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Computing Practice

Textbook

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Introduction

Since mathematics is both the most important working tool and the "language of expression" of physics, knowledge of the basic mathematical procedures presented in this textbook is the essential necessity for anyone who wants to study physics deeply. Combined lecture Computing practice 1, Computing practice 2 is a practical course suggested for undergraduate students directly following the lectures of Fundamental mathematical methods in physics 1, Fundamental mathematical methods in physics 2. The purpose of the Computing practice, as the name suggests, consists mainly in practical computations and the detailed practice of the knowledge gained in the above lectures. A prerequisite is also a complete and safe understanding of all topics of secondary school mathematics, which are no longer mentioned here.

This textbook is a comprehensive study material that helps you to select examples related to the given topics. It is divided into twelve essential chapters, arranged according to the chronological sequence of the lectures, supplemented by three appendices, intended for those interested in a wider knowledge of the important fields of mathematics, potentially useful in further studies and in physical practice. The individual chapters are always introduced by a brief theoretical summary of the given topic, which does not aim to provide a mathematically accurate and exhaustive explanation (supplemented by sentences, proofs, etc.), but to recap the main principles for the practical calculation of the problem in a simple and clear way. If the interpretation is simplified somewhere to the point that, for example, it neglects some assumptions or some solutions of an equation, this is noted in the text. The core of each chapter is then a set of examples that cover each topic to a sufficient extent. For each example, there is also the result that, in my opinion, allows students who are just getting familiar with a given field to be able to orient themselves correctly when calculating. Sections, paragraphs, and examples using more advanced maths that are primarily intended for more advanced or senior students are labeled ★. For easier handling, the entire collection is equipped with blue highlighted hyperlinks, which in electronic version enable immediately to move to the linked site and the same highlighted URL links, which after the click, automatically open the website.

Even the best study material will not substitute their own diligence and determination of those seeking knowledge and skills; it can only help them the subject to be more or less easier to understand. Therefore, I would very much welcome if those who will work with this collection give me their views, suggestions or reservations, for example on the clarity of the interpretation, or the difficulty of the examples, and to notify me at any time of any inaccuracy or deficiency they reveal in the examples or text.

I also thank Mgr. Lenka Czudková, Ph.D. and Mgr. Pavel Kočí, Ph.D. for useful advice and valuable comments.

Petr Kurfürst

Chapter 1

Differential and integral calculus[1]

1.1 Derivatives of functions of a single variable

- The *derivative* is one of the basic concepts of differential calculus and mathematical analysis in general. Using the predefined term limit, the derivative of a function of a single variable is defined as (see Figure 1.1)

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}, \tag{1.1}$$

where $h = \Delta x$ is an increment of an independent variable x.

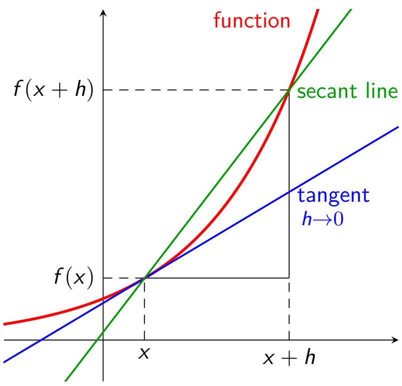

Figure 1.1: Schematic representation of the geometric meaning of a derivative of a function of a single variable, illustrating the formula (1.1). The graph of the function is plotted by the red curve. The green color represents the secant line of this function, passing through the points $[x, f(x)]$ and $[x+h, f(x+h)]$, whose slope (tangent of the angle between the secant line and the horizontal axis x) is given by the ratio $[f(x+h) - f(x)]/h$. If h gets smaller, the second intersection of the secant line with the given function gets closer to the first, until for $h \to 0$ the secant line becomes (blue) tangent, whose slope (the derivative of the given function $f(x)$ at the point x) is given by the formula (1.1).

So if we want to express derivative of elementary functions directly from the definition of (1.1), for example, in the case of a power-law function with an integer exponent, $y = x^n$, $n \in \mathbb{N}$, we can write

$$y' = \lim_{h\to 0} \frac{(x+h)^n - x^n}{h} = \lim_{h\to 0} \frac{x^n + nx^{n-1}h + \ldots - x^n}{h} = nx^{n-1}, \tag{1.2}$$

[1] Recommended literature for this chapter: Jarník (1974), Jarník (1984), Dĕmidovič (2003), Kvasnica (2004), Bartsch (2008), Rektorys (2009), Zemánek & Hasil (2012).

where the dotted term substitutes all terms with higher powers of h. Similarly, we can define the derivative of exponential function $y = \mathrm{e}^x$ as

$$y' = \lim_{h\to 0} \frac{\mathrm{e}^{(x+h)} - \mathrm{e}^x}{h} = \mathrm{e}^x \lim_{h\to 0} \frac{\mathrm{e}^h - 1}{h} = \mathrm{e}^x \tag{1.3}$$

and the derivative of trigonometric function $y = \sin x$ (using the relation $\sin\alpha - \sin\beta = 2\sin\frac{\alpha-\beta}{2}\cos\frac{\alpha+\beta}{2}$ and the theorem on limit of the product of functions: $\lim\limits_{x\to a}[f(x)g(x)] = \lim\limits_{x\to a} f(x) \lim\limits_{x\to a} g(x)$) as

$$y' = \lim_{h\to 0} \frac{\sin(x+h) - \sin x}{h} = \lim_{h\to 0} \frac{\sin\left(\frac{h}{2}\right)}{\frac{h}{2}} \lim_{h\to 0} \cos\left(x + \frac{h}{2}\right) = \cos x. \tag{1.4}$$

Derivative of a power function with a real exponent, $y = x^n$, $n \in \mathbb{R}$, we can define using the derivative of the exponential (1.3) and rule for differentiating a composite function (1.31),

$$y' = (x^n)' = \left(\mathrm{e}^{n\ln x}\right)' = x^n \frac{n}{x} = nx^{n-1}. \tag{1.5}$$

Derivatives of elementary *inverse* functions can be easily defined by derivatives of their original patterns, for example, for the function $y = \ln x$ holds $\mathrm{e}^y = x$ and thus $\mathrm{e}^y y' = 1$, or for the function $y = \arcsin x$ holds $\sin y = x$ hence $\cos y\, y' = 1$. For these two cases we get

$$y' = \frac{1}{\mathrm{e}^y} = \frac{1}{x}, \qquad y' = \frac{1}{\cos y} = \frac{1}{\sqrt{1-\sin^2 y}} = \frac{1}{\sqrt{1-x^2}}, \tag{1.6}$$

respectively. We can also define derivatives of other elementary functions of a single variable by some of these methods.

- The following list summarizes the derivatives of elementary functions of a single variable:

$$(Cx^n)' = Cnx^{n-1}, \text{ where } C \in \mathbb{R} \text{ is a constant, } n \in \mathbb{R} \text{ is a constant,} \tag{1.7}$$

$$(\mathrm{e}^x)' = \mathrm{e}^x, \tag{1.8}$$

$$(a^x)' = (\mathrm{e}^{x\ln a})' = a^x \ln a, \text{ where } a > 0 \text{ is a constant,} \tag{1.9}$$

$$(\ln x)' = \frac{1}{x},\ x > 0, \tag{1.10}$$

$$(\log_a x)' = \frac{1}{x\ln a},\ x > 0, \text{ where } a > 0,\ a \neq 1 \text{ is a constant,} \tag{1.11}$$

$$(\sin x)' = \cos x, \tag{1.12}$$

$$(\cos x)' = -\sin x, \tag{1.13}$$

$$(\tan x)' = \frac{1}{\cos^2 x},\ x \neq (2k+1)\frac{\pi}{2},\ k \in \mathbb{Z}, \tag{1.14}$$

$$(\cot x)' = -\frac{1}{\sin^2 x},\ x \neq k\pi,\ k \in \mathbb{Z}, \tag{1.15}$$

$$(\arcsin x)' = \frac{1}{\sqrt{1-x^2}},\ -1 < x < 1, \tag{1.16}$$

$$(\arccos x)' = -\frac{1}{\sqrt{1-x^2}},\ -1 < x < 1, \tag{1.17}$$

$$(\arctan x)' = \frac{1}{1+x^2}, \tag{1.18}$$

$$(\operatorname{arccot} x)' = -\frac{1}{1+x^2}, \tag{1.19}$$

$$(\sinh x)' = \left(\frac{\mathrm{e}^x - \mathrm{e}^{-x}}{2}\right)' = \frac{\mathrm{e}^x + \mathrm{e}^{-x}}{2} = \cosh x, \tag{1.20}$$

$$(\cosh x)' = \sinh x, \tag{1.21}$$

$$(\tanh x)' = \frac{1}{\cosh^2 x} = 1 - \tanh^2 x, \tag{1.22}$$

$$(\coth x)' = -\frac{1}{\sinh^2 x} = 1 - \coth^2 x,\ x \neq 0. \tag{1.23}$$

From Equation (1.20), the following identities for hyberbolometric functions (inverse to hyperbolic functions) can be derived:

$$\operatorname{argsinh} x = \ln\left(x + \sqrt{x^2+1}\right) \quad \text{and so} \quad (\operatorname{argsinh} x)' = \frac{1}{\sqrt{x^2+1}}, \tag{1.24}$$

$$\operatorname{argcosh} x = \ln\left(x + \sqrt{x^2-1}\right) \quad \text{and so} \quad (\operatorname{argcosh} x)' = \frac{1}{\sqrt{x^2-1}},\ x > 1, \tag{1.25}$$

$$\operatorname{argtanh} x = \frac{1}{2}\ln\left|\frac{1+x}{1-x}\right| \quad \text{and so} \quad (\operatorname{argtanh} x)' = \frac{1}{1-x^2},\ -1 < x < 1 \tag{1.26}$$

$$\operatorname{argcoth} x = \frac{1}{2}\ln\left|\frac{x+1}{x-1}\right| \quad \text{and so} \quad (\operatorname{argcoth} x)' = \frac{1}{1-x^2},\ |x| > 1. \tag{1.27}$$

- Rules for differentiation of a sum, product, and ratio of functions of a single variable:

$$(\alpha f + \beta g)' = \alpha f' + \beta g' \text{ for arbitrary functions } f,\ g \text{ and constants } \alpha,\ \beta, \tag{1.28}$$

$$(fg)' = f'g + fg' \text{ for arbitrary functions } f \text{ and } g, \tag{1.29}$$

$$\left(\frac{f}{g}\right)' = \left[f\left(\frac{1}{g}\right)\right]' = \frac{f'g - fg'}{g^2} \text{ for arbitrary functions } f \text{ and } g,\ g \neq 0. \tag{1.30}$$

- Rule for differentiation of a composite function $f(\phi(x))$, where f is outer and ϕ is inner function of the variable x (the so-called chain rule for derivatives):

$$[f(\phi)]' = \frac{\mathrm{d}f}{\mathrm{d}\phi}\frac{\mathrm{d}\phi}{\mathrm{d}x} = \frac{\mathrm{d}f}{\mathrm{d}\phi}\phi'. \tag{1.31}$$

  Proofs of the given rules (1.28) - (1.31) can be done quite simply using the definition of derivatives (1.1), I recommend to those interested in a deeper understanding of the principles mentioned above the literature listed below.

- For a deeper study of not only differential and integral calculus, but broader mathematical analysis covering a significant part of the stuff contained in this textbook, I especially recommend the collection of examples Děmidovič (2003).

For future practical computations (not only of derivatives, but more or less in all areas of mathematics), or for checking the correctness of mechanical calculations, analytical software packages can be employed, such as Wolfram Alpha: Computational Knowledge Engine `https://www.wolframalpha.com/`, whose basic applications are freely available; Sage (SageMath) is also very advanced `http://www.sagemath.org/`, etc. In any case, it does not substitute your skills; it only complements them and helps to quickly and correctly handle, simplify, and check even very large, on mechanical counting laborious expressions.

- **Examples:**

Calculate the derivatives of the functions and simplify the results. If D_f is only a subset of $\mathbb{R}$, find the intersection of the domains of definition of the specified and resulting functions. The result for each example is highlighted in red color.

1.1 $(2-x^2)(1-x^2+x^3)$ $\qquad -6x+6x^2+4x^3-5x^4$

1.2 $\dfrac{1-x}{1+x}$ $\qquad -\dfrac{2}{(1+x)^2}$

1.3 $(5x^2+1)^3$ $\qquad 30x(5x^2+1)^2$

1.4 $\sin(x^2+2x)$ $\qquad \cos(x^2+2x)(2x+2)$

1.5 $\dfrac{\sin x}{1-\cos x}$ $\qquad \dfrac{1}{\cos x-1}$

1.6 $6\,\mathrm{e}^{2x}+10x^2\ln x$ $\qquad 12\,\mathrm{e}^{2x}+10x(2\ln x+1)$

1.7 $\dfrac{3\,\mathrm{e}^{x}}{5\,\mathrm{e}^{3x}+1}$ $\qquad \dfrac{3(\,\mathrm{e}^{x}-10\,\mathrm{e}^{4x})}{(5\,\mathrm{e}^{3x}+1)^2}$

1.8 $\ln(1-7x)^3$ $\qquad \dfrac{21}{7x-1}$

1.9 $3\log_7[(x^2+1)^3]$ $\qquad \dfrac{18x}{(x^2+1)\ln 7}$

1.10 $\ln\left[\sin(3x^2)\sqrt{x^2+1}\right]$ $\qquad 6x\cot\left(3x^2\right)+\dfrac{x}{x^2+1}$

1.11 The sum of the two unknown numbers is 12. Find such two numbers

(a) so that the sum of their squares is minimal,

(b) so that the product of one number with the square of the second number is maximal.

(a) 6, 6

(b) 4, 8

1.12 Find a positive number for which the sum of 16 times this number and the inverse of the square of this number is minimal.

$\dfrac{1}{2}$

1.13 How high will a colored flare fly if fired from the ground vertically with the initial velocity $v_0 = 40\,\mathrm{m\,s^{-1}}$ (ignore air resistivity and other side effects)? How long will it take to reach this maximum height? For simplicity, consider the value of gravitational acceleration $g = 10\,\mathrm{m\,s^{-2}}$.

$80\,\mathrm{m}$, $4\,\mathrm{s}$

1.14 With what initial velocity must be fired the same flare if it is to reach the same height as in Example 1.13, with an elevation angle of $\alpha = 45°$? In what time it reaches the maximum height in this case? How far from the initial point the flare hits the ground? Consider the horizontal terrain and the value of gravitational acceleration $g = 10\,\mathrm{m\,s^{-2}}$.

$v_0 \approx 57\,\mathrm{m\,s^{-1}}$, $4\,\mathrm{s}$, approx. $325\,\mathrm{m}$

1.15 Find the dimensions of the swimming pool with the required volume of $972\,\mathrm{m}^3$ and with the required aspect ratio $a : b = 1 : 2$ (we denote its depth as h). Determine the dimensions of the pool with the required volume of $972\,\mathrm{m}^3$ and with the required aspect ratio $a : b = 1 : 2$ (its depth is denoted h), to minimize the cladding area of its walls and bottom.

$a = 9\,\mathrm{m}$, $b = 18\,\mathrm{m}$, $h = 6\,\mathrm{m}$

1.16 The steel cylindrical tank has a volume of $64\,\mathrm{m}^3$. Find its dimensions (radius of the base R and height H), at which the material consumption for its production will be minimal.

$R = \dfrac{4}{\sqrt[3]{2\pi}}\,\mathrm{m}$, $H = \dfrac{8}{\sqrt[3]{2\pi}}\,\mathrm{m}$

1.17 The farmer wants to enclose his rectangular field by fencing it around the perimeter and dividing it into two halves by a fence that runs parallel to one side. What maximum area does he enclose if he has $1200\,\mathrm{m}$ of fence wire mesh available?

$300\,\mathrm{m} \times 200\,\mathrm{m} = 60\,000\,\mathrm{m}^2$.

1.18 If the cough is severe, the trachea profile becomes narrower to achieve a higher speed of exhaled air. What is the optimal reduction of the trachea radius to maximize the speed? The formula giving the relationship between the exhalation rate v and the current trachea radius r has the form $v = c(r_0 - r)r^2$, where c is a positive constant (related to the length of the trachea), and r_0 is the radius of the trachea at rest.

$r = \dfrac{2}{3} r_0$

1.19 The Statue of Liberty, standing on the Island of Liberty in New York, USA, is $93\,\mathrm{m}$ high together with pedestal, while the height of the particular copper statue is $46\,\mathrm{m}$. From what distance do I have to photograph the entire monument if I want the copper statue to fill the maximum possible viewing angle (neglect the height of the human eye or the camera above the ground or sea level)? What would be the ratio of the angles $\varphi_{\mathcal{S}}$, which would fill the particular statue and $\varphi_{\mathcal{M}}$, which would fill the entire monument?

from the distance $D \approx 66\,\mathrm{m}$, the ratio $\varphi_{\mathcal{S}}/\varphi_{\mathcal{M}} \approx 0.35$ (the ratio will increase with distance)

1.20 Find the dimensions (base radius R and height H) of the minimum volume cone, circumscribed by a ball with the given radius r.

$R = \sqrt{2}r$, $H = 4r$

1.21 $\dfrac{1 + x - x^2}{1 - x + x^2}$ $\qquad$ $\dfrac{2(1-2x)}{(1 - x + x^2)^2}$

1.22 $\dfrac{1}{\sin 2} \ln \dfrac{1+x}{1-x} - \ln \dfrac{1 + x\cos 2}{1 - x\cos 2} \cot 2$ $\qquad$ $\dfrac{2\sin 2}{(1-x^2)\,(1 - x^2\cos^2 2)}$, $x \in (-1, 1)$

1.23 $\dfrac{1}{\sqrt{1+x^2}\left(x+\sqrt{1+x^2}\right)}$ $\qquad -\dfrac{1}{(x^2+1)^{3/2}}$

1.24 $\sin\left(\cos^2 x\right)\cdot\cos\left(\sin^2 x\right)$ $\qquad -\sin 2x\cdot\cos\left(\cos 2x\right)$

1.25 $\sqrt{x+\sqrt{x+\sqrt{x}}}$ $\qquad \dfrac{1+\sqrt{x}\left(2+4\sqrt{x+\sqrt{x}}\right)}{8\sqrt{x}\sqrt{x+\sqrt{x}}\sqrt{x+\sqrt{x+\sqrt{x}}}},\ x>0$

1.26 $x\left(\sin\ln x-\cos\ln x\right)$ $\qquad 2\sin\ln x,\ x>0$

1.27 $\sqrt{1+x^2}-\ln\left(\dfrac{1}{x}+\sqrt{1+\dfrac{1}{x^2}}\right)$ $\qquad \dfrac{\sqrt{x^2+1}}{x},\ x\neq 0$

1.28 $\dfrac{\arccos x}{x}+\dfrac{1}{2}\ln\dfrac{1-\sqrt{1-x^2}}{1+\sqrt{1-x^2}}$ $\qquad -\dfrac{\arccos x}{x^2},\ x\in\langle -1,1\rangle,\ x\neq 0$

1.29 x^{x^x} $\qquad x^{x^x}\left[x^{x-1}+x^x\ln x\left(\ln x+1\right)\right],\ x>0$

1.30 $x\arcsin\sqrt{\dfrac{x}{1+x}}+\operatorname{arccot}\sqrt{x}-\sqrt{x}$ $\qquad \arcsin\sqrt{\dfrac{x}{x+1}}-\dfrac{1}{\sqrt{x}\left(x+1\right)},\ x>0$

1.31 $x^{\sin^2 x}$ $\qquad x^{\sin^2 x}\left(\dfrac{\sin^2 x}{x}+2\sin x\cos x\ln x\right),\ x>0$

1.32 $x\arcsin\dfrac{x^2-1}{x^2+1}$ $\qquad \arcsin\dfrac{x^2-1}{x^2+1}+\dfrac{2x}{x^2+1}$

1.33 $5^{x\log_{10} x}$ $\qquad 5^{x\log x}\ln 5\left(\log x+\dfrac{1}{\ln 10}\right),\ x>0$

1.34 $\log_7\dfrac{x^2-1}{x-1}$ $\qquad \dfrac{1}{(x+1)\ln 7},\ x>-1$

1.35 $x-\ln\sqrt{1+e^{2x}}+e^{-x}\arctan e^x$ $\qquad \dfrac{2\,e^x-\left(1+e^{2x}\right)\arctan e^x}{e^{3x}+e^x}$

1.36 $x^{\sin x}+\ln\cos\sqrt{e^x+1}$

$$x^{\sin x}\left(\cos x\ln x+\frac{\sin x}{x}\right)-\frac{e^x\tan\sqrt{e^x+1}}{2\sqrt{e^x+1}},\ x>0$$

1.37 $x\ln^2(x+\sqrt{1+x^2})-2\sqrt{1+x^2}\ln(x+\sqrt{1+x^2})+2x$

$$\ln^2\left(x+\sqrt{1+x^2}\right)$$

1.38 $\dfrac{1+x^2}{\sqrt[3]{x^4}\sin^7 x}$

$$\frac{\frac{2}{3}\left(x^2-2\right)\sin x-7x\left(x^2+1\right)\cos x}{\sqrt[3]{x^7}\sin^8 x},\ x\neq 0$$

1.39 $f'(2\pi)$ of function $f(x) = x^2(\cos x)^{-\sin x}$.

$$f'(2\pi) = (\cos x)^{-\sin x}\left\{2x + x^2\left[\frac{\sin^2 x}{\cos x} - \cos x \ln(\cos x)\right]\right\}\bigg|_{2\pi} = 4\pi,\ x \in (4k-1, 4k+1)\frac{\pi}{2},$$
$k \in \mathbb{Z}$

1.40 $x^{\ln(\sin x)}\dfrac{x}{\sqrt{1+x^2}}$

$$x^{\ln(\sin x)}\left[\frac{\ln(\sin x) + x\ln x \cot x}{\sqrt{1+x^2}} + \frac{1}{(1+x^2)^{3/2}}\right],\ x > 0 \wedge x \in (2k, 2k+1)\,\pi,\ k \in \mathbb{Z}$$

1.41 $x^{\sin(\ln x)}\dfrac{\sqrt{1+x^2}}{x}$

$$x^{\sin(\ln x)}\frac{(x^2+1)\left[\sin(\ln x) + \ln x\cos(\ln x)\right] - 1}{x^2\sqrt{1+x^2}},\ x > 0$$

1.42 $\mathrm{e}^{ax\cos x}\dfrac{a\sin \mathrm{b}x - b\cos bx}{\sqrt{ax^2+b^2}}$, where a, b are positive constants.

$$\mathrm{e}^{ax\cos x}\left[\frac{a\sin bx - b\cos bx}{\sqrt{ax^2+b^2}}\left(a\cos x - ax\sin x - \frac{ax}{ax^2+b^2}\right) + \frac{ab\cos bx + b^2\sin bx}{\sqrt{ax^2+b^2}}\right]$$

1.43 $x^{ax\sin x}\dfrac{a\sin\sqrt{bx} - b\cos\sqrt{bx}}{\sqrt{a^2+b^2}}$, where a, b are positive constants.

$$\frac{\sqrt{b}\cos\sqrt{bx}}{\sqrt{a^2+b^2}}\,x^{ax\sin x}\left[\frac{a\sin x}{\sqrt{b}}\,(1 + \ln x + x\ln x\cot x)\left(a\tan\sqrt{bx} - b\right) + \frac{a + b\tan\sqrt{bx}}{2\sqrt{x}}\right],$$
$x > 0$. Why is the condition $x \neq (2k+1)\dfrac{\pi}{2}$, $k \in \mathbb{Z}$ not necessary?

1.44 $(ax\sin x)^{\frac{b\sin x}{x}}$, where a, b are positive constants.

$$b\,(ax\sin x)^{\frac{b\sin x}{x}}\left[\frac{\sin x + x\cos x}{x^2} + \ln(ax\sin x)\left(\frac{\cos x}{x} - \frac{\sin x}{x^2}\right)\right],$$
$$\begin{matrix} x > 0 \wedge x \in (2k, 2k+1)\pi \\ x < 0 \wedge x \in (2k-1, 2k)\pi \end{matrix},\ k \in \mathbb{Z}$$

1.45 $(ax\,\mathrm{e}^x)^{\frac{b\ln x}{x^2}}$, where a, b are positive constants.

$$\frac{b}{x^3}(ax\,\mathrm{e}^x)^{\frac{b\ln x}{x^2}}\left[(1+x)\ln x + \ln(ax\,\mathrm{e}^x)\,(1 - 2\ln x)\right],\ x > 0$$

1.46 $(x\,\mathrm{e}^x)^{\frac{a}{x\ln x}}$, where a is a positive constant.

$$-\frac{a(x + \ln^2 x)}{x^2\ln^2 x}\,\mathrm{e}^{\frac{a(x+\ln x)}{x\ln x}},\ x > 0,\ x \neq 1.$$

1.2 Indefinite integrals of functions of a single variable

- We call the *indefinite integral* an infinitely large set of functions consisting of the sum of any real constant C with the so-called *primitive function* $F(x)$ to the original function

$f(x)$ for which $F'(x) = f(x)$. In the case of a function of a single variable, we write

$$\int f(x)\,\mathrm{d}x = F(x) + C. \tag{1.32}$$

Integration is thus an inverse process to differentiation, indefinite integrals (in English, they are also called *antiderivatives*) of some elementary functions can be read directly from Equations (1.7) - (1.27).

- The following list summarizes indefinite integrals of elementary functions of a single variable[2]:

$$\int C_1 x^n\,\mathrm{d}x = C_1\frac{x^{n+1}}{n+1} + C_2,\ C_1, C_2 \in \mathbb{R},\ n \in \mathbb{R}\setminus\{-1\},\ \text{are constants}, \tag{1.33}$$

$$\int \mathrm{e}^x\,\mathrm{d}x = \mathrm{e}^x + C,\ C \in \mathbb{R}\ \text{is a constant}, \tag{1.34}$$

$$\int a^x\,\mathrm{d}x = \frac{a^x}{\ln a} + C,\ a > 0,\ a \neq 1\ \text{is a constant}, \tag{1.35}$$

$$\int \frac{1}{x}\,\mathrm{d}x = \ln|x| + C_1 = \ln(C_2|x|),\ x \neq 0,\ C_2 > 0,\ C_1 = \ln C_2, \tag{1.36}$$

$$\int \sin x\,\mathrm{d}x = -\cos x + C, \tag{1.37}$$

$$\int \cos x\,\mathrm{d}x = \sin x + C, \tag{1.38}$$

$$\int \frac{1}{\cos^2 x}\,\mathrm{d}x = \tan x + C,\ x \neq (2k+1)\frac{\pi}{2},\ k \in \mathbb{Z}, \tag{1.39}$$

$$\int \frac{1}{\sin^2 x}\,\mathrm{d}x = -\cot x + C,\ x \neq k\pi,\ k \in \mathbb{Z}, \tag{1.40}$$

$$\int \frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x = \arcsin x + C_1 = -\arccos x + C_2,\ -1 < x < 1, \tag{1.41}$$

$$\int \frac{1}{1+x^2}\,\mathrm{d}x = \arctan x + C_1 = -\operatorname{arccot} x + C_2, \tag{1.42}$$

$$\int \sinh x\,\mathrm{d}x = \cosh x + C, \tag{1.43}$$

$$\int \cosh x\,\mathrm{d}x = \sinh x + C, \tag{1.44}$$

$$\int \frac{1}{\cosh^2 x}\,\mathrm{d}x = \tanh x + C, \tag{1.45}$$

$$\int \frac{1}{\sinh^2 x}\,\mathrm{d}x = -\coth x + C,\ x \neq 0, \tag{1.46}$$

$$\int \frac{1}{\sqrt{x^2+1}}\,\mathrm{d}x = \ln\left(x + \sqrt{x^2+1}\right) + C = \operatorname{argsinh} x + C, \tag{1.47}$$

$$\int \frac{1}{\sqrt{x^2-1}}\,\mathrm{d}x = \ln\left(x + \sqrt{x^2-1}\right) + C = \operatorname{argcosh} x + C,\ x > 1, \tag{1.48}$$

$$\int \frac{1}{1-x^2}\,\mathrm{d}x = \begin{cases} \dfrac{1}{2}\ln\left|\dfrac{1+x}{1-x}\right| + C = \operatorname{argtanh} x + C,\ -1 < x < 1 \\ \dfrac{1}{2}\ln\left|\dfrac{x+1}{x-1}\right| + C = \operatorname{argcoth} x + C,\ |x| > 1, \end{cases} \tag{1.49}$$

[2]indefinite integrals are exhaustively tabulated, for example, in Bartsch (2008), Rektorys (2009).

$$\int \frac{1}{x^2-1}\,\mathrm{d}x \qquad = \frac{1}{2}\ln\left|\frac{x-1}{x+1}\right| + C. \tag{1.50}$$

- We can integrate the product of two functions $u(x)$ and $v'(x)$ of the independent variable x using the method *by parts* (per partes), which is the integral of Equation (1.29):

$$uv = \int (uv)'\,\mathrm{d}x = \int (u'v + uv')\,\mathrm{d}x \quad \text{and so} \quad \int uv'\,\mathrm{d}x = uv - \int u'v\,\mathrm{d}x. \tag{1.51}$$

- By *substitution method* we can integrate a composite function (see Equation (1.31)) where the internal function can be replaced by a new variable, or we can integrate a simple function by replacing the independent variable with a new internal function:
  - Type I substitution method can be used to integrate the composite function $f[\phi(x)]$ of the independent variable x in the form

$$\int f[\phi(x)]\phi'(x)\,\mathrm{d}x = \int f(z)\,\mathrm{d}z = F(z) + C = F[\phi(x)] + C, \tag{1.52}$$

    where we can replace (substitute) the internal function with a new variable: $\phi(x) = z$, $\phi'(x)\,\mathrm{d}x = \mathrm{d}z$. Type I substitution method is also the universal substitution $\tan(x/2) = z$, by which any trigonometric function can be converted to a rational function.
  - Type II substitution method can be used to integrate the simple function $f(x)$ of the independent variable x as follows

$$\int f(x)\,\mathrm{d}x = \int f[\phi(z)]\phi'(z)\,\mathrm{d}z = F(z) + C = F[\phi^{-1}(x)] + C, \tag{1.53}$$

    where we can substitute the original variable with a new internal function of the new variable: $x = \phi(z)$, $\mathrm{d}x = \phi'(z)\,\mathrm{d}z$ and where the expression ϕ^{-1} means the inverse of ϕ. A typical example of this method is the substitution $x = \sin z$, by means of which the irrational functions of type $\sqrt{1-x^2}\,\mathrm{d}x$ or $\mathrm{d}x/\sqrt{1-x^2}$ in the integrand can be replaced by the trigonometric function $\cos^2 z\,\mathrm{d}z$, in the second case only $\mathrm{d}z$.

- Rational function in the form

$$f(x) = \frac{P_m(x)}{Q_n(x)} = \frac{a_m x^m + a_{m-1}x^{m-1} + \cdots + a_1 x + a_0}{b_n x^n + b_{n-1}x^{n-1} + \cdots + b_1 x + b_0}, \tag{1.54}$$

  where $P_m(x)$ and $Q_n(x)$ are polynomials of degree m and n (where $m \geq n$), can be decomposed into sum of polynomial and a proper rational function (where $m < n$). The rational function can be expressed either as the sum of partial fractions, or, in the case where, for example, $f(x) = 1/Q_2(x)$, where $Q_2(x)$ is a degree 2 polynomial further irreducible in $\mathbb{R}$, we make the adjustment (the so-called completion to the square) $b_2x^2 + b_1x + b_0 = \left[\sqrt{b_2}x + b_1/(2\sqrt{b_2})\right]^2 + b_0 - b_1^2/(4b_2)$, leading to an integral in the form of Equation (1.42).

- Similarly, we can solve the integrals of irrational functions of the type $f(x) = 1/\sqrt{Q_2(x)}$, where $Q_2(x)$ is a second-degree polynomial whose completion to the square leads to integrals in the form of Equations (1.41), (1.47) or (1.48). The methods of analytical calculations of indefinite integrals of functions of all types are tabulated exhaustively, for example, in the following textbooks: Bartsch (2008), Rektorys (2009), etc.

- **Examples:**

1.47 $\displaystyle\int \left(4x^3-6x^2+8x-1\right)\,\mathrm{d}x$ $\qquad x\left(x^3-2x^2+4x-1\right)+C$

1.48 $\displaystyle\int \left(x^{-4}+x^{-3}+x^{-2}+x^{-1}\right)\,\mathrm{d}x$ $\qquad \displaystyle -\frac{1}{x}\left(\frac{1}{3x^2}+\frac{1}{2x}+1\right)+\ln|x|+C,\ x\neq 0$

1.49 $\displaystyle\int \left[\left(\sqrt{x}-1\right)^2-x\right]^2\,\mathrm{d}x$ $\qquad \displaystyle x\left(1-\frac{8}{3}\sqrt{x}+2x\right)+C,\ x\geq 0$

1.50 $\displaystyle\int \frac{\left(\sqrt{x}-1\right)^3}{x}\,\mathrm{d}x$ $\qquad \displaystyle \sqrt{x}\left(\frac{2}{3}x-3\sqrt{x}+6\right)-\ln|x|+C,\ x>0$

1.51 $\displaystyle\int \left(\sin^2 x-3\cos^2 x\right)\,\mathrm{d}x$ $\qquad -\left(x+\sin 2x\right)+C$

1.52 $\displaystyle\int \left(4^{2x}-\mathrm{e}^{-x}\right)\,\mathrm{d}x$ $\qquad \displaystyle \frac{4^{2x}}{4\ln 2}+\mathrm{e}^{-x}+C$

1.53 $\displaystyle\int \frac{x}{x^2+1}\,\mathrm{d}x$ $\qquad \displaystyle \frac{1}{2}\ln\left(x^2+1\right)+C$

1.54 $\displaystyle\int 4x\sqrt{7-2x^2}\,\mathrm{d}x$ $\qquad \displaystyle -\frac{2}{3}\left(7-2x^2\right)^{3/2}+C,\ |x|\leq\sqrt{\frac{7}{2}}$

1.55 $\displaystyle\int \frac{\mathrm{d}x}{x\ln x}$ $\qquad \ln|\ln x|+C,\ x>0,\ x\neq 1$

1.56 $\displaystyle\int \frac{1-\ln^2(ax)}{3x}\,\mathrm{d}x$, where a is a positive constant
$\displaystyle \frac{\ln(ax)}{3}\left[1-\frac{\ln^2(ax)}{3}\right]+C,\ x>1$

1.57 $\displaystyle\int \left(\cot x-\tan x\right)\,\mathrm{d}x$ $\qquad \displaystyle \ln\left(\frac{\sin 2x}{2}\right)+C,\ x\in\left(k,k+\frac{1}{2}\right)\pi,\ k\in\mathbb{Z}$

1.58 $\displaystyle\int \frac{1}{x^2}\cos\frac{1}{x}\,\mathrm{d}x$ $\qquad \displaystyle -\sin\frac{1}{x}+C,\ x\neq 0$

1.59 $\displaystyle\int x^2\sin x\,\mathrm{d}x$ $\qquad \left(2-x^2\right)\cos x+2x\sin x+C$

1.60 $\displaystyle\int x\ln x\,\mathrm{d}x$ $\qquad \displaystyle \frac{x^2}{4}\left(2\ln x-1\right)+C,\ x>0$

1.61 $\displaystyle\int \left(x^3+1\right)\mathrm{e}^{-3x}\,\mathrm{d}x$ $\qquad \displaystyle -\frac{\mathrm{e}^{-3x}}{3}\left(x^3+x^2+\frac{2}{3}x+\frac{11}{9}\right)+C$

1.62 $\displaystyle\int \mathrm{e}^{2x}\sin x\,\mathrm{d}x$ $\qquad \displaystyle \frac{\mathrm{e}^{2x}}{5}\left(2\sin x-\cos x\right)+C$

1.63 $\displaystyle\int \frac{\ln x}{x^2}\,\mathrm{d}x$ $\qquad \displaystyle -\frac{1}{x}\left(\ln x+1\right)+C,\ x>0$

1.64 $\displaystyle\int \cos(\ln x)\,\mathrm{d}x$ $\qquad$ $\displaystyle\frac{x}{2}\left[\sin(\ln x)+\cos(\ln x)\right]+C,\ x>0$

1.65 $\displaystyle\int \frac{x^4}{x^2-3}\,\mathrm{d}x$ $\qquad$ $\displaystyle\frac{x^3}{3}+3x+\frac{3\sqrt{3}}{2}\ln\left|\frac{x-\sqrt{3}}{x+\sqrt{3}}\right|+C,\ x\neq\pm\sqrt{3}$

1.66 $\displaystyle\int \frac{3x-4}{x^2-4}\,\mathrm{d}x$ $\qquad$ $\ln\left[(x+2)^{5/2}\sqrt{x-2}\right]+C,\ x>2$

1.67 $\displaystyle\int \frac{x^2}{\sqrt{1-x^6}}\,\mathrm{d}x$ $\qquad$ $\displaystyle\frac{1}{3}\arcsin\left(x^3\right)+C,\ x\in(-1,1)$

1.68 $\displaystyle\int \frac{\mathrm{d}x}{\sqrt{2+3x-2x^2}}$ $\qquad$ $\displaystyle\frac{1}{\sqrt{2}}\arcsin\left(\frac{4x-3}{5}\right)+C,\ x\in\left(-\frac{1}{2},2\right)$

1.69 $\displaystyle\int \frac{\mathrm{d}x}{x^2+3x+3}$ $\qquad$ $\displaystyle\frac{2}{\sqrt{3}}\arctan\left(\frac{2x+3}{\sqrt{3}}\right)+C$

1.70 $\displaystyle\int \left(-x^2+x\right)\mathrm{e}^{3x}\,\mathrm{d}x$ $\qquad$ $\displaystyle\left(-\frac{x^2}{3}+\frac{5x}{9}-\frac{5}{27}\right)\mathrm{e}^{3x}+C$

1.71 $\displaystyle\int \frac{1+x}{\sqrt{1+x^2}}\,\mathrm{d}x$ $\qquad$ $\sqrt{x^2+1}+\ln\left(x+\sqrt{x^2+1}\right)+C$

1.72 $\displaystyle\int \left(\frac{1}{\sqrt{2-x^2}}+\frac{1}{\sqrt{2+x^2}}\right)\mathrm{d}x$ $\qquad$ $\displaystyle\arcsin\frac{x}{\sqrt{2}}+\operatorname{argsinh}\frac{x}{\sqrt{2}}+C,\ |x|<\sqrt{2}$

1.73 $\displaystyle\int \frac{\mathrm{d}x}{\sin x}$ $\qquad$ $\displaystyle\ln\left|\tan\frac{x}{2}\right|+C,\ x\neq k\pi,\ k\in\mathbb{Z}$

1.74 $\displaystyle\int \tan^3 x\,\mathrm{d}x$ $\qquad$ $\displaystyle\frac{1}{2\cos^2 x}+\ln|\cos x|+C,\ x\neq(2k+1)\frac{\pi}{2},\ k\in\mathbb{Z}$

1.75 $\displaystyle\int \frac{\sin x}{2+\sin x}\,\mathrm{d}x$ $\qquad$ $\displaystyle x-\frac{4}{\sqrt{3}}\arctan\left(\frac{2\tan\frac{x}{2}+1}{\sqrt{3}}\right)+C,\ x\neq(2k+1)\frac{\pi}{2},\ k\in$ $\mathbb{Z}$

1.76 $\displaystyle\int \frac{1+\cos x}{\sin^3 x}\,\mathrm{d}x$ $\qquad$ $\displaystyle\ln\sqrt{\tan\frac{x}{2}}-\frac{1+\cos x}{2\sin^2 x}+C,\ x\in(2k,2k+1)\pi,\ k\in\mathbb{Z}$

1.77 $\displaystyle\int \frac{\mathrm{d}x}{1+\sin x+\cos x}$ $\qquad$ $\displaystyle\ln\left|1+\tan\frac{x}{2}\right|+C,\ x\neq(4k+2,4k+3)\frac{\pi}{2},\ k\in\mathbb{Z}$

1.78 $\displaystyle\int \arctan\sqrt{2x-1}\,\mathrm{d}x$ $\qquad$ $\displaystyle x\arctan\sqrt{2x-1}-\frac{\sqrt{2x-1}}{2}+C,\ x\geq\frac{1}{2}$

1.79 $\displaystyle\int \frac{\mathrm{d}x}{\sin^2 x\cos^2 x}$ $\qquad$ $\displaystyle-2\cot(2x)+C,\ x\neq k\frac{\pi}{2},\ k\in\mathbb{Z}$

1.80 $\displaystyle\int \frac{\mathrm{d}x}{\sqrt{(4-x^2)^3}}$ $\qquad$ $\displaystyle\frac{x}{4\sqrt{4-x^2}}+C,\ |x|<2$

1.81 $\displaystyle\int \ln\left(x^2+1\right)\mathrm{d}x$ $\qquad$ $x\ln\left(x^2+1\right)+2\arctan x-2x+C$

1.82 $\displaystyle\int \frac{\sqrt[3]{1+\sqrt[4]{x}}}{\sqrt{x}}\,\mathrm{d}x$ $\qquad \displaystyle\frac{3}{7}\left(\sqrt[4]{x}+1\right)^{4/3}\left(4\sqrt[4]{x}-3\right)+C,\ x>0$

1.83 $\displaystyle\int \frac{\sqrt{x-1}}{x+1}\,\mathrm{d}x$ $\qquad \displaystyle 2\sqrt{x-1}-2\sqrt{2}\arctan\sqrt{\frac{x-1}{2}}+C,\ x\geq 1$

1.84 $\displaystyle\int \frac{\sqrt[4]{x-1}}{x+1}\,\mathrm{d}x$

$$4\sqrt[4]{x-1}+\frac{1}{\sqrt[4]{2}}\ln\frac{\sqrt{2(x-1)}-2\sqrt[4]{2(x-1)}+2}{\sqrt{2(x-1)}+2\sqrt[4]{2(x-1)}+2}+2^{3/4}\arctan\left[1-\sqrt[4]{2(x-1)}\right]-$$
$$2^{3/4}\arctan\left[1+\sqrt[4]{2(x-1)}\right]+C,\ x\geq 1$$

1.85 $\displaystyle\int \frac{x}{x^3-1}\,\mathrm{d}x$ $\qquad \displaystyle\frac{1}{6}\ln\frac{(x-1)^2}{x^2+x+1}+\frac{1}{\sqrt{3}}\arctan\left(\frac{2x+1}{\sqrt{3}}\right)+C,\ x\neq 1$

1.86 (a) $\displaystyle\int \frac{\mathrm{d}x}{(x^3-1)^2}$, (b) $\displaystyle\int \frac{\mathrm{d}x}{\sin^4 x}$, (c) $\displaystyle\int \frac{\mathrm{d}x}{\cos^6 x}$

(a) $\displaystyle\frac{1}{9}\left[\ln\frac{x^2+x+1}{(x-1)^2}+\frac{6}{\sqrt{3}}\arctan\left(\frac{2x+1}{\sqrt{3}}\right)-\frac{3x}{x^3-1}\right]+C,\ x\neq 1$

(b) $\displaystyle -\mathrm{cotg}\,x\left(1+\frac{\mathrm{cotg}^2 x}{3}\right)+C,\ x\neq k\pi,\ k\in\mathbb{Z}$

(c) $\displaystyle \mathrm{tg}\,x+\frac{2\,\mathrm{tg}^3 x}{3}+\frac{\mathrm{tg}^5 x}{5}+C,\ x\neq(2k+1)\frac{\pi}{2},\ k\in\mathbb{Z}$

1.3 Definite integrals of functions of a single variable

Definite integral of the function $f(x)$ continuous in the interval $a\leq x\leq b$, is defined by the prescription

$$\int_a^b f(x)\,dx=F(b)-F(a), \tag{1.55}$$

where $F(a)$, $F(b)$ are function values of a primitive function $F(x)$ in points $x=a$, $x=b$. The geometric meaning of a definite integral of a function of a single variable is given by the size of the total area in the plane xy, where $y=f(x)$, that is bounded by the graph of a function $f(x)$, by the x-axis and by the straight lines $x=a$, $x=b$. The sizes of partial areas above the x-axis, that is, where $f(x)>0$, contribute to the total area size, the sizes of partial areas below the x-axis, where $f(x)<0$, are subtracted from the total area (see Figure 1.2).

Specific case represent the so-called *improper* integrals, whose limits are either formed by improper numbers ($-\infty$ and/or $+\infty$) or they are integrals of functions that are discontinuous within the interval $x=a$, $x=b$. In the first case, the following relationships apply,

$$\int_a^{\infty} f(x)\,dx=\lim_{b\to\infty}\int_a^b f(x)\,dx,\qquad \int_{-\infty}^{b} f(x)\,dx=\lim_{a\to-\infty}\int_a^b f(x)\,dx, \tag{1.56}$$

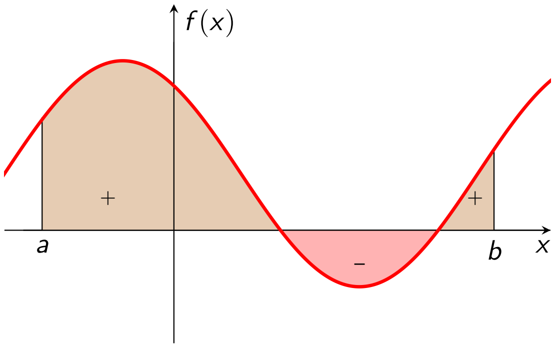

Figure 1.2: Schematic picture of the geometrical meaning of the definite integral of a function $f(x)$ of a single variable, illustrating the formula (1.55) and the previous explanation. The graph of a function is depicted by the red curve. Partial areas that contribute to the total area size (where $f(x) > 0$), given by the integral (1.55), are highlighted by the ochroid (brown) color, the partial area that is subtracted from the total area size (where $f(x) < 0$), is highlighted by red.

or any combinations thereof. If these limits exist, we consider them as improper integral values. For a function $f(x)$, discontinuous for example at the point $h \in (a, b)$, where $\lim_{x\to h} f(x) = \pm\infty$ (it can be a right, left, or two-sided limit), we define its integral (where a number $\epsilon > 0$) as

$$\int_a^b f(x)\,dx = \lim_{\epsilon\to 0^+} \int_a^{h-\epsilon} f(x)\,dx + \lim_{\epsilon\to 0^+} \int_{h+\epsilon}^b f(x)\,dx, \tag{1.57}$$

where again, if these limits exist, we consider them as integral values of a discontinuous function (calculating the integral according to the formula (1.57) is also called the determination of the *Cauchy principal value* of the integral; for example the definite integral of the function $f(x) = 1/x$ with singularity at the point $x = 0$, within the limits $a = -1, b = 1$, will be thus equal to zero).

- **Examples:**

1.87 $\displaystyle\int_{-3}^{3} \left(x^2 + x - 3\right)\,\mathrm{d}x$ $\quad 0$

1.88 $\displaystyle\int_{0}^{\pi/2} \sin x \cos x\,\mathrm{d}x$ $\quad \dfrac{1}{2}$

1.89 (a) $\displaystyle\int_{0}^{\pi/2} \sin^2 x\,\mathrm{d}x$, (b) $\displaystyle\int_{0}^{\pi/4} \sin^2 x\,\mathrm{d}x$ $\quad$ (a) $\dfrac{\pi}{4}$, (b) $\dfrac{\pi-2}{8}$

1.90 $\displaystyle\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x$ $\quad \pi$

1.91 $\displaystyle\int_{-\infty}^{\infty} \frac{1}{1+x^2}\,\mathrm{d}x$ $\quad \pi$

1.92 $\displaystyle\int_{-\infty}^{\infty} \frac{x^2}{1+x^6}\,\mathrm{d}x$ $\quad \dfrac{\pi}{3}$

1.93 $\displaystyle\int_0^1 \sqrt{1-\frac{x^2}{4}}\,\mathrm{d}x$ $\qquad \dfrac{\pi}{6}+\dfrac{\sqrt{3}}{4}$

1.94 (a) $\displaystyle\int_1^2 x\ln x\,\mathrm{d}x$, (b) $\displaystyle\int_0^1 x\ln x\,\mathrm{d}x$ $\qquad$ (a) $\ln 4-\dfrac{3}{4}$, (b) $-\dfrac{1}{4}$

1.95 (a) $\displaystyle\int_1^3 x^2\ln x\,\mathrm{d}x$, (b) $\displaystyle\int_0^1 x^2\ln x\,\mathrm{d}x$ $\qquad$ (a) $9\ln 3-\dfrac{26}{9}$, (b) $-\dfrac{1}{9}$

1.96 $\displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-|x|}\,\mathrm{d}x$ $\qquad 2$

1.97 (a) $\displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x$ *, (b) $\displaystyle\int_0^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x$ * $\qquad$ (a) $\sqrt{\pi}$, (b) $\dfrac{\sqrt{\pi}}{2}$

1.98 $\displaystyle\int_{\pi/6}^{\pi/3} \frac{x\,\mathrm{d}x}{\sin^2 x\cos^2 x}$ $\qquad \left[x\,(\tan x-\cot x)+\ln(\sin x\cos x)\right]_{\frac{\pi}{6}}^{\frac{\pi}{3}}=\dfrac{\pi}{\sqrt{3}}$

1.99 $\displaystyle\int_0^{\sqrt{\pi}} x\sin\left(\frac{x^2}{4}\right)\cos\left(\frac{x^2}{4}\right)\mathrm{d}x$ $\qquad \left[\sin^2\left(\dfrac{x^2}{4}\right)\right]_0^{\sqrt{\pi}}=\dfrac{1}{2}$

1.100 $\displaystyle\int_2^3 \frac{2x-1}{x^2-4x+5}\,\mathrm{d}x$ $\qquad \left[\ln(x^2-4x+5)+3\arctan(x-2)\right]_2^3=\ln 2+\dfrac{3\pi}{4}$

1.101 $\displaystyle\int_{-1}^1 \sqrt{4x^2+1}\,\mathrm{d}x$

$$\left[\frac{\ln(\sqrt{4x^2+1}+2x)}{4}+\frac{x\sqrt{4x^2+1}}{2}\right]_{-1}^{1}=\frac{\ln(\sqrt{5}+2)}{2}+\sqrt{5}\approx 2.96$$

1.102 $\displaystyle\int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} [(x\tan x+a)\tan x+1]\,\mathrm{d}x$, a is a constant. $\qquad \left[x\tan x+(1-a)\ln(\cos x)-\dfrac{x^2}{2}+x\right]_{-\frac{\pi}{4}}^{\frac{\pi}{4}}=\dfrac{\pi}{2}$

1.103 $\displaystyle\int_{-\pi/4}^{\pi/4} (x+a)\left(\frac{\sin x}{\cos x}\right)^2\mathrm{d}x$, a is a constant.

$$\left[x\tan x+\ln(\cos x)-\frac{x^2}{2}+a\tan x-ax\right]_{-\frac{\pi}{4}}^{\frac{\pi}{4}}=2a\left(1-\frac{\pi}{4}\right)$$

1.104 $\displaystyle\int_0^{\pi/6} \frac{x\,\mathrm{d}x}{(\cos^2 x-\sin^2 x)^2}$ $\qquad \left[\dfrac{x}{2}\tan(2x)+\ln\sqrt[4]{\cos(2x)}\right]_0^{\frac{\pi}{6}}=\dfrac{1}{4}\left(\dfrac{\pi}{\sqrt{3}}-\ln 2\right)$

1.105 $\displaystyle\int_0^1 x\arctan(x^2+1)\,\mathrm{d}x$

$$\left[\frac{x^2+1}{2}\arctan(x^2+1)-\ln\sqrt[4]{x^4+2x^2+2}\right]_0^1=\arctan 2-\frac{\pi}{8}+\frac{1}{4}\ln\frac{2}{5}$$

1.106 $\displaystyle\int_0^1 x^3 \ln\left(x^2+1\right) \mathrm{d}x$ $\displaystyle\left[\frac{(x^4-1)\ln(x^2+1)}{4} - \frac{x^4}{8} + \frac{x^2}{4}\right]_0^1 = \frac{1}{8}$

1.4 Simple geometric and physical applications of integration of a single variable function[3]

In the following examples, it is always necessary to construct a definite integral of a single variable function. If, within an example, a continuous quantity (called an *intensive* physical quantity - density, pressure, charge density, etc.) determines a corresponding extensive quantity (mass, pressure force, charge, ...) within a given geometrical structure (line, surface, volume, etc.), the calculation is performed as an integral of the intensive quantity over this structure. For example, the mass m of a circular plate with a radius R with a surface density $\sigma = \sigma(r)$, where r is the distance from the center of the plate, can be calculated from the integral

$$m = \int_S \sigma(r)\,\mathrm{d}S = \int_0^R \sigma(r)\,2\pi r\,\mathrm{d}r. \tag{1.58}$$

- **Examples:**

1.107 Calculate the size of the area enclosed "from the bottom" by the parabola $y = x^2$ and "from the top" by the curve $y = \sqrt{x}$.

$\dfrac{1}{3}$

1.108 Calculate the size of the area enclosed "from the bottom" by the parabola $y = x^2$ and "from the top" by the curve $y = x/2 + 5$.

$\dfrac{243}{16}$

1.109 Velocity of a point mass in a one-dimensional case is given by the formula

$$v = 3t - \frac{18}{(t+1)}.$$

Calculate the path that the point mass will go through in the time interval from $t = 0$ to stop. Will the point mass accelerate or brake at this time interval (i.e., will its speed increase or decrease)?

$s = 6\,(1 - 3\ln 3)$, the point mass will brake, the acceleration vector has the opposite direction to the velocity vector.

1.110 The dam is formed by a rectangular vertical concrete wall whose length is L. The depth of the water reservoir is exactly H in the whole length of the dam. What is the total pressure force exerted by the water on the dam?

$F_p = \left(\dfrac{\rho g H}{2} + p_0\right) LH$, where p_0 is the atmospheric pressure on the water surface.

* We solve the integrals in Example (1.97) by "completion to the square" in the Cartesian coordinate system, that is, by multiplying them by the same integral according to the independent variable y, then converting them to polar coordinates and taking the square root.

[3] We do not give the corresponding physical units in the results of the examples with geometric or physical quantities.

1.111 Cylindrical tank with radius R and height H is filled with gas whose density decreases with distance from the cylinder axis. The density drop is given by the function

$$\rho = \rho_0 \, \mathrm{e}^{-\frac{r^2}{10}},$$

where ρ_0 is the density of the gas in the cylinder axis, r is the distance from the cylinder axis.

(a) Calculate the mass of the gas in the tank.

(b) Calculate the total pressure force exerted by the gas on all tank walls if the pressure $p = a^2\rho$, where a is the constant (isothermal) speed of sound.

(c) What will be the total mass and the total pressure force if the radius increases "beyond all limits" ($R \to \infty$)?

(a) $m = 10\pi\rho_0 H \left(1 - \mathrm{e}^{-\frac{R^2}{10}}\right)$

(b) $F_p = 2\pi a^2 \rho_0 \left[10 + \mathrm{e}^{-\frac{R^2}{10}} (RH - 10)\right]$

(c) $m = 10\pi\rho_0 H$, $F_p = 20\pi a^2 \rho_0$

1.112 Cylindrical tank with radius R and height H is filled with gas, whose pressure decreases upwards. The pressure drop is expressed by the function

$$p = p_0 \, \mathrm{e}^{-\frac{h}{20}},$$

where p_0 is the gas pressure at the bottom of the cylinder and h is the vertical distance from the bottom. Calculate the total force that the gas exerts on all tank walls.

$F_p = 40 p_0 \pi R \left(1 - \mathrm{e}^{-\frac{H}{20}}\right) + p_0 \pi R^2 \left(1 + \mathrm{e}^{-\frac{H}{20}}\right)$

1.113 Cylindrical tank with radius R and height H is filled with gas whose pressure decreases with distance from the cylinder axis. The pressure drop is expressed by the function

$$p = \frac{p_0}{1 + \left(\frac{r}{10}\right)^2},$$

where p_0 is the pressure of the gas in the cylinder axis, and r is the distance from the axis. Calculate the total pressure force that the gas exerts on all tank walls.

$F_p = 200\pi p_0 \left[\frac{RH}{100 + R^2} + \ln\left(1 + \frac{R^2}{100}\right)\right]$

1.114 Rectangular container of a square-shaped base with side length A and height H is filled with gas, whose vertical pressure drop is expressed by the function

$$p = \frac{p_0}{\frac{h}{10} + 1},$$

where p_0 is the gas pressure at the bottom of the tank, and h is the vertical distance from the bottom. Calculate the total pressure force that gas exerts on (all) tank walls.

$F_p = p_0 A \left[2A \frac{H + 5}{H + 10} + 40 \ln\left(\frac{H}{10} + 1\right)\right]$

1.115 Circular plate with radius R is electrically charged with surface charge density σ. Calculate the total electric charge Q of the plate (in case of $\sigma = \text{const.}$, the total charge would be given by its product with the area of the surface, $Q = \sigma S$), if

(a) $\sigma = A\,\mathrm{e}^{Br^2}$,

(b) $\sigma = A\ln(r^2 + B)$,

(c) $\sigma = A\,\mathrm{e}^{-\frac{r^2}{3}} + Br$,

(d) $\sigma = A\ln\left(3r^2 + B\right) + Ar$,

where A, B are positive constants and r is the distance from the center of the plate.

(a) $Q = \dfrac{\pi A}{B}\left(\mathrm{e}^{BR^2} - 1\right)$

(b) $Q = \pi A\{(R^2 + B)[\ln(R^2 + B) - 1] - B(\ln B - 1)\}$

(c) $Q = 3\pi A\left(1 - \mathrm{e}^{-\frac{R^2}{3}}\right) + \dfrac{2}{3}\pi BR^3$

(d) $Q = \dfrac{\pi A}{3}\left[\left(3R^2 + B\right)\ln(3R^2 + B) - B\ln B + 2R^3 - 3R^2\right]$

1.116 A thin straight bar (of a negligible thickness) of length L is charged positively with a homogeneous linear (length) charge density τ. The endpoints of the bar are located at the points $[0, 0, 0]$, $[L, 0, 0]$. Calculate the electrostatic potential ϕ excited by the charge of the bar and the electric field intensity vector at the point $P = [-D, 0, 0]$, $D > 0$ (in case of a point charge Q, the electrostatic potential $\phi = Q/(4\pi\epsilon r)$, and the magnitude of the electric field intensity is determined as $E = Q/(4\pi\epsilon r^2)$, where the constant ϵ is the so-called permittivity, and r is the charge distance from the point P). Express the result in terms of the total electric charge Q of the bar.

$$\phi = \frac{Q}{4\pi\epsilon L}\ln\left(\frac{L + D}{D}\right), \qquad \vec{E} = \left(-\frac{Q}{4\pi\epsilon D(L + D)},\ 0,\ 0\right).$$

1.117 A thin straight bar (of a negligible thickness) of length L is charged positively with a homogeneous charge length density τ. The endpoints of the bar are located at the points $[0, 0, 0]$, $[L, 0, 0]$. Calculate the electrostatic potential ϕ excited by the charge of the bar at the point $P = [0, D, 0]$, $D > 0$.

$$\phi = \frac{Q}{4\pi\epsilon L}\ln\left(\frac{L + \sqrt{L^2 + D^2}}{D}\right)$$

1.118 For the same bar from Example 1.117 find the components E_x and E_y of the electric field intensity vector at the point $P = [0, D, 0]$, $D > 0$.

$$E_x = \frac{Q}{4\pi\epsilon L}\left(\frac{1}{\sqrt{L^2 + D^2}} - \frac{1}{D}\right), \qquad E_y = \frac{Q}{4\pi\epsilon D\sqrt{L^2 + D^2}}.$$

1.119 For the same bar from Example 1.117 find the electrostatic potential ϕ and the components E_x a E_y of the electric field intensity vector at the point $P = [L/2, D, 0]$, $D > 0$.

$$\phi = \frac{Q}{2\pi\epsilon L}\ln\left(\frac{L + \sqrt{L^2 + 4D^2}}{2D}\right), \qquad E_x = 0, \qquad E_y = \frac{Q}{2\pi\epsilon D\sqrt{L^2 + 4D^2}}.$$

1.120 A thin arc bar of a negligible thickness with a constant radius R is charged positively with a homogeneous charge length density τ. Endpoints of the bar are located (in polar coordinates) at the points $[R,\, 4\pi/3,\, 0]$, $[R,\, 5\pi/3,\, 0]$. Find the electrostatic potential ϕ and the components E_x and E_y of the electric field intensity vector excited by the charge of the bar at the point $P = [0, 0, 0]$. Express the result in terms of the length density τ and the total charge Q of the bar.

$$\phi = \frac{\tau}{12\epsilon} = \frac{Q}{4\pi\epsilon R}, \quad E_x = 0, \quad E_y = \frac{\tau}{4\pi\epsilon R} = \frac{3Q}{4\pi^2\epsilon R^2}.$$

1.121 Assume a hypothetical homogeneous ($\rho = \text{const.}$) spherical astronomical body with a radius R. The gravitational potential energy of any inner spherical shell of radius $r \in (0, R)$ is mgr, where m is the mass of the spherical shell, and $g = GM_r/r^2$ is the magnitude of the gravitational acceleration at the shell ($G \approx 6,67 \times 10^{-11}\,\mathrm{m^3\,kg^{-1}\,s^{-2}}$ is the gravitational constant). The quantity M_r is the mass of the sphere with the radius r. What will be the total gravitational potential energy of a homogeneous sphere with the radius R? Express the result in terms of the mass of the whole sphere M and its radius R.

$$E_p = \frac{3}{5}G\frac{M^2}{R}$$

Chapter 2

Basics of vector and tensor algebra[1]

2.1 Vectors and matrices

- **Vector calculus:**

Basic vector operations (in orthonormal bases - see Section 2.2) can be briefly written as follows:

- *Norm* (magnitude) of a vector $\vec{a}$ is defined (in $\mathbb{R}^3$) as

$$\|\vec{a}\| = \left(a_1^2 + a_2^2 + a_3^2\right)^{1/2} = \left(\sum_i a_i^2\right)^{1/2}, \tag{2.1}$$

  where the last term assumes that the index i progressively "runs" over all the components $1, 2, 3$, or alternatively x, y, z, of the vector $\vec{a}$. This convention for the so-called *free indexes* allows for much more compact notation of operations with vectors and matrices (for the sake of simplicity we do not introduce here the so-called *covariant* form of superscripts and subscripts yet).

- *Vector sum* of two vectors $\vec{a}$ and $\vec{b}$ whose explicit form of notation (in $\mathbb{R}^3$) is

$$\vec{c} = \vec{a} + \vec{b} = (a_1 + b_1, a_2 + b_2, a_3 + b_3) = (c_1, c_2, c_3), \tag{2.2}$$

  can be, using the given convention with free index i, written as

$$\vec{c} = \vec{a} + \vec{b} = a_i\vec{e}_i + b_i\vec{e}_i = c_i\vec{e}_i, \quad \text{with components} \quad a_i + b_i = c_i \text{ (vector)}, \tag{2.3}$$

  where $\vec{e}_i$ are vectors of the basis (see Section 2.2 for further details).

- *Scalar (dot) product* of two vectors $\vec{a}$ and $\vec{b}$ has the form

$$\vec{a} \cdot \vec{b} = a_i b_j \delta_{ij} = a_i b_i = \alpha \text{ (scalar)}, \tag{2.4}$$

  where indexes i, j again "run" over all components of the both vectors and where the symbol δ_{ij} (the so-called *Kronecker delta* - see Section 2.3 for further details) takes the values $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$. Also, the so-called *Einstein summation convention* is introduced, which states that if an index in any term of a vector equation

[1] Recommended literature for this chapter: Proskuryakov (1978), Young (1993), Kvasnica (2004), Arfken & Weber (2005), Musilová & Musilová (2006).

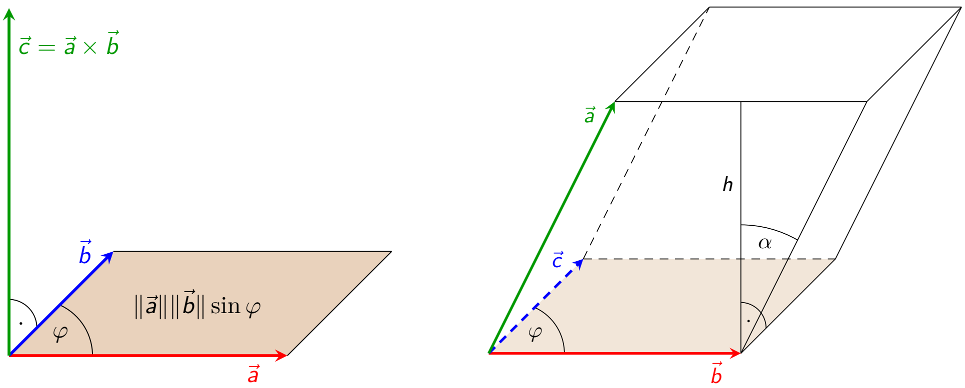

Figure 2.1: *Left panel*: Schematic representation of the geometric meaning of a vector (cross) product, illustrating Equations (2.6) - (2.7). Vector $\vec{c}$, which is the vector product of vectors $\vec{a}$ and $\vec{b}$, is perpendicular to the plane defined by them, and its orientation is given by the "right-hand rule". The color-highlighted area indicates a parallelogram, defined by the vectors $\vec{a}$ and $\vec{b}$, the size of which is equal to the magnitude of the vector $\vec{c}$. *Right panel*: Schematic representation of the geometric meaning of the triple (mixed) product. Vectors $\vec{a}$, $\vec{b}$, $\vec{c}$, form here a right-handed basis, their triple product according to the formula (2.8) gives the positive volume of the parallelepiped defined by them. The same volume is given by the product of the area of the color-highlighted surface (base) and the height h. Vector $\vec{b}\times\vec{c}$ is perpendicular to this base and is oriented upward, its area $\|\vec{b}\times\vec{c}\|$ corresponds to the area of the base. The scalar product of the vector $\vec{a}$ with the vector $\vec{b}\times\vec{c}$ is according to the formula (2.5) equal to $\|\vec{a}\|\|\vec{b}\times\vec{c}\|\cos\alpha$ where however $\|\vec{a}\|\cos\alpha = h$, and so $\vec{a}\cdot(\vec{b}\times\vec{c}) = \|\vec{b}\times\vec{c}\|h$.

repeats twice (*summation index*), we sum all the items with this index and the summation symbol $\sum$ can be omitted. The geometric meaning of a scalar product can be written as

$$\vec{a}\cdot\vec{b} = \|\vec{a}\|\|\vec{b}\|\cos\varphi, \tag{2.5}$$

where φ is the angle between the two vectors $(0 \le \varphi \le \pi)$.

- *Vector (cross) product* of two vectors $\vec{a}$ and $\vec{b}$ is defined as

$$\vec{c} = \vec{a}\times\vec{b} = \varepsilon_{ijk}a_j b_k \vec{e}_i = c_i\vec{e}_i \text{ (vector)}, \tag{2.6}$$

where indexes i, j, k denote particular components of the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$. Symbol ε_{ijk} (the so-called *Levi-Civita symbol* - see more details in Section 2.3) takes the values $\varepsilon_{ijk} = +1$ for even index permutations (i.e., 123, 231, 312), $\varepsilon_{ijk} = -1$ for odd index permutations (i.e., 132, 213, 321) and $\varepsilon_{ijk} = 0$ if ijk is not a permutation of 123 (that is, if any of the indexes repeat). The geometric meaning of the vector product (see left panel in Figure 2.1) can be written as

$$\vec{a}\times\vec{b} = \vec{n}\,\|\vec{a}\|\|\vec{b}\|\sin\varphi, \tag{2.7}$$

where φ is the angle between the vectors $\vec{a}$, $\vec{b}$ $(0 \le \varphi \le \pi)$ and $\vec{n}$ is a unit vector $(\|\vec{n}\| = 1)$ perpendicular to the plane, formed by the vectors $\vec{a}$, $\vec{b}$ (whose orientation is in the right-handed basis given by the right-hand rule). Thus, the magnitude of the vector product $\|\vec{a}\times\vec{b}\| = \|\vec{a}\|\|\vec{b}\|\sin\varphi$ expresses the magnitude of the area of the parallelogram formed by the vectors $\vec{a}$, $\vec{b}$.

- *Mixed (triple) product* of three vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ takes (analogously to Equations (2.4) and (2.6)) the form
$$\vec{a} \cdot (\vec{b} \times \vec{c}) = \varepsilon_{ijk} a_i b_j c_k = \alpha \text{ (scalar)}, \tag{2.8}$$
where indexes i, j, k denote particular components of the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$. Its value expresses the "oriented" volume of the parallelepiped (see right panel in Figure 2.1), formed by the three vectors, i.e., the volume is positive if the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ form a right-handed basis in a given order, it is zero if the vectors do not form a basis, while for a left-handed basis $\vec{a}$, $\vec{b}$, $\vec{c}$ the volume is negative.

- **Matrix calculus:**

The basic concepts of matrix calculus and basic operations with matrices can be briefly written as follows:

- *Matrix multiplication by a number*: If we multiply the matrix $\boldsymbol{A}$ of type $m \times n$ (m rows and n columns) by a number $\lambda \in \mathbb{C}$, the result will be the matrix $\boldsymbol{B} = \lambda \boldsymbol{A}$ of type $m \times n$, where for each element b_{ij} of the matrix $\boldsymbol{B}$ (element on ith row and jth column) holds
$$b_{ij} = \lambda\, a_{ij}. \tag{2.9}$$

- *Matrix summation*: The sum of two matrices $\boldsymbol{A}$ of type $m \times n$ and $\boldsymbol{B}$ of type $m \times n$ will be a matrix $\boldsymbol{C}$ of type $m \times n$, where for each element c_{ij} of the matrix $\boldsymbol{C}$ holds
$$c_{ij} = a_{ij} + b_{ij}. \tag{2.10}$$

- *Matrix multiplication*: The product of two matrices $\boldsymbol{A}$ of type $m \times \ell$ and $\boldsymbol{B}$ of type $\ell \times n$ will be a matrix $\boldsymbol{C} = \boldsymbol{AB}$ of type $m \times n$, where for each element c_{ij} of the matrix $\boldsymbol{C}$ holds
$$c_{ij} = \sum_{k=1}^{\ell} a_{ik} b_{kj} = a_{ik} b_{kj}, \tag{2.11}$$
where the last expression is written using Einstein's summation convention. If we write the formula (2.11) explicitly, we get $c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31}$, $c_{12} = a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32}$, etc. Multiplication of matrices is not commutative, so generally $\boldsymbol{AB} \neq \boldsymbol{BA}$ is true. In addition, matrix multiplication in both directions can only be performed if the matrix $\boldsymbol{A}$ is of type $m \times n$ and the matrix $\boldsymbol{B}$ is of type $n \times m$, so the resulting matrices will be of type $m \times m$ for the product $\boldsymbol{AB}$, or $n \times n$ for the product $\boldsymbol{BA}$.

- *Matrix rank* is defined as the number of linearly independent rows, i.e., the number of non-zero rows after the so-called Gaussian elimination (after matrix reduction to the echelon form). If the rank h of a square matrix $\boldsymbol{A}$ (of the type $n \times n$) $h(\boldsymbol{A}) < n$, it is the *singular* matrix, if $h(\boldsymbol{A}) = n$, it is the *regular* matrix.

- *Trace of the square matrix* $\boldsymbol{A}$ is defined as the sum of the elements on the main diagonal of the matrix, i.e., for each element a_{ij} of the matrix $\boldsymbol{A}$ holds
$$\mathrm{tr}(\boldsymbol{A}) = \sum_{i,j} a_{ij}\delta_{ij} = \sum_{i} a_{ii} = a_{ii}, \tag{2.12}$$
where the last expression is written using Einstein's summation convention. In addition, if $\boldsymbol{A} = (a_{ij}) = 0$ for all $i \neq j$, it is the so-called *diagonal* matrix, if $\boldsymbol{A} = (a_{ij}) = \delta_{ij}$, it is a unit matrix (denoted by $\boldsymbol{E}$ or $\mathbf{1}$).

- *Transposed matrix* $\boldsymbol{A}^T$ is created from the matrix $\boldsymbol{A}$ by interchanging rows and columns, for each element of the transposed matrix holds $a^T_{ij} = a_{ji}$. If $\boldsymbol{A}^T = \boldsymbol{A}$ holds, then the matrix $\boldsymbol{A}$ is called *symmetric*, where each element $a_{ij} = a_{ji}$. The matrix $\boldsymbol{A}$ is called *antisymmetric*, if $a_{ij} = -a_{ji}$ holds for each of its elements, then all the elements on the main diagonal will be zero and hence $\mathrm{tr}(\boldsymbol{A}) = 0$.

- *Determinant* of a square matrix $\boldsymbol{A}$ of the type $n \times n$ will be the scalar $\det \boldsymbol{A}$, which can be generally defined, e.g., using the Levi-Civita symbol:

$$\det \boldsymbol{A} = \sum_{j_1, j_2, \ldots, j_n} \varepsilon_{j_1 j_2 \cdots j_n} a_{j_1 1} a_{j_2 2} \cdots a_{j_n n}. \tag{2.13}$$

  So we have $\det \boldsymbol{A} = a_{11}$ for $n = 1$ while for $n = 2$ we have $\det \boldsymbol{A} = a_{11}a_{22} - a_{21}a_{12}$ and for $n = 3$ we have $\det \boldsymbol{A} = a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33} - a_{31}a_{22}a_{13}$ (the so-called *rule of Sarrus*). The Levi-Civita symbol can also be defined in an n-dimensional space in general. In this case, it will contain n different indexes, with even permutations being created by an even number of numeric exchanges, odd permutations by an odd number of numeric exchanges, the total number of permutations without repetition is $n!$ (see Section 12.1). For example, even permutations of ε_{ijkl} in four-dimensional space-time will be ε_{0123}, ε_{0231}, ε_{0312}, ε_{1032}, ε_{1320}, ε_{1203}, ε_{2130}, ε_{2301}, ε_{2013}, ε_{3210}, ε_{3102}, ε_{3021}. The other 12 permutations (without repetitions) will be odd. Determinant of a singular matrix $\det \boldsymbol{A} = 0$, determinant of a regular matrix $\det \boldsymbol{A} \neq 0$.

- *Inverse matrix* to the regular square matrix $\boldsymbol{A}$ will be a matrix $\boldsymbol{B} = \boldsymbol{A}^{-1}$ if it holds

$$\boldsymbol{AB} = \boldsymbol{BA} = \boldsymbol{E}. \tag{2.14}$$

- *Hermitian conjugate matrix* (usually denoted by $\boldsymbol{A}^H$ in linear algebra, $\boldsymbol{A}^\dagger$ or $\boldsymbol{A}^+$ in quantum mechanics) is a designation for a matrix that is complex conjugate and transposed,

$$\boldsymbol{A}^H = (\boldsymbol{A}^*)^T. \tag{2.15}$$

  If $\boldsymbol{A}^H = \boldsymbol{A}^T$, it is a real matrix. If $\boldsymbol{A}^H = \boldsymbol{A}$, we call it the *Hermitian matrix*.

- *Unitary matrix* $\boldsymbol{U}$ is a regular square matrix, whose hermitian conjugate matrix is simultaneously the inverse matrix, that is $\boldsymbol{U}^H = \boldsymbol{U}^{-1}$, and so

$$\boldsymbol{U}^H \boldsymbol{U} = \boldsymbol{U}\boldsymbol{U}^H = \boldsymbol{E}. \tag{2.16}$$

  Real unitary matrix $\boldsymbol{U}^H = \boldsymbol{U}^T$ is the so-called *orthogonal* matrix, where its rows or columns form an orthonormal system of vectors (see Section 2.2).

- A number λ is called *eigenvalue* and the nonzero vector $\vec{v}$ is called (right) *eigenvector* of a square matrix $\boldsymbol{A}$ of the type $n \times n$, if the condition

$$\boldsymbol{A}\vec{v} = \lambda\vec{v} \tag{2.17}$$

  is met, the matrix $\boldsymbol{A}$ thus acts on the eigenvector as a scalar, i.e., it does not change its direction (in case of the so-called left eigenvectors Equation (2.17) will take the form $\vec{v}\boldsymbol{A} = \lambda\vec{v}$). From Equation (2.17) results directly the relation for determining the eigenvalues of the matrix $\boldsymbol{A}$, where a system of n linear equations

$$(\boldsymbol{A} - \lambda\boldsymbol{E})\,\vec{v} = \vec{0} \wedge \vec{v} \neq \vec{0}, \qquad \text{so} \qquad \sum_{j=1}^{n} (a_{ij} - \lambda\delta_{ij}) v_j = 0 \quad \text{for} \quad i = 1, 2, \ldots, n \tag{2.18}$$

has a nonzero solution if and only if the matrix of this system is singular, that is, if

$$\det(\boldsymbol{A} - \lambda \boldsymbol{E}) = 0. \tag{2.19}$$

The eigenvectors corresponding to each eigenvalue are then determined by Equation (2.18). Right eigenvectors will thus take the form $c_r(v_{1r}, v_{2r}, \cdots, v_{nr})^T$ and left eigenvectors will be $c_l(v_{1\ell}, v_{2\ell}, \cdots, v_{n\ell})$, where c_r and c_ℓ are arbitrary constants.

- *Submatrix* of a matrix $\boldsymbol{A}$ is obtained by omitting selected rows and/or columns in the $\boldsymbol{A}$ matrix. Determinant of a regular square submatrix is called *subdeterminant* or *minor*.

- For a more detailed study of the problematic of calculation with vectors and matrices, I recommend, for example, the following textbooks: Proskuryakov (1978); Young (1993); Kvasnica (2004).

- **Examples:**

2.1 Given are the vectors $\vec{a} = (0, 2, 4)$, $\vec{b} = (1, 3, 5)$ and $\vec{c} = (6, 1, 3)$. Calculate $|\vec{a}|$, $|\vec{b}|$, $|\vec{c}|$, $\vec{a} \times (\vec{b} \times \vec{c})$, $(\vec{a} \times \vec{b}) \times \vec{c}$, $(\vec{a} + \vec{b}) \cdot (\vec{c} - \vec{a})$, $(\vec{b} + \vec{c}) \times (\vec{a} - \vec{b})$, $(\vec{a} \cdot \vec{b})^2 + (\vec{c} \times \vec{a})^2$.

$\sqrt{20}$, $\sqrt{35}$, $\sqrt{46}$, $(-142, 16, -8)$, $(14, -6, -26)$, -8, $(4, -1, -3)$, 1400

2.2 Calculate the area of a parallelogram whose vertices are defined by the points $A = [0, 0, 0]$, $B = [1, 2, 3]$, C, and $D = [3, 2, 1]$. Calculate the coordinates of the point C.

$4\sqrt{6}$, $C = [4, 4, 4]$

2.3 The points $A = [2, 1, 0]$, $B = [2, 2, 3]$, $C = [0, 1 + \sqrt{40}, 0]$ define vertices of a triangle. Use the vector product to find its area.

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2.4 The points $A = [4, 1, 0]$, $B = [4, -2, -3]$, $C = [1, -5, -3]$ define vertices of a triangle. Specify the magnitudes of the triangle's internal angles and using the vector product, calculate its area.

$\frac{\pi}{6}, \frac{2\pi}{3}, \frac{\pi}{6}, \frac{9\sqrt{3}}{2}$

2.5 The points $A = [2, -4, 9]$, $B = [-1, -4, 5]$, $C = [6, -4, 6]$ define vertices of a triangle. Calculate its area using the vector product and specify the magnitude of the angle α.

$\frac{25}{2}, \frac{\pi}{4}$

2.6 Given are the matrices $\boldsymbol{A} = \begin{pmatrix} 3 & -5 & 7 \\ -2 & 9 & 4 \end{pmatrix}$, $\boldsymbol{B} = \begin{pmatrix} -2 & 5 \\ 4 & -3 \\ 2 & 1 \end{pmatrix}$. Calculate $\boldsymbol{AB}$, $\boldsymbol{BA}$.

$\boldsymbol{AB} = \begin{pmatrix} -12 & 37 \\ 48 & -33 \end{pmatrix}$, $\quad \boldsymbol{BA} = \begin{pmatrix} -16 & 55 & 6 \\ 18 & -47 & 16 \\ 4 & -1 & 18 \end{pmatrix}$

2.7 Given are the matrices $\boldsymbol{A} = \begin{pmatrix} 2 & 1 & 3 \\ 0 & 1 & -7 \end{pmatrix}$, $\boldsymbol{B} = \begin{pmatrix} 3 & 2 & 0 \\ -2 & 1 & 2 \\ 4 & -2 & 1 \end{pmatrix}$, $\boldsymbol{C} = \begin{pmatrix} 2 & 1 \\ -1 & 3 \end{pmatrix}$. Calculate all matrix products of different matrices (in any order and number of them) and calculate also all determinants and inverse matrices.

$$\boldsymbol{AB} = \begin{pmatrix} 16 & -1 & 5 \\ -30 & 15 & -5 \end{pmatrix}, \ \boldsymbol{CA} = \begin{pmatrix} 4 & 3 & -1 \\ -2 & 2 & -24 \end{pmatrix}, \ \boldsymbol{CAB} = \begin{pmatrix} 2 & 13 & 5 \\ -106 & 46 & -20 \end{pmatrix},$$

$$\det \boldsymbol{B} = 35, \ \det \boldsymbol{C} = 7, \ \boldsymbol{B}^{-1} = \frac{1}{35}\begin{pmatrix} 5 & -2 & 4 \\ 10 & 3 & -6 \\ 0 & 14 & 7 \end{pmatrix}, \ \boldsymbol{C}^{-1} = \frac{1}{7}\begin{pmatrix} 3 & -1 \\ 1 & 2 \end{pmatrix}$$

2.8 Calculate inverse matrix to the matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 0 & -2 \\ -2 & 1 & 3 \\ 0 & 1 & -2 \end{pmatrix}$. $\quad \boldsymbol{A}^{-1} = \begin{pmatrix} 5 & 2 & -2 \\ 4 & 2 & -1 \\ 2 & 1 & -1 \end{pmatrix}$

2.9 Given are the matrices $\boldsymbol{A} = \begin{pmatrix} 3 & 1 & 2 \\ 0 & 2 & 1 \\ -1 & 3 & 3 \end{pmatrix}$, $\boldsymbol{B} = \begin{pmatrix} 0 & 1 & 1 \\ -1 & 0 & 2 \end{pmatrix}$. Calculate inverse matrix $\boldsymbol{A}^{-1}$ and the matrix $\boldsymbol{D} = \boldsymbol{BA}^{-1}$.

$$\boldsymbol{A}^{-1} = \frac{1}{12}\begin{pmatrix} 3 & 3 & -3 \\ -1 & 11 & -3 \\ 2 & -10 & 6 \end{pmatrix}, \qquad \boldsymbol{D} = \frac{1}{12}\begin{pmatrix} 1 & 1 & 3 \\ 1 & -23 & 15 \end{pmatrix}$$

2.10 Find the determinant of the matrix $\boldsymbol{A} = \begin{pmatrix} 2 & 3 & 0 & 4 \\ 1 & 2 & 1 & 1 \\ 3 & 4 & 1 & 1 \\ 1 & 2 & 2 & -1 \end{pmatrix}$. $\quad \det \boldsymbol{A} = 2$

2.11 Find the determinant of the matrix $\boldsymbol{A} = \begin{pmatrix} 2 & 0 & -3 & 3 \\ 1 & 4 & 3 & -1 \\ 1 & -4 & 8 & 0 \\ 0 & 3 & -1 & 2 \end{pmatrix}$. $\det \boldsymbol{A} = 294$

2.12 Find the determinant of the matrix $\boldsymbol{A} = \begin{pmatrix} 2 & 2 & 1 & 1 & 1 \\ 5 & 6 & 3 & 4 & 5 \\ 7 & 5 & 3 & 5 & 7 \\ 13 & 10 & 3 & 8 & 13 \\ 7 & 2 & 1 & 1 & 6 \end{pmatrix}$. $\det \boldsymbol{A} = 120$

2.13 Calculate the rank of the matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 1 \\ 0 & 5 & -1 \\ 2 & -1 & 3 \end{pmatrix}$. $\quad h(\boldsymbol{A}) = 2$

2.14 Calculate the rank of the matrix $\boldsymbol{A} = \begin{pmatrix} -1 & 1 & 2 & 4 \\ 0 & 1 & -1 & 2 \\ 2 & -1 & 0 & 3 \end{pmatrix}$. $\quad h(\boldsymbol{A}) = 3$

2.15 Given are the matrices $\boldsymbol{A} = \begin{pmatrix} 1 & -1 & 1 \\ 0 & 5 & 2 \\ 1 & -4 & 0 \end{pmatrix}$, $\boldsymbol{B} = \begin{pmatrix} 0 & 1 & 2 \\ -2 & 9 & 3 \\ 10 & 6 & 0 \end{pmatrix}$, $\boldsymbol{C} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 4 & 9 \\ 1 & 2 & 4 \end{pmatrix}$. Calculate the matrices $\boldsymbol{P} = \boldsymbol{A} - \boldsymbol{B}^T - 3\boldsymbol{C}$, $\boldsymbol{Q} = (3\boldsymbol{A}^T + \boldsymbol{B})\boldsymbol{C}$, $\boldsymbol{R} = \boldsymbol{C}^2\boldsymbol{B}$, $\boldsymbol{S} = \boldsymbol{CBC}$ and determinants of the matrices $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$.

$$\boldsymbol{P} = \begin{pmatrix} -2 & -5 & -18 \\ -4 & -16 & -31 \\ -4 & -13 & -12 \end{pmatrix}, \quad \boldsymbol{Q} = \begin{pmatrix} 9 & 20 & 38 \\ 10 & 68 & 165 \\ 25 & 74 & 147 \end{pmatrix}, \quad \boldsymbol{R} = \begin{pmatrix} 298 & 348 & 60 \\ 678 & 788 & 136 \\ 334 & 391 & 68 \end{pmatrix},$$

$$\boldsymbol{S} = \begin{pmatrix} 71 & 216 & 443 \\ 187 & 556 & 1121 \\ 87 & 260 & 527 \end{pmatrix}, \quad \det \boldsymbol{A} = 1, \quad \det \boldsymbol{B} = -174, \quad \det \boldsymbol{C} = 2$$

2.16 Calculate the minor of a submatrix $\boldsymbol{B}$ of the matrix $\boldsymbol{A}$ from Example 2.14, if the submatrix $\boldsymbol{B}$ is formed:

(a) by the 1st and 3rd rows, and the 1st and 2nd columns of the matrix $\boldsymbol{A}$,

(b) by the 2nd and 3rd rows, and the 2nd and 4th columns of the matrix $\boldsymbol{A}$,

(c) by the 1st and 3rd rows, and the 2nd and 4th columns of the matrix $\boldsymbol{A}$,

(d) by all the rows and the 1st, 3rd, and 4th columns of the matrix $\boldsymbol{A}$.

(a) $M = -1$, (b) $M = 5$, (c) $M = 7$, (d) $M = 19$

2.2 Bases and their transformations

Basis of a vector space V of a dimension n can be defined as an ordered n-tuple of linearly independent vectors that generate a vector space V, i.e., where each vector of the vector space V can be expressed as a linear combination of these (basis) vectors. Orthogonal and orthonormal bases play an important role in practical calculations. *Orthogonal basis* is a special case of a general basis where different basis vectors are perpendicular to each other. For basis vectors $\vec{x}_i$, $\vec{x}_j$, $i \neq j$ therefore holds

$$\vec{x}_i \cdot \vec{x}_j = 0, \quad \text{or} \quad (\vec{x}_i, \vec{x}_j) = 0 \quad \text{in the algebraic notation.} \tag{2.20}$$

Orthonormal basis is the special case of an orthogonal basis, where all the basis vectors (denoted in this case $\vec{e}_i$, while also the notation $\hat{\boldsymbol{x}}_i$ is often used) have a unit length,

$$\vec{e}_i \cdot \vec{e}_j = \delta_{ij}, \quad \text{or} \quad (\vec{e}_i, \vec{e}_j) = \delta_{ij}. \tag{2.21}$$

Within an example shown in Figure 2.2, we construct basis transition matrices and show the principles of representation of the vector in different bases in $\mathbb{R}^2$ (in case of a higher dimension of a vector space, the procedure will be completely analogous). Two bases $\mathcal{E}$ and $\mathcal{F}$ are introduced, black and red, with basis vectors $\vec{e}_1$, $\vec{e}_2$ and $\vec{f}_1$, $\vec{f}_2$, where the black basis is orthonormal and the red basis is quite general. The transition from the red basis $\mathcal{F}$ to the black basis $\mathcal{E}$ is given by the relations (corresponding to the vector sum)

$$\begin{aligned} \vec{f}_1 &= 2.5\,\vec{e}_1 + 0.5\,\vec{e}_2, \\ \vec{f}_2 &= 0.3\,\vec{e}_1 + \vec{e}_2. \end{aligned} \tag{2.22}$$

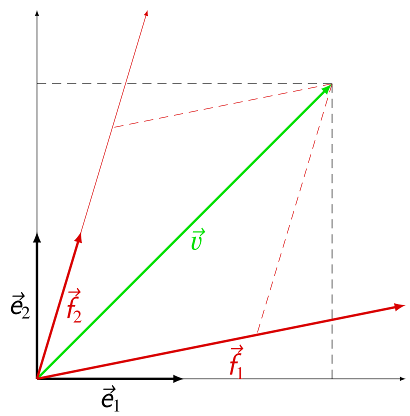

Figure 2.2: Schematic representation of the vector $\vec{v}$, denoted by green color, in two different bases in $\mathbb{R}^2$, in black orthonormal basis with basis vectors $\vec{e}_1$, $\vec{e}_2$ and in a red marked general basis with basis vectors $\vec{f}_1$, $\vec{f}_2$. The transition from the red to the black basis is given by the relations: $\vec{f}_1 = 2.5\,\vec{e}_1 + 0.5\,\vec{e}_2$, $\vec{f}_2 = 0.3\,\vec{e}_1 + \vec{e}_2$. In the black basis, the vector $\vec{v}$ has components $(2,2)$, the magnitude of the components is represented by the projection of vector $\vec{v}$ into the directions of each basis vector, highlighted by black dashed lines and means the ratio of the size of these projections to the length of the respective basis vectors. The same applies to the red-marked basis, where the magnitude of the components is given by the projection of the vector $\vec{v}$ into the directions of the particular basis vectors, highlighted by the red dashed lines. The magnitudes of the components of $\vec{v}$ in the red basis will be $\left(\frac{28}{47}, \frac{80}{47}\right) \approx (0.6,\ 1.7)$.

So we can immediately write the transition matrix $\boldsymbol{S}$ from the $\mathcal{F}$ basis to the $\mathcal{E}$ basis:

$$\boldsymbol{S}\,(\mathcal{F} \mapsto \mathcal{E}) = \begin{pmatrix} \frac{5}{2} & \frac{1}{2} \\ \frac{3}{10} & 1 \end{pmatrix}. \tag{2.23}$$

The transition matrix ((2.23) and all others) can also be written using the column formalism, i.e., the vectors $\vec{f}_1$, $\vec{f}_2$ can be written as column vectors. In this case, the transitional matrix, written as “column” (which means its transpose), will multiply any vector also written as column (see Equation (2.29) in the following explanation) written behind the matrix. The other principles described below will remain unchanged.

From Equations (2.22) we can easily derive equations for $\vec{e}_1$, $\vec{e}_2$, i.e., equations of the reverse transition from the black basis $\mathcal{E}$ to the red basis $\mathcal{F}$:

$$\begin{aligned} \vec{e}_1 &= \frac{20}{47}\vec{f}_1 - \frac{10}{47}\vec{f}_2, \\ \vec{e}_2 &= -\frac{6}{47}\vec{f}_1 + \frac{50}{47}\vec{f}_2. \end{aligned} \tag{2.24}$$

In the matrix notation it will be the matrix of reverse transition $\boldsymbol{T}$ which is inverse to the matrix $\boldsymbol{S}$, so $\boldsymbol{T} = \boldsymbol{S}^{-1}$:

$$\boldsymbol{T}\,(\mathcal{E} \mapsto \mathcal{F}) = \begin{pmatrix} \frac{20}{47} & -\frac{10}{47} \\ -\frac{6}{47} & \frac{50}{47} \end{pmatrix}. \tag{2.25}$$

The given (green) vector $\vec{v}$ has the horizontal and vertical component in the black basis $\mathcal{E}$ represented by projection of the vector into the horizontal and vertical axis, i.e., in the directions that correspond to the basis vectors $\vec{e}_1$, $\vec{e}_2$. The magnitudes of these components will correspond to the ratio of the lengths of these projections (black dashed lines) to the corresponding basis vectors, so we can write the vector $\vec{v}$ as a vector sum (in this case of the pre-selected) multiples of the basis vectors $\mathcal{E}$, or with use of only the components:

$$\vec{v} = 2\,\vec{e}_1 + 2\,\vec{e}_2, \quad \text{or} \quad \vec{v} = (2,2), \tag{2.26}$$

in the second case we implicitly assume that we "live" in the basis $\mathcal{E}$. Determining the components of the vector $\vec{v}$ in the red basis $\mathcal{F}$ will be quite similar. The projections of the vector $\vec{v}$ into the directions of the basis vectors $\vec{f}_1$, $\vec{f}_2$ are shown as the red dashed lines, the components magnitudes will again correspond to the ratio of the lengths of these projections and the corresponding basis vectors. Realizing that the vector $\vec{v}$ is the same in all the bases and therefore the vector sum of its components must be the same no matter from which basis we "observe" it, we can determine its components in the basis $\mathcal{F}$ by analogy to Equation (2.26), we can generally write

$$\vec{v} = a\vec{f}_1 + b\vec{f}_2 = 2\,\vec{e}_1 + 2\,\vec{e}_2. \tag{2.27}$$

Substituting for vectors $\vec{e}_1$, $\vec{e}_2$ from Equation (2.24), we calculate the length of the components a, b:

$$\vec{v} = \frac{28}{47}\vec{f}_1 + \frac{80}{47}\vec{f}_2, \quad \text{or} \quad \vec{v} = \left(\frac{28}{47}, \frac{80}{47}\right), \tag{2.28}$$

where in the second case, we again implicitly assume that we "live" in the basis $\mathcal{F}$. The same result is obtained by multiplying the vector $\vec{v}$, written using its components in the black basis $\mathcal{E}$, by the matrix $\boldsymbol{T}$ of the transition from the black basis $\mathcal{E}$ to the red basis $\mathcal{F}$:

$$(a,b) = (2,2)\begin{pmatrix} \dfrac{20}{47} & -\dfrac{10}{47} \\ -\dfrac{6}{47} & \dfrac{50}{47} \end{pmatrix} = \left(\frac{28}{47}, \frac{80}{47}\right). \tag{2.29}$$

The reverse transformation can be verified by multiplying the obtained components (a,b) of the vector $\vec{v}$ in the basis $\mathcal{F}$ by the matrix $\boldsymbol{S}$ of the transition from the red basis $\mathcal{F}$ to the black basis $\mathcal{E}$, the result must be the original components of the vector $\vec{v}$ in the basis $\mathcal{E}$:

$$\left(\frac{28}{47}, \frac{80}{47}\right)\begin{pmatrix} \dfrac{5}{2} & \dfrac{1}{2} \\ \dfrac{3}{10} & 1 \end{pmatrix} = (2,2). \tag{2.30}$$

Similarly, we would find that in another "red basis" $\mathcal{F}$, given for example by the transformation

$$\begin{aligned} \vec{f}_1 &= 2\,\vec{e}_1 + 0.5\,\vec{e}_2, \\ \vec{f}_2 &= \vec{e}_1 + \vec{e}_2, \end{aligned} \tag{2.31}$$

(where the basis $\mathcal{E}$ is again orthonormal) will a representation of the general vector $\vec{a} = 3\,\vec{e}_1 + 1.5\,\vec{e}_2 = \left(3, \frac{3}{2}\right)$ take the form (try to sketch yourself the corresponding image)

$$\vec{a} = \vec{f}_1 + \vec{f}_2 = (1,1)\,. \tag{2.32}$$

In case of orthonormal bases, the transition matrices between them will be rotational, i.e., orthogonal. So it must hold: $\boldsymbol{T}^{-1} = \boldsymbol{T}^T$ and at the same time: $\det \boldsymbol{T} = \det \boldsymbol{T}^{-1} = \pm 1$ (if $\det \boldsymbol{T} = \det \boldsymbol{T}^{-1} = -1$, this is a so-called false (improper) rotation, i.e., rotation associated with mirroring in a plane perpendicular to axis of rotation). For further details on vector and matrix calculations, including calculations with bases, follow the appropriate linear algebra courses.

- **Examples:**

2.17 In a vector space $\mathbb{R}^3$ there are given the vectors $\vec{v}_1 = (1,2,1)$, $\vec{v}_2 = (-1,1,1)$, and $\vec{v}_3 = (2,1,0)$. Do these vectors generate the basis of this vector space? no

2.18 Let the vectors $\vec{e}_1$, $\vec{e}_2$, $\vec{e}_3$, $\vec{e}_4$ form an orthonormal basis of the vector space $\mathbb{R}^4$. Decide if the vectors $\vec{u} = 2\vec{e}_1 + \vec{e}_2 + \vec{e}_3 - \vec{e}_4$, $\vec{v} = \vec{e}_1 - \vec{e}_2 + \vec{e}_3 + \vec{e}_4$, $\vec{w} = \vec{e}_2 - \vec{e}_3 - \vec{e}_4$, and $\vec{z} = \vec{e}_1 + \vec{e}_2 + \vec{e}_3$, form as well a basis of this vector space. yes

2.19 Find the transition matrices between the standard orthonormal basis (in the Cartesian system) and the orthonormal basis of the cylindrical system (for transformation equations see Section 4.2).

$$\begin{pmatrix} \vec{e}_r \\ \vec{e}_\phi \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix}, \quad \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{e}_r \\ \vec{e}_\phi \\ \vec{e}_z \end{pmatrix}$$

2.20 Find the transition matrices between the standard orthonormal basis (in the Cartesian system) and the orthonormal basis of the spherical system (for transformation equations see Section 4.3).

$$\begin{pmatrix} \vec{e}_r \\ \vec{e}_\theta \\ \vec{e}_\phi \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix},$$

$$\begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} \vec{e}_r \\ \vec{e}_\theta \\ \vec{e}_\phi \end{pmatrix}$$

2.21 Find the transition matrix for components of a position vector of a fixed point if you rotate the Cartesian coordinate system by an angle α about the z-axis (the so-called rotation matrix). The position vector of a general point in the rotated system is denoted by $\vec{r}\,' = (x', y', z')$, the position vector of the same point in the original system is $\vec{r} = (x, y, z)$.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

2.22 Find the matrix $\boldsymbol{G}$ of Galilean space-time transformation. Galilean space-time transformation is given by the transition $(t', x', y', z')^T \mapsto (t, x, y, z)^T$ where $t' = t$, $x' = x - v_x t$, $y' = y - v_y t$, and $z' = z - v_z t$, where the vector $\vec{v} = (v_x, v_y, v_z)$ is interpreted as velocity and $\vec{u}$ is a similar velocity vector in the primed system. Multiply the matrices to prove the relation $\boldsymbol{G}_{\vec{u}}\boldsymbol{G}_{\vec{v}} = \boldsymbol{G}_{\vec{u}+\vec{v}}$ and explain why this relation is called the *classical rule for velocity-addition.*

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -v_x & 1 & 0 & 0 \\ -v_y & 0 & 1 & 0 \\ -v_z & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ -v_x - u_x & 1 & 0 & 0 \\ -v_y - u_y & 0 & 1 & 0 \\ -v_z - u_z & 0 & 0 & 1 \end{pmatrix}$$

2.23 Vector $\vec{a}$ has in an *orthonormal* basis $\mathcal{B}$ in $\mathbb{R}^2$ the components $(11/2, -1)$. Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1\,' &= 4\,\vec{e}_1 + \vec{e}_2, \\ \vec{e}_2\,' &= \frac{3}{2}\vec{e}_1 - 2\,\vec{e}_2. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{B}$, and components of the vector $\vec{a}$ in the basis $\mathcal{B}'$. Is the basis $\mathcal{B}'$ orthonormal (specify the reason)? Draw a picture showing the length and direction of all the vectors, i.e., of basis vectors of both the bases and also the vector $\vec{a}$.

$$\boldsymbol{T} = \begin{pmatrix} \frac{4}{19} & \frac{2}{19} \\ \frac{3}{19} & -\frac{8}{19} \end{pmatrix}, \quad \boldsymbol{S} = \begin{pmatrix} 4 & 1 \\ \frac{3}{2} & -2 \end{pmatrix}, \quad \vec{a}_{(\mathcal{B}')} = (1,1), \quad \text{basis } \mathcal{B}' \text{ is not orthonormal.}$$

2.24 Vector $\vec{a}$ has in an *orthonormal* basis $\mathcal{B}$ the components $(1,0,-2)$. Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= -\vec{e}_1{}' + \vec{e}_2{}' - \vec{e}_3{}', \\ \vec{e}_2 &= \vec{e}_1{}' + 2\,\vec{e}_3{}', \\ \vec{e}_3 &= \vec{e}_1{}' + \vec{e}_2{}' + 2\,\vec{e}_3{}'. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{B}$, and components of the vector $\vec{a}$ in the basis $\mathcal{B}'$. Is the basis $\mathcal{B}'$ orthonormal (specify the reason)?

$\boldsymbol{T} = \begin{pmatrix} -1 & 1 & -1 \\ 1 & 0 & 2 \\ 1 & 1 & 2 \end{pmatrix}$, $\boldsymbol{S} = \begin{pmatrix} -2 & -3 & 2 \\ 0 & -1 & 1 \\ 1 & 2 & -1 \end{pmatrix}$, $\vec{a}_{(\mathcal{B}')} = (-3,-1,-5)$, basis $\mathcal{B}'$ is not orthonormal.

2.25 Vector $\vec{a}$ has in an *orthonormal* basis $\mathcal{B}'$ the components $(1,2,-1)$. Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \vec{e}_2{}' - \vec{e}_3{}', \\ \vec{e}_2 &= \vec{e}_1{}' + 2\,\vec{e}_3{}', \\ \vec{e}_3 &= \vec{e}_1{}' + \vec{e}_2{}' + 2\,\vec{e}_3{}'. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{B}$, and components of the vector $\vec{a}$ in the basis $\mathcal{B}$. Is the basis $\mathcal{B}$ orthonormal (specify the reason)?

$\boldsymbol{T} = \begin{pmatrix} 0 & 1 & -1 \\ 1 & 0 & 2 \\ 1 & 1 & 2 \end{pmatrix}$, $\boldsymbol{S} = \begin{pmatrix} 2 & 3 & -2 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \end{pmatrix}$, $\vec{a}_{(\mathcal{B})} = (3,2,-1)$, basis $\mathcal{B}$ is not orthonormal.

2.26 Vector $\vec{a}$ has in an *orthonormal* basis $\mathcal{B}'$ the components $(1,1,1)$. Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \vec{e}_1{}' - 2\,\vec{e}_2{}' - 3\,\vec{e}_3{}', \\ \vec{e}_2 &= 2\,\vec{e}_1{}' - \vec{e}_2{}' - \vec{e}_3{}', \\ \vec{e}_3 &= -\vec{e}_1{}' + \vec{e}_2{}' + \vec{e}_3{}'. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{B}$, and components of the vector $\vec{a}$ in the basis $\mathcal{B}$. Is the basis $\mathcal{B}$ orthonormal (specify the reason)?

$\boldsymbol{T} = \begin{pmatrix} 1 & -2 & -3 \\ 2 & -1 & -1 \\ -1 & 1 & 1 \end{pmatrix}$, $\boldsymbol{S} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 2 & 5 \\ -1 & -1 & -3 \end{pmatrix}$, $\vec{a}_{(\mathcal{B})} = (0,2,3)$, basis $\mathcal{B}$ is not orthonormal.

2.27 Vector $\vec{a}$ has in the standard Cartesian basis $\mathcal{E}$ the components $(1,-\sqrt{3},1)$. In addition, two bases $\mathcal{B}$ and $\mathcal{B}'$ are specified, where the matrix $\boldsymbol{R}^{-1}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{E}$ has the form

$$\boldsymbol{R}^{-1}(\mathcal{B}' \longmapsto \mathcal{E}) = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \vec{e}_1^{\,\prime} - \vec{e}_2^{\,\prime} - 2\,\vec{e}_3^{\,\prime}, \\ \vec{e}_2 &= 2\,\vec{e}_1^{\,\prime} - \vec{e}_2^{\,\prime} + \vec{e}_3^{\,\prime}, \\ \vec{e}_3 &= -\vec{e}_1^{\,\prime} + \vec{e}_2^{\,\prime} + 3\,\vec{e}_3^{\,\prime}. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{B}$, and components of the vector $\vec{a}$ in the bases $\mathcal{B}$ and $\mathcal{B}'$. Are the bases $\mathcal{B}$ and $\mathcal{B}'$ orthonormal (specify the reason)?

$\boldsymbol{T} = \begin{pmatrix} 1 & -1 & -2 \\ 2 & -1 & 1 \\ -1 & 1 & 3 \end{pmatrix}$, $\boldsymbol{S} = \begin{pmatrix} -4 & 1 & -3 \\ -7 & 1 & -5 \\ 1 & 0 & 1 \end{pmatrix}$, $\vec{a}_{(\mathcal{B}')} = (0,-2,1)$, $\vec{a}_{(\mathcal{B})} = (15,-2,11)$,

$\mathcal{B}'$ yes, $\mathcal{B}$ no.

2.28 Vector $\vec{a}$ has in the standard Cartesian basis $\mathcal{E}$ the components $(1,1,1)$. In addition, two bases $\mathcal{B}$ and $\mathcal{B}'$ are specified, where the matrix $\boldsymbol{R}^{-1}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{E}$ has the form

$$\boldsymbol{R}^{-1}(\mathcal{B}' \longmapsto \mathcal{E}) = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}. \qquad \boldsymbol{R} = \begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ 1 & 0 & \frac{1}{2} \end{pmatrix}$$

Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \vec{e}_2^{\,\prime} + \vec{e}_3^{\,\prime}, \\ \vec{e}_2 &= 2\,\vec{e}_1^{\,\prime} + \vec{e}_3^{\,\prime}, \\ \vec{e}_3 &= -\vec{e}_1^{\,\prime} + \vec{e}_2^{\,\prime} \quad . \end{aligned}$$

Find the matrix $\boldsymbol{R}$ of the transition from the basis $\mathcal{E}$ into the basis $\mathcal{B}'$, matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{E}$ into the basis $\mathcal{B}$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{E}$, and components of the vector $\vec{a}$ in the bases $\mathcal{B}$ and $\mathcal{B}'$. Are the bases $\mathcal{B}$ and $\mathcal{B}'$ orthonormal (specify the reason)?

$\boldsymbol{T} = \begin{pmatrix} -2 & \frac{3}{2} & 2 \\ -1 & 1 & 2 \\ 0 & \frac{1}{2} & 0 \end{pmatrix}$, $\boldsymbol{S} = \begin{pmatrix} -1 & 1 & 1 \\ 0 & 0 & 2 \\ -\frac{1}{2} & 1 & -\frac{1}{2} \end{pmatrix}$, $\vec{a}_{(\mathcal{B}')} = (2,1,0), \vec{a}_{(\mathcal{B})} = (-3,3,4)$,

$\mathcal{B}'$ no, $\mathcal{B}$ no.

2.29 Vector $\vec{a}$ has in the standard Cartesian basis $\mathcal{E}$ the components $(1,1,1)$. In addition, two bases $\mathcal{B}$ and $\mathcal{B}'$ are specified, where the matrix $\boldsymbol{R}^{-1}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{E}$ has the form

$$\boldsymbol{R}^{-1}(\mathcal{B}' \longmapsto \mathcal{E}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \phantom{2\,\vec{e}_1{}'} \quad \vec{e}_2{}' + \vec{e}_3{}', \\ \vec{e}_2 &= 2\,\vec{e}_1{}' \phantom{+ \vec{e}_2{}'} \quad + \vec{e}_3{}', \\ \vec{e}_3 &= -\vec{e}_1{}' + \vec{e}_2{}' \phantom{+ \vec{e}_3{}'} \quad . \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{E}$ into the basis $\mathcal{B}$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{E}$, and components of the vector $\vec{a}$ in the bases $\mathcal{B}$ and $\mathcal{B}'$. Are the bases $\mathcal{B}$ a $\mathcal{B}'$ orthonormal (specify the reason)?

$$\boldsymbol{T} = \begin{pmatrix} -1 & 1 & 2 \\ 1 & -1 & -1 \\ -2 & 1 & 2 \end{pmatrix}, \ \boldsymbol{S} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & -2 & -1 \\ 1 & 1 & 0 \end{pmatrix}, \ \vec{a}_{(\mathcal{B}')} = (-1,1,-1), \ \vec{a}_{(\mathcal{B})} = (-2,1,3),$$

$\mathcal{B}'$ yes, $\mathcal{B}$ no.

2.30 Vector $\vec{a}$ has in the standard Cartesian basis $\mathcal{E}$ the components $(1,1,2)$. In addition, two bases $\mathcal{B}$ and $\mathcal{B}'$ are specified, where the matrix $\boldsymbol{R}^{-1}$ of the transition from the basis $\mathcal{B}'$ into the basis $\mathcal{E}$ has the form

$$\boldsymbol{R}^{-1}(\mathcal{B}' \longmapsto \mathcal{E}) = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Transition between bases $\mathcal{B}$ and $\mathcal{B}'$ is given by the relations

$$\begin{aligned} \vec{e}_1 &= \phantom{\frac{1}{2}\,\vec{e}_1{}'} \quad -\vec{e}_2{}' - 2\,\vec{e}_3{}', \\ \vec{e}_2 &= \frac{1}{2}\,\vec{e}_1{}' - \frac{3}{2}\,\vec{e}_2{}' + \vec{e}_3{}', \\ \vec{e}_3 &= \phantom{\frac{1}{2}\,\vec{e}_1{}'} \quad \vec{e}_2{}' + 3\,\vec{e}_3{}'. \end{aligned}$$

Find the matrix $\boldsymbol{T}$ of the transition from the basis $\mathcal{E}$ into the basis $\mathcal{B}$, matrix $\boldsymbol{S}$ of the transition from the basis $\mathcal{B}$ into the basis $\mathcal{E}$, and components of the vector $\vec{a}$ in the bases $\mathcal{B}$ and $\mathcal{B}'$. Are the bases $\mathcal{B}$ and $\mathcal{B}'$ orthonormal (specify the reason)? Is the basis $\mathcal{B}'$ orthogonal (prove)?

$$\boldsymbol{T} = \begin{pmatrix} -4 & 1 & -3 \\ -7 & 1 & -5 \\ 1 & 0 & 1 \end{pmatrix}, \ \boldsymbol{S} = \begin{pmatrix} 1 & -1 & -2 \\ 2 & -1 & 1 \\ -1 & 1 & 3 \end{pmatrix}, \ \vec{a}_{(\mathcal{B})} = (-9,2,-6), \ \vec{a}_{(\mathcal{B}')} = (1,0,2),$$

$\mathcal{B}'$ no, $\mathcal{B}$ no. Yes.

2.3 Introduction to tensor calculus

In addition to scalars and vectors (i.e., zero and first-order tensors), there are more complicated algebraic structures, i.e., higher-order tensors. The most common of these are the so-called second-order tensors, which usually describe a physical field with the so-called shear effects (represented by non-diagonal elements in the corresponding tensor) in continuum mechanics, such as strain tensor, stress tensor, etc. A matrix $\boldsymbol{T} = (T_{ij})$, $i, j = 1, 2, \ldots, n$ is called the second-order Cartesian tensor if its elements T_{ij} are transformed in an *orthogonal coordinate transformation* (rotation in n-dimensional "space") $x_i' = a_{ij}x_j$ (see Example 2.21 where a_{ij} are elements of the orthogonal matrix) according to the relation

$$T_{ij}' = a_{ik}a_{jl}T_{kl}. \tag{2.33}$$

Just like every general vector $\vec{v}$ contains n scalar components $(v_1, v_2, \ldots, v_n)$, a general second-order tensor $\boldsymbol{T}$ consists of n "vector" components $(\vec{T}_1, \vec{T}_2, \ldots, \vec{T}_n)$ that are generally written as

$$\vec{T}_j = \begin{pmatrix} T_{1j} \\ T_{2j} \\ \vdots \\ T_{nj} \end{pmatrix}, \tag{2.34}$$

where each of the $\vec{T}_j$ vectors is written using n scalar components. If we generally write n-dimensional second-order tensor in the form of an explicit matrix notation, it will contain n^2 elements,

$$\boldsymbol{T} = (T_{ij}) = \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22} & \cdots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \cdots & T_{nn} \end{pmatrix}, \tag{2.35}$$

So if we write the three-dimensional (most common) second-order tensor in the form of an explicit matrix notation,

$$\boldsymbol{T} = (T_{ij}) = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix}, \tag{2.36}$$

each of the three vectors $\vec{T}_j$ is represented by one column of the matrix (2.36). In this paragraph, for the sake of simplicity, we do not yet introduce calculations with superscripts and subscripts, and we will also "live" here only in the Cartesian orthonormal basis.

We can illustrate the geometrical meaning of the second-order tensor from Equation (2.36) on the example of the stress tensor. A body of finite dimensions, unlike the point mass, can be subjected to force(s) in such a way that at different points of the body, the force vector (force resultant) has different directions and magnitudes. Let's imagine that this body consists of individual small volume elements bounded by surface elements (for simplicity, imagine small cubes with edges parallel to each Cartesian axis). The force applied to each such face of a selected cube can be divided into three independent directions: perpendicular (normal) to the face and parallel (tangential) to it in the direction of the two remaining axes. Because the faces are also oriented in three different directions, we denote by the first index the orientation of each face according to the direction of its normal, and the second index always denotes one of the three components of the force acting on the face. So we generally need nine tensor elements in total.

- **Symmetric and antisymmetric tensors:**

Second-order tensors (analogous to symmetric or antisymmetric matrices) can be decomposed into the sum of a symmetric and antisymmetric tensor of the second order. For each element T_{ij}, $i, j = 1, \ldots, n$ holds

$$T_{ij} = \frac{1}{2}\left(T_{ij} + T_{ji}\right) + \frac{1}{2}\left(T_{ij} - T_{ji}\right) = S_{ij} + Q_{ij}, \tag{2.37}$$

where (S_{ij}) is an n-dimensional symmetric second-order tensor, determined by $n(n+1)/2$ elements, (Q_{ij}) is an n-dimensional antisymmetric second-order tensor, determined by $n(n-1)/2$ elements. For higher-order tensors, symmetry or antisymmetry always applies only to a selected pair of indexes.

- **Summation of tensors:**

In the following, we implicitly assume tensors in "space" of the same dimension n. We sum (by analogy to matrix summation) individual elements with the same indexes (depending on their order), so we can only sum tensors of the same order, for example,

$$R_{ijk} = \alpha P_{ijk} + \beta Q_{ijk}, \tag{2.38}$$

where α and β are scalars.

- **Tensor contraction:**

By tensor contraction, we mean the sum over each pair of two identical indexes in the tensor $T_{ijk\ldots}$ (we will write hereafter the tensors according to the usual convention without brackets, i.e., using its elements). Contraction of the second-order tensor T_{ij} where we set $i = j$, will be (using Einstein summation convention) $T_{ii} = T_{11} + T_{22} + T_{33} = \mathrm{tr}(\boldsymbol{T}) = \alpha$, i.e., scalar (trace of the second-order tensor). Contraction of the third-order tensor T_{ijk} where we set, for example, $j = k$, will be $T_{ijj} = T_{i11} + T_{i22} + T_{i33} = \beta T_i$, i.e., vector, contraction of the fourth-order tensor T_{ijkl}, where we set, for example, $k = l$ will be $T_{ijkk} = T_{ij11} + T_{ij22} + T_{ij33} = \gamma T_{ij}$, i.e., second-order tensor, etc. Any contraction of any tensor $T_{ijkl\ldots}$ of any order (but at least second-order with two indexes) reduces the order of this tensor by two.

- **Tensor multiplication:**

Analogously to the way of writing a vector using a component and a unit basis vector (in Einstein notation) $\vec{v} = v_i \vec{e}_i$, we can write the second-order tensor as

$$\boldsymbol{T} = T_{ij}\vec{e}_i\vec{e}_j \qquad \text{or} \qquad \boldsymbol{T} = T_{ij}\vec{e}_i \otimes \vec{e}_j. \tag{2.39}$$

Equation (2.39) expresses the so-called *tensor product* of Cartesian basis vectors, i.e., the tensor product of two vectors of the same dimension, the first one being a column vector and the second a row vector. This special case of the tensor product is also called the dyadic product. This is the product of matrices of $n \times 1$ and $1 \times n$ with the resulting matrix of the type of $n \times n$, unlike a scalar product, which can be similarly expressed as the product of a row and column matrix of type $1 \times n$ and $n \times 1$ with the resulting matrix of type 1×1, i.e., a scalar. Individual, the so-called *basis tensors*, of the second-order (dyads) $\vec{e}_i\vec{e}_j$ in Equation (2.39) can be in Cartesian system (where $n = 3$) explicitly expressed by the following matrix notation,

$$\begin{aligned}
\vec{e}_1\vec{e}_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \vec{e}_1\vec{e}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \vec{e}_1\vec{e}_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\vec{e}_2\vec{e}_1 &= \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \vec{e}_2\vec{e}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \vec{e}_2\vec{e}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \\
\vec{e}_3\vec{e}_1 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \vec{e}_3\vec{e}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \vec{e}_3\vec{e}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{aligned} \tag{2.40}$$

From Equation (2.39) it is also possible to deduce that every element of the second-order tensor T_{ij} can be determined (similarly to a component v_i of a vector $\vec{v}$ by the scalar product, $v_i = \vec{v}\cdot\vec{e}_i$) using a double dot product

$$T_{ij} = \vec{e}_i \cdot \boldsymbol{T} \cdot \vec{e}_j, \tag{2.41}$$

where the individual scalar products represent in this case the matrix multiplication, i.e., $\vec{e}_i$ will be the row vector, and $\vec{e}_j$ will be the column vector. A tensor product of two vectors $\vec{v}$ and $\vec{w}$ is thus a second-order tensor, where for each its element T_{ij} holds

$$T_{ij} = v_i w_j. \tag{2.42}$$

For a dyadic product also hold the following identities,

$$(\vec{u} \otimes \vec{v}) \cdot \vec{w} = (\vec{v} \cdot \vec{w})\, \vec{u}, \qquad \vec{u} \cdot (\vec{v} \otimes \vec{w}) = (\vec{u} \cdot \vec{v})\, \vec{w}, \tag{2.43}$$

where the scalar product again represents matrix multiplication.

The result of a tensor product of general-order tensors will always be a tensor of the order, corresponding to the sum of orders of the original tensors (whose dimension will correspond to their product). For example, the tensor product of the second-order tensor $\boldsymbol{P}$ with elements P_{ij} and the first-order tensor (vector) $\vec{q}$ with elements q_k would be a third-order tensor $\boldsymbol{R}$ with elements R_{ijk}, the tensor product of the second-order tensor $\boldsymbol{P}$ with elements P_{ij} and the second-order tensor $\boldsymbol{Q}$ with elements Q_{kl} would be a fourth-order tensor $\boldsymbol{R}$ with elements R_{ijkl}, etc. Tensor product of general tensors $\boldsymbol{P}, \boldsymbol{Q}, \boldsymbol{R}$ (of any order) has the following properties:

- $\boldsymbol{P} \otimes \boldsymbol{Q} \neq \boldsymbol{Q} \otimes \boldsymbol{P},$ (2.44)
- $\boldsymbol{P} \otimes (\boldsymbol{Q} \otimes \boldsymbol{R}) = (\boldsymbol{P} \otimes \boldsymbol{Q}) \otimes \boldsymbol{R},$ (2.45)
- $\boldsymbol{P} \otimes (\alpha\boldsymbol{Q} + \beta\boldsymbol{R}) = \alpha\boldsymbol{P} \otimes \boldsymbol{Q} + \beta\boldsymbol{P} \otimes \boldsymbol{R}, \quad (\alpha\boldsymbol{P} + \beta\boldsymbol{Q}) \otimes \boldsymbol{R} = \alpha\boldsymbol{P} \otimes \boldsymbol{R} + \beta\boldsymbol{Q} \otimes \boldsymbol{R},$ (2.46)

where Equation (2.44) expresses the general non-commutativity of the tensor product (in particular cases, for example, for zero-order tensors or if $\boldsymbol{P} \equiv \boldsymbol{Q}$, this need not apply) and where Equations (2.45) and (2.46) express the associativity and linearity of the tensor product.

- **Kronecker delta:**

The so-called Kronecker delta is a mathematical function denoted by δ_{ij}, determined as follows:

$$\delta_{ij} = \begin{cases} 1, & \text{if} \quad i = j, \\ 0, & \text{if} \quad i \neq j. \end{cases} \tag{2.47}$$

Some important features of the Kronecker delta function:

- Orthonormality of vectors $\vec{e}_i, \vec{e}_j$ can be expressed as $e_i e_j \delta_{ij}$.
- $\delta_{ii} = 3$.
- Kronecker delta δ_{ij} interchanges indexes of vector components or tensor elements, for example

$$v_i \delta_{ij} = v_j, \qquad \text{or generally} \qquad T_{ij\,\dots\,k\,\dots\,z}\delta_{kl} = T_{ij\,\dots\,l\,\dots\,z}. \tag{2.48}$$

- Contraction (reduction) of the product of two functions $\delta_{ij}\delta_{jk}$ with one common index j to the resulting function δ_{ik}, reducing of the product of two functions with two common indexes i, j to the resulting function $\delta_{ij}\delta_{ij} = \delta_{ii} = 3$.
- Kronecker delta δ_{ij} reduces the summation (that is, removes one sum) where, for example,

$$\sum_i \sum_j A_{ij}\delta_{ij} = \sum_i A_{ii}, \qquad \sum_j \sum_k A_{jk}\delta_{jk}\delta_{ij} = \sum_j A_{jj}\delta_{ij} = A_{ij}. \tag{2.49}$$

- **Antisymmetric** (permutation or Levi-Civita) **symbol:**

The so-called *antisymmetric* (or Levi-Civita - see also Section 2.1) symbol, denoted as ε_{ijk}, is in $\mathbb{R}^3$ defined as

$$\varepsilon_{ijk} = \begin{cases} +1, & \text{if } ijk \text{ are even permutations, so } ijk = 123, 231, 312, \\ -1, & \text{if } ijk \text{ are odd permutations, so } ijk = 132, 213, 321, \\ 0, & \text{if any of the indexes repeats, so if } i = j \vee j = k \vee k = i. \end{cases} \tag{2.50}$$

Some essential features of the Levi-Civita symbol ε_{ijk}:

- It enables us to determine the expression for the determinant of a general regular square matrix $\boldsymbol{A}$ of any dimension (it is described in Equation (2.13)). For example, for matrix $\boldsymbol{A}$ of dimension 3×3, we get

$$\det \boldsymbol{A} = \sum_{i,j,k} \varepsilon_{ijk}\, A_{i1}\, A_{j2}\, A_{k3}. \tag{2.51}$$

- Also very useful in calculations (for example vector identities or differential operators) is the relationship between the Levi-Civita symbol ε_{ijk} and the Kronecker function δ_{ij}. It is clear from the definition of the Levi-Civita symbol (2.50) that by combining two symbols ε_{ijk} and ε_{lmn}, we get the identity

$$\varepsilon_{ijk}\varepsilon_{lmn} = \delta_{il}\delta_{jm}\delta_{kn} + \delta_{im}\delta_{jn}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km} - \delta_{il}\delta_{jn}\delta_{km} - \delta_{im}\delta_{jl}\delta_{kn} - \delta_{in}\delta_{jm}\delta_{kl}, \tag{2.52}$$

which can be compactly written using matrix formalism in the form

$$\varepsilon_{ijk}\varepsilon_{lmn} = \det \begin{pmatrix} \delta_{il} & \delta_{im} & \delta_{in} \\ \delta_{jl} & \delta_{jm} & \delta_{jn} \\ \delta_{kl} & \delta_{km} & \delta_{kn} \end{pmatrix}. \tag{2.53}$$

- Equation (2.53) and contraction of two Kronecker delta functions with common indexes further show that the action of two Levi-Civita symbols $\varepsilon_{ijk}\varepsilon_{klm}$ with one common index k simplifies Equation (2.52) to the form

$$\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}. \tag{2.54}$$

- In the case of two or all three common indexes, we get

$$\varepsilon_{ijk}\varepsilon_{jkl} = 2\delta_{il}, \qquad \varepsilon_{ijk}\varepsilon_{ijk} = 6. \tag{2.55}$$

- The Levi-Civita symbol can also be defined in $\mathbb{R}^n$ (also described in Section 2.1), even permutations will be created by an even number of numeric exchanges for n of different indexes, odd permutations by an odd number of numeric exchanges. For example, even permutations of the symbol ε_{1234} will be ε_{0123}, ε_{0231}, ε_{0312}, ε_{1032}, ε_{1320}, ε_{1203}, ε_{2130}, ε_{2301}, ε_{2013}, ε_{3210}, ε_{3102}, ε_{3021}. The other 12 permutations (without repetitions) will be odd.

- **Gradient and divergence of tensor:**

  - Differentiation of scalar functions is described in Section 1.1. The meaning of gradient, divergence and curl operators and their effects on zero and first-order tensors are explained in detail in Section 5.3.

  - Gradient (see Section 5.3) of tensor increases the so-called tensor order by one, i.e., for example, from a vector (first-order tensor), it creates a second-order tensor, from a second-order tensor, it creates a third-order tensor, etc. For example, the gradient of a second-order tensor $\boldsymbol{T}$ can be generally written in the Cartesian coordinate system as

$$\vec{\nabla}\boldsymbol{T} = \frac{\partial T_{jk}}{\partial x_i} = R_{ijk}, \tag{2.56}$$

with a corresponding representation using a matrix with 27 elements. In the resulting tensor (third-order, but this generally applies to any order) in Equation (2.56), we draw attention to the ordering of indexes, where the first index denotes the variable by which we derive while the other indexes denote the particular tensor element.

If we explicitly write the gradient of a vector (in the Cartesian coordinate system in $\mathbb{R}^3$), we get

$$\vec{\nabla}\vec{A} = \frac{\partial A_j}{\partial x_i} = T_{ij}, \text{ where } T_{ij} = \begin{pmatrix} \dfrac{\partial A_x}{\partial x} & \dfrac{\partial A_y}{\partial x} & \dfrac{\partial A_z}{\partial x} \\ \dfrac{\partial A_x}{\partial y} & \dfrac{\partial A_y}{\partial y} & \dfrac{\partial A_z}{\partial y} \\ \dfrac{\partial A_x}{\partial z} & \dfrac{\partial A_y}{\partial z} & \dfrac{\partial A_z}{\partial z} \end{pmatrix}. \tag{2.57}$$

  - The tensor divergence can be understood as a contraction of the gradient, for example, if we set $i = k$ in Equation (2.56), we get instead of the third-order tensor a first-order tensor (vector) with components $A_j = \partial T_{jk}/\partial x_k$. Divergence (see also Section 5.3) of a tensor thus reduces the tensor order by one, i.e., it creates, for example, a vector from a second-order tensor, a scalar from a vector, etc. Divergence of a second-order tensor $\boldsymbol{T}$ can be generally written in the Cartesian coordinate system in $\mathbb{R}^3$ as

$$\vec{\nabla}\cdot\boldsymbol{T} = \frac{\partial T_{ij}}{\partial x_j}\,\vec{e}_i = \vec{A}. \tag{2.58}$$

The explicitly written resulting vector will take the form

$$\vec{A} = \left(\frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{\partial T_{xz}}{\partial z}, \frac{\partial T_{yx}}{\partial x} + \frac{\partial T_{yy}}{\partial y} + \frac{\partial T_{yz}}{\partial z}, \frac{\partial T_{zx}}{\partial x} + \frac{\partial T_{zy}}{\partial y} + \frac{\partial T_{zz}}{\partial z}\right). \tag{2.59}$$

We can also write Equation (2.58) by the form of matrix multiplication of the gradient vector with the tensor $\boldsymbol{T}$,

$$\vec{\nabla} \cdot \boldsymbol{T} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \begin{pmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{pmatrix}^T , \tag{2.60}$$

where the resulting vector is given by Equation (2.59).

- **Examples** (we always consider the Cartesian orthonormal basis of a given vector space) **:**

2.31 Write the explicit form of the scalar product $\vec{u} \cdot \vec{v}$ with a common parameter a and also the tensor (dyadic) products $\vec{u} \otimes \vec{v}$ and $\vec{v} \otimes \vec{u}$ of the vectors $\vec{u} = (1, 5, -5, 2)$ and $\vec{v} = (2, -1, a, 4)$ in $\mathbb{R}^4$, where both the vectors will be perpendicular to each other. Perform the tensor contraction of the resulting second-order tensors.

$$\vec{u} \cdot \vec{v} = 5(1-a), \quad \vec{u} \otimes \vec{v} = \begin{pmatrix} 2 & -1 & 1 & 4 \\ 10 & -5 & 5 & 20 \\ -10 & 5 & -5 & -20 \\ 4 & -2 & 2 & 8 \end{pmatrix}, \quad \vec{v} \otimes \vec{u} = \begin{pmatrix} 2 & 10 & -10 & 4 \\ -1 & -5 & 5 & -2 \\ 1 & 5 & -5 & 2 \\ 4 & 20 & -20 & 8 \end{pmatrix}$$

By contracting both second-order tensors, we obtain the (identical) scalar product of both vectors, if $\vec{u} \perp \vec{v}$, then $\vec{u} \cdot \vec{v} = 0$

2.32 Write the explicit form of a tensor product of the second-order tensor $\boldsymbol{T}$ and the vector $\vec{v}$ in $\mathbb{R}^3$,

$$T_{ij} = \begin{pmatrix} 1 & 1 & -1 \\ 2 & 1 & 2 \\ 3 & 1 & 1 \end{pmatrix}, \quad \vec{v} = (4, 2, 2),$$

and then perform the tensor contraction by setting an index denoting the vector components to j.

$$T_{ij} \otimes v_k = S_{ijk} = \begin{pmatrix} R_{111} & R_{112} & R_{113} & R_{121} & R_{122} & R_{123} & R_{131} & R_{132} & R_{133} \\ R_{211} & R_{212} & R_{213} & R_{221} & R_{222} & R_{223} & R_{231} & R_{232} & R_{233} \\ R_{311} & R_{312} & R_{313} & R_{321} & R_{322} & R_{323} & R_{331} & R_{332} & R_{333} \end{pmatrix} =$$

$$= \begin{pmatrix} 4 & 2 & 2 & 4 & 2 & 2 & -4 & -2 & -2 \\ 8 & 4 & 4 & 4 & 2 & 2 & 8 & 4 & 4 \\ 12 & 6 & 6 & 4 & 2 & 2 & 4 & 2 & 2 \end{pmatrix}, \quad S_i = (4, 14, 16)$$

2.33 Write the explicit form of a tensor product of two second-order tensors $\boldsymbol{P}$ and $\boldsymbol{Q}$ in $\mathbb{R}^2$, $P_{ij} = \begin{pmatrix} 2 & 2 \\ 1 & 3 \end{pmatrix}$, $Q_{kl} = \begin{pmatrix} 1 & -1 \\ 1 & 2 \end{pmatrix}$, and then perform the tensor contraction by setting $l = k$.

$$P_{ij} \otimes Q_{kl} = R_{ijkl} = \begin{pmatrix} R_{1111} & R_{1112} & R_{1211} & R_{1212} \\ R_{1121} & R_{1122} & R_{1221} & R_{1222} \\ R_{2111} & R_{2112} & R_{2211} & R_{2212} \\ R_{2121} & R_{2122} & R_{2221} & R_{2222} \end{pmatrix} = \begin{pmatrix} 2 & -2 & 2 & -2 \\ 2 & 4 & 2 & 4 \\ 1 & -1 & 3 & -3 \\ 1 & 2 & 3 & 6 \end{pmatrix}, \; R_{ij} = \begin{pmatrix} 6 & 6 \\ 3 & 9 \end{pmatrix}$$

2.34 Components y_i of the vector $\vec{y}$ are given by equation $y_i = b_{ij} z_j$, where components z_i of the vector $\vec{z}$ are given by equation $z_i = a_{ij} x_j$, $i, j = 1, 2, 3$. Write explicitly and also using Einstein notation, the transformation equations of the components of the vector $\vec{y}$ directly using the components of the vector $\vec{x}$.

$$y_1 = (b_{11}a_{11}+b_{12}a_{21}+b_{13}a_{31})z_1+(b_{11}a_{12}+b_{12}a_{22}+b_{13}a_{32})z_2+(b_{11}a_{13}+b_{12}a_{23}+b_{13}a_{33})z_3,$$
$$y_2 = (b_{21}a_{11}+b_{22}a_{21}+b_{23}a_{31})z_1+(b_{21}a_{12}+b_{22}a_{22}+b_{23}a_{32})z_2+(b_{21}a_{13}+b_{22}a_{23}+b_{23}a_{33})z_3,$$
$$y_3 = (b_{31}a_{11}+b_{32}a_{21}+b_{33}a_{31})z_1+(b_{31}a_{12}+b_{32}a_{22}+b_{33}a_{32})z_2+(b_{31}a_{13}+b_{32}a_{23}+b_{33}a_{33})z_3$$

$y_i = b_{im}a_{mj}z_j$

2.35 Adjust the following expressions $(i, j, \ldots = 1, 2, 3)$:

(a) $\delta_{ii}\delta_{kk}$, (b) $\delta_{ij}\delta_{ik}\delta_{jl}$, (c) $\delta_{il}\delta_{jl}\delta_{mm}\delta_{qj}\delta_{qk}$, (d) $\delta_{i1}\delta_{j2}\delta_{k3}$, (e) $\delta_{il}\delta_{jj}\delta_{kk} - \delta_{kj}\delta_{jk}\delta_{il}$

(a) 9, (b) δ_{kl}, (c) $3\delta_{ik}$, (d) 1, (e) $6\delta_{il}$

2.36 Prove that:

(a) $\varepsilon_{ij}\,\varepsilon_{ij} = 2!$
(b) $\varepsilon_{ijk}\,\varepsilon_{ijk} = 3!$
(c) $\varepsilon_{ijkl}\,\varepsilon_{ijkl} = 4!$
(d) Estimate the result $\varepsilon_{i_1\,i_2\,i_3\,\ldots\,i_n}\,\varepsilon_{i_1\,i_2\,i_3\,\ldots\,i_n}$
(e) Write the complete form of the so-called Levi-Civita tensor (given by Equation (2.50)).

(a)-(d) using Equations (2.52) and (2.53), (e) $\varepsilon_{ijk} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

2.37 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the vector identity $\vec{A} \times \vec{B} = -\vec{B} \times \vec{A}$.

Using identities $\varepsilon_{ijk}A_jB_k\vec{e}_i = -\varepsilon_{ikj}A_jB_k\vec{e}_i = -\varepsilon_{ikj}B_kA_j\vec{e}_i = -\varepsilon_{ijk}B_jA_k\vec{e}_i$, when passing from the third to the fourth term, we interchange the indexes j and k.

2.38 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the identity for the triple product $\vec{A} \cdot (\vec{B} \times \vec{C}) = \vec{B} \cdot (\vec{C} \times \vec{A}) = \vec{C} \cdot (\vec{A} \times \vec{B})$.

By adjustment of the expression $(A_i\vec{e}_i) \cdot (\varepsilon_{ijk}B_jC_k\vec{e}_i)$ and following even permutations.

2.39 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the identity for the triple product $\vec{A} \cdot (\vec{B} \times \vec{A}) = 0$.

Analogously to Example 2.38, we get $A_i\varepsilon_{ijk}B_jA_k = B_i\varepsilon_{ijk}A_jA_k = \vec{B} \cdot (\vec{A} \times \vec{A}) = 0$.

2.40 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the vector identity $\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\,\vec{B} - (\vec{A} \cdot \vec{B})\,\vec{C}$.

Using the expression $(A_j\vec{e}_j) \times (\varepsilon_{klm}B_lC_m\vec{e}_k) = \varepsilon_{ijk}A_j\varepsilon_{klm}B_lC_m\vec{e}_i$ and by using Equation (2.54).

2.41 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the vector identity $(\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C})$.

Using the expression $(\varepsilon_{ijk}A_jB_k\vec{e}_i) \cdot (\varepsilon_{ilm}C_lD_m\vec{e}_i)$ and by using Equation (2.54).

2.42 Using the Kronecker delta and Levi-Civita symbol in Einstein notation, verify the vector identity $(\vec{A}\times\vec{B})\times(\vec{C}\times\vec{D}) = \vec{C}\,[\vec{D}\cdot(\vec{A}\times\vec{B})] - \vec{D}\,[\vec{C}\cdot(\vec{A}\times\vec{B})]$.

Using further adjustments of the expression $\varepsilon_{ijk}(\vec{A}\times\vec{B})_j(\vec{C}\times\vec{D})_k\vec{e}_i$ and by using Equations (2.6) and (2.54).

2.43 Use the Einstein and vector notation, write expicitly the vector identity $\vec{\nabla}\cdot\left(\vec{A}\cdot\vec{\nabla}\right)\vec{B}$.

$$A_j\frac{\partial}{\partial x_j}\frac{\partial B_i}{\partial x_i} + \frac{\partial A_j}{\partial x_i}\frac{\partial B_i}{\partial x_j} = \left(\vec{A}\cdot\vec{\nabla}\right)\left(\vec{\nabla}\cdot\vec{B}\right) + \mathrm{tr}\left(\vec{\nabla}\vec{A}\cdot\vec{\nabla}\vec{B}\right)$$

2.44 Particular elements of the so-called Cauchy deformation tensor E_{ij} (describing small deformations) can be written using index notation as

$$E_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right),$$

where $i,j = 1,2,3$ and v_i, v_j are components of the velocity vector. In Einstein notation, write an expression for the divergence of this tensor, and also write the explicit expression for the first vectorial component of this divergence.

$$\frac{\partial E_{ij}}{\partial x_j} = \frac{1}{2}\left(\frac{\partial^2 v_i}{\partial x_j^2} + \frac{\partial^2 v_j}{\partial x_i \partial x_j}\right), \quad \frac{\partial E_{xx}}{\partial x} + \frac{\partial E_{xy}}{\partial y} + \frac{\partial E_{xz}}{\partial z} = \frac{1}{2}\left[\Delta v_x + \frac{\partial}{\partial x}\left(\vec{\nabla}\cdot\vec{v}\right)\right]$$

2.45 Particular elements of the so-called Green-Lagrange deformation tensor E_{ij} (describing arbitrarily large deformations) can be written using index notation as

$$E_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} + \frac{\partial v_k}{\partial x_j}\frac{\partial v_k}{\partial x_i}\right),$$

where $i,j,k = 1,2,3$ and v_i, v_j, v_k are components of the velocity vector. In Einstein notation, write an expression for the divergence of this tensor.

$$\frac{\partial E_{ij}}{\partial x_j} = \frac{1}{2}\left(\frac{\partial^2 v_i}{\partial x_j^2} + \frac{\partial^2 v_j}{\partial x_i \partial x_j} + \frac{\partial v_k}{\partial x_j}\frac{\partial^2 v_k}{\partial x_i \partial x_j} + \frac{\partial v_k}{\partial x_i}\frac{\partial^2 v_k}{\partial x_j^2}\right)$$

2.46 The so-called strain tensor T_{ij} can be written in the form

$$T_{ij} = -p\,\delta_{ij} + \eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right),$$

where $i,j = 1,2,3$ and v_i, v_j are components of the velocity vector, p is the scalar quantity (scalar pressure), and η is constant (dynamical viscosity coefficient). Using Einstein and vector notation, write an expression for the divergence of this tensor.

$$\frac{\partial T_{ij}}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \eta\left(\frac{\partial^2 v_i}{\partial x_j^2} + \frac{\partial^2 v_j}{\partial x_i \partial x_j}\right) = -\vec{\nabla}p + \eta\left[\Delta\vec{v} + \vec{\nabla}\left(\vec{\nabla}\cdot\vec{v}\right)\right]$$

2.47 The so-called tensor of viscous (shear) strain σ_{ij} can be written, for example, in the form

$$\sigma_{ij} = \eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + \lambda\frac{\partial v_k}{\partial x_k}\delta_{ij},$$

where $i, j, k = 1, 2, 3$, v_i, v_j, v_k are components of the velocity vector, and η i λ are constants (dynamical viscosity coefficient, dilatation viscosity coefficient). Using Einstein and vector notation, write the expression for the divergence of this tensor.

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \eta \left(\frac{\partial^2 v_i}{\partial x_j^2} + \frac{\partial^2 v_j}{\partial x_i \partial x_j} \right) + \lambda \frac{\partial^2 v_k}{\partial x_i \partial x_k} = \eta \Delta \vec{v} + (\eta + \lambda) \vec{\nabla} \left(\vec{\nabla} \cdot \vec{v} \right)$$

2.4 Covariant and contravariant transformations: ★

By acting the metric tensor of a given coordinate system (see, for example, Equations (B.4), (B.3), (B.36), and (B.63) in Section B), we transform the vector and tensor quantities between the so-called *covariant* and *contravariant* bases, which distinguish the quantitative behavior of a given geometric or physical entity when changing the basis. To preserve the length of a vector as such, the components of vectors (for example, position or velocity), whose length is proportional to the scale of the basis, must be *contra-variant* to basis vectors, we write them $\vec{V} = V^i \vec{e}_i$. On the contrary, the components of the so-called *dual* vectors, also called *co-vectors* (for example, the gradient vector that has the dimension of the inverse of the distance), must be *co-variant* to change of the basis, we write them $\vec{V} = V_i \vec{e}^{\,i}$. In this notation, we formally distinguish them by the *lower* or *upper* position of the indexes. In orthogonal coordinate systems, the so-called *covariant metric tensor* $\boldsymbol{\eta}$ has the elements g_{ij} only on main diagonal (see the so-called *Lamé coefficients* in Equation (B.11)). For the so-called *contravariant metric tensor* $\boldsymbol{\eta}'$ with elements g^{ij} always holds $\boldsymbol{\eta}\boldsymbol{\eta}' = \boldsymbol{E}$ and so $\boldsymbol{\eta}' = \boldsymbol{\eta}^{-1}$, for their elements always holds (following the Einstein summation convention) $g_{ij} g^{ij} = \dim V$, that is, the dimension of the corresponding vector space V. A metric tensor is always symmetrical, that is, $g_{ij} = g_{ji}$, $g^{ij} = g^{ji}$. A general expression of the transformation of a vector V_i from covariant to contravariant basis thus can be written as follows (see Einstein summation convention):

$$V^j = g^{ji} V_i = g^{j1} V_1 + g^{j2} V_2 + g^{j3} V_3. \tag{2.61}$$

Transformation of the second-order covariant tensor T_{ij} into a contravariant basis we write as follows:

$$T_i^j = g^{jk} T_{ki} = g^{j1} T_{1i} + g^{j2} T_{2i} + g^{j3} T_{3i} \qquad \text{(mixed co- and contravariant tensor)}, \tag{2.62}$$

$$T^{ij} = g^{im} g^{jn} T_{mn} = g^{i1} g^{j1} T_{11} + g^{i1} g^{j2} T_{12} + g^{i1} g^{j3} T_{13} + g^{i2} g^{j1} T_{21} + \ldots + g^{i3} g^{j3} T_{33}. \tag{2.63}$$

Any higher-order tensors will be transformed analogously. A mixed metric tensor with elements $g_i^j = g_j^i$ is always represented by unit matrix.

Three-dimensional space distinguishes the so-called *axial vectors* (*pseudovectors*) which do not mirror together with the coordinate system (unlike the so-called *polar* or *true* vectors that are mirrored) and which can be defined as a pseudovector V_i dual to antisymmetric tensor T_{jk},

$$V_i = \frac{1}{2} \varepsilon_{ijk} T_{jk}, \quad \text{and so} \quad V_i = \frac{1}{2} \left(T_{jk} - T_{kj} \right) = T_{jk} \quad (\text{where } i \neq j \neq k), \tag{2.64}$$

where the particular elements of the tensor T_{jk} are defined as $T_{jk} = A_j B_k - A_k B_j$, that is, we can regard them in $\mathbb{R}^3$ as the corresponding components of the vector product $\vec{A} \times \vec{B}$. In a

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

similar way, we define in a flat four-dimensional space-time, whose metric (*Minkowski*) tensor is of the form

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{2.65}$$

a second-order antisymmetric pseudotensor (the so called *Hodge dual tensor*, denoted by $^\star\boldsymbol{T}$) that is dual to second-order antisymmetric tensor and a third-order antisymmetric pseudotensor that is dual to vector:

$$^\star T^{\mu\nu} = \frac{1}{2}\varepsilon^{\mu\nu\rho\sigma}T_{\rho\sigma}, \qquad ^\star T^{\mu\nu\rho} = \varepsilon^{\mu\nu\rho\sigma}V_\sigma. \tag{2.66}$$

For the initial permutation of the Levi-Civita symbol in a covariant basis (within the convention introduced here, cf. also the textbook Lenc (2001)) holds $\varepsilon_{0123} = 1$. For the initial permutation in the contravariant basis must then apply $\varepsilon^{0123} = g^{00}g^{11}g^{22}g^{33}\varepsilon_{0123}$, where $g^{\mu\nu}$ are the non-zero elements of the Minkowski metric tensor from Equation (2.65), and so $\varepsilon^{0123} = -1$ (in a similar way, with use of Equation (B.4), we can derive that in a flat three-dimensional space holds $\varepsilon_{123} = \varepsilon^{123} = 1$). For a more detailed study of tensor calculus, I recommend, for example, the textbooks Young (1993); Kvasnica (2004); Arfken & Weber (2005).

- **Examples** (we always consider the Cartesian orthonormal basis of a given vector space) **:**

2.48 ★ Covariant metric tensor g_{ij} of the cylindrical coordinate system where the order of coordinate directions is r, ϕ, z, is expressed by matrix (see Equation (B.36))

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Similar covariant metric tensor of the spherical coordinate system with the order of coordinate directions r, θ, ϕ is expressed by matrix (see Equation (B.63))

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2\sin^2\theta \end{pmatrix}.$$

Calculate:

(a) All nonzero the so-called *Christoffel symbols* $\Gamma^\rho_{\mu\nu}$ of the cylindrical coordinate system (defining the *curvature* of a given metric) that are generally defined by the formula (unlike in Eqs (B.12), we have to distinguish in spacetime the covariant and contravariant four-vectors $x_\mu = (ct, -\vec{r})$ and $x^\mu = (ct, \vec{r})$, respectively)

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2}g^{\rho\lambda}\left(\frac{\partial g_{\nu\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu\lambda}}{\partial x^\nu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda}\right),$$

(b) all nonzero spherical Christoffel symbols, also defined by the formula (B.12),

(c) explicit form of a vector curl of the vector $\vec{A}$ in a cylindrical system generally given by the formula (see also Equation (B.20))

$$\vec{\nabla} \times \vec{A} = \epsilon_{ijk}\,\frac{1}{h_j h_k}\left[\frac{\partial}{\partial x_j}(h_k A_k)\right]\vec{e}_i,$$

(d) explicit form of the vector curl of vector $\vec{A}$ in the spherical system, given generally by the same formula.

(a) $\Gamma^r_{\phi\phi} = -r$, $\Gamma^\phi_{\phi r} = \Gamma^\phi_{r\phi} = \dfrac{1}{r}$,

(b) $\Gamma^r_{\theta\theta} = -r$, $\Gamma^\theta_{\theta r} = \Gamma^\theta_{r\theta} = \Gamma^\phi_{\phi r} = \Gamma^\phi_{r\phi} = \dfrac{1}{r}$, $\Gamma^r_{\phi\phi} = -r\sin^2\theta$, $\Gamma^\theta_{\phi\phi} = -\sin\theta\cos\theta$, $\Gamma^\phi_{\phi\theta} = \Gamma^\phi_{\theta\phi} = \cot\theta$,

(c) see relation (B.45) in Appendix B,

(d) see relation (B.71) in Appendix B.

2.49 ★ Covariant tensor A_{ij} and covariant metric tensor g_{ij} of the given coordinate system are specified in the order of the coordinate directions r, θ, ϕ, in the form

$$A_{ij} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \qquad g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2\sin^2\theta \end{pmatrix}.$$

Calculate:

(a) mixed metric tensor g^i_j and mixed tensor A^i_j,

(b) contravariant tensor A^{ij}.

(a) $$g^i_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \delta^i_j, \quad A^i_j = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ \dfrac{a_{21}}{r^2} & \dfrac{a_{22}}{r^2} & \dfrac{a_{23}}{r^2} \\ \dfrac{a_{31}}{r^2\sin^2\theta} & \dfrac{a_{32}}{r^2\sin^2\theta} & \dfrac{a_{33}}{r^2\sin^2\theta} \end{pmatrix},$$

(b) $$A^{ij} = \begin{pmatrix} a_{11} & \dfrac{a_{12}}{r^2} & \dfrac{a_{13}}{r^2\sin^2\theta} \\ \dfrac{a_{21}}{r^2} & \dfrac{a_{22}}{r^4} & \dfrac{a_{23}}{r^4\sin^2\theta} \\ \dfrac{a_{31}}{r^2\sin^2\theta} & \dfrac{a_{32}}{r^4\sin^2\theta} & \dfrac{a_{33}}{r^4\sin^4\theta} \end{pmatrix}.$$

2.50 ★ The covariant tensor is specified in the four-dimensional space (space-time) $A_{\mu\nu}$ and the covariant metric tensor $g_{\alpha\beta}$ of a given coordinate system, in the order of coordinate directions t, u, v, w in the form

$$A_{\mu\nu} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix}, \qquad g_{\alpha\beta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & w \\ 0 & 0 & u^2 & 0 \\ 0 & w & 0 & u^2 \end{pmatrix}.$$

Calculate:

(a) contravariant metric tensor $g^{\alpha\beta}$ and mixed metric tensor g^α_β,

(b) mixed tensor A^μ_ν,

(c) contravariant tensor $A^{\mu\nu}$.

We write the covariant four-vector of the coordinates of an event as $x_\mu = (ct, -\vec{r})$.

(a) $g^{\alpha\beta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & \dfrac{u^2}{u^2-w^2} & 0 & \dfrac{w}{w^2-u^2} \\ 0 & 0 & \dfrac{1}{u^2} & 0 \\ 0 & \dfrac{w}{w^2-u^2} & 0 & \dfrac{1}{u^2-w^2} \end{pmatrix}, \quad g^{\alpha}_{\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \boldsymbol{E} = \delta^{\alpha}_{\beta},$

(b) $A^{\mu}_{\nu} = \begin{pmatrix} -a_{00} & -a_{01} & -a_{02} & -a_{03} \\ \dfrac{u^2\,a_{10} - w\,a_{30}}{u^2-w^2} & \dfrac{u^2\,a_{11} - w\,a_{31}}{u^2-w^2} & \dfrac{u^2\,a_{12} - w\,a_{32}}{u^2-w^2} & \dfrac{u^2\,a_{13} - w\,a_{33}}{u^2-w^2} \\ \dfrac{a_{20}}{u^2} & \dfrac{a_{21}}{u^2} & \dfrac{a_{22}}{u^2} & \dfrac{a_{23}}{u^2} \\ \dfrac{w\,a_{10} - a_{30}}{w^2-u^2} & \dfrac{w\,a_{11} - a_{31}}{w^2-u^2} & \dfrac{w\,a_{12} - a_{32}}{w^2-u^2} & \dfrac{w\,a_{13} - a_{33}}{w^2-u^2} \end{pmatrix},$

(c) $A^{\mu\nu} = \begin{pmatrix} a_{00} & \dfrac{u^2 a_{10} - w\,a_{30}}{w^2-u^2} & -\dfrac{a_{20}}{u^2} & \dfrac{w\,a_{10} - a_{30}}{u^2-w^2} \\ \dfrac{u^2 a_{01} - w\,a_{03}}{w^2-u^2} & \dfrac{u^4 a_{11} + w^2 a_{33} - u^2 w\,\mathcal{S}}{(w^2-u^2)^2} & \dfrac{u^2 a_{21} - w\,a_{23}}{u^2(u^2-w^2)} & \dfrac{u^2 a_{31} + w^2 a_{13} - w\,\mathcal{T}}{(u^2-w^2)^2} \\ -\dfrac{a_{02}}{u^2} & \dfrac{u^2 a_{12} - w\,a_{32}}{u^2(u^2-w^2)} & \dfrac{a_{22}}{u^4} & \dfrac{a_{32} - w\,a_{12}}{u^2(u^2-w^2)} \\ \dfrac{w\,a_{01} - a_{03}}{u^2-w^2} & \dfrac{u^2 a_{13} + w^2 a_{31} - w\,\mathcal{T}}{(u^2-w^2)^2} & \dfrac{a_{23} - w\,a_{21}}{u^2(u^2-w^2)} & \dfrac{a_{33} + w^2 a_{11} - w\,\mathcal{S}}{(w^2-u^2)^2} \end{pmatrix},$

where $\mathcal{T} = u^2 a_{11} + a_{33}$, and $\mathcal{S} = a_{13} + a_{31}$.

2.51 ★ Covariant tensor of electromagnetic field $F_{\mu\nu}$ is defined as

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu},$$

where the so-called *four-potential* (four-vector of an electromagnetic potential) $A_\mu = \left(\dfrac{\phi}{c}, -\vec{A}\right)$. The component $A_0 = \dfrac{\phi}{c}$ expresses the scaled scalar potential of the electric field, and the components A_1, A_2, A_3 express the so-called vector (magnetic) potential. We write the covariant four-vector of the coordinates of an event as $x_\mu = (ct, -\vec{r})$. Metric tensor (*Minkowski tensor*) of the flat four-space (space-time) is given by Equation (2.65), and the formalism of the Levi-Civita symbol ϵ is described within the explanatory text of this section. Vectors of electric intensity and magnetic induction are defined as

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}, \qquad \vec{B} = \vec{\nabla} \times \vec{A}.$$

Write:

(a) explicit form of the tensor $F_{\mu\nu}$ and the tensor $F^{\mu\nu}$,

(b) dual tensor ${}^\star F_{\mu\nu}$ and dual tensor ${}^\star F^{\mu\nu}$,

(c) the so-called *invariants* of electromagnetic field $F_{\mu\nu}F^{\mu\nu}$ and $F_{\mu\nu}\,{}^\star F^{\mu\nu}$,

(d) with use of "four-dimensional" divergence

$$\varepsilon^{\mu\nu\rho\sigma}\frac{\partial F_{\rho\sigma}}{\partial x^\nu} = \frac{\partial\,{}^\star F^{\mu\nu}}{\partial x^\nu} = 0$$

derive the first pair of Maxwell equations;

(e) with use of "four-dimensional" divergence

$$\frac{\partial F^{\mu\nu}}{\partial x^\nu} = -\mu_0\, j^\mu,$$

where j^μ is the contravariant four-vector of current density $j^\mu = (c\rho, \vec{j})$, derive the second pair of Maxwell equations.

(a) $F_{\mu\nu} = \begin{pmatrix} 0 & \dfrac{E_x}{c} & \dfrac{E_y}{c} & \dfrac{E_z}{c} \\ -\dfrac{E_x}{c} & 0 & -B_z & B_y \\ -\dfrac{E_y}{c} & B_z & 0 & -B_x \\ -\dfrac{E_z}{c} & -B_y & B_x & 0 \end{pmatrix}$, $\quad F^{\mu\nu} = \begin{pmatrix} 0 & -\dfrac{E_x}{c} & -\dfrac{E_y}{c} & -\dfrac{E_z}{c} \\ \dfrac{E_x}{c} & 0 & -B_z & B_y \\ \dfrac{E_y}{c} & B_z & 0 & -B_x \\ \dfrac{E_z}{c} & -B_y & B_x & 0 \end{pmatrix}$,

(b) ${}^\star F_{\mu\nu} = \begin{pmatrix} 0 & -B_x & -B_y & -B_z \\ B_x & 0 & -\dfrac{E_z}{c} & \dfrac{E_y}{c} \\ B_y & \dfrac{E_z}{c} & 0 & -\dfrac{E_x}{c} \\ B_z & -\dfrac{E_y}{c} & \dfrac{E_x}{c} & 0 \end{pmatrix}$, $\quad {}^\star F^{\mu\nu} = \begin{pmatrix} 0 & B_x & B_y & B_z \\ -B_x & 0 & -\dfrac{E_z}{c} & \dfrac{E_y}{c} \\ -B_y & \dfrac{E_z}{c} & 0 & -\dfrac{E_x}{c} \\ -B_z & -\dfrac{E_y}{c} & \dfrac{E_x}{c} & 0 \end{pmatrix}$,

(c) $F_{\mu\nu}F^{\mu\nu} = -2\left(\dfrac{E^2}{c^2} - B^2\right)$, $F_{\mu\nu}\,{}^\star F^{\mu\nu} = 4\,\dfrac{\vec{E}\cdot\vec{B}}{c}$,

(d) $\dfrac{\partial\,{}^\star F^{0\nu}}{\partial x^\nu} = \vec{\nabla}\cdot\vec{B} = 0$, $\dfrac{\partial\,{}^\star F^{i\nu}}{\partial x^\nu} = -\vec{\nabla}\times\vec{E} - \dfrac{\partial\vec{B}}{\partial t} = \vec{0}$, $i = 1, 2, 3$,

(e) $\dfrac{\partial F^{0\nu}}{\partial x^\nu} = -\vec{\nabla}\cdot\vec{E} = -\dfrac{\rho}{\epsilon_0}$, $\dfrac{\partial F^{i\nu}}{\partial x^\nu} = \mu_0\epsilon_0\dfrac{\partial\vec{E}}{\partial t} - \vec{\nabla}\times\vec{B} = -\mu_0\,\vec{j}$, $i = 1, 2, 3$, $c = (\mu_0\epsilon_0)^{-1/2}$.

2.52 ★ Contravariant tensor of energy-momentum $T^{\alpha\beta}$ for macroscopic ideal fluid is defined as

$$T^{\alpha\beta} = (\varepsilon + p)\, u^\alpha u^\beta - p\, g^{\alpha\beta},$$

where $\varepsilon = \rho c^2$ is the energy density (ρ is the mass density), p is the scalar pressure, and u^μ is the so-called *four-velocity* (four-vector of velocity), defined as a tangent to the so-called *worldline* s, that is, $u^\mu = \mathrm{d}x^\mu/\mathrm{d}s$, where $s = c\,\tau$. The so-called *proper time* τ in a system associated with a moving body is related to the so-called coordinate time t (i.e., "normal" time of an observer) as $t = \gamma\tau$, where the so-called Lorentz factor $\gamma = (1 - v^2/c^2)^{-1/2}$ (see also Example 9.8). The four-vector of an event x^μ and the metric tensor of the Minkowski space-time $g^{\mu\nu}$ can be specified with the use of their definition in Example 2.51 and in Equation (2.65). Write:

(a) the explicit form of tensor $T^{\alpha\beta}$ and tensor $T_{\alpha\beta}$,

(b) the explicit form of these tensors in the coordinate system (0), associated with the moving fluid.

(c) using the "four-divergence" of an energy-momentum tensor $T^{\alpha\beta}$ for "dust", that is, an ensemble of particles that do not interact with each other,

$$\frac{\partial T^{\alpha\beta}}{\partial x^{\beta}} = 0,$$

derive the continuity and momentum equations of a "collisionless" fluid.

Using the expression: $W = \gamma^2 \left(\varepsilon + \frac{v^2}{c^2}\, p\right)$, $S^i = \gamma^2\,(\varepsilon + p)\,v^i$, $\sigma^{ij} = \frac{\gamma^2}{c^2}\,(\varepsilon + p)\,v^i v^j + p\,\delta^{ij}$, $\sigma_{ij} = \frac{\gamma^2}{c^2}\,(\varepsilon + p)\,v_i v_j + p\,\delta_{ij}$, we can write,

(a) $$T^{\alpha\beta} = \begin{pmatrix} W & -\frac{S_x}{c} & -\frac{S_y}{c} & -\frac{S_z}{c} \\ -\frac{S_x}{c} & \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\frac{S_y}{c} & \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ -\frac{S_z}{c} & \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}, \quad T_{\alpha\beta} = \begin{pmatrix} W & \frac{S_x}{c} & \frac{S_y}{c} & \frac{S_z}{c} \\ \frac{S_x}{c} & \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \frac{S_y}{c} & \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \frac{S_z}{c} & \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix},$$

where $S_i = -S^i$ and $\sigma_{ij} = \sigma^{ij}$ for $i, j = 1, 2, 3$,

(b) $$T^{\alpha\beta}(0) = T_{\alpha\beta}(0) = \begin{pmatrix} \varepsilon & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix},$$

(c) $$\frac{\partial T^{0\beta}}{\partial x^{\beta}} = \frac{\partial \tilde{\rho}}{\partial t} + \vec{\nabla}\cdot(\tilde{\rho}\vec{v}) = 0, \quad \left.\frac{\partial T^{i\beta}}{\partial x^{\beta}}\right|_{i=1,2,3} = \frac{\partial \tilde{\rho}\vec{v}}{\partial t} + \vec{\nabla}\cdot(\tilde{\rho}\vec{v}\otimes\vec{v}) = 0,$$

where "collisionless" means $p = 0$, the density $\tilde{\rho} = \gamma^2 \rho$, corresponding to a frame where $\vec{v} \neq 0$, is given by the ratio of a mass $\tilde{m} = \gamma m$ (cf. Example 9.8) and a volume $\tilde{V} = V/\gamma$ (quantities ρ, m and V are associated to a frame where $\vec{v} = 0$).

• Curved space-time metrics

In general relativity (GR), there are the commonly introduced and used curved space-time metrics. For example, the well-known Schwarzschild metric describes the space-time geometry within a strong gravitational field, e.g., in the vicinity of a (spherically symmetric, nonrotating) black hole (BH). According to the already selected convention $+---$, the Schwarzschild metric tensor (in the coordinate order t, r, θ, ϕ) has the canonic form

$$g_{\mu\nu} = \begin{pmatrix} 1 - \frac{2GM_\bullet}{c^2 r} & 0 & 0 & 0 \\ 0 & -\left(1 - \frac{2GM_\bullet}{c^2 r}\right)^{-1} & 0 & 0 \\ 0 & 0 & -r^2 & 0 \\ 0 & 0 & 0 & -r^2 \sin^2\theta \end{pmatrix}, \tag{2.67}$$

where $M_\bullet$ is the mass of a spherical gravitating object, G is the gravitational constant, and c is the speed of light (often used expressions $1-\frac{2M_\bullet}{r}$ in the so-called “natural unit system” set the constants G and c equal to one). As before, the contravariant form $g^{\mu\nu}$ of the metric tensor will simply invert the diagonal terms.

The Christoffel symbols $\Gamma^\rho_{\mu\nu}$ of the Schwarzschild metric (describing the curvature) that are generally defined as (see also Equations (B.12), however, we distinguish here the covariant and contravariant four-vectors $x_\mu = (ct, -\vec{r})$ and $x^\mu = (ct, \vec{r})$, respectively)

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2} g^{\rho\lambda} \left(\frac{\partial g_{\nu\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu\lambda}}{\partial x^\nu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda} \right), \tag{2.68}$$

will be (introducing only the nonzero terms)

$$\begin{aligned}
&\Gamma^t_{tr} = \Gamma^t_{rt} = \frac{GM_\bullet}{r\left(c^2 r - 2GM_\bullet\right)},\ \Gamma^r_{tt} = \frac{GM_\bullet\left(c^2 r - 2GM_\bullet\right)}{c^4 r^3},\ \Gamma^r_{rr} = -\frac{GM_\bullet}{r\left(c^2 r - 2GM_\bullet\right)},\\
&\Gamma^r_{\theta\theta} = -\left(r - \frac{2GM_\bullet}{c^2}\right),\ \Gamma^r_{\phi\phi} = -\frac{\left(c^2 r - 2GM_\bullet\right)\sin^2\theta}{c^2},\ \Gamma^\theta_{\theta r} = \Gamma^\theta_{r\theta} = \Gamma^\phi_{\phi r} = \Gamma^\phi_{r\phi} = \frac{1}{r},\\
&\Gamma^\theta_{\phi\phi} = -\sin\theta\cos\theta,\ \Gamma^\phi_{\phi\theta} = \Gamma^\phi_{\theta\phi} = \cot\theta.
\end{aligned} \tag{2.69}$$

We can also construct the Christoffel symbols with low indices (sometimes called the Christoffel symbols of the first kind in the literature, while the above are called the Christoffel symbols of the second kind) where the index lowering is done via $\Gamma_{\rho\mu\nu} = g_{\rho\lambda}\Gamma^\lambda_{\mu\nu}$,

$$\begin{aligned}
&\Gamma_{ttr} = \Gamma_{trt} = \frac{GM_\bullet}{c^2 r^2},\ \Gamma_{rtt} = -\frac{GM_\bullet}{c^2 r^2},\ \Gamma_{rrr} = -\frac{GM_\bullet c^2}{\left(c^2 r - 2GM_\bullet\right)^2},\ \Gamma_{r\theta\theta} = r,\ \Gamma_{r\phi\phi} = r\sin^2\theta,\\
&\Gamma_{\theta\theta r} = \Gamma_{\theta r\theta} = -r,\ \Gamma_{\phi\phi r} = \Gamma_{\phi r\phi} = -r\sin^2\theta,\ \Gamma_{\theta\phi\phi} = r^2\sin\theta\cos\theta,\\
&\Gamma_{\phi\phi\theta} = \Gamma_{\phi\theta\phi} = -r^2\sin\theta\cos\theta.
\end{aligned} \tag{2.70}$$

Using the Christoffel symbols, we construct the fourth-order *Riemann (curvature) tensor* $R^\alpha{}_{\mu\beta\nu}$ as the central mathematical tool in the GR theory which represents the tidal force experienced by a rigid body moving along a *geodesic* (the shortest path between two points in an *arbitrarily curved spacetime*). The general formula is $R^\alpha{}_{\mu\beta\nu} = \partial_\beta\Gamma^\alpha_{\mu\nu} - \partial_\nu\Gamma^\alpha_{\mu\beta} + \Gamma^\alpha_{\beta\lambda}\Gamma^\lambda_{\mu\nu} - \Gamma^\alpha_{\nu\lambda}\Gamma^\lambda_{\mu\beta}$, (noting that the simplified expression ∂_α hereafter means $\frac{\partial}{\partial\alpha}$) involving the first two linear terms (partial derivatives) and the last two terms as the nonlinear products of Christoffel symbols. Following this and substituting $\frac{2GM_\bullet}{c^2} = r_\mathrm{s}$ (the so-called *Schwarzschild radius* or *radius of the event horizon*), the nonzero terms of the Schwarzschild metric Riemann tensor will be

$$\begin{aligned}
&R^t{}_{rtr} = 2R^\theta{}_{rr\theta} = 2R^\phi{}_{rr\phi} = -R^t{}_{rrt} = -2R^\theta{}_{r\theta r} = -2R^\phi{}_{r\phi r} = \frac{r_\mathrm{s}}{r^2\left(r - r_\mathrm{s}\right)},\\
&2R^t{}_{\theta\theta t} = 2R^r{}_{\theta\theta r} = R^\phi{}_{\theta\phi\theta} = -2R^t{}_{\theta t\theta} = -2R^r{}_{\theta r\theta} = -R^\phi{}_{\theta\theta\phi} = \frac{r_\mathrm{s}}{r},\\
&2R^t{}_{\phi\phi t} = 2R^r{}_{\phi\phi r} = R^\theta{}_{\phi\theta\phi} = -2R^t{}_{\phi t\phi} = -2R^r{}_{\phi r\phi} = -R^\theta{}_{\phi\phi\theta} = \frac{r_\mathrm{s}\sin^2\theta}{r},\\
&R^r{}_{ttr} = 2R^\theta{}_{t\theta t} = 2R^\phi{}_{t\phi t} = -R^r{}_{trt} = -2R^\theta{}_{tt\theta} = -2R^\phi{}_{tt\phi} = c^2\frac{r_\mathrm{s}\left(r - r_\mathrm{s}\right)}{r^4}.
\end{aligned} \tag{2.71}$$

By contraction $R^\alpha{}_{\mu\alpha\nu}$ of the Riemann tensor, we obtain the symmetric *Ricci (curvature) tensor* $R_{\mu\nu} = R_{\nu\mu}$ which reflects a measure of local deformation of a given metric tensor comparing with ordinary Euclidean (or pseudo-Euclidean) space. From the definition of the tensor contraction, we can construct the Ricci tensor directly by using the Christoffel symbols as $R_{\mu\nu} = \partial_\rho \Gamma^\rho_{\mu\nu} - \partial_\nu \Gamma^\rho_{\mu\rho} + \Gamma^\rho_{\rho\lambda}\Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\mu\lambda}\Gamma^\lambda_{\nu\rho}$. In case of the Schwarzchild metric, the Ricci tensor $R_{\mu\nu} = 0$.

We can assign to each point in the Riemannian manifold (a real, smooth manifold equipped with a positive-definite inner product on the tangent space at each point) a single real number determined by the geometry of the metric near that point, the so-called *Ricci scalar* R, defined as $R = g^{\mu\nu} R_{\mu\nu}$. All the above-described mathematical formalism allows us to construct the complete Einstein field equations (omitting here for simplicity the cosmological constant Λ)

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = \frac{8\pi G}{c^4} T_{\mu\nu}, \tag{2.72}$$

where the complete LHS is often denoted as the *Einstein tensor* $G_{\mu\nu}$ and $T_{\mu\nu}$ is the energy-momentum tensor (see example 2.52). "Manual" calculations of such extensive tensor structures are very laborious and often lead to mistakes and omitting; several programs currently enable analytical or numerical calculations of tensors within an arbitrary metric (for example, MATHEMATICA, Python applications, etc.).

Chapter 3

Ordinary differential equations[1]

3.1 First-order ordinary differential equations

Ordinary differential equations contain derivatives of a function of a single independent variable (usually denoted x, while the dependent variable is usually denoted as $y(x)$). An ordinary differential equation of nth-order can be in general written in the form

$$f(y^{(n)}, \ldots, y'', y', y, x) = 0, \tag{3.1}$$

where $y^{(k)}$ denotes kth derivative of the function $y(x)$. Ordinary *linear* differential equations are called equations in the form

$$y^{(n)} + a_{n-1}(x)y^{(n-1)} + \ldots + a_1(x)y' + a_0(x)y = f(x). \tag{3.2}$$

If the ordinary differential equation cannot be written in the form (3.2), it is the *nonlinear* ordinary differential equation. The terms $a_k(x)$ in Equation (3.2) are *coefficients*, which can be functions of the variable x, if they are constant, we speak about the differential equation with *constant coefficients*, and the function $f(x)$ represents the right-hand side of the differential equation. If $f(x) = 0$, then it is the *homogeneous differential equation* (equation without the right-hand side). We call *partial* differential equations the differential equations with derivatives of functions of several independent variables. The *order* of a differential equation is given by the highest order of the derivative of the dependent variable $y(x)$, which occurs in the equation, in case of the first-order equations, it will be the first derivative $y' = \mathrm{d}y/\mathrm{d}x$.

3.1.1 Separable and homogeneous equations

If the first-order differential equation can be expressed in a simple form $y' = f(x)$, we solve it by direct integration, i.e.,

$$y = \int f(x)\,\mathrm{d}x. \tag{3.3}$$

If the first-order differential equation can be expressed as $y' = f(x)g(y)$, where $g(y) \neq 0$, we solve it by dividing the functions by the independent variable x and by the dependent variable y on different sides of equation (*by separating variables*), that is

$$\int \frac{\mathrm{d}y}{g(y)} = \int f(x)\,\mathrm{d}x. \tag{3.4}$$

[1]Solved examples of various types of ordinary differential equations it is possible to find in literature, for example in the publications: Tenenbaum & Pollard (1985), Ráb (1989), Plch (2002), Bartsch (2008), Rektorys (2009).

We call $f(x, y)$ a *homogeneous*, nth-order function, if for all x, y and for all $z > 0$, where z is an arbitrary parameter, holds $f(zx, zy) = z^n f(x, y)$. Ordinary first-order differential equation

$$M(x, y)\,\mathrm{d}x + N(x, y)\,\mathrm{d}y = 0 \tag{3.5}$$

is homogeneous if $M(x, y)$ and $N(x, y)$ are homogeneous functions of the same degree. If the homogeneous equation is written in the general form (3.5) or also in the form

$$y' = f\left(\frac{y}{x}\right), \tag{3.6}$$

we solve it by using an appropriate substitution, for example $y = zx$, and convert it to a separable equation. Similarly, the equation in the form

$$y' = f\left(ax + by + c\right), \tag{3.7}$$

where a, b, c, are constants, we convert to the equation with separable variables using the substitution $z = ax + by + c$. Equations in the form of a rational function (where A, B, C, are also constants),

$$y' = \frac{ax + by + c}{Ax + By + C}, \tag{3.8}$$

if expressions $ax+by$, $Ax+By$ are not linearly dependent, we solve by eliminating the absolute terms c, C by substituting $u = x - x_0$, $v = y - y_0$, where x_0, y_0 are the roots of the system of equations $ax + by + c = 0$, $Ax + By + C = 0$ and then by converting them to the form of Equation (3.6). If the expressions $ax + by$, $Ax + By$ are linearly dependent (the system has no solution), we solve the system by substitution $ax + by = z$ (or $Ax + By = z$), which will enable its subsequent conversion to the form of Equation (3.6).

Solutions of the first-order differential equations always contain one independent (integration) constant. We get its value from the so-called *initial* (Cauchy) *condition*, where $y(x_p) = y_p$.

- **Examples:**

3.1 $y' + 2y = 0$ $\quad y = C\,\mathrm{e}^{-2x},\ y = 0$

3.2 $y' + 3y - 7 = 0$ $\quad y = C\,\mathrm{e}^{-3x} + \dfrac{7}{3}$

3.3 $y' + y + xy = 0$ $\quad y = C\,\mathrm{e}^{-x(1+x/2)},\ y = 0$

3.4 $y'xy^2 = \ln x$ $\quad y^3 = \dfrac{3}{2}\ln^2 x + C,\ x > 0$

3.5 $y' = y^2 + 1,\ y(0) = 1$ $\quad y = \tan\left(x + \dfrac{\pi}{4}\right),\ x \neq \left(k + \dfrac{1}{4}\right)\pi,\ k \in \mathbb{Z}$

3.6 $y' = y\,\mathrm{e}^{3x},\ y(0) = 1$ $\quad y = \mathrm{e}^{\left(\mathrm{e}^{3x}-1\right)/3}$

3.7 $y' = \dfrac{y+1}{x^{3/2}}$ $\quad y = C\,\mathrm{e}^{-2/\sqrt{x}} - 1,\ x > 0$

3.8 $y' = \left(y^2 - 1\right) x,\ y(0) = 0$ $\qquad y = \dfrac{1 - \mathrm{e}^{x^2}}{1 + \mathrm{e}^{x^2}}$

3.9 $y' = 2\dfrac{y}{x},\ y(1) = 2$ $\qquad y = 2x^2,\ y = 0,\ x \neq 0$

3.10 $y' = \dfrac{y}{x} + x,\ y(1) = 0$ $\qquad y = x^2 - x,\ x \neq 0$

3.11 The number of bacteria n in a bacterial strain increases with time proportionally to their total amount ($\Delta n/\Delta t \propto n$). If at a specific time their number is $n = 10^6$ and two hours later $n = 4 \times 10^6$, find the function that describes the time dependence of the number of bacteria.

$n = 10^6\,\mathrm{e}^{t \ln 2}$, where t is the time in hours

3.12 The radioactive element decays with half-time of 100 years. If, at a particular time, the mass of this element within the sample is $m = 2\,\mathrm{kg}$, find the function describing the time dependence of this element mass in the sample. How long will it take from the initial time to have only $0.1\,\mathrm{kg}$ of the radioactive element left in this sample?

$m = 2\,\mathrm{e}^{-t\,(\ln 2)/100}\,\mathrm{kg}$, where t is the time in years; after about $432\,\mathrm{years}$

3.13 Hydrostatic equilibrium equation for fluid (liquid, gas) in the homogeneous gravitational field has the form $\mathrm{d}P(z)/\mathrm{d}z = -\rho(z)g$, where $P(z)$ is the pressure, z is the height above some fixed reference level z_0, $\rho(z)$ is the density, and g is constant gravitational acceleration. In the case of an ideal gas, its equation of state is $P = \rho RT/M$, where R is the molar gas constant, T is the temperature, and M is the so-called molar mass of the gas. Find the functions describing the dependence of the pressure and density of an ideal gas on altitude if we consider a constant temperature for simplicity and denote $P(z_0) = P_0$ and $\rho(z_0) = \rho_0$ (the so-called barometric equation).

$P = P_0\,\mathrm{e}^{-Mgz/(RT)},\ \rho = \rho_0\,\mathrm{e}^{-Mgz/(RT)}$

3.14 A body with the mass $5\,\mathrm{kg}$ falls from rest by free fall, while the force induced by the air resistance is proportional to the instantaneous fall velocity. Determine the constant of proportionality b of the resistance force, if the terminal velocity $v_\infty = 100\,\mathrm{m\,s^{-1}}$ of the free fall was measured. For simplicity, consider the magnitude of gravitational acceleration $g = 10\,\mathrm{m\,s^{-2}}$.

$b = 0.5\ \mathrm{kg\ s^{-1}}$

3.15 A body of an arbitrary mass falls from rest by free fall, with force induced by air resistance being

(a) proportional to the instantaneous fall velocity,

(b) proportional to the square of the instantaneous velocity of the fall.

In both cases, the terminal fall velocity v_∞ with the magnitude $100\,\mathrm{m\,s^{-1}}$ was measured. How long will it take for this body to reach an instantaneous velocity equal to one half of the terminal velocity v_∞? For simplicity, consider the magnitude of gravitational acceleration $g = 10\,\mathrm{m\,s^{-2}}$. How long will it take for this body to reach an instantaneous velocity equal to 90% of the terminal velocity v_∞? For comparison, calculate the times in which this body would reach the corresponding velocities in the vacuum.

(a) $0.5\,v_\infty$ reaches after $10\ln 2\,\mathrm{s} \approx 6.93\,\mathrm{s}$, $0.9\,v_\infty$ reaches after $10\ln 10\,\mathrm{s} \approx 23\,\mathrm{s}$

(b) $0.5\,v_\infty$ reaches after $5\ln 3\,\mathrm{s} \approx 5.49\,\mathrm{s}$, $0.9\,v_\infty$ reaches after $5\ln 19\,\mathrm{s} \approx 14.72\,\mathrm{s}$

Why are the times achieved in the case (b) shorter than in the case (a), if the resistivity force should be expected to be larger (since it is proportional to the square of the instantaneous velocity)?

3.16 $\dfrac{yy'}{\sqrt{1+y^2}} + \dfrac{x}{\sqrt{1+x^2}} = 0$ $\qquad \sqrt{1+y^2} = C - \sqrt{1+x^2}$

3.17 $(x^2-1)y^3 - \mathrm{e}^x y' = 0$ $\qquad y = 0 \vee \dfrac{1}{2y^2} - (x+1)^2\,\mathrm{e}^{-x} = C,\ y \neq 0$

3.18 $y' = 3^{3x+2y},\ y(0) = 1$ $\qquad y = -\dfrac{\log_3\left(\frac{7}{9} - \frac{2}{3}\cdot 3^{3x}\right)}{2},\ x < \dfrac{1}{3}\log_3\dfrac{7}{6}$

3.19 $x^2(y^3+5)\,\mathrm{d}x + (x^3+5)y^2\,\mathrm{d}y = 0,\ y(0) = 1$ $\qquad (y^3+5)(x^3+5) = 30$

3.20 $y' = \cos(x-y),\ y(0) = \dfrac{\pi}{2}$ $\qquad y = x + 2\,\mathrm{arccot}\,(x+1)$

3.21 $x^2\left(y' - \dfrac{1}{\ln x}\right) = xy$ $\qquad y = x\ln(C|\ln x|),\ x > 0,\ C > 0,\ x \neq 1$

3.22 $y' = \sqrt{2x+y-3},\ y(0) = 3$

$2(\sqrt{2x+y-3}+2) - 4\ln(\sqrt{2x+y-3}+2) = x - (4\ln 2 - 4),\ 2x+y-3 \geq 0$

3.23 $(x+y)^2 y' = 4,\ y(0) = 2$ $\qquad y = 2\arctan\left(\dfrac{x+y}{2}\right) - \dfrac{\pi}{2} + 2$

3.24 $y' = \dfrac{y}{x}\left(1 + \ln\dfrac{y}{x}\right)$ $\qquad y = x\,\mathrm{e}^{Cx},\ \dfrac{y}{x} > 0$

3.25 $y' = \dfrac{y}{x} + \tan\dfrac{y}{x}$

$y = 0 \vee \sin\dfrac{y}{x} = Cx,\ x \neq 0,\ y \neq (2k+1)\dfrac{\pi}{2}x,\ k \in \mathbb{Z}$

3.26 $x^2 y' = xy + \ln x$ $\qquad y = -\dfrac{2\ln x + 1}{4x} + Cx,\ x > 0$

3.27 $xy' = y + \dfrac{y}{x}$ $\qquad y = Cx\,\mathrm{e}^{-1/x} \vee y = 0,\ x \neq 0$

3.28 $x^3 y' = x^2[y + \ln(x^2)]$ $\qquad y = -2\left(\ln|x| + 1\right) + Cx,\ x \neq 0$

3.29 $y' = 1 + (x-y)^2$ $\qquad y = x - \dfrac{1}{x+C},\ x \neq -C$

3.30 $y' = (y+x)\ln(y+x) - 1$ $\qquad y = \mathrm{e}^{C\,\mathrm{e}^x} - x,\ x \in \mathbb{R}$

3.31 $y' = \dfrac{\mathrm{e}^{(x+y)^2}}{x+y} - 1$ $\qquad y = \pm\sqrt{\ln\left(\dfrac{1}{C-2x}\right)} - x,\ x \in (-\infty, C/2).$

3.32 $y' = \mathrm{e}^{y+x^2} - 2x$ $\quad y = \ln\left[(C-x)^{-1}\right] - x^2,\ x \in (-\infty, C).$

3.33 $y' = \dfrac{x+2y-7}{x-3}$ $\quad x + y - 5 = C(x-3)^2,\ x \neq 3$

3.34 $y' = \dfrac{1+9x-3y}{3x-y}$ $\quad (3x-y)^2 + 2x = C,\ y \neq 3x$

3.35 $y' = \dfrac{2x-y+3}{x-2y+3}$ $\quad x^2 + y^2 - xy + 3x - 3y = C,\ 2y \neq x+3$

3.36 $y' = \dfrac{x-y}{x+y}$ $\quad y = \pm\sqrt{C+2x^2} - x,\ 2x^2 + C \geq 0$

3.1.2 Linear inhomogeneous equations

We solve *inhomogeneous* linear first-order differential equations (also called "equations with the right-hand side"), written in the general form

$$y' + P(x)y = Q(x), \tag{3.9}$$

where $Q(x) \neq 0$, by the method of *variation of parameter* or by the method of *integrating factor*. In the first case of *variation of parameter*, we first solve a homogeneous equation $y' + P(x)y = 0$ where its constant of integration C will be a common function $C(x)$ of independent variable; a *general* solution will thus be

$$y = C(x)\,\mathrm{e}^{-\int P(x)\,\mathrm{d}x}. \tag{3.10}$$

The function $C(x)$ can be found by substituting Equation (3.10) into Equation (3.9), its form will be

$$C(x) = \int Q(x)\,\mathrm{e}^{\int P(x)\,\mathrm{d}x}\,\mathrm{d}x + K \tag{3.11}$$

where K is a constant. We substitute this expression for the function $C(x)$ into Equation (3.10); the resulting *particular* solution will be

$$y = \left(\int Q(x)\,\mathrm{e}^{\int P(x)\,\mathrm{d}x}\,\mathrm{d}x + K\right)\mathrm{e}^{-\int P(x)\,\mathrm{d}x}. \tag{3.12}$$

The method of *integrating factor* is the designation for multiplying the complete equation by the expression $\mathrm{e}^{\int P(x)\,\mathrm{d}x}$; Equation (3.9) thus becomes the form

$$y'\,\mathrm{e}^{\int P(x)\,\mathrm{d}x} + P(x)y\,\mathrm{e}^{\int P(x)\,\mathrm{d}x} = Q(x)\,\mathrm{e}^{\int P(x)\,\mathrm{d}x}. \tag{3.13}$$

However, the left-hand side of Equation (3.13) represents the derivative of the product, so we can rewrite the whole equation to the form

$$\left(y\,\mathrm{e}^{\int P(x)\,\mathrm{d}x}\right)' = Q(x)\,\mathrm{e}^{\int P(x)\,\mathrm{d}x}, \tag{3.14}$$

whose direct integration again gives us a solution in the form of Equation (3.12).

- **Examples:**

3.37 $y' + 2xy = x\,\mathrm{e}^{-x^2}\sin x,\ y(0) = 1$ $\qquad y = (\sin x - x\cos x + 1)\,\mathrm{e}^{-x^2}$

3.38 $y' + y\cos x = \cos x$ $\qquad y = C\,\mathrm{e}^{-\sin x} + 1$

3.39 $(1+x^2)y' - 2xy = (1+x^2)^2$ $\qquad y = (x+C)(1+x^2)$

3.40 $y' - 6xy = 4x\,\mathrm{e}^{3x^2},\ y(0) = 1$ $\qquad y = \left(2x^2+1\right)\,\mathrm{e}^{3x^2}$

3.41 $y' + 3x\,\mathrm{e}^{3x} = -y + 7,\ y(0) = 7$ $\qquad y = 7 + \left(\frac{3}{16} - \frac{3}{4}x\right)\,\mathrm{e}^{3x} - \frac{3}{16}\,\mathrm{e}^{-x}$

3.42 $xy' + y = x\sin x,\ y\left(\frac{\pi}{2}\right) = 0$ $\qquad y = \dfrac{\sin x - 1}{x} - \cos x,\ x \neq 0$

3.43 $y' = 2x + 3y + 2,\ \ y(0) = 0$ $\qquad y = \dfrac{8}{9}\left(\mathrm{e}^{3x} - 1\right) - \dfrac{2x}{3}$

3.44 $y' = 4x^2 + 3y - 1,\ y(0) = 0$ $\qquad y = \dfrac{1}{27}\left(1 - \mathrm{e}^{3x}\right) - \dfrac{4}{3}x^2 - \dfrac{8}{9}x$

3.45 $y' = 2x^2 - y + 1,\ y(0) = 0$ $\qquad y = 2x^2 - 4x + 5\left(1 - \mathrm{e}^{-x}\right)$

3.46 $y' = 2x^3 - y + 1,\ y'(0) = 0$ $\qquad y = 2x^3 - 6x^2 - 11 + 12(x + \mathrm{e}^{-x})$

3.47 $y' = -\dfrac{4x}{x^2+1}y + \dfrac{1}{x^2+1},\ y(0) = 1$ $\qquad y = \dfrac{1}{3}\left(x^3 + 3x + 3\right)\left(x^2+1\right)^{-2}$

3.48 A metal coin is heated to the temperature of 1200° C, and then it cools freely. After 2 minutes, its temperature drops to 900° C, with the constant ambient temperature of 20° C. After how long will it be possible to pick up a coin by hand (i.e., when its temperature drops below 50° C)? Consider the change in temperature of a coin being proportional to the difference between its temperature and the constant ambient temperature.

after about 25 minutes

3.49 A paste has temperature 20° C of an ambient environment, and it is placed in an oven where the internal temperature is 200° C. After two hours at the temperature of 90° C, it is pulled out and allowed to cool for 30 minutes. What will be the resulting temperature? Consider the same thermal conductivity coefficient and other physical parameters inside and outside the oven. Follow the same procedure as in Example 3.48.

about 82° C

3.1.3 Bernoulli equation

We call the *Bernoulli (differential) equation* a first-order differential equation with nth power of the dependent variable $y(x)$ in the form

$$y' + p(x)\,y + q(x)\,y^n = 0,\ \text{ where } n \in \mathbb{R}, \tag{3.15}$$

which, despite its non-linearity, has an analytical solution. If $n = 0$, the Bernoulli equation becomes the inhomogeneous linear Equation (3.9), for $n = 1$, it becomes the easily separable homogeneous linear Equation (3.4). Using substitution

$$z = y^{1-n} \text{ for } n \neq 0, 1, \tag{3.16}$$

we get a first-order inhomogeneous linear differential equation of type (3.9) in the form

$$z' + (1-n)\, p(x) z + (1-n)\, q(x) = 0. \tag{3.17}$$

- **Examples:**

3.50 $y' = 6x^2y^3$ $\quad$ $y^2 = \dfrac{1}{C - 4x^3},\ y = 0,\ 4x^3 < C$

3.51 $xy' - y = -xy^2$ $\quad$ $y = \dfrac{2x}{x^2 + C},\ y = 0,\ x^2 \neq -C$

3.52 $y' + \dfrac{4}{x}y = x^3y^2$ $\quad$ $y = \dfrac{1}{x^4\,(C - \ln|x|)},\ y = 0,\ x \neq 0$

3.53 $y' + \dfrac{y}{x} - \sqrt{y} = 0$ $\quad$ $y = \left(\dfrac{x}{3} + \dfrac{C}{\sqrt{x}}\right)^2,\ y = 0,\ x > 0,\ x^{\frac{3}{2}} \geq -3C$

3.54 $y' + xy = xy^3,\ y^2(0) = \dfrac{1}{2}$ $\quad$ $y^2 = \left(\mathrm{e}^{x^2} + 1\right)^{-1},\ y = 0$

3.55 $xy' + y = y^2 \ln x,\ y(1) = -1$ $\quad$ $y = \dfrac{1}{1 + \ln x - 2x},\ y = 0,\ x > 0$

3.56 $2xyy' - y^2 = x^2,\ y(1) = 0$ $\quad$ $y^2 - x^2 = x$

3.57 $x^2y^2y' + xy^3 = 1,\ y(-2) = -1$ $\quad$ $y^3 = \dfrac{2}{x^3} + \dfrac{3}{2x},\ x \neq 0$

3.1.4 Exact differential equation

We call the equation of type (3.5) *exact*, if the expression on its left-hand side is the total differential of a scalar (the so-called *scalar potential*) function $F(x, y)$, that is (see Section 5.2 for details),

$$\mathrm{d}F(x, y) = \frac{\partial F(x, y)}{\partial x}\,\mathrm{d}x + \frac{\partial F(x, y)}{\partial y}\,\mathrm{d}y. \tag{3.18}$$

The functions $M(x, y)$, $N(x, y)$ in Equation (3.5) correspond to individual partial derivatives (i.e., the components of the *gradient* - see Section 5.1) of the scalar function $F(x, y)$ ordered according to Equation (3.18). If both the functions $M(x, y)$, $N(x, y)$ are continuously differentiable, then according to the *Schwarz theorem* about the equality of mixed derivatives must hold,

$$\frac{\partial M(x, y)}{\partial y} = \frac{\partial N(x, y)}{\partial x}. \tag{3.19}$$

To solve Equation (3.5), it is necessary to find the scalar potential function $F(x,y)$, whose general solution is usually written in the form $F(x,y)=C$. If Equation (3.19) does not hold, Equation (3.5) is not an exact equation. However, if we find a function $R(x,y)$ (the so-called *integrating factor*) such that

$$R(x,y)\left[M(x,y)\,\mathrm{d}x+N(x,y)\,\mathrm{d}y\right]=0,\quad \frac{\partial}{\partial y}\left[R(x,y)M(x,y)\right]=\frac{\partial}{\partial x}\left[R(x,y)N(x,y)\right], \tag{3.20}$$

Equation (3.20) will be exact. For the continuously differentiable functions $M(x,y)\neq 0, N(x,y)\neq 0$ such an integrating factor $R(x,y)$ always exists.

- **Examples:**

3.58 $2xy-9x^2+\left(2y+x^2+1\right)y'=0$ $\quad$ $y^2+\left(x^2+1\right)y-3x^3=C$

3.59 $\left(2xy+6x\right)\mathrm{d}x+\left(x^2+4y^3\right)\mathrm{d}y=0$ $\quad$ $x^2y+3x^2+y^4=C$

3.60 $\left(8y-x^2y\right)y'+x-xy^2=0$ $\quad$ $\frac{1}{2}x^2\left(1-y^2\right)+4y^2=C$

3.61 $\left(\mathrm{e}^{4x}+2xy^2\right)\mathrm{d}x+\left(\cos y+2x^2y\right)\mathrm{d}y=0$ $\quad$ $\frac{1}{4}\mathrm{e}^{4x}+x^2y^2+\sin y=C$

3.62 $\left(3x^2+y\cos x\right)\mathrm{d}x+\left(\sin x-4y^3\right)\mathrm{d}y=0$ $\quad$ $x^3+y\sin x-y^4=C$

3.63 $x\arctan y\,\mathrm{d}x+\dfrac{x^2}{2(1+y^2)}\,\mathrm{d}y=0$ $\quad$ $\frac{x^2}{2}\arctan y=C$

3.64 $\left(2x+x^2y^3\right)\mathrm{d}x+\left(x^3y^2+4y^3\right)\mathrm{d}y=0$ $\quad$ $x^2+\frac{x^3y^3}{3}+y^4=C$

3.65 $\left(2x^3-3x^2y+y^3\right)y'=2x^3-6x^2y+3xy^2$ $\quad$ $\frac{x^4}{2}-2x^3y+\frac{3}{2}x^2y^2-\frac{y^4}{4}=C$

3.66 $\left(y^2\cos x-\sin x\right)\mathrm{d}x+\left(2y\sin x+2\right)\mathrm{d}y=0$ $\quad$ $y^2\sin x+\cos x+2y=C$

3.67 $2xy^2\,\mathrm{d}x+\left(3x^2y+4\right)\mathrm{d}y=0$ $\quad$ $x^2y^3+2y^2=C$

3.68 $\left(2y+4x^2y^2\right)\mathrm{d}x+\left(x+2yx^3\right)\mathrm{d}y=0$ $\quad$ $x^2y+x^4y^2=C$

3.69 $2xy\,\mathrm{d}x+\left(y^2-3x^2\right)\mathrm{d}y=0$ $\quad$ $\frac{x^2}{y^3}-\frac{1}{y}=C$

3.1.5 Riccati equation ★

Although it is a first-order equation, it may require knowledge of the procedures referred to in Section 3.2.2. The nonlinear first-order differential equation in the form of

$$y'=a_0(x)+a_1(x)y+a_2(x)y^2, \tag{3.21}$$

where $a_0(x)\neq 0$ and $a_2(x)\neq 0$, which contains the quadratic function of the dependent variable $y(x)$, we call the Riccati equation (this term may have also a broader meaning, which I do not

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

mention here). If $a_0(x) = 0$, the equation becomes the Bernoulli differential equation (Section 3.1.3); if $a_2(x) = 0$, the equation becomes an ordinary linear first-order differential equation (see Section 3.1.2).

We solve Equation (3.21) by the substitution $u = a_2(x)y$. In that case $u' = a_2'y + a_2y'$, and the equation (3.21) becomes the form

$$u' = a_0a_2 + \left(a_1 + \frac{a_2'}{a_2}\right) u + u^2. \tag{3.22}$$

Using another substitution $u = -v'/v$, we get $u' = -v''/v + (v'/v)^2$, so Equation (3.22) becomes the form of a homogeneous linear second-order differential equations (with non-constant coefficients),

$$v'' - \left(a_1 + \frac{a_2'}{a_2}\right) v' + a_0a_2v = 0. \tag{3.23}$$

We solve the equation according to the principles introduced in Section 3.2.2, then we can find the original function y as $y = -v'/(a_2v)$.

However, if we know or somehow guess one solution of the original equation (3.21) (we denote it, for example, y_1), then by the substitution $y = y_1 + u$ the Riccati equation becomes the Bernoulli equation. By substituting the given substitution into Equation (3.21), we get

$$y_1' + u' = a_0 + a_1y_1 + a_2y_1^2 + a_1u + a_2\left(2y_1u + u^2\right). \tag{3.24}$$

Since y_1 is also a solution of the equation (3.21), then $y_1' = a_0 + a_1y_1 + a_2y_1^2$ must hold, so

$$u' = (a_1 + 2a_2y_1)\, u + a_2u^2, \tag{3.25}$$

which is the Bernoulli equation for $n = 2$ with unknown function u.

3.2 Linear ordinary second-order differential equations

3.2.1 Equations with constant coefficients

Linear ordinary second-order differential equations (i.e., containing the second derivative of the dependent variable $y(x)$) with constant coefficients p, q are solved in the first step as a homogeneous equation, where the equation in the form

$$y'' + py' + qy = 0, \tag{3.26}$$

we solve by the so-called *characteristic equation* $\lambda^2 + p\lambda + q = 0$. For the roots of the characteristic equation $\lambda_1, \lambda_2 \in \mathbb{R}$ will take Equation (3.26) solution in the form

$$y = C_1\,\mathrm{e}^{\lambda_1 x} + C_2\,\mathrm{e}^{\lambda_2 x} \qquad \text{for } \lambda_1 \neq \lambda_2, \tag{3.27}$$

$$y = C_1\,\mathrm{e}^{\lambda_1 x} + C_2\,x\,\mathrm{e}^{\lambda_2 x} \qquad \text{for } \lambda_1 = \lambda_2. \tag{3.28}$$

For the roots of the characteristic equation $\lambda_1, \lambda_2 = \alpha \pm \beta\,\mathrm{i} \in \mathbb{C}$ will take Equation (3.26) solution in the form

$$y = C_1\,\mathrm{e}^{(\alpha-\beta\mathrm{i})\,x} + C_2\,\mathrm{e}^{(\alpha+\beta\mathrm{i})\,x} = A\,\mathrm{e}^{\alpha x}\cos\beta x + B\,\mathrm{e}^{\alpha x}\sin\beta x. \tag{3.29}$$

These solutions can be generalized also for higher-order differential equations: for each root of the characteristic equation of nth-order $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}$ with the multiplicity Π will take Equation (3.26) Π solutions in the form

$$y = C_1\,\mathrm{e}^{\lambda_1 x} + C_2\,x\,\mathrm{e}^{\lambda_2 x} + \cdots + C_\Pi\,x^{\Pi-1}\,\mathrm{e}^{\lambda_\Pi x}. \tag{3.30}$$

For each pair of roots of the characteristic equation of nth-order $\lambda_1, \lambda_2 = \alpha \pm \beta\,\mathrm{i} \in \mathbb{C}$ with multiplicity Π will take Equation (3.26) Π solutions in the form

$$y = \mathrm{e}^{\alpha x}\cos\beta x\left(A_1 + A_2 x + \cdots + A_\Pi x^{\Pi-1}\right) + \mathrm{e}^{\alpha x}\sin\beta x\left(B_1 + B_2 x + \cdots + B_\Pi x^{\Pi-1}\right). \tag{3.31}$$

The sequence of linearly independent terms $y_1(x), \ldots, y_n(x)$ within the solution of a homogeneous equation represents the so-called *fundamental system*.

Analogously to the method described in Section 3.1.2, we search a particular solution of an inhomogeneous equation (equation with the right-hand side) in the form of

$$y'' + py' + qy = R(x) \tag{3.32}$$

by the method of *variation of parameters*, where Equations (3.27), (3.28), or (3.29) are written as the general solution of the differential equation, that is

$$y = C_1(x)\,\mathrm{e}^{\lambda_1 x} + C_2(x)\,\mathrm{e}^{\lambda_2 x} = C_1 u_1 + C_2 u_2. \tag{3.33}$$

Functions $C_1(x)$, $C_2(x)$, $\mathrm{e}^{\lambda_1 x}$, $\mathrm{e}^{\lambda_2 x}$, which we will hereafter write for the sake of simplicity as C_1, C_2, u_1, u_2, we find again by substituting Equation (3.33) into Equation (3.32). Thus we get one equation for two unknown functions C_1, C_2,

$$\begin{aligned} R(x) &= (C_1u_1 + C_2u_2)'' + p\,(C_1u_1 + C_2u_2)' + q\,(C_1u_1 + C_2u_2) \\ &= C_1\left(u_1'' + pu_1' + qu_1\right) + C_2\left(u_2'' + pu_2' + qu_2\right) + \left(C_1''u_1 + 2C_1'u_1' + C_2''u_2 + 2C_2'u_2'\right) \\ &\quad + p\left(C_1'u_1 + C_2'u_2\right), \end{aligned} \tag{3.34}$$

where the first two terms in brackets (multiplied by the non-differentiated functions C_1, C_2) represent the homogeneous Equations (3.26). We thus have one equation for two unknown functions C_1' and C_2', where the third plus the fourth bracket (multiplied by coefficient p) from equation (3.34) are equal to its right-hand side $R(x)$. Setting the expression in the fourth bracket, $C_1'u_1 + C_2'u_2$, equal to a completely arbitrary function $f(x)$ that we may always regard as a common subset of a complete solution of the right-hand side, then $C_1''u_1 + C_1'u_1' + C_2''u_2 + C_2'u_2' = f'(x)$, and the equation (3.34) can be rewritten as $C_1'u_1' + C_2'u_2' + p \cdot f(x) + f'(x) = R(x)$. However, if the function $f(x)$ can be selected absolutely arbitrarily, then its simplest choice will be $f(x) = 0$, and therefore:

$$C_1'u_1 + C_2'u_2 = 0. \tag{3.35}$$

Since the function $f'(x)$ must also be equal to zero, substitution into Equation (3.34) gives the resulting system of two equations for the two unknown functions C_1', C_2', written as

$$\begin{aligned} C_1'u_1 + C_2'u_2 &= 0, \\ C_1'u_1' + C_2'u_2' &= R(x). \end{aligned} \tag{3.36}$$

If we write the system of Equations (3.36) using the so-called *Wronski matrix*, i.e., in the form

$$\begin{pmatrix} u_1 & u_2 \\ u_1' & u_2' \end{pmatrix}\begin{pmatrix} C_1' \\ C_2' \end{pmatrix} = \begin{pmatrix} 0 \\ R(x) \end{pmatrix}, \tag{3.37}$$

whose determinant $u_1u_2' - u_2u_1'$ (the so-called *Wronskian*) denoted W, we can easily find the solution

$$C_1 = -\int \frac{u_2 R(x)}{W}\,\mathrm{d}x, \quad C_2 = \int \frac{u_1 R(x)}{W}\,\mathrm{d}x \tag{3.38}$$

of the system of Equations (3.36). Substituting Equation (3.38) into the general solution (3.33) gives the particular solution of the ordinary second-order differential equation. In the case of an ordinary differential equation of a general (nth) order, Equation (3.37) becomes:

$$\begin{pmatrix} u_1 & u_2 & \cdots & u_n \\ u_1' & u_2' & \cdots & u_n' \\ \vdots & \vdots & & \vdots \\ u_1^{(n-1)} & u_2^{(n-1)} & \cdots & u_n^{(n-1)} \end{pmatrix} \begin{pmatrix} C_1' \\ C_2' \\ \vdots \\ C_n' \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ R(x) \end{pmatrix}. \tag{3.39}$$

If the right-hand side $R(x)$ of an inhomogeneous equation takes the form (the so-called *special right-hand side*), generally written as

$$R(x) = [P_n(x)\cos\beta x + Q_n(x)\sin\beta x]\,\mathrm{e}^{\alpha x}, \tag{3.40}$$

where P_n and Q_n are polynomials of maximum nth degree (where n is equal to the higher degree of both polynomials P, Q), it is often easier to find the solution of the differential equation by the so-called *method of undetermined coefficients*. When looking for a particular solution, we start (regardless of the values of the coefficients α and β, which can be zero, or regardless of whether one of the polynomials P_n, Q_n is zero) from the equation

$$y = \left[(A_p x^n + B_p x^{n-1} + \ldots + C_p)\cos\beta x + (A_q x^n + B_q x^{n-1} + \ldots + C_q)\sin\beta x\right] x^{\Pi}\,\mathrm{e}^{\alpha x}, \tag{3.41}$$

where Π is the multiplicity of the root $\lambda = \alpha + \beta\,\mathrm{i}$ of the characteristic equation (where again α, β can be zero). We substitute Equation (3.40) into Equation (3.32) and compare general coefficients $A_p, \ldots, C_p$, $A_q, \ldots, C_q$ with the coefficients of function $R(x)$, given by Equation (3.40).

General solutions of second-order differential equations always contain two independent constants. Their values are obtained by solving the so-called boundary problem, given in the form of *boundary conditions*, where for two different x_1, x_2 holds $y(x_1) = y_1$, $y(x_2) = y_2$ (*Dirichlet* boundary conditions) or $y'(x_1) = y_1$, $y'(x_2) = y_2$ (*Neumann* boundary conditions), or their various combinations, for example, $y(x_1) = y_1$, $y'(x_1) = \alpha y_1$ or $y(x_1) = y_1$, $y'(x_2) = y_2$ where $\alpha \neq 0$ is a constant, etc. For a detailed listing of types of boundary conditions and their classification, see, for example, (Arfken & Weber, 2005; Franců, 2011; Pospíšil, 2006).

- **Examples:**

3.70 $y'' - 2y' + y = \dfrac{\mathrm{e}^x}{x}$, $y(1) = 0$, $y'(1) = 0$ $\qquad y = \mathrm{e}^x + x\,\mathrm{e}^x\left(\ln|x| - 1\right),\ x \neq 0$

3.71 $y'' - 7y' + 12y = 5$ $\qquad y = C_1\,\mathrm{e}^{3x} + C_2\,\mathrm{e}^{4x} + \dfrac{5}{12}$

3.72 $y'' - 3y' + 2y = \dfrac{\mathrm{e}^{3x}}{1 + \mathrm{e}^{2x}}$

$$y = C_1\,\mathrm{e}^x + C_2\,\mathrm{e}^{2x} - \frac{1}{2}\mathrm{e}^x \ln\left(1 + \mathrm{e}^{2x}\right) + \mathrm{e}^{2x}\arctan\left(\mathrm{e}^x\right)$$

3.73 $y'' + y = \dfrac{1}{\sin x}$, $y\left(\frac{\pi}{2}\right) = 1$, $y'\left(\frac{\pi}{2}\right) = 0$

$y = \left(\dfrac{\pi}{2} - x\right)\cos x + \sin x\,(1 + \ln|\sin x|)\,,\ x \neq k\pi,\ k \in \mathbb{Z}$

3.74 $y'' - 2y' = x^2 - x$ $\qquad y = C_1 + C_2\,\mathrm{e}^{2x} - \dfrac{x^3}{6}$

3.75 $y'' + y' = \dfrac{1}{1+\mathrm{e}^x}$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = 1 + x + (1 + \mathrm{e}^{-x})\ln\dfrac{2}{1+\mathrm{e}^x}$

3.76 $y'' + y = \cos x$, $y(0) = 1$, $y\left(\frac{\pi}{2}\right) = 1 + \dfrac{\pi}{4}$ $\qquad y = \cos x + \sin x\left(1 + \dfrac{x}{2}\right)$

3.77 $y'' - 2y' + 5y = \mathrm{e}^x\cos x$, $y(0) = \dfrac{4}{3}$, $y'(0) = \dfrac{10}{3}$ $\qquad y = \left(\cos 2x + \sin 2x + \dfrac{1}{3}\cos x\right)\mathrm{e}^x$

3.78 $y'' - 6y' + 9y = 4x\,\mathrm{e}^{3x}\cos x$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = (1 - 7x + 8\sin x - 4x\cos x)\,\mathrm{e}^{3x}$

3.79 $y'' + y' - 6y = 12x^2 + 2x + 1$ $\qquad y = C_1\,\mathrm{e}^{-3x} + C_2\,\mathrm{e}^{2x} - 2x^2 - x - 1$

3.80 $y'' + y' - 6y = 12x^2 - 2x + 1$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = \dfrac{31}{45}\,\mathrm{e}^{-3x} + \dfrac{6}{5}\,\mathrm{e}^{2x} - 2x^2 - \dfrac{x}{3} - \dfrac{8}{9}$

3.81 $y'' + 4y' + 4y = \mathrm{e}^{-2x}\ln x$

$y = C_1\,\mathrm{e}^{-2x} + C_2 x\,\mathrm{e}^{-2x} + \dfrac{x^2}{4}\,\mathrm{e}^{-2x}(2\ln x - 3),\ x > 0$

3.82 $y'' + 4y' + 4y = \mathrm{e}^{-2x}\ln^2 x$

$y = C_1\,\mathrm{e}^{-2x} + C_2 x\,\mathrm{e}^{-2x} + \dfrac{x^2}{2}\mathrm{e}^{-2x}\left(\ln^2 x - 3\ln x + \dfrac{7}{2}\right),\ x > 0$

3.83 $y'' - 4y' + 5y = 0$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = \mathrm{e}^{2x}(\cos x - 2\sin x)$

3.84 $y'' - 2y' + 5y = 0$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = \mathrm{e}^x\left(\cos 2x - \dfrac{1}{2}\sin 2x\right)$

3.85 $y'' - 8y' + 32y = 0$, $y\left(\frac{\pi}{2}\right) = 1$, $y'\left(\frac{\pi}{2}\right) = 0$ $\qquad y = \mathrm{e}^{4x-2\pi}(\cos 4x - \sin 4x)$

3.86 $y'' - 3y' + 2y = (x^4 + 1)\,\mathrm{e}^x$

$y = \left(C_1 - \dfrac{x^5}{5} - x^4 - 4x^3 - 12x^2 - 25x\right)\mathrm{e}^x + C_2\,\mathrm{e}^{2x}$

3.87 $y'' - 4y' + 5y = (x^2 + 2x)\,\mathrm{e}^{2x}\cos x$

$y = \mathrm{e}^{2x}\left[\left(C_1 + \dfrac{x^2}{4} + \dfrac{x}{2}\right)\cos x + \left(C_2 + \dfrac{x^3}{6} + \dfrac{x^2}{2} - \dfrac{x}{4}\right)\sin x\right]$

3.88 $y'' - 3y' + 2y = (1 - 2x)\,\mathrm{e}^x$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = 3\,\mathrm{e}^x - 2\,\mathrm{e}^{2x} + (x^2 + x)\,\mathrm{e}^x$

3.89 $y'' - 2y' + y = (x + 1)\,\mathrm{e}^x$, $y(0) = 1$, $y'(0) = 0$ $\qquad y = \mathrm{e}^x\left(\dfrac{x^3}{6} + \dfrac{x^2}{2} - x + 1\right)$

3.90 $y'' + 4y' + 4y = (6x+2)\,\mathrm{e}^{-2x}$, $y(0) = 1$, $y'(0) = 0$ $\quad y = \mathrm{e}^{-2x}\left(x^3 + x^2 + 2x + 1\right)$

3.91 $y'' + 4y' + 4y = \mathrm{e}^{-2x}\sin x$, $y(0) = 1$, $y'(0) = 0$ $\quad y = \mathrm{e}^{-2x}(3x - \sin x + 1)$

3.92 $y'' - 2y' + 2y = \mathrm{e}^{x}\sin x$, $y(0) = 1$, $y'(0) = 0$ $\quad y = \frac{\mathrm{e}^x}{2}\left[(2-x)\cos x - \sin x\right]$

3.93 $y'' - 2y' + 2y = x^2 + x + \mathrm{e}^x\sin x$, $y(0) = 2$, $y'(0) = 3$

$$y = \mathrm{e}^x\left[\left(1 - \frac{x}{2}\right)\cos x + \sin x\right] + \frac{x^2}{2} + \frac{3x}{2} + 1$$

3.94 A body with mass 3 kg hangs on a massless spring. The acting of a force of 5.4 N on the body will extend the spring by 0.2 m. Then the spring and the body are allowed to oscillate freely with zero initial velocity. Find the (one-dimensional) equations of the dependence of the position and velocity of the oscillating body on time, where we denote the equilibrium position coordinate as $x_0 = 0$ (we start from Hook's law $\vec{F} = -k\vec{x}$ where $F = ma = m\ddot{x}$ and the oscillation velocity $\vec{v}$ can be expressed as $v = \dot{x}$).

$$x(t) = \frac{1}{5}\cos 3t, \quad v(t) = -\frac{3}{5}\sin 3t$$

3.95 Equation of motion of mathematical pendulum has the nonlinear form

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} + \frac{g}{L}\sin\theta = 0,$$

where θ is the angle of its deviation from the equilibrium (vertical) position, L is its length (length of the rod), and g is the magnitude of gravitational acceleration. For small displacements, we can use linear approximation $\sin\theta \approx \theta$, and the differential equation will become linear. Consider a mathematical pendulum with the rod length of 2.5 m that is at the time $t = 0$ deflected by the (growing) angle $\theta = 0.1\,\mathrm{rad}$ and the magnitude of its initial angular velocity is $\dot{\theta} = 0.25\,\mathrm{rad\,s^{-1}}$ (consider for simplicity $g = 10$ m s^{-2}) :

(a) Find equations of the time dependence of angular displacement θ and angular velocity ω of the pendulum, where the equilibrium coordinate is denoted as $\theta_0 = 0$.

(b) What will be the maximum pendulum displacement?

(c) At what time will the pendulum reach its equilibrium position for the first time, and what will be its circumferential velocity?

(a) $\theta(t) = \frac{1}{10}\cos 2t + \frac{1}{8}\sin 2t, \quad \omega(t) = -\frac{1}{5}\sin 2t + \frac{1}{4}\cos 2t$

(b) $\theta_{\max} \approx 0.160\,\mathrm{rad}$

(c) $t(\theta_0) \approx 1.233\,\mathrm{s}, \quad v(\theta_0) \approx 0.8\,\mathrm{m\,s^{-1}}$

3.96 Suppose that the spring oscillations from Example 3.94 are damped, where the damping force is proportional to the velocity (magnitude) and counteracts the direction of its motion, with a proportionality constant $c = 1$ kg s^{-1} (we thus get the equation $m\ddot{x} + c\dot{x} + kx = 0$). Find the equation of position dependence $x(t)$ on time in this case. What is the limitation of the proportionality constant c for the spring to oscillate at all (see Figure 3.1)?

$$x(t) = \mathrm{e}^{-\frac{1}{6}t}\left[\frac{1}{5}\cos\left(\frac{\sqrt{323}}{6}\,t\right) + \frac{1}{5\sqrt{323}}\sin\left(\frac{\sqrt{323}}{6}\,t\right)\right], \quad c < 18$$

3.97 Suppose that the spring oscillations with the parameters from Example 3.94 are excited by the harmonic driven force $F_b = F_0 \sin(2t)$ where the amplitude of the driven force $F_0 = 21\,\mathrm{N}$. We thus obtain the equation $m\ddot{x} + kx = F_0 \sin(2t)$. Find equations of the time dependence of the position and velocity of the oscillating body in this case.

$$x(t) = \frac{21\sin 2t - 14\sin 3t + 3\cos 3t}{15}, \quad v(t) = \frac{14\,(\cos 2t - \cos 3t) - 3\sin 3t}{5}$$

3.98 Suppose that the damped oscillations of the spring with stiffness k, with a hung body of mass m and with the damping proportionality constant c, are excited by the harmonic driven force $F_b = F_0 \sin(2t)$. Find the general equation of the time dependence of the oscillating body position on time with the condition for the damping proportionality constant.

$$x(t) = \frac{F_0\,[(k-4m)\sin 2t - 2c\cos 2t]}{4c^2 + (k-4m)^2} + \mathrm{e}^{-\frac{c}{2m}t}\left(C_1\,\mathrm{e}^{\frac{\sqrt{c^2-4km}}{2m}t} + C_2\,\mathrm{e}^{-\frac{\sqrt{c^2-4km}}{2m}t}\right),\ c^2 < 4km$$

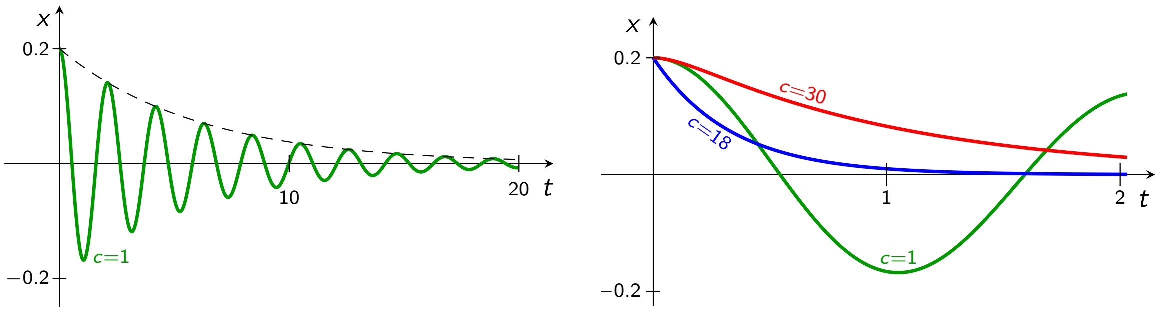

Figure 3.1: *Left panel*: Graph of the damped oscillation illustrating the result of Example 3.96 with the damping force proportionality constant $c = 1$ (subcritical damping, $c^2 < 4km$), plotted in the time interval from $t = 0$ to $t = 20$. The dashed line enveloping the damped vibration graph (indicated by a thick green line) represents the function $x(t) = \frac{1}{5}\,\mathrm{e}^{-ct/2m} = \frac{1}{5}\,\mathrm{e}^{-t/6}$. *Right panel*: Part of the same graph according to Example 3.96, plotted in the time interval from $t = 0$ to $t = 2$. The blue line shows the so-called critical damping ($c^2 = 4km$), given in this case by the function $x(t) = \frac{1}{5}\,\mathrm{e}^{-3t}$ when the oscillator no longer oscillates but settles in the equilibrium position in the shortest possible time. The red line shows the so-called supercritical damping ($c^2 > 4km$), given in this case by the function $x(t) = \mathrm{e}^{-t}(9 - \mathrm{e}^{-8t})/40$ when it is again a non-periodic movement, at which the oscillator returns to its equilibrium position more slowly.

3.2.2 Equations with non-constant coefficients ★

Ordinary second-order differential equations of the type of Equation (3.32), where the coefficient $p = p(x)$ and $q = q(x) = 0$, we can solve by converting them to first-order equations of the dependent variable $z = y'$. We solve the equations of the type

$$y'' + p(x)y' + q(x)y = R(x), \tag{3.42}$$

by searching for a function $I(x)$ (integrating factor) such that for $z = I(x)y$ Equation (3.42) transforms to the form of the equation with constant coefficients,

$$z'' + pz' + qz = R(x). \tag{3.43}$$

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

Ordinary second-order differential equations of the type

$$y'' + p(y')^m y^n + qy^r = R(x)y^s \tag{3.44}$$

where m, n, r, s are constants can be solved by finding such $z = f(y)$ for which Equation (3.43) again holds.

- **Examples:** ★

3.99 $y'' - \dfrac{2y'}{x} = x^2 + 1,\ y(1) = -\dfrac{11}{12},\ y'(1) = 1$ $\quad y = \dfrac{x^4}{4} + \dfrac{x^3}{3} - \dfrac{x^2}{2} - 1,\ x \neq 0$

3.100 $xy'' + (x+2)y' + y = 0$ $\quad y = \dfrac{1}{x}\left(C_1 + C_2\,\mathrm{e}^{-x}\right),\ y = 0,\ x \neq 0$

3.101 $xy'' - (3x-2)y' + (2x-3)y = 0$ $\quad y = \dfrac{1}{x}\left(C_1\,\mathrm{e}^{x} + C_2\,\mathrm{e}^{2x}\right),\ y = 0,\ x \neq 0$

3.102 $x^2y'' - 2x(x+2)y' + (x^2+4x+6)y = 0$ $\quad y = \mathrm{e}^{x}\left(C_1x^2 + C_2x^3\right),\ y = 0$

3.103 $x^2y'' + x(x+4)y' + (x^2+2x+2)y = 0$ $\quad y = \dfrac{\mathrm{e}^{-\frac{x}{2}}}{x^2}\left(C_1\cos\dfrac{\sqrt{3}}{2}x + C_2\sin\dfrac{\sqrt{3}}{2}x\right),\ y = 0$

3.104 $x^2y'' - 4xy' + 4y = x + 1$ $\quad y = C_1x + C_2x^4 - \dfrac{x\ln x}{3} + \dfrac{1}{4},\ x > 0$

3.105 $x^2y'' - xy' + y = 2x - 4$ $\quad y = C_1x + C_2x\ln x + x\ln^2 x - 4,\ x > 0$

3.106 $y'' - \left(\dfrac{3}{\sqrt{x}} - \dfrac{1}{2x}\right)y' + \dfrac{2}{x}y = 2\sqrt{x}$

$y = C_1\,\mathrm{e}^{2\sqrt{x}} + C_2\,\mathrm{e}^{4\sqrt{x}} + x^{\frac{3}{2}} + \dfrac{9x}{4} + \dfrac{21\sqrt{x}}{8} + \dfrac{45}{32},\ x > 0$

3.107 $y'' + \dfrac{2x-6}{x^2}y' + \dfrac{8}{x^4}y = 0$ $\quad y = C_1\,\mathrm{e}^{-2/x} + C_2\,\mathrm{e}^{-4/x},\ y = 0,\ x \neq 0$

3.108 $\dfrac{1}{16x^2}y'' - \left(\dfrac{1}{16x^3} + \dfrac{1}{x}\right)y' + 4y = 4x^4 + 1$ $\quad y = C_1\,\mathrm{e}^{4x^2} + C_2x^2\,\mathrm{e}^{4x^2} + x^4 + x^2 + \dfrac{5}{8},\ x \neq 0$

3.109 $y'' - \dfrac{2}{2x-1}y' = 2x(2x-1)^2$ $\quad y = C_1 + C_2(x^2 - x) + \dfrac{8}{15}x^5 - \dfrac{5}{6}x^4 + \dfrac{x^3}{3},\ x \neq \dfrac{1}{2}$

3.110 $2yy'' + 2y'(y' - 4y) + 4y^2 = x$

$y = \pm\dfrac{1}{2}\sqrt{C_1\,\mathrm{e}^{2x} + C_2x\,\mathrm{e}^{2x} + x + 1} = \sqrt{D},\ D \geq 0$

3.111 $\dfrac{y''}{2y} - \dfrac{y'}{y}\left(\dfrac{3y'}{4y} + 1\right) = 2 - \mathrm{e}^{x}\sqrt{y}$ $\quad y = \mathrm{e}^{-2x}\left(C_1\cos x + C_2\sin x + 1\right)^{-2},\ y \geq 0$

3.3 Solutions of linear ordinary second-order and higher-order differential equations by converting them to a system of first-order linear ordinary differential equations

Like "common" equations, the ordinary (linear) differential equations can also form a system. Consider a system of linear differential equations of the first-order only (higher-order equations can always be easily converted to such system, for example, the second-order equation $y'' + a_1 y' + a_0 y = f$ we write as two first-order equations: $y' = z$, $z' = -a_1 z - a_0 y + f$)

$$\begin{aligned} y_1' &= a_{11}(x)y_1 + a_{12}(x)y_2 + \cdots + a_{1n}(x)y_n + f_1(x), \\ y_2' &= a_{21}(x)y_1 + a_{22}(x)y_2 + \cdots + a_{2n}(x)y_n + f_2(x), \\ &\dots \\ y_n' &= a_{n1}(x)y_1 + a_{n2}(x)y_2 + \cdots + a_{nn}(x)y_n + f_n(x). \end{aligned} \tag{3.45}$$

The system of Equations (3.45) we write in vectorial form as

$$\vec{y}\,' = \boldsymbol{A}\vec{y} + \vec{f} \quad (\text{or, if } \vec{f}(x) = 0, \text{ like a homogeneous system } \vec{y}\,' = \boldsymbol{A}\vec{y}), \tag{3.46}$$

where the matrix

$$\boldsymbol{A}(x) = \begin{bmatrix} a_{11}(x) & a_{12}(x) & \cdots & a_{1n}(x) \\ a_{21}(x) & a_{22}(x) & \cdots & a_{2n}(x) \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1}(x) & a_{n2}(x) & \cdots & a_{nn}(x) \end{bmatrix} \tag{3.47}$$

and where $\vec{y}\,'$, $\vec{y}$, and $\vec{f}$ are column vectors. Solving systems of equations with non-constant coefficients $\boldsymbol{A}(x)$ can be very complicated in practice and represents the particular discipline that is beyond the scope of this textbook, so in the following sections, we will focus only on the systems of equations with constant coefficients $\boldsymbol{A}(x) = \boldsymbol{A}$.

3.3.1 Homogeneous systems with constant coefficients

In case of the homogeneous system with constant coefficients a_{ij} (according to Equation (3.46)) where a matrix $\boldsymbol{A}$ of the type $n \times n$ has n of *various real* eigenvalues λ_i, $i = 1 \dots n$ (see Equation (2.17)), we can write the solution in the general vector form

$$\vec{y}(x) = C_1\,\mathrm{e}^{\lambda_1 x}\vec{v}_1 + C_2\,\mathrm{e}^{\lambda_2 x}\vec{v}_2 + \cdots + C_n\,\mathrm{e}^{\lambda_n x}\vec{v}_n, \tag{3.48}$$

where v_i are the particular eigenvectors according to Equations (2.17) and (2.18), corresponding to the eigenvalues λ_i. Equation (3.48) would also be reached, for example, by successive substitutions, i.e., by replacing n first-order equations with one nth-order equation. However, especially in the case of higher n, it may be very complicated and difficult. As a simple example, we show a system of two homogeneous equations

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 1 & 6 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}. \tag{3.49}$$

The eigenvalues of a matrix $\boldsymbol{A}$ will be $\lambda_1, \lambda_2 = -1, 4$, the corresponding eigenvectors will be $\vec{v}_1 = (-3, 1)^T$ and $\vec{v}_2 = (2, 1)^T$. From Section 2.1, it is evident that the eigenvectors are also all the vectors $\vec{v}_1$, $\vec{v}_2$ multiplied by an arbitrary constant (we will only present its elemental form in the following text). If no other conditions are specified, we can write the resulting solution of the system of equations as

$$\vec{y}(x) = C_1 \begin{pmatrix} -3 \\ 1 \end{pmatrix} \mathrm{e}^{-x} + C_2 \begin{pmatrix} 2 \\ 1 \end{pmatrix} \mathrm{e}^{4x}. \tag{3.50}$$

If the eigenvalues of a matrix $\boldsymbol{A}$ are represented by (complex conjugate) pairs of *complex numbers*, we will search for solutions similarly as in the case of real eigenvalues. As a simple example, we show the system of two homogeneous equations

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 2 & -5 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}. \tag{3.51}$$

The eigenvalues of a matrix $\boldsymbol{A}$ will be in this case $\lambda_1, \lambda_2 = \pm\mathrm{i}$, the corresponding eigenvectors will be $\vec{v}_1 = (2-\mathrm{i}, 1)^T$, and $\vec{v}_2 = (2+\mathrm{i}, 1)^T$. The resulting solution of the system of the equations will be

$$\vec{y}(x) = C_1 \begin{pmatrix} 5 \\ 2-\mathrm{i} \end{pmatrix} \mathrm{e}^{\mathrm{i}x} + C_2 \begin{pmatrix} 5 \\ 2+\mathrm{i} \end{pmatrix} \mathrm{e}^{-\mathrm{i}x} = A \begin{pmatrix} 5\cos x \\ 2\cos x + \sin x \end{pmatrix} + B \begin{pmatrix} 5\sin x \\ 2\sin x - \cos x \end{pmatrix}, \tag{3.52}$$

where the relation between the exponential and the trigonometric form of the equation (3.52) is given by the *Euler identity* $\mathrm{e}^{\pm\mathrm{i}x} = \cos x \pm \mathrm{i}\sin x$ and where the coefficients $A = C_1 + C_2$, $B = \mathrm{i}\,(C_2 - C_1)$.

If any *real* eigenvalue of the matrix $\boldsymbol{A}$ is *multiple*, then the solution will depend on the number of eigenvectors corresponding to it, where there are two possibilities:

(a) Multiple (k-fold) eigenvalue ρ corresponds to k of linearly independent eigenvectors, then the part of the general solution following this eigenvalue will have the form

$$\vec{y}_\rho(x) = C_1 \mathrm{e}^{\rho x} \vec{v}_1 + C_2 \mathrm{e}^{\rho x} \vec{v}_2 + \cdots + C_k \mathrm{e}^{\rho x} \vec{v}_k. \tag{3.53}$$

A simple example might be the following system,

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \tag{3.54}$$

with the double eigenvalue $\rho = 3$ and with the two linearly independent eigenvectors $\vec{v}_1 = (1, 0)^T$ and $\vec{v}_2 = (0, 1)^T$. The resulting solution of the system in the sense of Equation (3.53) will be

$$\vec{y}_\rho(x) = C_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \mathrm{e}^{3x} + C_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \mathrm{e}^{3x}. \tag{3.55}$$

(b) Multiple (k-fold) eigenvalue ρ corresponds to j of linearly independent eigenvectors where $1 \le j < k$, that is, $s = k - j$ eigenvalues ρ correspond to only one linearly independent eigenvector $\vec{u}$. Such a matrix is called *defective*, and it is not *diagonalizable*, i.e., convertible to a diagonal matrix by multiplying it by the matrix of row left eigenvectors from the left and by the matrix of column right eigenvectors from the right. Then the piece of the general solution following this eigenvector $\vec{u}$ will have the form

$$\vec{y}_\rho(x) = C_1 \vec{u}\, \mathrm{e}^{\rho x} + C_2 \left(\vec{w}_1 + x\vec{u}\right) \mathrm{e}^{\rho x} + \cdots \tag{3.56}$$

$$\cdots + C_s \left(\vec{w}_{s-1} + x\vec{w}_{s-2} + \frac{x^2}{2!}\vec{w}_{s-3} + \cdots + \frac{x^{s-2}}{(s-2)!}\vec{w}_1 + \frac{x^{s-1}}{(s-1)!}\vec{u} \right) \mathrm{e}^{\rho x}, \tag{3.57}$$

where the vector $\vec{w}_i$ corresponds to any solution of the algebraic equations

$$(\boldsymbol{A} - \rho \boldsymbol{E})\,\vec{w}_i = \vec{w}_{i-1}, \quad \ldots \quad (\boldsymbol{A} - \rho \boldsymbol{E})\,\vec{w}_1 = \vec{u}. \tag{3.58}$$

The following example illustrates the described principle of the solution: consider a system

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 3 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \tag{3.59}$$

with the double eigenvalue $\rho = 2$ but with the only one corresponding linearly independent eigenvector $\vec{u} = (1,1)^T$. The vector $\vec{w}$ is determined by Equation (3.58),

$$\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \text{so} \quad \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.60}$$

The resulting solution of the system in the sense of Equation (3.56) will be

$$\vec{y}_\rho(x) = C_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \mathrm{e}^{2x} + C_2 \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + x \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right] \mathrm{e}^{2x}. \tag{3.61}$$

The solution of systems with more than two first-order linear equations is analogous to the above-mentioned simple examples with two equations; some principles will be made more evident by the following examples, while including also systems of three equations.

- **Examples:**

3.112 $\vec{y}' = \begin{pmatrix} 4 & 10 \\ 1 & 1 \end{pmatrix} \vec{y}$ $\qquad \vec{y} = C_1 \begin{pmatrix} 5 \\ 1 \end{pmatrix} \mathrm{e}^{6x} + C_2 \begin{pmatrix} 2 \\ -1 \end{pmatrix} \mathrm{e}^{-x}$

3.113 $\vec{y}' = \begin{pmatrix} 7 & 13 \\ -1 & 1 \end{pmatrix} \vec{y}$

$$\vec{y} = C_1 \begin{pmatrix} 13 \\ -3+2\mathrm{i} \end{pmatrix} \mathrm{e}^{(4+2\mathrm{i})x} + C_2 \begin{pmatrix} 13 \\ -3-2\mathrm{i} \end{pmatrix} \mathrm{e}^{(4-2\mathrm{i})x} = \\ = \left[A \begin{pmatrix} 13\cos 2x \\ -3\cos 2x - 2\sin 2x \end{pmatrix} + B \begin{pmatrix} 13 \sin 2x \\ 2\cos 2x - 3 \sin 2x \end{pmatrix} \right] \mathrm{e}^{4x}$$

3.114 $\vec{y}' = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \vec{y}$ $\qquad \vec{y} = C_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + C_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \mathrm{e}^{x} + C_3 \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \mathrm{e}^{3x}$

3.115 $\vec{y}' = \begin{pmatrix} 5 & 8 & 16 \\ 4 & 1 & 8 \\ -4 & -4 & -11 \end{pmatrix} \vec{y}$ $\qquad \vec{y} = C_1 \begin{pmatrix} -2 \\ -1 \\ 1 \end{pmatrix} \mathrm{e}^{x} + \left[C_2 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} + C_3 \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} \right] \mathrm{e}^{-3x}$

3.116 $\vec{y}' = \begin{pmatrix} -2 & 0 & 0 \\ 1 & -3 & -1 \\ -1 & 1 & -1 \end{pmatrix} \vec{y}$

$$\vec{y} = \left\{ C_1 \begin{pmatrix} 0 \\ 2 \\ -2 \end{pmatrix} + C_2 \begin{pmatrix} 2 \\ 0 \\ 2 \end{pmatrix} + C_3 \left[\begin{pmatrix} 0 \\ -1 \\ -1 \end{pmatrix} + x \begin{pmatrix} 0 \\ 2 \\ -2 \end{pmatrix} \right] \right\} \mathrm{e}^{-2x}$$

3.117 $\vec{y}\,' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 2 \\ 2 & -2 & -1 \end{pmatrix} \vec{y}$

$$\vec{y} = \left\{ C_1 \begin{pmatrix} 0 \\ 4 \\ -4 \end{pmatrix} + C_2 \left[\begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix} + x \begin{pmatrix} 0 \\ 4 \\ -4 \end{pmatrix} \right] + C_3 \left[\begin{pmatrix} 1 \\ 4 \\ -4 \end{pmatrix} + x \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix} + \frac{x^2}{2} \begin{pmatrix} 0 \\ 4 \\ -4 \end{pmatrix} \right] \right\} \mathrm{e}^{x}$$

3.118 $\vec{y}\,' = \begin{pmatrix} -1 & 1 & 0 \\ -2 & -3 & 1 \\ 1 & 1 & -2 \end{pmatrix} \vec{y}$

$$\vec{y} = \left\{ C_1 \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} + C_2 \left[\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + x \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \right] + C_3 \left[\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} + x \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + \frac{x^2}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \right] \right\} \mathrm{e}^{-2x}$$

3.3.2 Inhomogeneous systems with constant coefficients

A solution of linear systems with a right-hand side will be in principle analogous to the methods of solving ordinary second-order differential equations (see Section 3.2.1), i.e., to the methods of *variation of parameters* and *undetermined coefficients*. The method of *variation of parameters* can be applied as follows: suppose that the particular solution of the inhomogeneous Equation (3.46) in the form

$$\vec{y}_{\mathrm{p}} = \boldsymbol{Y}(x)\vec{t}(x) \tag{3.62}$$

where $\boldsymbol{Y}(x)$ is a matrix whose columns are formed by individual linearly independent solutions of the corresponding homogeneous equation (3.46), now rewritten into the form $\boldsymbol{Y}' = \boldsymbol{A}\boldsymbol{Y}$, then $\vec{t}(x)$ is the generally written searched column vector. Because Equation (3.46) must also hold for the particular solutions, i.e., $\vec{y}_{\mathrm{p}}\,' = \boldsymbol{A}\vec{y}_{\mathrm{p}} + \vec{f}$, the first derivative of the particular solution in such a case will be

$$\vec{y}_{\mathrm{p}}\,' = \boldsymbol{Y}'\vec{t} + \boldsymbol{Y}\vec{t}\,' = \boldsymbol{A}\boldsymbol{Y}\vec{t} + \vec{f} = \boldsymbol{Y}'\vec{t} + \vec{f}, \quad \text{so} \quad \boldsymbol{Y}\vec{t}\,' = \vec{f}. \tag{3.63}$$

We find the vector $\vec{t}$ by integrating Equation (3.63),

$$\vec{t} = \int \boldsymbol{Y}^{-1}\vec{f}\,\mathrm{d}x, \quad \vec{y}_{\mathrm{p}} = \boldsymbol{Y} \int \boldsymbol{Y}^{-1}\vec{f}\,\mathrm{d}x. \tag{3.64}$$

This method is illustrated by the following solved example: we use the homogeneous system from the solved example (see Equation (3.49)) with the right-hand side added,

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 1 & 6 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \end{pmatrix} x. \tag{3.65}$$

We immediately see from Equation (3.50) that the matrix $\boldsymbol{Y}(x)$ will be

$$\boldsymbol{Y} = \begin{pmatrix} -3\mathrm{e}^{-x} & 2\mathrm{e}^{4x} \\ \mathrm{e}^{-x} & \mathrm{e}^{4x} \end{pmatrix}, \quad \text{from which} \quad \boldsymbol{Y}^{-1} = \frac{1}{5} \begin{pmatrix} -\mathrm{e}^{x} & 2\mathrm{e}^{x} \\ \mathrm{e}^{-4x} & 3\mathrm{e}^{-4x} \end{pmatrix}. \tag{3.66}$$

According to Equation (3.64), we thus get the particular solution by integration (by integrating each component of the vector $\vec{y}_\mathrm{p}$ separately)

$$\vec{y}_\mathrm{p} = \frac{1}{5}\begin{pmatrix} -3\mathrm{e}^{-x} & 2\mathrm{e}^{4x} \\ \mathrm{e}^{-x} & \mathrm{e}^{4x} \end{pmatrix} \int \begin{pmatrix} -\mathrm{e}^{x} & 2\mathrm{e}^{x} \\ \mathrm{e}^{-4x} & 3\mathrm{e}^{-4x} \end{pmatrix} \begin{pmatrix} 3x \\ x \end{pmatrix} \mathrm{d}x = \begin{bmatrix} -3/4 \\ (1-4x)/8 \end{bmatrix}. \tag{3.67}$$

The complete solution will be the sum of Equations (3.50) and (3.67). In the result of Equation (3.67), we do not introduce the integration constant, assuming that it is already included in the constants of the homogeneous solution in Equation (3.50).

The method of *undetermined coefficients* for the system of equations is completely analogous to the solution given for the second-order equations; the only difference is that the coefficients will now be vectors. If, for example, in Section 3.2.1, the right-hand side of the equation was a polynomial of the first degree and the general notation of the particular solution was $y_\mathrm{p} = Ax + B$; now it will be $\vec{y}_\mathrm{p} = \vec{A}x + \vec{B}$. We will show the method on the same solved example: suppose the general form of a particular solution, i.e.,

$$\vec{y}_\mathrm{p} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} x + \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \quad \text{which gives} \quad \vec{y}_\mathrm{p}^{\,\prime} = \vec{A} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}. \tag{3.68}$$

Equation (3.46) must again hold also for the particular solution, $\vec{y}_\mathrm{p}^{\,\prime} = \boldsymbol{A}\vec{y}_\mathrm{p} + \vec{f}$ so that $\vec{A} = \boldsymbol{A}(\vec{A}x + \vec{B}) + \vec{f}$. If we rewrite the (vector) polynomial of the first degree to the following explicit form

$$\left[\boldsymbol{A}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \end{pmatrix}\right] x + \boldsymbol{A}\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} - \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \vec{0}, \tag{3.69}$$

we get the following equations for both linear and absolute terms (both must be zero):

$$\begin{pmatrix} 1 & 6 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = -\begin{pmatrix} 3 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 6 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}. \tag{3.70}$$

Now we easily calculate the individual undetermined coefficients, we get $A_1 = 0$, $A_2 = -1/2$, $B_1 = -3/4$, $B_2 = 1/8$, which after substitution and adjustment gives the identical result to Equation (3.67).

Somewhat more complicated is the case when the sum of the coefficients $\alpha + \beta\mathrm{i}$ on the right-hand side of the equation (see the similarity with the equation (3.41)) is equal to one of the eigenvalues of the system of equations. In this case, we again multiply the general vector of the right-hand side by the factor x^ρ, where ρ is the degree of degeneracy of the eigenvalue (analogous to the multiplicity of the root of a characteristic equation), but we must also "extend" the general vector by the lower powers of the general polynomial (to include its possible nonzero terms in higher derivatives), usually up to the absolute term. We will illustrate this procedure in the following example (which includes more such eventualities from the previous discussion):

$$y'''' + 3y''' = x^2 + x + 1. \tag{3.71}$$

A fourth order equation can be thought of as a system of four first order equations of four variables, where in a homogeneous equation $y_1' = y_2$, $y_2' = y_3$, $y_3' = y_4$ a $y_4' = -3y_4$. The explicit matrix notation of the homogeneous system will take the form

$$\vec{y}^{\,\prime} \equiv \begin{pmatrix} y_4' \\ y_3' \\ y_2' \\ y_1' \end{pmatrix} = \begin{pmatrix} -3 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} y_4 \\ y_3 \\ y_2 \\ y_1 \end{pmatrix} \equiv \boldsymbol{A}\vec{y} \tag{3.72}$$

and its solution will be

$$\begin{pmatrix} y_4 \\ y_3 \\ y_2 \\ y_1 \end{pmatrix} = C_1 \begin{pmatrix} -27 \\ 9 \\ -3 \\ 1 \end{pmatrix} \mathrm{e}^{-3x} + C_2 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} + C_3 \left[\begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} + x \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] + C_4 \left[\begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} + x \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} + \frac{x^2}{2} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] . \quad (3.73)$$

Since the eigenvalue $\lambda_{2,3,4} = 0$ is triple and corresponds to the parameter α of the right-hand side of the given equation, the general equation of the right-hand side must be multiplied by x^3. This general equation, given the above, in this case will be

$$\vec{y}_{\mathrm{p}} = \vec{A}x^5 + \vec{B}x^4 + \vec{C}x^3 + \vec{D}x^2 + \vec{E}x + \vec{F} \quad (3.74)$$

and the whole matrix notation of the general solution of the right side will be

$$\vec{y_{\mathrm{p}}}' = \boldsymbol{A}\,\vec{y}_{\mathrm{p}} + \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \left(x^2 + x + 1\right) . \quad (3.75)$$

From the general solution of the right-hand side it follows (see equation (3.41)) that the equation for y_{p1} will contain only the coefficients A_1, B_1 and C_1, i.e., $D_1 = 0$, $E_1 = 0$, $F_1 = 0$ (numbered "from bottom to top", consistently with the homogeneous system). Furthermore, the expression of the vector equation for the coefficients of the fifth power of the variable x implies $A_1 = A_1$, $A_2 = 0$, $A_3 = 0$, $A_4 = 0$. By comparing all other coefficients for the same powers, we get a unique right-hand side solution,

$$\vec{y}_{\mathrm{p}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{180} \end{pmatrix} x^5 + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{36} \\ \frac{1}{216} \end{pmatrix} x^4 + \begin{pmatrix} 0 \\ \frac{1}{9} \\ \frac{1}{54} \\ \frac{4}{81} \end{pmatrix} x^3 + \begin{pmatrix} \frac{1}{3} \\ \frac{1}{18} \\ \frac{4}{27} \\ 0 \end{pmatrix} x^2 + \begin{pmatrix} \frac{1}{9} \\ \frac{8}{27} \\ 0 \\ 0 \end{pmatrix} x + \begin{pmatrix} \frac{8}{27} \\ 0 \\ 0 \\ 0 \end{pmatrix} . \quad (3.76)$$

This can be easily verified by setting the bottom row as the solution of given Equation (3.71) where we identify y_{p1} to the original y (the same applies for the homogeneous solution). The higher rows then correspond successively to the first, second and third derivatives of y.

- **Examples:**

3.119 $\vec{y}' = \begin{pmatrix} 1 & 3 \\ 1 & -1 \end{pmatrix} \vec{y} + \begin{pmatrix} 2 \\ 1 \end{pmatrix} \mathrm{e}^{-5x}$

$$\vec{y} = C_1 \begin{pmatrix} 3 \\ 1 \end{pmatrix} \mathrm{e}^{2x} + C_2 \begin{pmatrix} -1 \\ 1 \end{pmatrix} \mathrm{e}^{-2x} - \begin{pmatrix} 5/21 \\ 4/21 \end{pmatrix} \mathrm{e}^{-5x}$$

3.120 $\vec{y}' = \begin{pmatrix} 3 & -1 \\ 1 & 1 \end{pmatrix} \vec{y} + \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\vec{y} = C_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \mathrm{e}^{2x} + C_2 \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + x \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right] \mathrm{e}^{2x} - \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$$

3.121 $\vec{y}\,' = \begin{pmatrix} 2 & -1 & -1 \\ 0 & -1 & 0 \\ 0 & 2 & 1 \end{pmatrix} \vec{y} + \begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} x^2$

$$\vec{y} = C_1 \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \mathrm{e}^{-x} + C_2 \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \mathrm{e}^{x} + C_3 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \mathrm{e}^{2x} + \begin{pmatrix} -2 \\ 1 \\ -3 \end{pmatrix} x^2 - \begin{pmatrix} 4 \\ 2 \\ 2 \end{pmatrix} x + \begin{pmatrix} -4 \\ 2 \\ -6 \end{pmatrix}$$

3.122 $\vec{y}\,' = \begin{pmatrix} 1 & -3 & 3 \\ 3 & -5 & 3 \\ 6 & -6 & 4 \end{pmatrix} \vec{y} + \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} (x+1)\,\mathrm{e}^{2x}$

$$\vec{y} = C_1 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \mathrm{e}^{-2x} + C_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \mathrm{e}^{-2x} + C_3 \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix} \mathrm{e}^{4x} + \left[\begin{pmatrix} 1/4 \\ 0 \\ -1/4 \end{pmatrix} x + \begin{pmatrix} 3/16 \\ 0 \\ -3/16 \end{pmatrix} \right] \mathrm{e}^{2x}$$

3.123 $\vec{y}\,' = \begin{pmatrix} 1 & 3 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \vec{y} + \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} x^2$

$$\vec{y} = C_1 \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \mathrm{e}^{-x} + C_2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \mathrm{e}^{x} + C_3 \left[\begin{pmatrix} 1 \\ 1/4 \\ 1/4 \end{pmatrix} + x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right] \mathrm{e}^{x} + \begin{pmatrix} -4 \\ 1 \\ 0 \end{pmatrix} x^2 - \begin{pmatrix} 10 \\ 0 \\ -2 \end{pmatrix} x - \begin{pmatrix} 16 \\ -2 \\ 0 \end{pmatrix}$$

3.124 Find the solution of the 3rd-order ordinary differential equation

$$y''' + y'' - y' - y = x^2 + 1$$

using its transformation into a system of 1st-order equations. Verify the result using one of the methods given in paragraph 3.2.1.

$y = C_1 \mathrm{e}^{-x} + C_2 x\,\mathrm{e}^{-x} + C_3\,\mathrm{e}^{x} - x^2 + 2x - 5$

3.125 Find the solution of the 3rd-order ordinary differential equation

$$y''' + 3y'' - 7y' - 9y = \sin x$$

using its transformation into a system of 1st-order equations. Verify the result using one of the methods given in paragraph 3.2.1.

$y = C_1 \mathrm{e}^{-x} + C_2\,\mathrm{e}^{\left(-1+\sqrt{10}\right)x} + C_3\,\mathrm{e}^{-\left(1+\sqrt{10}\right)x} + \frac{1}{26}\cos x - \frac{3}{52}\sin x$

3.126 Find the solution of the 4th-order ordinary differential equation

$$y'''' - 4y''' + 3y'' + 4y' - 4y = x^4 + \cos x$$

using its transformation into a system of 1st-order equations. Verify the result using one of the methods given in paragraph 3.2.1.

$y = C_1 \mathrm{e}^{2x} + C_2 x\,\mathrm{e}^{2x} + C_3\,\mathrm{e}^{x} + C_4\,\mathrm{e}^{-x} - \frac{1}{8}\left(2x^4 + 8x^3 + 42x^2 + 72x + 99\right) - \frac{3}{50}\cos x + \frac{2}{25}\sin x$

3.127 Find the solution of the 3rd-order ordinary differential equation

$$y''' + y'' + y' + y = (x^2 + 1)\,\mathrm{e}^{-x} \tag{3.77}$$

using its transformation into a system of 1st-order equations. Verify the result using one of the methods given in paragraph 3.2.1.

$$y = C_1 \cos x + C_2 \sin x + \left(\frac{x^3}{6} + \frac{x^2}{2} + x + C_3\right)\mathrm{e}^{-x}$$

Chapter 4

Introduction to curvilinear coordinates[1]

Most phenomena in nature (and hence in physical processes) are not strictly rectangular, and it is not appropriate nor often even feasible to simply describe them using the Cartesian coordinates. In this case, it is advantageous to select a coordinate system (usually curvilinear) that best matches the geometry of the described process. The most commonly used curvilinear coordinate systems are the *cylindrical* system and the *spherical* system. Furthermore, there are numerous specific curvilinear coordinate systems, e.g., elliptical, parabolic, conical, etc.

4.1 Cartesian coordinates

Although the Cartesian system is in fact not regarded as curvilinear, it is described here as the simplest orthogonal coordinate system within which we introduce the basic concepts. We further apply these within the true curvilinear coordinate systems by analogy (we continue to assume implicitly that we "live" in $\mathbb{R}^3$). The orthonormal Cartesian basis vectors, $\vec{e}_x = (1,0,0)$, $\vec{e}_y = (0,1,0)$, $\vec{e}_z = (0,0,1)$, are constant (they are always of the same size and the same direction), so the derivatives of these basis vectors are zero.

Viewing from any point of the positive half-axis $+z$, if the positive half-axis $+x$ may be transferred by an angle of $\pi/2$ in the mathematically positive sense (counterclockwise) to the positive half-axis $+y$, it is a *right-handed* (positively oriented) system otherwise it is a *left-handed* (negatively oriented) system. Curves (straight lines in this case) created by the points whose two coordinates are constant and only one changes continuously are the so-called *coordinate curves*. The surfaces created by the points whose one coordinate is constant are called *coordinate surfaces*.

For the square of the distance of two points in the Cartesian system (Pythagorean theorem in the differential form, which can also be regarded as the square of the length of diagonal of an elementary cuboid with edges $\mathrm{d}x, \mathrm{d}y, \mathrm{d}z$) holds

$$\mathrm{d}s^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2. \tag{4.1}$$

At the same time, the distance $\mathrm{d}s$ must be the same for all coordinate systems. The factors that scale the lengths of the particular edges of an elementary cuboid (the lengths, not their squares) are called the *Lamé coefficients* denoted by h_i. Thus, in the Cartesian system, the Lamé coefficients (not to be confused with the coefficients of the same name used in mechanics of continua) will be $h_x = 1, h_y = 1, h_z = 1$. The definition of the Cartesian system implies that the so-called *surface elements* (where the subscript means a constant coordinate on a given

[1]Recommended literature for this chapter: Kvasnica (2004), Arfken & Weber (2005).

surface) $\mathrm{d}S_x = \mathrm{d}y\,\mathrm{d}z$, $\mathrm{d}S_y = \mathrm{d}z\,\mathrm{d}x$, $\mathrm{d}S_z = \mathrm{d}x\,\mathrm{d}y$ and the *volume element* $\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ have a constant size.

- **Examples:**

4.1 Calculate the magnitude $\|\vec{u}\| = u$ of the vector $\vec{u} = 12\vec{e}_x - 3\vec{e}_y + 7\vec{e}_z$ and also the vector $\vec{u}_x$, the unit vector $\vec{v}$ in the direction $\vec{u}$ and the vector $\vec{w}$ with the length 7 in the direction $-\vec{u}$.

$$u = \sqrt{202}, \quad \vec{u}_x = 12\vec{e}_x, \quad \vec{v} = \frac{1}{\sqrt{202}}(12\vec{e}_x - 3\vec{e}_y + 7\vec{e}_z), \quad \vec{w} = -\frac{7}{\sqrt{202}}(12\vec{e}_x - 3\vec{e}_y + 7\vec{e}_z)$$

4.2 There are 3 points in space, $A = [12, 1, -3]$, $B = [7, -5, 8]$ and $C = [4, 11, -2]$. Write the vector sum of the vectors $\vec{u} = \overrightarrow{AB}$, $\vec{v} = \overrightarrow{AC}$, $\vec{w} = \overrightarrow{CB}$ and determine its magnitude. Check if the given 3 points are not in one line; if not, write the general equation of their plane σ.

$$\vec{u}+\vec{v}+\vec{w} = -10\vec{e}_x - 12\vec{e}_y + 22\vec{e}_z, \quad \|\vec{u}+\vec{v}+\vec{w}\| = 2\sqrt{182}, \quad \sigma : 116x + 83y + 98z - 1181 = 0$$

4.3 Determine the distance d of the origin of the coordinate system, i.e., of the point $O = [0, 0, 0]$ from the plane σ given by Example 4.2.

$$d \approx 6.82$$

4.4 Write the Cartesian equation of the spherical surface with center at the point $x, y, z = [2, 1, 7]$ and with radius $r = 3$ as a function of $z = f(x, y)$. Determine the coordinates of the intersections P_1 and P_2 of this surface with a line passing through the point $x, y, z = [1, 1, 1]$, whose direction vector $\vec{u} = (0, 0, 1)$.

$$z = 7 \pm \sqrt{4 - x(x-4) - y(y-2)}, \quad P_1 = [1, 1, 7 + 2\sqrt{2}], \quad P_2 = [1, 1, 7 - 2\sqrt{2}]$$

4.5 In the Cartesian system has the position vector the form $\vec{r} = (x, y, z)$. Consider a completely general non-orthogonal coordinate system with coordinate directions α, β, γ, with constant basis vectors (cf. Figure 2.2 and its accompanying explanation), in which the same position vector ("seen" from the Cartesian system) would take the form $\vec{r} = (\alpha, \alpha + 3\beta, \gamma - \alpha - 2\beta)$. What would then be the basis vectors $\vec{e}_\alpha, \vec{e}_\beta, \vec{e}_\gamma$, "seen" from the Cartesian system? (Basis vectors of orthogonal coordinate systems can be obtained using the relation $h_i\vec{e}_i = \partial x_j/\partial q_i$, where q_i are new coordinates).

$$\vec{e}_\alpha = (1, 1, -1), \quad \vec{e}_\beta = (0, 3, -2), \quad \vec{e}_\gamma = (0, 0, 1)$$

4.2 Cylindrical coordinates

The cylindrical coordinate system is appropriate for describing axially symmetric (rotational) phenomena. The coordinate directions are: ρ - distance from the axis of cylindrical symmetry, ϕ - azimuthal angle, z - height (if we consider only the system in $\mathbb{R}^2$ where $z = 0$, then the system is commonly called *polar*), where $\rho \in \langle 0, \infty)$, $\phi \in \langle 0, 2\pi)$, $z \in (-\infty, \infty)$. Thus, the cylindrical system is orthogonal. The conversion between the cylindrical and Cartesian system

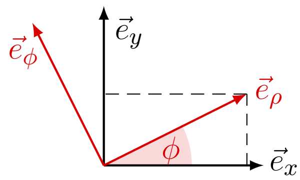

Figure 4.1: Scheme of mutual transformation of unit basis vectors of the Cartesian and cylindrical coordinate system (see Equation (4.4)). The z-axis is the same for both the systems, and it points towards us from the origin.

is given by the relations[2]

$$x = \rho\cos\phi, \quad y = \rho\sin\phi, \quad z = z. \tag{4.2}$$

For the reverse transformation holds

$$\rho = \sqrt{x^2+y^2}, \quad \phi = \arccos\frac{x}{\sqrt{x^2+y^2}}, \quad \phi = \arcsin\frac{y}{\sqrt{x^2+y^2}}, \quad \phi = \arctan\frac{y}{x}. \tag{4.3}$$

The unit vectors of the cylindrical basis will in the Cartesian system take the form (see Figure 4.1)

$$\vec{e}_\rho = \vec{e}_x\cos\phi + \vec{e}_y\sin\phi, \quad \vec{e}_\phi = -\vec{e}_x\sin\phi + \vec{e}_y\cos\phi, \quad \vec{e}_z = \vec{e}_z. \tag{4.4}$$

The only constant basis vector will be $\vec{e}_z$; the other basis vectors will change direction depending on the angle ϕ.

Coordinate curves in the cylindrical system will be:

- half-lines s_ρ with origin on the axis z, lying in a plane perpendicular to the axis z ($\phi =$ const., $z =$ const.),
- circles s_ϕ centered on the axis z, lying in a plane perpendicular to the axis z ($\rho =$ const., $z =$ const., $\rho = 0$ gives a point on the axis z),
- straight lines s_z parallel to the axis z ($\rho =$ const., $\phi =$ const., $\rho = 0$ gives the axis z).

Coordinate surfaces in the cylindrical system will be:

- rotational cylindrical surfaces S_ρ whose axis of rotation coincides with the axis z ($\rho =$ const.; $\rho = 0$ gives the axis z),
- half-planes S_ϕ passing through the axis z ($\phi =$ const.),
- planes S_z, parallel with the plane ρ-ϕ ($z =$ const.).

For the square of the distance of two points in the differential form (substituting Equation (4.2) into Equation (4.1)) in the cylindrical system holds

$$\mathrm{d}s^2 = \mathrm{d}\rho^2 + \rho^2\,\mathrm{d}\phi^2 + \mathrm{d}z^2, \tag{4.5}$$

which can again be regarded as the square of diagonal of an elementary "cuboid" or "wedge" with edges $\mathrm{d}s_\rho = \mathrm{d}\rho$, $\mathrm{d}s_\phi = \rho\,\mathrm{d}\phi$, $\mathrm{d}s_z = \mathrm{d}z$. In the cylindrical system, we get the Lamé coefficients

[2] In the following description, we will distinguish ρ for the radial cylindrical coordinate and r for the radial spherical coordinate. For unit basis vectors, we distinguish $\vec{e}_\rho$ for the cylindrical system and $\vec{e}_r$ for the spherical system.

$h_\rho = 1, h_\phi = \rho, h_z = 1$. From the infinitesimal, mutually perpendicular edge lines or curves, we construct the surface elements

$$\mathrm{d}S_\rho = \mathrm{d}s_\phi\,\mathrm{d}s_z = \rho\,\mathrm{d}\phi\,\mathrm{d}z, \quad \mathrm{d}S_\phi = \mathrm{d}s_z\,\mathrm{d}s_\rho = \mathrm{d}z\,\mathrm{d}\rho, \quad \mathrm{d}S_z = \mathrm{d}s_\rho\,\mathrm{d}s_\phi = \rho\,\mathrm{d}\rho\,\mathrm{d}\phi \tag{4.6}$$

and also the volume element of the cylindrical system

$$\mathrm{d}V = \mathrm{d}s_\rho\,\mathrm{d}s_\phi\,\mathrm{d}s_z = \rho\,\mathrm{d}\rho\,\mathrm{d}\phi\,\mathrm{d}z. \tag{4.7}$$

Unlike the Cartesian system, all these elements are not constant, their size (except the surface element $\mathrm{d}S_\phi$) obviously increases proportionally to the distance ρ from the axis z.

Detailed description of the cylindrical coordinate system is given in Section B.2 in Appendix B.

- **Examples:**

4.6 Write the cylindrical coordinates of the point A, whose Cartesian coordinates are $x, y, z = [6, -2\sqrt{3}, 3]$.

$A:\ \rho, \phi, z = \left[4\sqrt{3}, \frac{11\pi}{6}, 3\right]$

4.7 Write the Cartesian coordinates of the point B, whose cylindrical coordinates are $\rho, \phi, z = \left[4, \frac{5\pi}{3}, -2\right]$.

$B:\ x, y, z = [2, -2\sqrt{3}, -2]$

4.8 Write the equation of the surface $z = 5 - 2\sqrt{x^2+y^2}$, $z \geq 0$ in cylindrical coordinates. Sketch the given surface.

$z = 5 - 2\rho$, $z \in \langle 0, 5\rangle$; part of a rotational conical surface whose axis of rotation is the z-axis common to both systems, with the radius $\rho = 5/2$ in the $z = 0$ plane and with vertex at the point [0,0,5].

4.9 Write the equation of the surface $z - \sqrt{x^2+y^2-4x-2y+5} = 0$, $z \leq 4$ in cylindrical coordinates. Sketch the given surface.

$z = \rho$, $z \in \langle 0, 4\rangle$; part of a rotational conical surface, whose axis of rotation passes through the origin of the cylindrical system at the point $O: x, y, z = [2, 1, 0]$, with the directional vector $\vec{z} = (0, 0, 1)$, with radius $\rho = 4$ in the plane $z = 4$ and with vertex at the origin.

4.10 Write the equation of the surface $2z - x^2 - y^2 = 0$, $z \leq 8$ in cylindrical coordinates. Sketch the given surface.

$z = \rho^2/2$, $z \in \langle 0, 8\rangle$; part of a rotational paraboloid, whose axis of rotation is the z-axis that is common to both systems, with radius $\rho = 4$ in the plane $z = 8$ and with vertex in the common origin.

4.11 Write the equation of the surface $x - y^2 - z^2 + 8y + 2z - 17 = 0$, $x \leq 4$ in cylindrical coordinates. Sketch the given surface.

$x = \rho^2$, $x \in \langle 0, 4\rangle$; part of a rotational paraboloid, whose axis of rotation passes through the zero point of the cylindrical system at the point $O: x, y, z = [0, 4, 1]$, with directional vector $\vec{x} = (1, 0, 0)$, with radius $\rho = 2$ in the plane $x = 4$ and with vertex at the origin.

4.3 Spherical coordinates

The spherical system is appropriate for describing point-like (centrally) symmetric phenomena. Coordinate directions are: r - distance from the central point - the origin of the system, θ

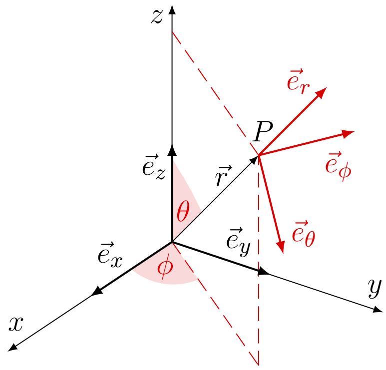

Figure 4.2: Scheme of mutual transformation of unit basis vectors of the Cartesian and spherical coordinate system (see Equation (4.8)). The basis vectors of the orthonormal Cartesian basis are drawn in bold black, the basis vectors of the orthonormal spherical basis are drawn in bold red. The general point P is determined by its position vector $\vec{r}$, the direction of the basis vector $\vec{e}_r$ is identical to the direction of the vector $\vec{r}$. Part of the half-plane S_ϕ passing through the z-axis with the constant coordinate ϕ (increasing from the x-axis to the half-plane S_ϕ) is drawn by the dashed red line, the basis vector $\vec{e}_\phi$ is perpendicular to this half-plane and is (in the right-handed system) positively oriented towards it. The basis vector $\vec{e}_\theta$ is also perpendicular to the two previous basis vectors and is oriented in the direction of increasing coordinate θ (increasing from the axis z to the vector $\vec{r}$) so that the basis vectors of the spherical system, ordered according to Equation (4.10), form a right-handed system.

- polar angle, ϕ - azimuthal angle (in this ordering of coordinate directions is the system right-handed - representation of particular directions and basis vectors is shown in Figure 4.2), where $r \in \langle 0, \infty)$, $\theta \in \langle 0, \pi \rangle$, $\phi \in \langle 0, 2\pi)$. The spherical system is again orthogonal. The transformation between the spherical and the Cartesian system is given by the relations

$$x = r \sin\theta \cos\phi, \quad y = r \sin\theta \sin\phi, \quad z = r\cos\theta. \tag{4.8}$$

For the reverse transformation, we get

$$\begin{gathered} r = \sqrt{x^2 + y^2 + z^2}, \\ \theta = \arccos \frac{z}{\sqrt{x^2+y^2+z^2}}, \\ \phi = \arccos \frac{x}{\sqrt{x^2+y^2}}, \quad \phi = \arcsin \frac{y}{\sqrt{x^2+y^2}}, \quad \phi = \arctan \frac{y}{x}. \end{gathered} \tag{4.9}$$

The unit vectors of the spherical basis will have in the Cartesian system (see Figure 4.2) the form

$$\begin{aligned} \vec{e}_r &= \vec{e}_x \sin\theta\cos\phi + \vec{e}_y \sin\theta \sin\phi + \vec{e}_z \cos\theta, \\ \vec{e}_\theta &= \vec{e}_x \cos\theta \cos\phi + \vec{e}_y \cos\theta \sin\phi - \vec{e}_z \sin\theta, \\ \vec{e}_\phi &= -\vec{e}_x \sin\phi + \vec{e}_y \cos\phi. \end{aligned} \tag{4.10}$$

Thus, in the spherical system, none of the basis vectors is constant.

Coordinate curves in the spherical system will be:

- half-lines (rays) r pointing in any direction from the origin of the system ($\theta =$ const., $\phi =$ const.),
- semicircles s_θ centered at the origin of the system, lying in the half-plane passing through the axis z ($r =$ const., $\phi =$ const., the analogy of the geographical meridians),
- circles s_ϕ centered on the z-axis, lying in a plane perpendicular to the z-axis ($r =$ const., $\theta =$ const., the analogy of the geographical parallels).

Coordinate surfaces in the spherical system will be:

- spherical surfaces S_r centered at the origin of the system ($r =$ const.),
- rotational conical (or semi-conical) surfaces S_θ with vertex at the origin of the system and with the axis of rotation in the z-axis ($\theta =$ const.),
- half-planes S_ϕ, passing through the z-axis ($\phi =$ const.).

For the square of the distance of two points in the differential form (by substituting Equation (4.8) to Equation (4.1)) in the spherical system holds,

$$\mathrm{d}s^2 = \mathrm{d}r^2 + r^2\,\mathrm{d}\theta^2 + r^2 \sin^2\theta\,\mathrm{d}\phi^2, \tag{4.11}$$

which again can be regarded as the square of the diagonal of the elementary "cuboid" or "spherical wedge" with edges $\mathrm{d}s_r = \mathrm{d}r$, $\mathrm{d}s_\theta = r\,\mathrm{d}\theta$, $\mathrm{d}s_\phi = r\sin\theta\,\mathrm{d}\phi$. In the spherical system we get the Lamé coefficients $h_r = 1, h_\theta = r, h_\phi = r\sin\theta$. From infinitesimal, mutually perpendicular edge lines or curves, we construct the surface elements

$$\mathrm{d}S_r = \mathrm{d}s_\theta\,\mathrm{d}s_\phi = r^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi,\;\; \mathrm{d}S_\theta = \mathrm{d}s_\phi\,\mathrm{d}s_r = r\sin\theta\,\mathrm{d}\phi\,\mathrm{d}r,\;\; \mathrm{d}S_\phi = \mathrm{d}s_r\,\mathrm{d}s_\theta = r\,\mathrm{d}r\,\mathrm{d}\theta \tag{4.12}$$

and also the volume element of the spherical system

$$\mathrm{d}V = \mathrm{d}s_r\,\mathrm{d}s_\theta\,\mathrm{d}s_\phi = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi. \tag{4.13}$$

None of these elements is constant, their sizes increase proportionally to the second ($\mathrm{d}S_r$, $\mathrm{d}V$) or the first ($\mathrm{d}S_\theta$, $\mathrm{d}S_\phi$) power of the distance r from the beginning of the system and also (except the surface element $\mathrm{d}S_\phi$) proportionally to the sine of polar angle θ.

A detailed description of the spherical coordinate system is given in Section B.3 in Appendix B.

- **Examples:**

4.12 Write the spherical coordinates of the point A whose Cartesian coordinates are $x, y, z = [1, 1, 1]$.

$$A:\; r, \theta, \phi = \left[\sqrt{3}, \arccos\frac{1}{\sqrt{3}}, \frac{\pi}{4}\right]$$

4.13 Write the Cartesian coordinates of the point B whose spherical coordinates are $r, \theta, \phi = \left[12, \frac{\pi}{3}, -\frac{\pi}{6}\right]$.

$$B:\; x, y, z = \left[9, -3\sqrt{3}, 6\right]$$

4.14 Write the equation of the surface $z = \pm\sqrt{25 - x^2 - y^2}$ in the spherical coordinates. Sketch the given surface.

$r = 5$; spherical surface centered at the common origin of both systems

4.15 Write the equation of the surface $x^2 + y^2 + z^2 - 14x - 6y - 10z = 61$ in the spherical coordinates. Sketch the given surface.

$r = 12$; spherical surface centered at the beginning of the spherical system located at the point $[7, 3, 5]$, given in the Cartesian coordinates

4.16 Write the vector $\vec{u}$, given in the Cartesian orthonormal basis as $\vec{u} = 2\vec{e}_x + \vec{e}_y + \vec{e}_z$, in terms of orthonormal spherical basis vectors.

$\vec{u} = (2\sin\theta\cos\phi + \sin\theta\sin\phi + \cos\theta)\,\vec{e}_r + (2\cos\theta\cos\phi + \cos\theta\sin\phi - \sin\theta)\,\vec{e}_\theta + (\cos\phi - 2\sin\phi)\,\vec{e}_\phi$

4.17 Write the components of the vector $\vec{u}$ (the expressions in parentheses) in the result of Example 4.16 using the Cartesian coordinates.

$$\vec{u} = \frac{2x + y + z}{\sqrt{x^2 + y^2 + z^2}}\,\vec{e}_r + \frac{z(2x + y) - x^2 - y^2}{\sqrt{x^2 + y^2}\sqrt{x^2 + y^2 + z^2}}\,\vec{e}_\theta + \frac{x - 2y}{\sqrt{x^2 + y^2}}\,\vec{e}_\phi$$

4.18 According to Equation (4.13), derive the formula for calculation of the volume V of a sphere with radius R.

$V = \dfrac{4}{3}\pi R^3$

Chapter 5

Scalar and vector functions of several variables[1] [2]

5.1 Partial and directional derivatives, total differential

Partial derivatives of a function of two or more independent variables $f(x_1, x_2, \ldots, x_n)$ is a derivative of this function according to one of these variables, i.e., we derive the given function as a function of only this *single* variable according to which we calculate the derivative. The other independent variables have, at this moment, a constant value (they behave like constants). The spatial image (see Figure 5.1) can be done using a function of two variables $f(x, y)$, whose geometric meaning can be described as the surface given by the formula $z = f(x, y)$. The partial derivative of this function, for example, according to the variable x that we write as

$$\frac{\partial f(x,y)}{\partial x} \quad \text{or only} \quad \frac{\partial f}{\partial x} \quad \text{or also} \quad f_x\,, \tag{5.1}$$

expresses the slope of the tangent of this surface, which lies in the plane parallel to the plane xz and which is oriented in the positive sense of the x-axis. The value of the second independent variable y is thus constant for this tangent. The same applies to partial derivatives according to other independent variables.

Of course, we can generalize the partial derivatives for a completely arbitrary direction, not just for the directions of the coordinate axes, which represent the direction of the increase of only one particular independent variable. In this case, we call them the directional derivatives (or derivatives in a given direction). The selected direction can be defined, for example, by the vector $\vec{u} = (u_1, u_2, \ldots, u_n)$, whose norm is denoted by $\|\vec{u}\| = u$. Thus, the directional derivative in case of a function of two variables, analogous to the example described in the previous paragraph, expresses the slope of the tangent of this surface, which lies in the plane parallel to the plane defined by this vector and the z-axis. The directional derivative of a continuously differentiable scalar function in the direction of the vector $\vec{u}$ can be generally defined as

$$\frac{\mathrm{d}f(x_1, x_2, \ldots, x_n)}{\mathrm{d}u} = \vec{\nabla} f(x_1, x_2, \ldots, x_n) \cdot \frac{\vec{u}}{u}, \tag{5.2}$$

where the symbol (the so-called *operator Nabla*) $\vec{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n}\right)$ denotes in this case the vector of partial derivatives according to all independent variables. So, Equation (5.2) can

[1] We do not give the corresponding physical units in the results of the examples with geometric or physical quantities.

[2] Recommended literature for this chapter: Dĕmidovič (2003), Kvasnica (2004), Bartsch (2008), Rektorys (2009).

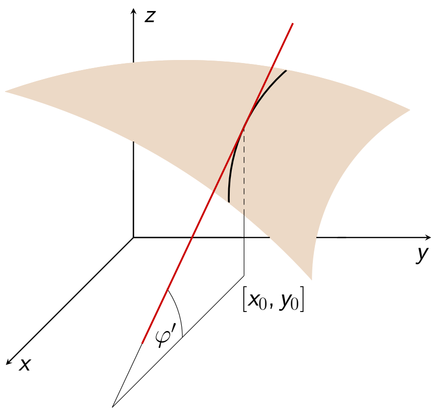

Figure 5.1: Geometric meaning of the partial derivative of a function two variables $z = f(x, y)$ at the point $[x_0, y_0]$. The segment of the function $f(x, y)$ is highlighted in the illustration by the colored area. The partial derivative (in this case, by x) of the function of the two variables $f(x, y)$ gives the slope of the tangent line to the curve that corresponds to the section of the graph (surface) of the function $f(x, y)$ by the plane that is parallel to the corresponding axis; in this case by the plane parallel to the plane xz, passing through the point $[x_0, y_0]$. The sectional curve of the respective surface is shown in this figure by a thick black line passing through the colored area, its tangent at the point $[x_0, y_0]$ is shown in red. In this case, the partial derivative $\partial f/\partial x$ will correspond to $\tan\varphi$, where $\varphi = -\varphi'$. The geometric meaning of partial derivatives, according to other variables or directional derivatives, is analogous.

be explicitly written

$$\frac{\mathrm{d}f(x_1, x_2, \ldots, x_n)}{\mathrm{d}u} = \frac{\partial f}{\partial x_1}\frac{u_1}{u} + \frac{\partial f}{\partial x_2}\frac{u_2}{u} + \ldots + \frac{\partial f}{\partial x_n}\frac{u_n}{u}. \tag{5.3}$$

The complete (total) differential of a general scalar function $f(\vec{x}) = f(x_1, x_2, \ldots, x_n)$ of several *independent* variables is called a function

$$\mathrm{d}f = \frac{\partial f}{\partial x_1}\,\mathrm{d}x_1 + \frac{\partial f}{\partial x_2}\,\mathrm{d}x_2 + \ldots + \frac{\partial f}{\partial x_n}\,\mathrm{d}x_n = \vec{\nabla} f(\vec{x}) \cdot \mathrm{d}\vec{x}. \tag{5.4}$$

If the total differential of a function $f(\vec{x})$ exists at the given point, we say that the function $f(\vec{x})$ is differentiable at this point. If the total differential of a function $f(\vec{x})$ exists at all points of this function, we say that the function $f(\vec{x})$ is continuously differentiable (smooth). If the total differential of a function $f(\vec{x})$ exists in limited areas of this function only, we say that the function $f(\vec{x})$ is differentiable by parts.

The higher (nth) order total differential of a function $f(x, y)$ of two *independent* variables x, y will be the function given by the general formula

$$\mathrm{d}^n f(x, y) = \sum_{k=0}^{n} \binom{n}{k} \frac{\partial^n f}{\partial x^k\, \partial y^{n-k}}\, \mathrm{d}x^k\, \mathrm{d}y^{n-k}, \tag{5.5}$$

where the expression in parentheses after the sum is the so-called *combination number* (see Equation (12.1)). The total differential of a higher (nth) order of a function $f(x_1, x_2, x_3, ..., x_{m-1}, x_m)$ of an arbitrary number of m independent variables $x_1, x_2, ..., x_m$ will be the function given by the prescription

$$\mathrm{d}^n f(x_1, x_2, ..., x_m) = \sum_{k_1+k_2+\ldots+k_m=n} \binom{n}{k_1, k_2, ..., k_m} \frac{\partial^n f}{\partial x_1^{k_1} \partial x_2^{k_2} ... \partial x_m^{k_m}}\, \mathrm{d}x_1^{k_1}\, \mathrm{d}x_2^{k_2} ...\, \mathrm{d}x_m^{k_m}, \tag{5.6}$$

where the expression in parentheses after the sum is the so-called *multinomial coefficient* (see Equation (12.6)) and where the meaning and the use of all other expressions and symbols corresponds to the so-called *multinomial theorem* (12.7).

- **Examples:**

5.1 Calculate the partial derivatives $\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}$ of the scalar function $f(x, y) = x^2 + x - y$.

$2x + 1,\ -1$

5.2 Calculate the partial derivatives $\dfrac{\partial^2 f}{\partial x^2}, \dfrac{\partial^2 f}{\partial y^2}$ of the scalar function $f(x, y) = x \ln y + x^y$.

$\left(y^2 - y\right) x^{y-2},\ -\dfrac{x}{y^2} + x^y \ln^2 x$

5.3 Calculate the mixed partial derivative $\dfrac{\partial^3 f}{\partial x\, \partial y\, \partial z}$ of the scalar function $f(x, y, z) = xyz + x^2 \sin(xy) + yz$.

1

5.4 Calculate the mixed partial derivative $\dfrac{\partial^4 f}{\partial x\, \partial y\, \partial z^2}$ of the scalar function $f(x, y, z) = xy^2z^3 + x^2 \sin^2(xz) + yz + x + y + z$.

$12yz$

5.5 Prove that from the equation of state of an ideal gas $pV = n\mathcal{R}T$, where p is the pressure, V is the volume, T is the thermodynamic temperature, n is the amount of substance, and $\mathcal{R}$ is the molar gas constant, follows: $\dfrac{\partial p}{\partial V} \dfrac{\partial V}{\partial T} \dfrac{\partial T}{\partial p} = -1$.

5.6 Show that the function $u = \dfrac{1}{2a\sqrt{\pi t}}\, \mathrm{e}^{-\frac{(x-b)^2}{4a^2 t}}$, where a, b are constants, satisfies the heat conduction equation $\dfrac{\partial u}{\partial t} = a^2 \dfrac{\partial^2 u}{\partial x^2}$.

5.7 Show that the function $u = \dfrac{1}{r}$, where $r = \sqrt{(x-a)^2 + (y-b)^2 + (z-c)^2}$, where a, b, c are constants, satisfies the Laplace equation $\Delta u = 0$ for $r \neq 0$.

Examples 5.5, 5.6, 5.7 - using the partial derivatives of the functions.

5.8 Calculate the derivative of the function $f(x, y) = \dfrac{x}{y}$ at the point $[4, -1]$ in the direction of the vector $\vec{u} = (-2, 3)$.

$-\dfrac{10}{\sqrt{13}}$

5.9 Calculate the derivative of the function $f(x, y, z) = \cos(xy) + \ln z^2$ at the point $[\pi, 1, 1]$ in the direction of the vector $\vec{u} = (1, 1, 1)$.

$\dfrac{2}{\sqrt{3}}$

5.10 Calculate the derivative of the function $f(x,y) = x^2 - y^2$ at the point $[1,1]$ in the direction of the vector $\vec{u} = (1,-1)$.

$2\sqrt{2}$

5.11 Calculate the derivative of the function $f(x,y) = x + 2y$ at the point $[2,1]$ in the direction of the vector $\vec{u} = (1,2)$.

$\sqrt{5}$

5.12 Calculate the derivative of the function $f(x,y,z) = x + y^2 + z^3$ at the point $[0,1,2]$ in the direction of the vector $\vec{u} = (1,0,1)$.

$\dfrac{13}{\sqrt{2}}$

5.13 Calculate the derivative of the function $f(x,y) = x^3 - y^2 + 2xy$ at the point $[2,3]$ in the direction of the vector $\vec{u} = (-3,2)$.

$-\dfrac{58}{\sqrt{13}}$

5.14 Find the value of the derivative of the function $f(x,y) = x^2 - xy - y^2$ in the direction of its maximum growth at the point $[1,-3]$.

$5\sqrt{2}$

5.15 Find the first and second differential of the function $f(x) = x\cos x$ and evaluate them at the point $\pi/4$.

$\dfrac{1}{\sqrt{2}}\left(1 - \dfrac{\pi}{4}\right)\mathrm{d}x, \; -\dfrac{1}{\sqrt{2}}\left(2 + \dfrac{\pi}{4}\right)\mathrm{d}x^2$

5.16 Find the first and second differential of the function $f(x,y) = \left(x + y^3\right)^2$ and evaluate them at the point $[2,3]$.

$58\,\mathrm{d}x + 1566\,\mathrm{d}y, \; 2\,\mathrm{d}x^2 + 108\,\mathrm{d}x\,\mathrm{d}y + 2502\,\mathrm{d}y^2$

5.17 Find the first and second differential of the function $f(x,y) = xy + x\cos y + y^x$ and evaluate them at the point $[1,\mathrm{e}]$.

$(2\mathrm{e} + \cos\mathrm{e})\,\mathrm{d}x + (2 - \sin\mathrm{e})\,\mathrm{d}y, \; \mathrm{e}\,\mathrm{d}x^2 + (6 - 2\sin\mathrm{e})\,\mathrm{d}x\,\mathrm{d}y - (\cos\mathrm{e})\,\mathrm{d}y^2$

5.18 Find the first and second differential of the function $f(x,y) = \ln\left(x + y^2\right)$ and evaluate them at the point $[1,1]$.

$\dfrac{1}{2}\,\mathrm{d}x + \mathrm{d}y, \; -\dfrac{1}{4}\,\mathrm{d}x^2 - \mathrm{d}x\,\mathrm{d}y$

5.19 Calculate the value of the product 1.03×1.98 by using the first differential and compare it to the value specified by the calculator.

2.04 (by calculator 2.0394)

5.20 Calculate the value of the ratio $\left(\dfrac{3.96}{2.01}\right)^3$ by using the first differential and compare it to the value specified by the calculator.

7.64 (by calculator 7.64711...)

5.21 Calculate the value of the function $\arctan\left(\dfrac{1.01}{0.98}\right)$ by using the first differential and compare it to the value specified by the calculator.

$\dfrac{\pi}{4} + 0.015 \approx 0.8004$ (by calculator 0.80047...)

5.2 Scalar potential function

We have already met the *scalar potential* function when calculating the exact differential equations in Section 3.1.4. The term scalar potential function is closely related to the concepts of the total differential and the conservative vector field. The general vector field $\vec{A}(\vec{x})$ is said to be conservative if there is such a scalar function $\varphi(\vec{x})$ that

$$\vec{A}(\vec{x}) = \vec{\nabla}\varphi(\vec{x}), \qquad \text{or alternatively,} \qquad \mathrm{d}\varphi(\vec{x}) = \vec{A}(\vec{x}) \cdot \mathrm{d}\vec{x}. \tag{5.7}$$

The left expression (considering a three-dimensional case) $\vec{\nabla}\varphi = \left(\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}, \frac{\partial\varphi}{\partial z}\right)$ of Equation (5.7) means the *gradient* of the function φ (see also Section 5.3), the right expression $\mathrm{d}\varphi$ of Equation (5.7) is the total differential of the function φ. If Equation (5.7) holds, the function φ is called the scalar potential function (in fact it is the negative of the "physical" scalar potential, where the "physical" meaning of the scalar potential $\phi = -\varphi$) of the conservative vector field $\vec{A}$. The intensity $\vec{E}$ of the general conservative field will then be $\vec{E} = -\vec{\nabla}\phi$ and the corresponding force field $\vec{F} = -\vec{\nabla}E_p$, where E_p is the potential energy. We can check by the Schwarz theorem if the given vector field is conservative, the analogous procedure is given in Equation (3.19). We can generalize this procedure to any number of variables, i.e.,

$$\frac{\partial A_j(x_1, x_2, \ldots, x_j, \ldots, x_k, \ldots, x_n)}{\partial x_k} = \frac{\partial A_k(x_1, x_2, \ldots, x_j, \ldots, x_k, \ldots, x_n)}{\partial x_j}, \tag{5.8}$$

where A_j, A_k denote jth and kth components of the vector $\vec{A}$, respectively, and the free indices j, k successively take all the values from 1 to n. Then we can find the scalar potential function (for example, in three-dimensional case) using the integral

$$\varphi(x, y, z) = \int_{x_0}^{x} A_x(t, y, z)\,\mathrm{d}t + \int_{y_0}^{y} A_y(x_0, t, z)\,\mathrm{d}t + \int_{z_0}^{z} A_z(x_0, y_0, t)\,\mathrm{d}t. \tag{5.9}$$

For a different number of dimensions, formula (5.9) will be truncated or extended correspondingly.

- **Examples:**

Decide if the expression is the total differential, if yes, find the corresponding scalar potential function:

5.22 $(\sin x + y)\,\mathrm{d}x + \left(x^2 + \cos y\right)\mathrm{d}y$ It is not the total differential.

5.23 $(x^2 + y)\,\mathrm{d}x + (x + y^2)\,\mathrm{d}y$ $\qquad \dfrac{x^3}{3} + xy + \dfrac{y^3}{3} - \left(\dfrac{x_0^3}{3} + x_0\,y_0 + \dfrac{y_0^3}{3}\right)$

5.24 $xy^2\,\mathrm{d}x + (y^2 + x^2y + 4)\,\mathrm{d}y$ $\qquad \dfrac{x^2y^2}{2} + \dfrac{y^3}{3} + 4y - \left(\dfrac{x_0^2\,y_0^2}{2} + \dfrac{y_0^3}{3} + 4y_0\right)$

5.25 $(x + 2xy)\,\mathrm{d}x + (\cos y + x^2)\,\mathrm{d}y$ $\qquad \dfrac{x^2}{2} + x^2y + \sin y - \left(\dfrac{x_0^2}{2} + x_0^2\,y_0 + \sin y_0\right)$

5.26 $y'\left(\dfrac{\ln x}{y^2} - y\right) = \dfrac{1}{xy},\ y(1) = 2$ $\qquad 2 - \dfrac{\ln x}{y} - \dfrac{y^2}{2}$

5.27 $\left(3x^2 - 2xy + \dfrac{1}{y}\right) - \left(x^2 + \dfrac{x}{y^2} + \dfrac{2}{y^3}\right)y',\ y(0) = 1$ $\qquad x^3 - x^2y + \dfrac{x}{y} + \dfrac{1}{y^2} - 1$

5.28 $(6x^3y^2 + 3x^2)\,\mathrm{d}x + (3x^4y + \cos y)\,\mathrm{d}y,\ y(1) = \dfrac{\pi}{2}$ $\qquad \dfrac{3}{2}x^4y^2 + x^3 + \sin y - \dfrac{3\pi^2}{8} - 2$

5.29 $-\dfrac{2x}{x^2 + y^2}\,\mathrm{d}x - \dfrac{2y}{x^2 + y^2}\,\mathrm{d}y,\ y(1) = 1$ $\qquad \ln 2 - \ln(x^2 + y^2)$

5.30 $\dfrac{1}{y^2}\,\mathrm{d}x + \left(-\dfrac{2x}{y^3} + \mathrm{e}^y\right)\mathrm{d}y,\ y(0) = 1$ $\qquad \dfrac{x}{y^2} + \mathrm{e}\left(\mathrm{e}^{y-1} - 1\right)$

5.31 $\dfrac{3x^2}{2\sqrt{x^3 + y^3}}\,\mathrm{d}x + \dfrac{3y^2}{2\sqrt{x^3 + y^3}}\,\mathrm{d}y,\ y(1) = 2$ $\qquad \sqrt{x^3 + y^3} \pm 3$

Prove that the force field is conservative and determine the corresponding potential energy V (k is constant, Q_1 and Q_2 are the constant electric charges):

5.32 $\vec{F} = -k\vec{r}$ (elastic force) $\qquad V = \dfrac{kr^2}{2} = \dfrac{k}{2}\left(x^2 + y^2 + z^2\right)$

5.33 $\vec{F} = k\dfrac{Q_1Q_2}{r^3}\vec{r}$ (electrostatic force) $\qquad V = k\dfrac{Q_1Q_2}{r} = k\dfrac{Q_1Q_2}{\sqrt{x^2 + y^2 + z^2}}$

5.34 Find the potential of the vector field $\vec{A} = (2xy, x^2)$. Is this potential determined unambiguously?

$\phi = -x^2y + C$

5.35 The intensity of a physical field is determined by the vector $\vec{A} = \left[\ln(x - y) + \dfrac{x}{x - y}, -\dfrac{x}{x - y}, 0\right]$. Can this potential be determined for this field? If so, find it. Will this potential be determined unambiguously?

$\phi = -x\ln(x - y) + C$

5.36 Prove that the central force field $\vec{F} = -k\,\vec{r}\,r$ is conservative. Determine the corresponding potential energy V at the point $x, y, z = [X_0, Y_0, Z_0]$ if its value at the point $x, y, z =$

$[0,0,0]$ is equal to V_0. The quantity k is a constant, $\vec{r}$ is the position vector, and r is its magnitude.

$$V(X_0, Y_0, Z_0) = \frac{k}{3}\left(X_0^2 + Y_0^2 + Z_0^2\right)^{3/2} + V_0$$

5.37 Prove that the given central force field $\vec{F} = -\frac{k\,\vec{r}}{r}$ defined for $r \geq 1$ is conservative. Determine the corresponding potential energy V at the point $x, y, z = [X_0, Y_0, Z_0]$ if its value at the minimum defined distance from the point $x, y, z = [0,0,0]$ is equal to V_0. The quantity k is a constant, $\vec{r}$ is the position vector, and r is its magnitude.

$$V(X_0, Y_0, Z_0) = k\left(\sqrt{X_0^2 + Y_0^2 + Z_0^2} - 1\right) + V_0$$

5.38 Prove that the given force field $\vec{F} = -k\frac{\vec{r}}{r^3}$ defined for $r \geq 1$ is conservative. Determine the corresponding potential energy V at the point $x, y, z = [2,2,1]$ if the value of the potential energy at the distance $r = 1$ from the point $x, y, z = [0,0,0]$ is denoted as $E_0 = 0$. The quantity $k = 1.5$ is a constant, r is the magnitude of the position vector $\vec{r} = (x, y, z)$.

$$V(2,2,1) = k\left(1 - \frac{1}{\sqrt{X_0^2 + Y_0^2 + Z_0^2}}\right) + E_0 = 1$$

5.39 Prove that the central force field $\vec{F}$ defined for $r \geq 1$ is conservative. Determine the corresponding potential energy V of the field at the point $x, y, z = [X_0, Y_0, Z_0]$ if we set its value at the minimum defined distance from the point $x, y, z = [0,0,0]$ as zero:

(a) $\vec{F} = -k\,\vec{r}\ln r$,

(b) $\vec{F} = -k\,\vec{r}\ln r^2$,

(c) $\vec{F} = -k\,\vec{r}\ln r^3$.

The quantity k is a constant, $\vec{r}$ is the position vector, and r is its magnitude.

(a) $V(X_0, Y_0, Z_0) = \frac{k}{2}\left[\left(X_0^2 + Y_0^2 + Z_0^2\right)\left(\ln\sqrt{X_0^2 + Y_0^2 + Z_0^2} - \frac{1}{2}\right) + \frac{1}{2}\right]$

(b) $V(X_0, Y_0, Z_0) = \frac{k}{2}\left\{\left(X_0^2 + Y_0^2 + Z_0^2\right)\left[\ln\left(X_0^2 + Y_0^2 + Z_0^2\right) - 1\right] + 1\right\}$

(c) $V(X_0, Y_0, Z_0) = \frac{k}{2}\left\{\left(X_0^2 + Y_0^2 + Z_0^2\right)\left[\ln\left(X_0^2 + Y_0^2 + Z_0^2\right)^{\frac{3}{2}} - \frac{3}{2}\right] + \frac{3}{2}\right\}$

5.40 Prove that the given force field $\vec{F} = -k\,(x, y, z)\ln r^{-2}$ defined for $r \geq 1$ is conservative. Determine the corresponding potential energy V at the point $x, y, z = [X_0, Y_0, Z_0]$ if the potential energy at the distance $r = 1$ from the point $x, y, z = [0,0,0]$ is equal to E_0. The quantity k is a constant, r is the magnitude of the position vector $\vec{r} = (x, y, z)$.

$$V(X_0, Y_0, Z_0) = -\frac{k}{2}\left\{\left(X_0^2 + Y_0^2 + Z_0^2\right)\left[\ln\left(X_0^2 + Y_0^2 + Z_0^2\right) - 1\right] + 1\right\} + E_0$$

5.41 Prove that the given central force field $\vec{F} = -k\,\vec{r}\,\mathrm{e}^r$ is conservative. Determine its corresponding potential energy V at the point $x, y, z = [X_0, Y_0, Z_0]$ if the value of the potential energy at the point $x, y, z = [0, 0, 0]$ is equal to $-V_0 = -k$. The quantity k is a constant, $\vec{r}$ is the position vector, and r is its magnitude.

$V(X_0, Y_0, Z_0) = V_0\, \mathrm{e}^{\sqrt{X_0^2+Y_0^2+Z_0^2}} \left(\sqrt{X_0^2 + Y_0^2 + Z_0^2} - 1\right)$

5.3 Differential operators

Differential operators control the acting of the nabla operator (see also Sections 5.1 and 5.2) on a scalar or vector field in any of the following ways:

- *gradient* of a scalar function f: $\operatorname{grad} f = \vec{\nabla} f$, the result is a vector (5.10)
- *divergence* of a vector field $\vec{A}$: $\operatorname{div} \vec{A} = \vec{\nabla} \cdot \vec{A}$, the result is a scalar (5.11)
- *curl* of a vector field $\vec{A}$ (only in $\mathbb{R}^3$): $\operatorname{rot} \vec{A} = \vec{\nabla} \times \vec{A}$, the result is a vector (5.12)
- Laplace operátor (*Laplacian*): $\Delta = \vec{\nabla} \cdot \vec{\nabla}$, conserves the tensor type (5.13)

The Laplace operator does not change the tensor order, i.e., if it acts on a scalar, the result is a scalar, if it acts on a vector, the result remains a vector, etc. (see Appendix B). A variant form of writing differential operators using free indexes (in the Einstein convention) can look in the Cartesian coordinate system like this (the meaning of the symbols δ_{ij} and ε_{ijk} is explained in Section 2.3):

- *gradient* of a scalar function f: $\operatorname{grad} f = \vec{e}_i \dfrac{\partial f}{\partial x_i}$, (5.14)
- *divergence* of a vector field $\vec{A}$: $\operatorname{div} \vec{A} = \dfrac{\partial}{\partial x_i} A_j\, \delta_{ij} = \dfrac{\partial}{\partial x_i} A_i$, (5.15)
- *curl* of a vector field $\vec{A}$: $\operatorname{rot} \vec{A} = \varepsilon_{ijk}\, \vec{e}_i \dfrac{\partial}{\partial x_j} A_k$, (5.16)
- Laplace operator (*Laplacian*): $\Delta f = \dfrac{\partial}{\partial x_i} \dfrac{\partial}{\partial x_i} f, \quad \Delta \vec{A} = \vec{e}_i \dfrac{\partial}{\partial x_j} \dfrac{\partial}{\partial x_j} A_i.$ (5.17)

A gradient of a scalar function represents a vector field indicating the magnitude and the direction of its steepest increase. Divergence of a vector can be interpreted, for example, as the "expansion rate" ("intensity of its outflow rate") of a given vector quantity, or as its behavior as a "fountain", i.e., a measure of how much the given vector field behaves as the "source". For example, if the vector field at the same time "appears" (source) and "disappears" (sink), its divergence is zero (magnetic induction case); the homogeneous vector field (constant vector) must have zero divergences, etc. The curl of a vector field (as it follows from the title) describes the infinitesimal rotation of the field at a general point in space; if the curl is zero, we speak about the "non-vortex" flow of the vector variable. A curl of a vector field is defined only in the three-dimensional case.

A detailed description of the derivation of the particular differential operators in the essential coordinate systems, including related mathematics, is given in Appendix B. We give here only the basic overview of the explicit forms of the differential operators in Cartesian, cylindrical, and spherical coordinate systems in $\mathbb{R}^3$ (We introduce again ρ instead of r in the cylindrical

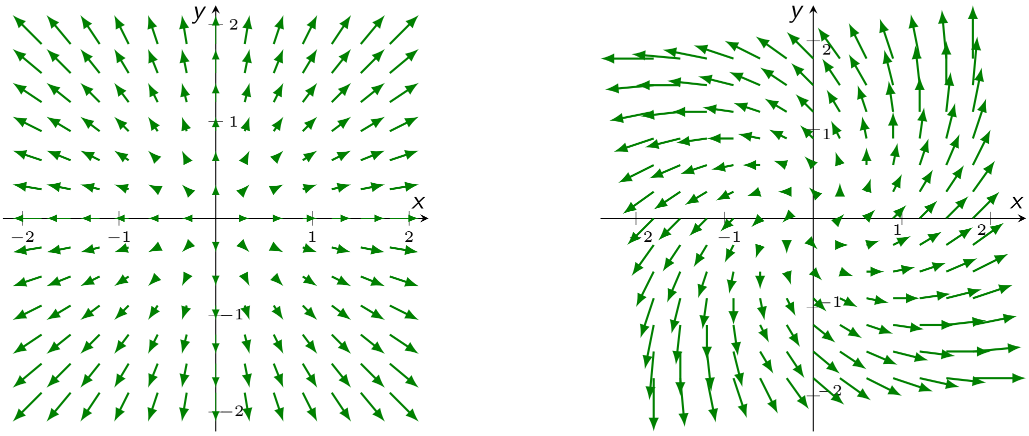

Figure 5.2: *Left panel*: Two-dimensional representation of the vector field $\vec{F}(x,y,z) = a(x,y,0)$, where the scaling constant $a = 1/6$ is introduced for graphical clarity. The divergence of this field $\operatorname{div} \vec{F} = 2a$, the curl of this field is zero. We see in this case (the divergence is constant) that the magnitude of the vector (the length of the arrows) increases proportionally with the distance from the origin, but the vector does not change its direction with the distance. If the divergence was a function of only one of the coordinates, the direction of the vector would change in some way depending on the distance from the origin. *Right panel*: Two-dimensional representation of the vector field $\vec{F}(x,y,z) = a(x-y, x+y, 0)$, where the same scaling constant $a = 1/6$ is introduced. The divergence of this field is again $2a$ but also the curl of this field is now nonzero, $\|\operatorname{rot} \vec{F}\| = 2a$.

system), where the Laplacian operator can act either on a scalar function or on the particular components of a vector:

- Cartesian coordinate system (x_1, x_2, $x_3 = x, y, z$):

$$\operatorname{grad} f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right), \tag{5.18}$$

$$\operatorname{div} \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}, \tag{5.19}$$

$$\operatorname{rot} \vec{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}, \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}, \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right), \tag{5.20}$$

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}, \tag{5.21}$$

$$\Delta \vec{A} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)(A_x, A_y, A_z) = \tag{5.22}$$

$$= \left(\frac{\partial^2 A_x}{\partial x^2} + \frac{\partial^2 A_x}{\partial y^2} + \frac{\partial^2 A_x}{\partial z^2}, \frac{\partial^2 A_y}{\partial x^2} + \frac{\partial^2 A_y}{\partial y^2} + \frac{\partial^2 A_y}{\partial z^2}, \frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} + \frac{\partial^2 A_z}{\partial z^2}\right). \tag{5.23}$$

- cylindrical coordinate system (x_1, x_2, $x_3 = \rho, \phi, z$):

$$\operatorname{grad} f = \left(\frac{\partial f}{\partial \rho}, \frac{1}{\rho}\frac{\partial f}{\partial \phi}, \frac{\partial f}{\partial z}\right), \tag{5.24}$$

$$\operatorname{div} \vec{A} = \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho A_\rho) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}, \tag{5.25}$$

$$\operatorname{rot} \vec{A} = \left\{\frac{1}{\rho}\frac{\partial A_z}{\partial \phi} - \frac{\partial A_\phi}{\partial z}, \frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial \rho}, \frac{1}{\rho}\left[\frac{\partial}{\partial \rho}(\rho A_\phi) - \frac{\partial A_\rho}{\partial \phi}\right]\right\}, \tag{5.26}$$

$$\Delta f = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial f}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2}, \tag{5.27}$$

$$\Delta \vec{A} = \left[\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}\right](A_\rho, A_\phi, A_z)\,. \tag{5.28}$$

- spherical coordinate system (x_1, x_2, $x_3 = r, \theta, \phi$):

$$\operatorname{grad} f = \left(\frac{\partial f}{\partial r}, \frac{1}{r}\frac{\partial f}{\partial \theta}, \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\right), \tag{5.29}$$

$$\operatorname{div} \vec{A} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 A_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}, \tag{5.30}$$

$$\operatorname{rot} \vec{A} = \left\{\frac{1}{r\sin\theta}\left[\frac{\partial}{\partial \theta}(\sin\theta\, A_\phi) - \frac{\partial A_\theta}{\partial \phi}\right], \frac{1}{r}\left[\frac{1}{\sin\theta}\frac{\partial A_r}{\partial \phi} - \frac{\partial}{\partial r}(rA_\phi)\right], \frac{1}{r}\left[\frac{\partial}{\partial r}(rA_\theta) - \frac{\partial A_r}{\partial \theta}\right]\right\}, \tag{5.31}$$

$$\Delta f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}, \tag{5.32}$$

$$\Delta \vec{A} = \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right](A_r, A_\theta, A_\phi)\,. \tag{5.33}$$

- **Examples:**

5.42 Prove the following relations (all examples in this Section are considered in $\mathbb{R}^3$), where $\vec{r}$ is a position vector, $r{=}\|\vec{r}\|$ is its magnitude, $\vec{A}$ is a constant vector, $\vec{B}$ is an arbitrary vector, $\boldsymbol{E}$ is a unit matrix, and $n \in \mathbb{R}$ is a constant:

(a) $\operatorname{div}\vec{r} = 3$,

(b) $\operatorname{rot}\vec{r} = \vec{0}$,

(c) $\Delta\,\vec{r} = \vec{0}$,

(d) $\operatorname{grad} r = \dfrac{\vec{r}}{r}$,

(e) $\operatorname{grad}(\vec{A}\cdot\vec{r}) = \vec{A}$,

(f) $\operatorname{grad}\,(r^n) = nr^{n-2}\,\vec{r}$,

(g) $\operatorname{grad}\vec{r} = \boldsymbol{E}$ in Cartesian system

(h) $\operatorname{grad}(\vec{B}\cdot\vec{r}) = \vec{B} + (\vec{\nabla}\vec{B})\cdot\vec{r}$,

Using the vector identities in Cartesian coordinates.

5.43 Calculate: $\operatorname{div}\operatorname{rot}\vec{F}$, $\vec{F} = \left[xyz, y\left(x^2 - z^2\right), xy + zx + yz\right]$. 0

5.44 Calculate: $\operatorname{div}\operatorname{rot}\vec{F}$, $\vec{F}=\left(x^2y, y^2, z^2x\right)$. 0

5.45 Calculate: $\operatorname{grad} f$, $f(x,y,z)=2xyz+x^2y+y^2z+z^2x$.

$\operatorname{grad} f=(2yz+2xy+z^2, 2xz+x^2+2yz, 2xy+y^2+2xz)$

5.46 Calculate: $\operatorname{grad} f$, $f(x,y,z)=x^2y+x\cosh(yz)$.

$\operatorname{grad} f=\left[2xy+\cosh(yz), x^2+xz\sinh(yz), xy\sinh(yz)\right]$

5.47 Show that $\operatorname{div}\vec{F}=(x-y^2, y^5z^2, 3\,\mathrm{e}^{y^2z})$ is positive. $\operatorname{div}\vec{F}=1+5y^4z^2+3y^2\,\mathrm{e}^{y^2z}$

For the scalar functions f, g and the vectors $\vec{A}, \vec{B}$ prove that:

5.48 $\vec{\nabla}(fg)=(\vec{\nabla}f)g+f\vec{\nabla}g$

5.49 $\vec{\nabla}\times\vec{\nabla}f=\vec{0}$

5.50 $\vec{\nabla}\cdot\left(\vec{\nabla}\times\vec{A}\right)=0$

5.51 $\vec{\nabla}\cdot f\vec{A}=\vec{A}\cdot\vec{\nabla}f+f\vec{\nabla}\cdot\vec{A}$

5.52 $\vec{\nabla}\cdot\left(\vec{A}\times\vec{B}\right)=\vec{B}\cdot\left(\vec{\nabla}\times\vec{A}\right)-\vec{A}\cdot\left(\vec{\nabla}\times\vec{B}\right)$

5.53 $\vec{\nabla}\times\left(\vec{A}\times\vec{B}\right)=\vec{A}\left(\vec{\nabla}\cdot\vec{B}\right)-\vec{B}\left(\vec{\nabla}\cdot\vec{A}\right)+\left(\vec{B}\cdot\vec{\nabla}\right)\vec{A}-\left(\vec{A}\cdot\vec{\nabla}\right)\vec{B}$

5.54 $\vec{\nabla}\times f\vec{A}=(\vec{\nabla}f)\times\vec{A}+f\vec{\nabla}\times\vec{A}$

5.55 Prove the validity of the vector identity $\vec{\nabla}\times\left(\vec{\nabla}\times\vec{A}\right)=\vec{\nabla}\left(\vec{\nabla}\cdot\vec{A}\right)-\Delta\vec{A}$.

5.56 Prove the validity of the vector identity $\vec{A}\times\left(\vec{\nabla}\times\vec{A}\right)=\frac{1}{2}\vec{\nabla}A^2-\left(\vec{A}\cdot\vec{\nabla}\right)\vec{A}$.

Examples 5.48 - 5.56 - using the vector identities in Cartesian coordinates.

5.57 Centrally symmetrical (isotropic) physical field is determined by the vector $\vec{A}=\frac{\vec{r}}{r}$, where $\vec{r}$ is the position vector, and r is its magnitude. Prove that the divergence of this field $\vec{\nabla}\cdot\vec{A}=\frac{2}{r}$.

$$\vec{A}=\frac{\vec{r}}{r}=\frac{(x,y,z)}{\sqrt{x^2+y^2+z^2}},\ \vec{\nabla}\cdot\vec{A}=\frac{2}{\sqrt{x^2+y^2+z^2}}=\frac{2}{r}$$

5.58 Hypothetical centrally symmetrical physical field is determined by the potential $\phi=\ln\left(\frac{A}{r}\right)+B$, where A is a positive constant r is the position vector magnitude $\vec{r}$. A constant B scales the value of the potential ϕ in the distance A from the point $x,y,z=[0,0,0]$. Determine the vector $\vec{E}$ of intensity of this field and prove that the divergence of this field $\vec{\nabla}\cdot\vec{E}=\frac{1}{r^2}$.

$$\vec{E} = \frac{\vec{r}}{r^2} = \frac{(x, y, z)}{x^2 + y^2 + z^2}, \; \vec{\nabla} \cdot \vec{E} = \frac{1}{r^2} = \frac{1}{x^2 + y^2 + z^2}$$

5.59 A hypothetical centrally symmetrical physical field is determined by the potential $\phi = -Ar^3 + B$, where a constant A scales the magnitude r of the position vector $\vec{r}$ and a constant B scales the value of the potential ϕ at the point $x, y, z = [0, 0, 0]$. Determine the vector $\vec{E}$ of the intensity of this field and prove that the divergence of this field $\vec{\nabla} \cdot \vec{E} = 12A\sqrt{x^2 + y^2 + z^2} = 12Ar$.

$$\vec{E} = 3A\vec{r}\,r = 3A\,(x, y, z)\sqrt{x^2 + y^2 + z^2}, \; \vec{\nabla} \cdot \vec{E} = 12Ar = 12A\sqrt{x^2 + y^2 + z^2}$$

5.60 A hypothetical centrally symmetrical physical field, defined at the distance $r \geq 1$, is determined by the potential $\phi = -Ar^2 \ln r^2 + B$, where a constant A scales the magnitude r of the position vector $\vec{r}$ and a constant B scales the value of the potential ϕ at the minimum defined distance from the point $x, y, z = [0, 0, 0]$. Determine the vector $\vec{E}$ of the intensity of this field and prove that the divergence of this field $\vec{\nabla} \cdot \vec{E} = A\left(6 \ln r^2 + 10\right)$.

$$\vec{E} = 2A\vec{r}\left(\ln r^2 + 1\right) = 2A\,(x, y, z)\left[\ln(x^2 + y^2 + z^2) + 1\right], \; \vec{\nabla} \cdot \vec{E} = A\left(6 \ln r^2 + 10\right)$$

5.61 A hypothetical physical field is determined by the asymmetric potential $\phi = \frac{Ax}{r}$, where A is a positive constant and r is the magnitude of the position vector $\vec{r}$. Determine the vector $\vec{E}$ of the intensity of this field and prove that the divergence of this field $\vec{\nabla} \cdot \vec{E} = \frac{2\phi}{r^2}$.

$$\vec{E} = \frac{-A\,(y^2 + z^2), Axy, Axz}{r^3}, \quad \vec{\nabla} \cdot \vec{E} = \frac{2Ax}{(x^2 + y^2 + z^2)^{3/2}} = \frac{2Ax}{r^3}$$

5.62 A hypothetical centrally symmetrical physical field is determined by the potential $\phi = A\,\mathrm{e}^{-r}$, where A is a positive constant and r is the magnitude of the position vector $\vec{r}$. Determine the vector $\vec{E}$ of the intensity of this field and prove that the divergence of this field $\vec{\nabla} \cdot \vec{E} = A\,\mathrm{e}^{-r}\left(\frac{2}{r} - 1\right)$.

$$\vec{E} = A\mathrm{e}^{-r}\frac{\vec{r}}{r} = A\,\mathrm{e}^{-\sqrt{x^2+y^2+z^2}}\frac{(x, y, z)}{\sqrt{x^2 + y^2 + z^2}}, \vec{\nabla} \cdot \vec{E} = A\mathrm{e}^{-\sqrt{x^2+y^2+z^2}}\left(\frac{2}{\sqrt{x^2 + y^2 + z^2}} - 1\right)$$

5.63 A hypothetical centrally symmetrical physical field is determined by the potential $\phi = A^{-r}$, where A is a positive constant and r is the magnitude of the position vector $\vec{r}$. Determine the vector $\vec{E}$ of the intensity of this field and prove that the divergence of this field $\vec{\nabla} \cdot \vec{E} = A^{-r} \ln A\left(\frac{2}{r} - \ln A\right)$.

$$\vec{E} = A^{-r} \ln A\,\frac{\vec{r}}{r}, \quad \vec{\nabla} \cdot \vec{E} = A^{-\sqrt{x^2+y^2+z^2}} \ln A\left(\frac{2}{\sqrt{x^2 + y^2 + z^2}} - \ln A\right)$$

5.64 Use the Kronecker delta and Levi-Civita symbols to verify the vector identities from Examples 5.48-5.56 in the Einstein notation.

Using Equations (2.54) and (5.14)-(5.17).

Chapter 6

Line integral[1] [2]

6.1 Line integral of type I

The line (path) integral of type I is called the integral $\int_{\mathcal{C}} f \, \mathrm{d}s$, where (in $\mathbb{R}^3$) $f(x, y, z)$ is a smooth (smooth in parts[3]) scalar function along the curve $\mathcal{C}$, and $\mathrm{d}s$ is the length element of the curve: $\mathrm{d}s^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2$ (Pythagorean theorem in the differential form). If the curve $\mathcal{C}$ is *closed*, it is marked by the circle over the integration symbol, that is $\oint$. For example, if we set the x-coordinate as independent variable and $y(x)$, $z(x)$ as dependent variables, we can write

$$\int_{\mathcal{C}} f \, \mathrm{d}s = \int_{x_1}^{x_2} f(x, y, z) \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 + \left(\frac{\mathrm{d}z}{\mathrm{d}x}\right)^2} \, \mathrm{d}x. \tag{6.1}$$

If we find the appropriate parameter t, then the parameterized Equation (6.1) with functions $f(t) = f\,[x(t), y(t), z(t)]$, $s(t) = s\,[x(t), y(t), z(t)]$ will take the form

$$\int_{\mathcal{C}} f(t) \frac{\mathrm{d}s(t)}{\mathrm{d}t} \, \mathrm{d}t = \int_{t_1}^{t_2} f(t) \sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)^2 + \left(\frac{\mathrm{d}z}{\mathrm{d}t}\right)^2} \, \mathrm{d}t. \tag{6.2}$$

We can determine various geometric and physical characteristics of the given curve using the line integral of type I. If we set $f = 1$, the result will be the length of the curve $\mathcal{C}$. If we set $f = \tau$ (linear density of the curve), we get $\tau \, \mathrm{d}s = \mathrm{d}m$, that is the mass of the length element of the curve, the result of the integration will be the mass of the curve $\mathcal{C}$,

$$m = \int_{\mathcal{C}} \mathrm{d}m = \int_{\mathcal{C}} \tau \, \mathrm{d}s. \tag{6.3}$$

If we set, for example, $f = z\tau$, we get the so-called static moment S_z of the curve relative to the axis z. By dividing it by its mass, we get the z-coordinate of the centre of mass z_T of the curve $\mathcal{C}$ (similarly for other coordinate directions), thus

$$x_T = \frac{1}{m} \int_{\mathcal{C}} x \, \mathrm{d}m = \frac{1}{m} \int_{\mathcal{C}} x\tau \, \mathrm{d}s, \quad y_T = \frac{1}{m} \int_{\mathcal{C}} y \, \mathrm{d}m, \quad z_T = \frac{1}{m} \int_{\mathcal{C}} z \, \mathrm{d}m. \tag{6.4}$$

[1] We do not give the corresponding physical units in the results of the examples with geometric or physical quantities.

[2] Recommended literature for this chapter: Děmidovič (2003), Kvasnica (2004), Bartsch (2008), Rektorys (2009).

[3] The smooth curve in parts consists of a finite number of smooth curves. The same applies to surfaces, functions, etc.

If we set $f = r^2\tau$, where r is the distance of the general point of the curve from the selected line in space (from the axis o in general), we get the moment of inertia J_o of the curve $\mathcal{C}$ relative to this axis. Moments of inertia of the curve $\mathcal{C}$, for example, relative to the particular Cartesian coordinate axes, will then be

$$J_x = \int_{\mathcal{C}} (y^2 + z^2)\,\mathrm{d}m = \int_{\mathcal{C}} (y^2 + z^2)\,\tau\,\mathrm{d}s, \quad J_y = \int_{\mathcal{C}} (z^2 + x^2)\,\mathrm{d}m, \quad J_z = \int_{\mathcal{C}} (x^2 + y^2)\,\mathrm{d}m. \tag{6.5}$$

- **Examples:**

6.1 Calculate the length of the circle with the radius R in Cartesian coordinates and using appropriate parameterization.

$s = 2\pi R$

6.2 Calculate the length of the curve $s = \displaystyle\int_{\mathcal{C}} \left(x^2 + y^2\right) \mathrm{d}s$ where $\mathcal{C}$ is the curve with parameterization $x = a\sin t$, $y = a\cos t$, $t \in \langle 0, \pi\rangle$.

$s = \pi a^3$

6.3 Calculate the length of the curve $s = \displaystyle\int_{\mathcal{C}} \left(x^2 + y^2\right) \mathrm{d}s$, where $\mathcal{C}$ is the curve with parameterization $x = a(\cos t + t\sin t)$, $y = a(\sin t - t\cos t)$, $t \in \langle 0, 2\pi\rangle$.

$s = a^3\left(2\pi^2 + 4\pi^4\right)$

6.4 Calculate the length of one arc of the cycloid $x = a(t - \sin t)$, $y = a(1 - \cos t)$, $t \in \langle 0, 2\pi\rangle$.

$s = 8a$

6.5 Calculate the length of the section of the parabola $y = x^2$, bounded by the points $[-2, 4]$ and $[2, 4]$.

$s = 2\sqrt{17} + \ln\sqrt{4 + \sqrt{17}} \approx 9.2936$

6.6 How many times longer will be the actual trajectory s of a projectile motion (with the start and endpoint at the same level)

(a) with the maximum possible range D,

(b) if the starting (elevation) angle $\alpha = 30°$,

(c) if the elevation angle $\alpha = 60°$,

(d) if the elevation angle is such that the maximum trajectory height equals the range,

than the corresponding range? Prove that for $\alpha = \frac{\pi}{2}$, $\frac{s}{D} \to \infty$, and also for $\alpha = 0$, $\frac{s}{D} \to 1$.

$$s = \frac{1}{2}\left[\frac{1}{\cos\alpha} + \ln\left(\frac{1 + \sin\alpha}{\cos\alpha}\right)\cot\alpha\right] D$$

(a) $s = \left(\frac{1}{\sqrt{2}} + \ln\sqrt{1 + \sqrt{2}}\right) D \approx 1.15D$, (b) $s = \left(\frac{1}{\sqrt{3}} + \frac{\sqrt{3}\ln\sqrt{3}}{2}\right) D \approx 1.05D$,

(c) $s = \left(1 + \dfrac{\ln\sqrt{2+\sqrt{3}}}{\sqrt{3}}\right) D \approx 1.38D,$ (d) $s = \left(\dfrac{\sqrt{17}}{2} + \dfrac{\ln\sqrt{4+\sqrt{17}}}{4}\right) D \approx 2.32D$

6.7 By direct calculation in Cartesian coordinates and also by using appropriate parameterization, calculate the mass of the astroid $x^{2/3} + y^{2/3} = a^{2/3}$ with the linear density $\tau = x^{4/3} + y^{4/3}$ (see Figure 6.1). Parameterization of the astroid can be, for example: $x = a\cos^3 t$, $y = a\sin^3 t$ where t does not denote time but the angular parameter.

$m = 4a^{7/3}$

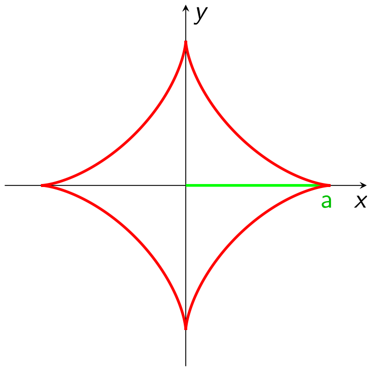

Figure 6.1: Astroid. The geometrical meaning of the constant a is highlighted by green color.

6.8 Using parameterization $x = a\cos t$, $y = a\sin t$, $z = bt$, calculate the mass of one "thread" of a cylindrical helix with the length (linear) density $\tau = \dfrac{z^2}{x^2+y^2}$.

$$m = \frac{8\pi^3}{3}\left(\frac{b}{a}\right)^2 \sqrt{a^2+b^2}$$

6.9 Using appropriate parameterization and using general coefficients, calculate the mass of one "thread" of a cylindrical helix with the length density $\tau = \dfrac{1}{x^2+y^2+z^2}$.

$$m = \frac{\sqrt{a^2+b^2}}{ab} \arctan\frac{2\pi b}{a}$$

6.10 Using the parameterization $x = at\cos t$, $y = at\sin t$, $z = bt$, calculate the mass of one "thread" of a conical helix with the length density $\tau = 2\sqrt{x^2+y^2} - z$.

$$m = \frac{2a-b}{3a^2}\left[\sqrt{(a^2+b^2+4\pi^2a^2)^3} - \sqrt{(a^2+b^2)^3}\right]$$

6.11 Prove the relation $s = \displaystyle\int_{\phi_1}^{\phi_2} \sqrt{f^2+\dot{f}^2}\,\mathrm{d}\phi$ where s is the length of a smooth curve, expressed in the polar coordinates as $r = f(\phi)$, and where $\dot{f} = \mathrm{d}f/\mathrm{d}\phi$.

using the transformation relations for polar coordinates and the line integral definition

6.12 Prove the relation $s = \int_{\theta_1}^{\theta_2} \sqrt{f^2 + \dot{g}^2 \left(f^2 \sin^2\theta + \dot{f}^2\right)}\, \mathrm{d}\theta$, where s is the length of a smooth curve, expressed in the spherical coordinates as $r = f(\phi)$, $\phi = g(\theta)$, and where $\dot{f} = \mathrm{d}f/\mathrm{d}\phi$, $\dot{g} = \mathrm{d}g/\mathrm{d}\theta$.

using the transformation relations for spherical coordinates and the line integral definition

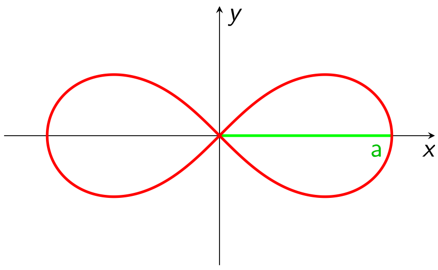

Figure 6.2: Lemniscate of Bernoulli. The geometrical meaning of the constant a is highlighted by green color.

6.13 Use the appropriate coordinate transformation to calculate the mass of the Lemniscate of Bernoulli (Figure 6.2) with the Cartesian equation $(x^2 + y^2)^2 = a^2(x^2 - y^2)$, with the length density $\tau = |y|$. Follow the principle introduced in Example 6.11 or use the transformation equation: $x = a\cos t/(1 + \sin^2 t)$, $y = a \sin t \cos t/(1 + \sin^2 t)$, where $t = \arcsin(\tan\phi)$ is angular parameter (always consider the correct integration limits for the selected parameter within the particular quadrant).

$m = 2a^2\left(2 - \sqrt{2}\right)$

6.14 By direct intersection in Cartesian coordinates as well as by the appropriate coordinate transformation, calculate the mass of an inhomogeneous curve with the linear density $\tau = x + y$, resulting from the intersection of surfaces $x^2 + y^2 + z^2 = a^2$, $x = y$, in the 1st octant.

$m = \sqrt{2}a^2$

6.15 Calculate the mass of the arc of an ellipse $\frac{x^2}{9} + \frac{y^2}{4} = 1$ in the 1st quadrant. The linear density $\tau = xy$.

$m = \frac{38}{5}$

6.16 Calculate the total length s and the mass m of the cardioid (Figure 6.3) with the polar equation $r = a\,(1 - \sin\phi)$, with the linear density $\tau = |x|$.

$s = 8a, \quad m = \frac{32\,a^2}{5}$

6.17 Specify the coordinates of the center of gravity T of a semicircle (passing through the 1st and 2nd quadrants) and a quarter circle (passing through the 1st quadrant), both with the length density $\tau = y$. Determine their moments of inertia if they rotate around their geometrical axes.

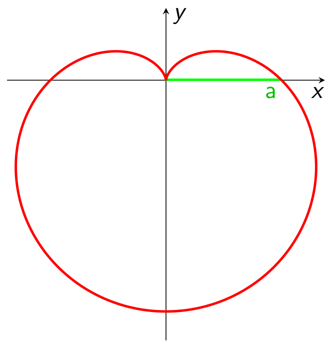

Figure 6.3: Cardioid. The geometrical meaning of the constant a is highlighted by green color.

$T = \left[0, \frac{\pi a}{4}\right]$, $T = \left[\frac{a}{2}, \frac{\pi a}{4}\right]$, $J = 2a^4$, $J = a^4$

6.18 Find the coordinates of the center of gravity T of one arc of the cycloid from Example 6.4 with the homogeneous length density $\tau(x, y) = 1$.

$T = \left[\pi a, \frac{4a}{3}\right]$

6.19 The wire has the circular shape, $x^2 + y^2 = a^2$. Calculate its moment of inertia J, if the wire rotates around its diameter. Its length density $\tau = |x| + |y|$.

$J = 4a^4$

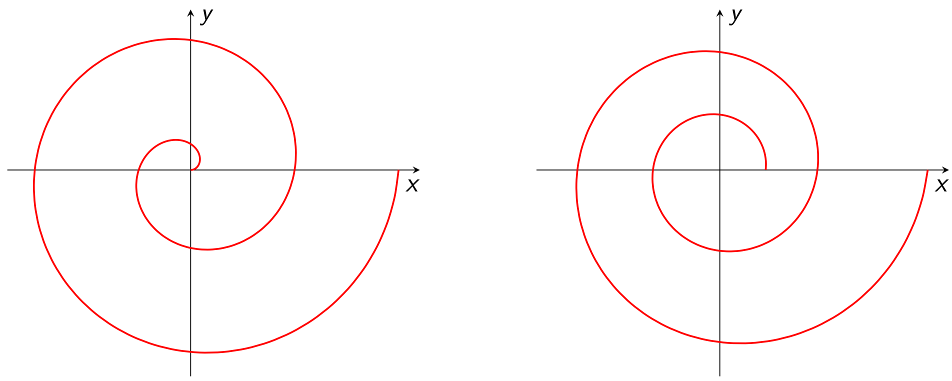

Figure 6.4: "Two threads" of a spiral with the polar angle $\phi \in \langle 0, 4\pi \rangle$. Left: Archimedean spiral, right: logarithmic spiral.

6.20 Calculate the length ℓ of "two threads" (see Figure 6.4) and the moment of inertia J of the following curves with the constant length density τ, rotating around the z-axis (that passes through the origin of the coordinates, perpendicular to the plane drawn):

(a) of the Archimedean spiral, given in polar coordinates by the prescription $r = \alpha\phi$, where α is a positive constant and the polar angle $\phi \in \langle 0, 4\pi \rangle$,

(b) of the logarithmic spiral, given in polar coordinates by the prescription $r = \alpha\, \mathrm{e}^{\beta\phi}$, where α and β are positive constants and the polar angle $\phi \in \langle 0, 4\pi \rangle$.

(c) how the case (b) changes if the origin of the spiral moves to the point $[0, 0]$?

Express the result also as a function of the mass of the curve $m = \tau\ell$ and the maximum distance of the curve from the axis of rotation $R = r_{\max}$.

(a) $\ell = \frac{\alpha}{2}\left[4\pi\sqrt{16\pi^2+1} + \ln\left(4\pi + \sqrt{16\pi^2+1}\right)\right]$,
$J = \frac{\tau\alpha^3}{8}\left[4\pi\left(32\pi^2+1\right)\sqrt{16\pi^2+1} - \ln\left(4\pi+\sqrt{16\pi^2+1}\right)\right] \approx 0,492\, mR^2$,

(b) $\ell = \frac{\alpha}{\beta}\sqrt{\beta^2+1}\left(\mathrm{e}^{4\pi\beta}-1\right)$, $J = \frac{\tau\alpha^3}{3\beta}\sqrt{\beta^2+1}\left(\mathrm{e}^{12\pi\beta}-1\right) = \left(1+\mathrm{e}^{-4\pi\beta}+\mathrm{e}^{-8\pi\beta}\right)\frac{mR^2}{3}$,

(c) $\ell = \frac{\alpha}{\beta}\sqrt{\beta^2+1}\,\mathrm{e}^{4\pi\beta}$, $J = \frac{\tau\alpha^3}{3\beta}\sqrt{\beta^2+1}\,\mathrm{e}^{12\pi\beta} = \frac{mR^2}{3}$

6.2 Line integral of type II

The line integral of type II is called the integral $\int_{\mathcal{C}} \vec{F}\cdot \mathrm{d}\vec{s}$ of a general vector field $\vec{F}(x, y, z)$ along a curve $\mathcal{C}$, where $\mathrm{d}\vec{s}$ is the tangent vector of the element $\mathrm{d}s$ of the given curve (see Section 6.1). The explicit notation of the type II integral in the Cartesian coordinate system (in $\mathbb{R}^3$) will take the form

$$\int_{x_1}^{x_2} F_x\,\mathrm{d}x + \int_{y_1}^{y_2} F_y\,\mathrm{d}y + \int_{z_1}^{z_2} F_z\,\mathrm{d}z, \tag{6.6}$$

where F_x, F_y, F_z are the particular components of the vector $\vec{F}$. Analogously to Equation (6.2), the parameterized line integral of type II will take the form

$$\int_{t_1}^{t_2}\left[F_x(t)\frac{\mathrm{d}x(t)}{\mathrm{d}t} + F_y(t)\frac{\mathrm{d}y(t)}{\mathrm{d}t} + F_z(t)\frac{\mathrm{d}z(t)}{\mathrm{d}t}\right]\mathrm{d}t. \tag{6.7}$$

A typical example of the line integral of type II is the calculation of the work performed as the integral of the force vector $\vec{F}$ along the oriented curve $\mathcal{C}$.

- **Examples:**

6.21 By direct calculation in Cartesian coordinates and using appropriate parameterization, calculate the line integral of type II, $\oint_{\mathcal{C}} x\,\mathrm{d}x + y\,\mathrm{d}y$, where $\mathcal{C}$ is the positively oriented circle with radius a.

0

6.22 By direct calculation in Cartesian coordinates and using appropriate parameterization, calculate the line integral of type II, $\int_{\mathcal{C}} x^2\,\mathrm{d}x + y^2\,\mathrm{d}y$, where a curve $\mathcal{C}$ is the positively oriented circle with radius a in the 1st and 2nd quadrant.

$-\frac{2a^3}{3}$

6.23 Calculate the line integral of type II, $\int_{\mathcal{C}} (x+1)\,\mathrm{d}y + y\,\mathrm{d}x$, by direct calculation in Cartesian coordinates and using appropriate parameterization, where the curve $\mathcal{C}$ is the positively oriented circle with radius a in the 1st quadrant.

a

6.24 Calculate the line integral of type II, $\int_{\mathcal{C}} x\,\mathrm{d}x + y\,\mathrm{d}y + (xz - y)\,\mathrm{d}z$, where the curve $\mathcal{C}$ is given parametrically, $x = t^2$, $y = 2t$, $z = 4t^3$, $t \in \langle 0, 1\rangle$.

$\frac{5}{2}$

6.25 Calculate the line integral of type II, $\oint_{\mathcal{C}} (2 - y)\,\mathrm{d}x + (1 + x)\,\mathrm{d}y$, where the curve $\mathcal{C}$ is the triangle circumference in the direction of the vertices $A = [0, 0]$, $B = [1, 1]$, and $C = [0, 2]$.

2

6.26 Calculate the work done by the force $\vec{F} = (y, z, x)$, acting along the positively oriented closed curve that is given by the intersection of the surfaces $z = xy$ and $x^2 + y^2 = 1$.

$W = -\pi$

6.27 Calculate the work done by the force $\vec{F} = \left(\frac{y}{x}, x\right)$, acting along the curve $xy = 1$ from point $\left[3, \frac{1}{3}\right]$ to point $\left[\frac{1}{2}, 2\right]$.

$W = \ln 6 - \frac{5}{3}$

6.28 Calculate the work done by the force $\vec{F} = (x - y, x + y)$, acting along the trajectory $y = x^2$, $x \in \langle 0, 2\rangle$.

$W = \frac{38}{3}$

6.29 Calculate the work done by the force $\vec{F} = (y, -x, z)$, acting along the circumference of a triangle, whose vertices are given by the intersections of the plane $3x + 2y + 6z = 6$ with the coordinate axes in the order x, y, z.

$W = -6$

6.30 Calculate the work done by the force $\vec{F} = (yz, xy, yz)$, acting along the circumference of a triangle, whose vertices are given by the intersections of the plane $2x + 3y + 4z = 12$ with the coordinate axes in the order x, y, z.

$W = 22$

6.31 Calculate the work done by the force $\vec{F} = (x^2 + y, 3y^2, 0)$, acting along the closed curve, consisting of the positively oriented semicircle of radius a in the 1st and 2nd quadrant, and from the abscissa (its diameter).

$W = -\frac{\pi a^2}{2}$

6.32 Calculate the work that would be done by the gravitational field when riding a water slide with exactly three turns if the gravitational field would be $\vec{F}_g = -mg(0, 0, z)$. The water slide can be simplified as a cylindrical helix, use the general coefficients.

$W = 18\pi^2 b^2 mg$

6.33 Calculate the work done by the force $\vec{F} = \left(x^2 + y, 3y^2, 0\right)$, which acts in the mathematically positive sense along a semicircle of the radius a. The center of the semicircle is at the origin of the coordinate system and passes through the 2nd and 3rd quadrants of the plane xy in the Cartesian coordinate system. Is this force field conservative?

$W = -\dfrac{\pi a^2}{2} - 2a^3$, the field is not conservative.

6.34 Calculate the work done by the force $\vec{F} = \left(x^2, -y, z\right)$, which acts in the mathematically positive sense along a curve given by the prescription $(x-1)^2 + y^2 = 1$, $z = 2$, from the initial point $[1, -1, 2]$ to the endpoint $[0, 0, 2]$. Is this force field conservative?

$W = \dfrac{1}{6}$, the field is conservative.

6.35 Calculate the work done by the force $\vec{F} = \left(2x^2 - y, x, z\right)$, which acts in the mathematically negative sense along one half of the thread of a cylindrical helix of the radius R, with the axis $(0, 0, z)$ that passes through the origin of the coordinate system. The starting point of the acting force has the coordinates $\left[0, R, \frac{\pi b}{2}\right]$, the endpoint has the coordinates $\left[0, -R, -\frac{\pi b}{2}\right]$. Is this force field conservative?

$W = -\pi R^2$, the field is not conservative.

6.36 Calculate the work done by the force $\vec{F} = (3x - y, x, z)$, which acts in the mathematically positive sense along one thread of a cylindrical helix of the radius R, with the axis $(0, 0, z)$ that passes through the origin of the coordinate system. The starting point of the acting force has the coordinates $\left[0, -R, -\frac{\pi b}{2}\right]$, the endpoint has the coordinates $\left[0, -R, \frac{3\pi b}{2}\right]$, the transformation equations of the helix are $x = R\cos t$, $y = R\sin t$, $z = bt$. Is this force field conservative?

$W = \pi\left(2R^2 + \pi b^2\right)$, the field is not conservative.

6.37 Calculate the work done by the force $\vec{F} = \left(x^3, y, z^3\right)$, which acts first in the mathematically positive sense along a curve given by the prescription $x^2 + (y-3)^2 = 4$, $z = 5$ from the point [0,1,5] to the point [2,3,5], and then along the straight line to the point [3,1,5]. Is this force field conservative?

$W = \dfrac{81}{4}$, the field is conservative.

6.38 Calculate the work done by the force $\vec{F}(x, y) = (x - y, x)$, which acts along the following closed curve: first along the straight line from the point $[1, 1]$ to the point $[1, 2]$, then along a quarter circle with the center at the point $[1, 1]$ in the mathematically negative sense to the point $[2, 1]$, and finally along the straight line back to the starting point. Is this force field conservative?

$W = -\dfrac{\pi}{2}$, the field is not conservative.

6.39 Calculate the work done by the force $\vec{F}(x,y) = (-y,x)$, which acts along the following closed curve: first along the straight line from the point $[0,0]$ to the point $[2,1]$, then along the straight line to the point $[2,2]$, and finally along the quarter circle with the center at the point $[2,0]$ in the mathematically positive sense back to the starting point. How does the work change if the applied force $\vec{F}(x,y) = (y,x)$?

$W = 2(\pi - 1)$, the work of the conservative force along the closed curve would be zero.

6.40 Calculate the work done by the force $\vec{F}(x,y) = (-y,x)$, which acts along the following closed curve: at first along the straight line from the point $[0,0]$ to the point $[1,0]$, then along the straight line to the point $[1,1]$, and finally along the quarter circle with center at the point $[1,0]$ in the mathematically positive sense back to the starting point. How does the work change if the applied force $\vec{F}(x,y) = (y,x)$?

$W = \dfrac{\pi}{2}$, conservative force - work is zero.

Chapter 7

Double and triple integral[1] [2]

To the integral of the function $f(x,y)$ of two variables x, y (double integral), which is continuous on two-dimensional area (domain) $\mathcal{S} = (a,b) \times (c,d)$ where $a \le x \le b$ and $c \le y \le d$, it is possible to apply the so-called *Fubini's theorem* to calculate n-dimensional integrals using n calculations of simple integrals,

$$\iint_{\mathcal{S}} f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_a^b \left[\int_c^d f(x,y)\,\mathrm{d}y\right] \mathrm{d}x = \int_c^d \left[\int_a^b f(x,y)\,\mathrm{d}x\right] \mathrm{d}y.^{3} \tag{7.1}$$

If $f(x,y) = g(x) \cdot h(y)$ applies in this case, Equation (7.1) is simplified into the expression

$$\iint_{\mathcal{S}} f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_a^b g(x)\,\mathrm{d}x \cdot \int_c^d h(y)\,\mathrm{d}y. \tag{7.2}$$

Now let's define another area $\mathcal{S}$ that is no longer rectangular and is bounded by the lines $x = a$, $x = b$ where $a \le x \le b$ and graphs of the functions $\phi_1(x)$, $\phi_2(x)$, continuous on the interval $\langle a,b\rangle$, i.e., $\mathcal{S} = (a,b) \times [\phi_1(x), \phi_2(x)]$. Integral of the function $f(x,y)$, continuous on the area $\mathcal{S}$, is then defined as

$$\iint_{\mathcal{S}} f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_a^b \left[\int_{\phi_1(x)}^{\phi_2(x)} f(x,y)\,\mathrm{d}y\right] \mathrm{d}x. \tag{7.3}$$

If in case (7.3) holds the inequality on the interval $\langle a,b\rangle$, or on its part $\phi_1(x) < y < \phi_2(x)$, then this area contributes positively to the overall integral while it is the negative contribution to the total integral otherwise [if $\phi_2(x) < y < \phi_1(x)$, see Figure 7.1]. This can also be compared with the integral of the function of a single variable in Figure 1.2, which can be regarded as a double integral of the Cartesian surface element $\mathrm{d}x\,\mathrm{d}y$ on the area $\mathcal{S} = (a,b) \times [0, f(x)]$.

Quite similar principles also apply in three-dimensional domains $\mathcal{V} = (a,b) \times (a,b) \times (e,f)$ where $a \le x \le b$, $c \le y \le d$, $e \le z \le f$. Here the integral of the continuous function $f(x,y,z)$ of three variables (triple integral) is defined as

$$\iiint_{\mathcal{V}} f(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_a^b \left\{\int_c^d \left[\int_e^f f(x,y,z)\,\mathrm{d}z\right] \mathrm{d}y\right\} \mathrm{d}x, \tag{7.4}$$

[1] We do not give the corresponding physical units in the results of the examples with geometric or physical quantities.

[2] Recommended literature for this chapter: Děmidovič (2003), Kvasnica (2004), Bartsch (2008), Rektorys (2009), Plch et al. (2012).

[3] Equation (7.1) does not apply if the integral of the absolute value of the function in the integrand diverges, that is, $\iint_{\mathcal{S}} |f(x,y)|\,\mathrm{d}x\,\mathrm{d}y \to \pm\infty$. Details of such cases go beyond the scope of this textbook, I recommend the literature to those interested.

where the ordering of the integration can be again interchanged analogously to Equation 7.1. If $f(x, y, z) = g(x) \cdot h(y) \cdot k(z)$ holds in this case, Equation (7.4) is simplified to the product

$$\iiint_{\mathcal{V}} f(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_a^b g(x)\,\mathrm{d}x \cdot \int_c^d h(y)\,\mathrm{d}y \cdot \int_e^f k(z)\,\mathrm{d}z. \tag{7.5}$$

Similarly to Equation (7.3), on a three-dimensional domain $\mathcal{V}$ which is not a rectangular body and is bounded by $\mathcal{V} = (a, b) \times [\phi_1(x), \phi_2(x)] \times [\psi_1(x, y), \psi_2(x, y)]$ where $a \le x \le b$ and where the functions $\phi_1(x)$, $\phi_2(x)$ are continuous on the interval $\langle a, b\rangle$ and the functions $\psi_1(x, y)$, $\psi_2(x, y)$ are continuous on the interval $\mathcal{S} = (a, b) \times [\phi_1(x), \phi_2(x)]$, the integral of a function $f(x, y, z)$ is continuous on an area $\mathcal{V}$ defined as

$$\iiint_{\mathcal{V}} f(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_a^b \left[\int_{\phi_1(x)}^{\phi_2(x)} \left(\int_{\psi_1(x,y)}^{\psi_2(x,y)} f(x, y, z)\,\mathrm{d}z\right)\mathrm{d}y\right]\mathrm{d}x. \tag{7.6}$$

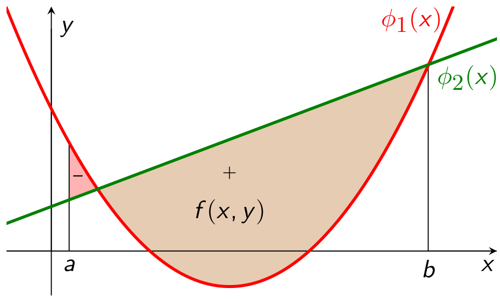

Figure 7.1: Graphical representation of the integration domain $\mathcal{S} = (a, b) \times [\phi_1(x), \phi_2(x)]$ of a continuous function $f(x, y)$, illustrating Equation (7.3). Graph of a function $\phi_1(x)$ is represented by the red curve; graph of a function $\phi_2(x)$ is drawn by the green curve. A sub-region that positively contributes to the overall integral (where $\phi_2(x) > \phi_1(x)$), is marked by ocher (brown) color, the sub-region that contributes negatively to the total integral size $\phi_2(x) < \phi_1(x)$ is drawn in red.

Transformation of the double integral coordinates can be defined (see Figure 7.2) using a unique map Φ, given by the transformation equations $x = \xi(u, v)$, $y = \eta(u, v)$. If $A \subset \mathbb{R}^2(x, y)$ and $B \subset \mathbb{R}^2(u, v)$ are closed surfaces (highlighted in Figure 7.2 by colored areas), and the function $f(x, y)$ is continuous on area $A = \Phi(B)$, then holds

$$\iint_A f(x, y)\,\mathrm{d}x\,\mathrm{d}y = \iint_B f\,[\xi(u, v), \eta(u, v)]\,J(u, v)\,\mathrm{d}u\,\mathrm{d}v. \tag{7.7}$$

The expression

$$J(u, v) = |\mathrm{det}| \begin{pmatrix} \dfrac{\partial x}{\partial u} & \dfrac{\partial x}{\partial v} \\ \dfrac{\partial y}{\partial u} & \dfrac{\partial y}{\partial v} \end{pmatrix}, \tag{7.8}$$

in Equation (7.7) is the *Jacobian* of two-dimensional coordinate transformation. The triple integral of a function $f(x, y, z)$ can be transformed using the bijection of Ψ with the transformation equations $x = \xi(u, v, w)$, $y = \eta(u, v, w)$, $z = \zeta(u, v, w)$ with similarly enclosed surfaces $A \subset \mathbb{R}^3(x, y, z)$ and $B \subset \mathbb{R}^3(u, v, w)$ where the function $f(x, y, z)$ is continuous on the area $A = \Phi(B)$. By analogy to Equation (7.7) then holds

$$\iiint_A f(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \iiint_B f\,[\xi(u, v, w), \eta(u, v, w), \zeta(u, v, w)]\,J(u, v, w)\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w. \tag{7.9}$$

The expression

$$J(u, v, w) = |\det| \begin{pmatrix} \dfrac{\partial x}{\partial u} & \dfrac{\partial x}{\partial v} & \dfrac{\partial x}{\partial w} \\ \dfrac{\partial y}{\partial u} & \dfrac{\partial y}{\partial v} & \dfrac{\partial y}{\partial w} \\ \dfrac{\partial z}{\partial u} & \dfrac{\partial z}{\partial v} & \dfrac{\partial z}{\partial w} \end{pmatrix} \tag{7.10}$$

in Equation (7.9) is the Jacobian of three-dimensional coordinate transformation. Significant and often used are the Jacobians of coordinate transformations from Cartesian to the cylindrical coordinate system where $(u, v, w) = (\rho, \phi, z)$, with the transformation equations $x = \rho \cos \phi$, $y = \rho \sin \phi$, $z = z$ where $J = \rho$, and from Cartesian to spherical coordinate system where $(u, v, w) = (r, \theta, \phi)$, with the transformation equations $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$ where $J = r^2 \sin \theta$ (compare with the surface and volume elements of particular coordinate systems derived in Chapter 4).

7.1 Surface integral of type I

Integral of a scalar function $\iint_S f(x, y, z)\, \mathrm{d}S$ is (analogously to the line integral of type I in Section 6.1) called the surface integral of type I which is continuous on smooth (smooth in parts) surface S where $\mathrm{d}S$ is the surface element of the surface S. For example, if we specify x and y as the independent variables and the function $z = \varphi(x, y)$ as the dependent variable, we can find tangent vectors $\vec{t}_x, \vec{t}_y$ to the surface S in the directions of the coordinate axes x, y as partial derivatives of all variables (see Section 5.1) with respect to the corresponding independent variables, i.e.,

$$\vec{t}_x = \left[\frac{\partial x}{\partial x}, \frac{\partial y}{\partial x}, \frac{\partial \varphi(x, y)}{\partial x}\right] = \left(1, 0, \frac{\partial \varphi}{\partial x}\right), \quad \vec{t}_y = \left[\frac{\partial x}{\partial y}, \frac{\partial y}{\partial y}, \frac{\partial \varphi(x, y)}{\partial y}\right] = \left(0, 1, \frac{\partial \varphi}{\partial y}\right). \tag{7.11}$$

We determine the normal vector $\vec{\nu}$ to the surface S (i.e., the vector perpendicular to the surface S) as the vector product of the tangent vectors $\vec{t}_x \times \vec{t}_y$ (whose order in the vector product depends on the desired orientation of the normal), whose magnitude (see Equation (2.1)) will be $\|\vec{\nu}\| = \|\vec{t}_x \times \vec{t}_y\|$, so

$$\vec{\nu} = \vec{t}_x \times \vec{t}_y = \left(-\frac{\partial \varphi}{\partial x}, -\frac{\partial \varphi}{\partial y}, 1\right), \quad \|\vec{\nu}\| = \|\vec{t}_x \times \vec{t}_y\| = \sqrt{1 + \left(\frac{\partial \varphi}{\partial x}\right)^2 + \left(\frac{\partial \varphi}{\partial y}\right)^2}. \tag{7.12}$$

The surface element itself is thus a vector oriented in the direction of the normal vector $\vec{\nu}$, where the area of the surface element is determined by the maximum possible length of the normal vector $\|\vec{\nu}\|_{\max}$, that is, of the one that is constructed as a vector product of two mutually perpendicular tangent vectors (in orthogonal coordinate systems, partial derivatives according to any two selected coordinate directions meet this requirement). Thus, in the selected Cartesian parameterization, we can write

$$\mathrm{d}\vec{S} = \vec{\nu}\, \mathrm{d}x\, \mathrm{d}y = \left(-\frac{\partial \varphi}{\partial x}, -\frac{\partial \varphi}{\partial y}, 1\right) \mathrm{d}x\, \mathrm{d}y, \quad \mathrm{d}S = \|\vec{\nu}\|\, \mathrm{d}x\, \mathrm{d}y = \sqrt{1 + \left(\frac{\partial \varphi}{\partial x}\right)^2 + \left(\frac{\partial \varphi}{\partial y}\right)^2}\, \mathrm{d}x\, \mathrm{d}y. \tag{7.13}$$

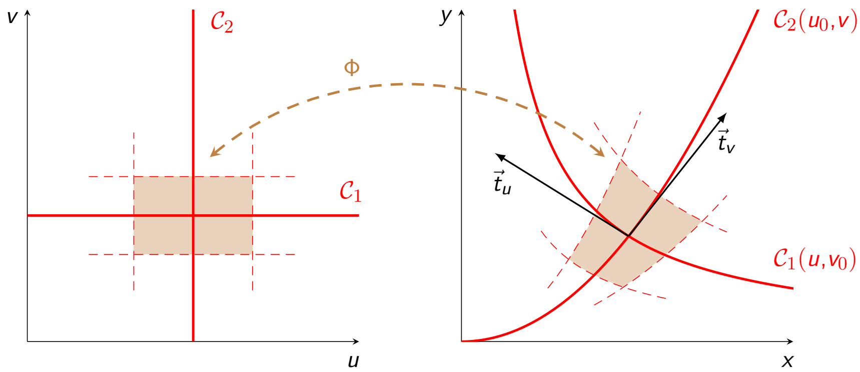

Figure 7.2: Scheme of transformation of general coordinates in $\mathbb{R}^2$ described by Equation (7.7) where Φ symbolizes the bijection. $\mathcal{C}_1$, $\mathcal{C}_2$ are the coordinates curves to which there applies $\mathcal{C}_1 : x = x(u, v_0), y = y(u, v_0)$, $\mathcal{C}_2 : x = x(u_0, v), y = y(u_0, v)$; the dashed lines enclosing the highlighted area can be expressed as $\mathcal{C}_1^+(u, v_0+\Delta v)$, $\mathcal{C}_1^-(u, v_0-\Delta v)$, $\mathcal{C}_2^+(u_0+\Delta u, v)$, $\mathcal{C}_2^-(u_0-\Delta u, v)$. We can determine the tangent vectors to the coordinate curves $\mathcal{C}_1, \mathcal{C}_2$ at the point $[u_0, v_0]$, as $\vec{t}_u\big|_{u_0,v_0} = \left(\frac{\partial x}{\partial u}, \frac{\partial y}{\partial u}\right)_{u_0,v_0}$, $\vec{t}_v\big|_{u_0,v_0} = \left(\frac{\partial x}{\partial v}, \frac{\partial y}{\partial v}\right)_{u_0,v_0}$.

Obviously, there applies $\mathrm{d}\vec{S} = \dfrac{\vec{\nu}}{\|\vec{\nu}\|}\,\mathrm{d}S = \vec{n}\,\mathrm{d}S$, where $\vec{n}$ is a normal unit vector. Explicit notation of the surface integral of type I in the orthonormal Cartesian basis on an area $\mathcal{S} = (a, b) \times [\phi_1(x), \phi_2(x)]$ and $z = \varphi(x, y)$ will be (compare Equations (7.1) and (7.3)):

$$\iint_S f(x, y, \varphi)\,\mathrm{d}S = \int_a^b \int_{\phi_1(x)}^{\phi_2(x)} f(x, y, \varphi)\sqrt{1 + \left(\frac{\partial \varphi}{\partial x}\right)^2 + \left(\frac{\partial \varphi}{\partial y}\right)^2}\,\mathrm{d}x\,\mathrm{d}y. \tag{7.14}$$

If we find appropriate parameters u, v (e.g., θ, ϕ on the spherical surface), we can parameterize the function f as well as the surface S using transformation equations $x = \xi(u, v)$, $y = \eta(u, v)$, $z = \zeta(u, v)$ (see Equation (7.9)). Tangent vectors $\vec{t}_u$, $\vec{t}_v$ to the given surface S in coordinate directions u, v (see Figure 5.1) are determined as partial derivatives of a function of the given surface (see Section 5.1) according to the corresponding directions, that is,

$$\vec{t}_u = \left(\frac{\partial \xi}{\partial u}, \frac{\partial \eta}{\partial u}, \frac{\partial \zeta}{\partial u}\right), \quad \vec{t}_v = \left(\frac{\partial \xi}{\partial v}, \frac{\partial \eta}{\partial v}, \frac{\partial \zeta}{\partial v}\right). \tag{7.15}$$

Normal vector $\vec{\nu}\,'$ (which is not identical to the vector $\vec{\nu}$ from Equation (7.12), it will have the same direction but different length) is determined again as a vector product of the two tangent vectors $\vec{\nu}\,' = \vec{t}_u \times \vec{t}_v$, whose magnitude $\|\vec{\nu}\,'\| = \|\vec{t}_u \times \vec{t}_v\|$. Analogously to Equation (7.13) we get:

$$\mathrm{d}\vec{S} = \vec{\nu}\,'\,\mathrm{d}u\,\mathrm{d}v, \quad \mathrm{d}S = \|\vec{\nu}\,'\|\,\mathrm{d}u\,\mathrm{d}v = \|\vec{t}_u \times \vec{t}_v\|\,\mathrm{d}u\,\mathrm{d}v. \tag{7.16}$$

Parametric expression of the surface integral of type I will have the explicit form

$$\int_{u_1}^{u_2}\int_{v_1}^{v_2} f(\xi, \eta, \zeta)\left\|\left(\frac{\partial \xi}{\partial u}, \frac{\partial \eta}{\partial u}, \frac{\partial \zeta}{\partial u}\right) \times \left(\frac{\partial \xi}{\partial v}, \frac{\partial \eta}{\partial v}, \frac{\partial \zeta}{\partial v}\right)\right\|\mathrm{d}u\,\mathrm{d}v. \tag{7.17}$$

Correlation between Equations (7.13) and (7.16) is given by Equation (7.7), which implies: $\vec{\nu}\,\mathrm{d}x\,\mathrm{d}y = \vec{\nu}\,'J(u, v)\,\mathrm{d}u\,\mathrm{d}v$ and simultaneously $\|\vec{\nu}\|\,\mathrm{d}x\,\mathrm{d}y = \|\vec{\nu}\,'\|J(u, v)\,\mathrm{d}u\,\mathrm{d}v$, where $J(u, v)$ is the Jacobian of the coordinate transformation given by Equation (7.8).

For example, for a spherical surface of radius R with center at the origin of the coordinate system, with a Cartesian equation $z(x,y) = \sqrt{R^2 - x^2 - y^2}$, with an outer normal, Equation (7.13) will take the form

$$\mathrm{d}\vec{S} = \left(\frac{x}{\sqrt{R^2 - x^2 - y^2}}, \frac{y}{\sqrt{R^2 - x^2 - y^2}}, 1 \right) \mathrm{d}x\,\mathrm{d}y, \quad \mathrm{d}S = \frac{R\,\mathrm{d}x\,\mathrm{d}y}{\sqrt{R^2 - x^2 - y^2}}, \tag{7.18}$$

by integrating it within the limits $x \in \langle -R, R\rangle$, $y \in \left\langle -\sqrt{R^2 - x^2}, \sqrt{R^2 - x^2} \right\rangle$ we get $S = 2\pi R^2$ which is the part of the sphere above $z = 0$. The parameterized Equation (7.16) will take the form

$$\mathrm{d}\vec{S} = \left(R^2 \sin^2\theta\cos\phi,\, R^2\sin^2\theta\sin\phi,\, R^2\sin\theta\cos\theta \right) \mathrm{d}\theta\,\mathrm{d}\phi, \quad \mathrm{d}S = R^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi, \tag{7.19}$$

by integrating it according to the variables $\theta \in \langle 0, \pi\rangle$ and $\phi \in \langle 0, 2\pi)$; we get $S = 4\pi R^2$. Since the Jacobian corresponding to Equation (7.8) will be $R^2 \sin\theta\cos\theta$ in this case, it is easy to see from Equations (7.18) and (7.19) that the relation $\|\vec{\nu}\|\,\mathrm{d}x\,\mathrm{d}y = \|\vec{\nu}\,'\| J(\theta,\phi)\,\mathrm{d}\theta\,\mathrm{d}\phi$ holds.

Using the surface integral of type I, some geometric and physical characteristics of a given surface can be determined: Setting $f = 1$ results in a total area of the surface S. Setting $f = \sigma$ (surface density), we get $\sigma\,\mathrm{d}S = \mathrm{d}m$, i.e., mass of the surface element S, its integration will result in the total mass m of the surface,

$$m = \iint_S \mathrm{d}m = \iint_S \sigma\,\mathrm{d}S. \tag{7.20}$$

If we set, for example, $f = z\sigma$, we get the so-called static moment S_z of a given surface relative to the z-axis, dividing it by its masses, we get z-coordinate of the center of mass z_T of the surface (similarly for other coordinate directions), i.e.,

$$x_T = \frac{1}{m}\iint_S x\,\mathrm{d}m = \frac{1}{m}\iint_S x\sigma\,\mathrm{d}S, \quad y_T = \frac{1}{m}\iint_S y\,\mathrm{d}m, \quad z_T = \frac{1}{m}\iint_S z\,\mathrm{d}m. \tag{7.21}$$

If we set $f = r^2\sigma$ where r is the distance of a general point of the surface from a selected line in space (axis o), we get the moment of inertia J_o of that surface with respect to this axis. Moments of inertia of the surface S, for example, relative to individual Cartesian coordinate axes will then be

$$J_x = \iint_S (y^2+z^2)\,\mathrm{d}m = \iint_S (y^2+z^2)\,\sigma\,\mathrm{d}S,\ J_y = \iint_S (z^2+x^2)\,\mathrm{d}m,\ J_z = \iint_S (x^2+y^2)\,\mathrm{d}m. \tag{7.22}$$

- **Examples:**

Calculate the area of the surface $S \in \mathbb{R}^2$ bounded by the following curves in Cartesian coordinates and also using an appropriate parameterization:

7.1 $y = x^2,\ y = \mathrm{e}x^2,\ y = \dfrac{1}{x},\ y = \dfrac{4}{x}$ 1

7.2 $y = x^2,\ y = 16\,x^2,\ y = \dfrac{2\sqrt[3]{2}}{x^2},\ y = \dfrac{16}{x^2}$ 8

7.3 $y = x^3,\ y = \dfrac{x^3}{3},\ y = \dfrac{1}{x},\ y = \dfrac{\mathrm{e}}{x}$ $\qquad \dfrac{(\mathrm{e}-1)\ln 3}{4}$

7.4 $y = 1,\ y = \mathrm{e},\ y = \mathrm{e}^{0.2x},\ y = \mathrm{e}^{0.4x}$ $\qquad 2.5$

7.5 Calculate the type I surface integral $\displaystyle\iint_S xyz\,\mathrm{d}S$, where S is the Cartesian coordinate surface S_z (see Chapter 4), $z = 3,\ x \in \langle 0, 1\rangle,\ y \in \langle 2, 3\rangle$.
$\dfrac{15}{4}$

7.6 Calculate the type I surface integral $\displaystyle\iint_S \mathrm{d}S$, where S is the cylindrical coordinate surface $S_\rho,\ \rho = 2,\ z \in \langle 0, 5\rangle$.
20π

7.7 Calculate the type I surface integral $\displaystyle\iint_S (x-y)\,\mathrm{d}S$, where S is the spherical coordinate surface $S_\phi,\ \phi = \dfrac{\pi}{4},\ r \le 2$.
0

Calculate the surface integrals of type I in Cartesian coordinates and using appropriate parameterization:

7.8 $\displaystyle\iint_S x^2 z\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 + z^2 = R^2,\ z \ge 0\big\}$. $\qquad \dfrac{\pi R^5}{4}$

7.9 $\displaystyle\iint_S \sqrt{2}\,x^2 z\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 - z^2 = 0,\ z \in \langle 0, H\rangle\big\}$. $\qquad \dfrac{2\pi R^5}{5},\ R = H$

7.10 $\displaystyle\iint_S \big(x^2 + y^2\big)\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 + z^2 = R^2,\ z \ge 0\big\}$. $\qquad \dfrac{4}{3}\pi R^4$

7.11 $\displaystyle\iint_S x^2 y^2\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 + z^2 = R^2,\ z \ge 0\big\}$. $\qquad \dfrac{2}{15}\pi R^6$

7.12 $\displaystyle\iint_S x^2 z^2\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 + z^2 = R^2,\ z \ge 0\big\}$. $\qquad \dfrac{2}{15}\pi R^6$

7.13 $\displaystyle\iint_S y^2\,\mathrm{d}S$, where $S = \left\{z = H - \dfrac{H}{R}\sqrt{x^2 + y^2},\ z \in \langle 0, H\rangle\right\}$. $\qquad \dfrac{\pi R^3}{4}\sqrt{R^2 + H^2}$

7.14 $\displaystyle\iint_S z\,\mathrm{d}S$, where $S = \{x + y + z = 1,\ x \in \langle 0, 1\rangle,\ y \in \langle 0,\ 1 - x\rangle\}$. $\qquad \dfrac{1}{2\sqrt{3}}$

7.15 $\displaystyle\iint_S \dfrac{1}{x^2 + y^2 + z}\,\mathrm{d}S$, where $S = \big\{x^2 + y^2 + z = H,\ z \ge 0\big\}$. $\qquad \dfrac{\pi}{6H}\left[(1 + 4H)^{\frac{3}{2}} - 1\right]$

Calculate the surface area using appropriate parameterization or in Cartesian coordinates $S \in \mathbb{R}^3$ alternatively:

7.16 $S=\{x^2+y^2+z^2=R^2,\ x^2+y^2 \le a^2,\ z \ge 0,\ a \le R\}$ (spherical cap) $2\pi R\left[R-\sqrt{R^2-a^2}\right]$

7.17 $S = \{x^2 + z^2 = a^2,\ z \ge 0\}$

(a) $|x| \le |y| \le a$ $2a^2(\pi - 2)$

(b) $|x| > |y|$ $4a^2$

7.18 $S = \{x^2 + z^2 = a^2,\ x^2 + y^2 \le a^2,\ z \ge 0\}$ $4a^2$

7.19 A spatial curve, given by intersection of the spherical surface $S = \{x^2 + y^2 + z^2 = R^2\}$ and the cylindrical surface $S' = \{(x-a)^2 + y^2 = a^2\}$ where $a = R/2$, delimits a closed sub-surface within the surface of the sphere (the so-called Viviani window). Calculate the area of this sub-surface.

$2R^2(\pi - 2)$

7.20 Calculate the area of a part of the Earth's surface bounded in one direction by two adjacent meridians (for example, 15 and 16) and in the other direction by two adjacent parallel lines:

(a) 0th (equator) and 1st,

(b) 49th a 50th,

(c) 89th a 90th (pole).

Give the areas of the surfaces in km^2. Regard the radius of the Earth $R = 6371\,\mathrm{km}$ as constant.

(a) approx. $12\,364\,\mathrm{km}^2$

(b) approx. $8\,030\,\mathrm{km}^2$

(c) approx. $108\,\mathrm{km}^2$

7.21 Calculate the mass of the spherical cap $S = \left\{x^2 + y^2 + z^2 = R^2,\ x^2 + y^2 \le \frac{R^2}{4},\ z \ge 0\right\}$ with the surface density $\sigma(x, y, z) = |x| + |y| + |z|$.

$R^3\left(\frac{11}{12}\pi + \sqrt{3}\right)$

7.22 Calculate the position of the center of mass of the surface $S = \{x^2 + y^2 + z^2 = R^2,\ z \ge 0\}$ whose surface density σ is given by the function $\sigma = x^2 + z^2$.

$x_T = 0,\ y_T = 0,\ z_T = \frac{9R}{16}$

7.23 Calculate the position of the center of mass of the surface $S = \{x^2 + y^2 - z^2 = 0,\ z \in \langle 0, H\rangle\}$ whose surface density σ is given by the function $\sigma = x^2 + z^2$.

$x_T = 0,\ y_T = 0,\ z_T = \frac{4H}{5}$

7.24 Spiral surface with a constant surface density σ is given parametrically in the form $x = u\cos v$, $y = u\sin v$, $z = v$, $u \in \langle 0, a\rangle$, $v \in \langle 0, 2\pi\rangle$. Calculate:

(a) mass of the surface,

(b) position of its center of mass,

(c) moment of inertia with respect to its geometrical axis.

(a) $\pi\sigma\left[a\sqrt{1+a^2} + \ln\left(a + \sqrt{1+a^2}\right)\right]$

(b) $(0, 0, \pi)$

(c) $\dfrac{\pi\sigma}{4}\left[\left(2a^3 + a\right)\sqrt{1+a^2} - \ln\left(a + \sqrt{1+a^2}\right)\right]$

7.25 Calculate the following parameters of the surface from Example 7.13 if its surface density $\sigma = x^2 z$:

(a) mass of the surface,

(b) position of its center of mass,

(c) moment of inertia with respect to its geometrical axis.

(a) $\dfrac{\pi}{20} H R^3 \sqrt{R^2 + H^2}$

(b) $z_T = \dfrac{H}{3}$

(c) $\dfrac{\pi}{42} H R^5 \sqrt{R^2 + H^2}$

7.26 Calculate the following parameters of the surface from Example 7.14 if its surface density $\sigma = x^2 + y^2$:

(a) mass of the surface,

(b) position of its center of mass.

(a) $\dfrac{1}{2\sqrt{3}}$

(b) $\left(\dfrac{2}{5}, \dfrac{2}{5}, \dfrac{1}{5}\right)$

7.27 Calculate the mass of the surface from Example 7.15 if its surface density $\sigma = x^2$.

$$\frac{\pi}{16}\left[\left(4R^2 + 1\right)^{\frac{3}{2}}\left(\frac{4}{5}R^2 - \frac{2}{15}\right) + \frac{2}{15}\right]$$

7.28 Calculate the total pressure force exerted by a liquid with a constant density ρ on all walls of the closed container formed by the surface from Example 7.13 and the corresponding base (neglecting atmospheric pressure).

$$\pi\rho g H\left(\frac{2}{3}R\sqrt{R^2 + H^2} + R^2\right)$$

7.29 Calculate the total pressure force exerted by a liquid with a constant density ρ on all walls of the closed container formed by the surface from Example 7.15 and the corresponding base (neglecting atmospheric pressure).

$\frac{\pi}{8}\rho g\left[\left(4R^2+1\right)^{\frac{3}{2}}\left(\frac{4}{5}R^2-\frac{2}{15}\right)+\frac{2}{15}\right]+\pi\rho g R^4$

7.30 The cone-shaped water tank, standing "tip" down with the radius of a top horizontal base $R = 3\,\mathrm{m}$, and the height $H = 4\,\mathrm{m}$ is designed to withstand a total pressure force $10^6\,\mathrm{N}$. Is it designed sufficiently, insufficiently, or is it approximately at the structural limit? Consider the values of the constants $\rho = 1000\,\mathrm{kg\,m^{-3}}$, $g = 9.81\,\mathrm{m\,s^{-2}}$. Neglect the effects of atmospheric pressure.

$F_p \approx 6,3 \times 10^5\,\mathrm{N}$. The shell of the tank is designed sufficiently.

7.31 The cone-shaped water tank, standing "tip" down, is filled with a special liquid in which the pressure increases with depth as $p = \rho_0 g h^2$ where ρ_0 is the density of the liquid at the surface, and h is the depth of a given point in the liquid. The radius of the top horizontal base surface of the tank $R = 0.5\,\mathrm{m}$ and its height $H = 1\,\mathrm{m}$. Determine the pressure force that the tank must withstand. Consider the values of the constants $\rho_0 = 1000\,\mathrm{kg\,m^{-3}}$, $g = 9.81\,\mathrm{m\,s^{-2}}$. Neglect the effects of atmospheric pressure.

$F_p \approx 3000\,\mathrm{N}$.

7.32 The shell of a spherical water tank with radius $R = 2\,\mathrm{m}$ is designed to withstand a total pressure force of $10^6\,\mathrm{N}$. Is it designed sufficiently, insufficiently, or is it approximately at the structural limit? Consider the values of the constants $\rho = 1000\,\mathrm{kg\,m^{-3}}$, $g = 9.81\,\mathrm{m\,s^{-2}}$. Neglect the effects of atmospheric pressure.

$F_p \approx 10^6\,\mathrm{N}$. The shell of the tank is designed approximately at the structural limit.

7.33 A bowl in the shape of a hemisphere with a radius $R = 1\,\mathrm{m}$ is filled with a special liquid in which the pressure increases with depth as $p = \rho_0 g h^{\frac{3}{2}}$ where ρ_0 is the density of the liquid at the surface, and h is the depth of a given point in the liquid. Determine the pressure force that the tank must withstand. Consider the values of the constants $\rho_0 = 1000\,\mathrm{kg\,m^{-3}}$, $g = 9.81\,\mathrm{m\,s^{-2}}$. Neglect the effects of atmospheric pressure.

$F_p \approx 25\,000\,\mathrm{N}$.

7.2 Surface integral of type II

Surface integral of type II is called the integral $\iint_S \vec{F}\cdot \mathrm{d}\vec{S} = \iint_S \vec{F}\cdot\vec{n}\,\mathrm{d}S$ of a general vector field $\vec{F}(x,y,z)$ defined by parts on a smooth surface S whose orientation is determined by the normal unit vector $\vec{n} = (n_x, n_y, n_z)$. The explicit notation of the surface integral of type II on a smooth by parts surface, formed by the coordinate surfaces of the Cartesian system, will have the form

$$\int_y\int_z F_x\,\mathrm{d}y\,\mathrm{d}z\Big|_{x=\text{const.}} + \int_z\int_x F_y\,\mathrm{d}z\,\mathrm{d}x\Big|_{y=\text{const.}} + \int_x\int_y F_z\,\mathrm{d}x\,\mathrm{d}y\Big|_{z=\text{const.}}, \tag{7.23}$$

where F_x, F_y, F_z are particular components of the vector $\vec{F}$. Analogously to Equation (7.17), a parameterized surface integral of type II where $x = \xi(u,v)$, $y = \eta(u,v)$, $z = \zeta(u,v)$ will take the form

$$\int_{u_1}^{u_2}\int_{v_1}^{v_2}\left[F_x(\xi,\eta,\zeta)\,\det\begin{pmatrix}\dfrac{\partial\eta}{\partial u} & \dfrac{\partial\zeta}{\partial u}\\ \dfrac{\partial\eta}{\partial v} & \dfrac{\partial\zeta}{\partial v}\end{pmatrix} + F_y(\xi,\eta,\zeta)\,\det\begin{pmatrix}\dfrac{\partial\zeta}{\partial u} & \dfrac{\partial\xi}{\partial u}\\ \dfrac{\partial\zeta}{\partial v} & \dfrac{\partial\xi}{\partial v}\end{pmatrix} + \right.$$
$$\left. + F_z(\xi,\eta,\zeta)\,\det\begin{pmatrix}\dfrac{\partial\xi}{\partial u} & \dfrac{\partial\eta}{\partial u}\\ \dfrac{\partial\xi}{\partial v} & \dfrac{\partial\eta}{\partial v}\end{pmatrix}\right]\mathrm{d}u\,\mathrm{d}v\,. \tag{7.24}$$

The order of the parameters u and v in vector products is determined by the desired orientation of the surface normal. A typical physical application of type II surface integral is the computation of the flux Φ of a vector field $\vec{F}$ through a given surface $\vec{S}$.

- **Examples:**

7.34 Calculate the flux of the vector field $\vec{F} = (1,1,1)$ through the Cartesian coordinate surface S_z (see Chapter 4) where $z = 3$, $x \in \langle 0,1\rangle$, and $y \in \langle 2,3\rangle$ in the direction of the positively oriented normal of this surface.

$\Phi_F = 1$

7.35 Calculate the flux of the vector field $\vec{F} = (x, xy, xz)$ through the Cartesian coordinate surface S_x where $x = 5$, $y \in \langle 0,5\rangle$, and $z \in \langle 0,5\rangle$ in direction of the negatively oriented normal of this surface.

$\Phi_F = 125$

7.36 Calculate the flux of the vector field $\vec{F} = (x,2,3)$ through the cylindrical coordinate surface S_ρ where $\rho = 2$ and $z \in \langle 0,5\rangle$ in the direction of the outer normal of this surface.

$\Phi_F = 20\pi$

7.37 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through the closed surface $S = \{(x,y,z)\,|\,x \in \langle A,\,2A\rangle,\, y \in \langle B,\,2B\rangle,\, z \in \langle C,\,2C\rangle\}$.

$\Phi_F = 3ABC(A+B+C)$

7.38 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through the closed surface $S = \left\{(x,y,z)\,|\,x^2+y^2 = R^2,\, z \in \langle 0,\,H\rangle\right\}$.

$\Phi_F = \pi R^2 H^2$

7.39 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = (x^3, y^3, z^3)$ through the surface given by the prescription $S = \left\{(x,y,z)\,|\,x^2+y^2+z^2 = R^2\right\}$.

$\Phi_F = \dfrac{12}{5}\pi R^5$

7.40 The force field $\vec{F} = (x^3 - x^2,\, y^3 - y^2,\, z^3 - z^2)$ is given. Using the surface integral of type II, calculate its flux through the surface of the body $\mathcal{V} = \left\{(x,y,z)\,|\,x,y,z \in \langle 0,R\rangle,\, x^2+y^2+z^2 \le R^2\right\}$.

$\Phi_F = \dfrac{3\pi R^4}{40}\,(4R - 5)$

7.41 Calculate the flux of the vector field $\vec{F} = (z^2, x^2, y^2)$ through a circular surface with radius R with center at the point $x, y, z = [A, B, C]$ lying in the plane $z = C$ in the direction of its positively oriented normal.

$\dfrac{\pi R^4}{4} + \pi B^2 R^2$

7.42 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through a closed surface formed by the surface of the body from Example 7.15.

$\Phi_F = \dfrac{\pi R^2 H^2}{3}$

7.43 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = \left(x^3 - y^3, x^3 + y^3, z\right)$ through a surface of the body $\mathcal{V} = \left\{(x, y, z)\,|\, z \in \langle 0,\ H\rangle,\ x^2 + y^2 \leq \dfrac{R^2}{H^2}(H - z)^2\right\}$.

$\Phi_F = \dfrac{\pi R^2 H}{30}\left(9R^2 + 10\right)$

7.44 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = (x, y, z)$ through a surface of the body from Example 8.42. Why is the resulting value three times the result of the Example mentioned above?

$\Phi_F = \dfrac{3\pi^2 a^3}{4}$

7.45 Using the surface integral of type II, calculate the flux of the vector field $\vec{F} = (x^3, y^3, z^3)$ through a closed surface formed by the surface of the body from Example 8.42.

$\Phi_F = \dfrac{27}{64}\pi^2 a^5 = \left(\dfrac{3}{4}\right)^3 \pi^2 a^5$

7.46 Calculate the flux of the vector field $\vec{F} = (y, z, x)$ through a planar rectangular surface with vertices at the points $[1, 0, 0]$, $[3, 0, 1]$, $[3, 2, 1]$, $[1, 2, 0]$ in the direction of normal $\vec{\nu}$ of this surface whose component ν_x is positively oriented.

-6

7.47 Calculate the flux of the vector field $\vec{F} = (3, z, y)$ through a planar rectangular surface with vertices at the points $[0, 0, 1]$, $[0, 1, 3]$, $[2, 1, 3]$, $[2, 0, 1]$ in the direction of a normal $\vec{\nu}$ of this surface whose component ν_y is positively oriented.

7

7.48 Calculate the flux of the vector field $\vec{F} = (3, z, y)$ through a planar rectangular surface with vertices at the points $[0, 0, 1]$, $[0, 2, 2]$, $[5, 2, 2]$, $[5, 0, 1]$ in the direction of normal $\vec{\nu}$ of this surface whose component ν_y is positively oriented.

$-\dfrac{5}{2}$

7.49 Calculate the flux of the vector field $\vec{F} = (y, z, x)$ through a planar trapezoid surface with vertices in the points $[1, 1, 1]$, $[1, 3, 3]$, $[2, 4, 5]$, $[2, 1, 2]$ in the direction of a normal $\vec{\nu}$ of this surface whose component ν_y is positively oriented.

$\frac{53}{6}$

7.50 Calculate the flux of the vector field $\vec{F} = (x, z, y)$ through a planar triangular surface with vertices at the points $[3, 0, 2]$, $[1, 2, 0]$, $[0, 0, 7]$ in the direction of normal $\vec{\nu}$ of this surface whose component ν_y is positively oriented.

$\frac{98}{3}$

7.3 Volume integral

The volume integral is a triple integral of a scalar function $f(x, y, z)$ over a domain (body) $\mathcal{T} \in \mathbb{R}^3$ with volume V:

$$\iiint_V f(x, y, z)\,\mathrm{d}V = \iiint_V f(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z. \tag{7.25}$$

Using the volume integral it is possible to determine specific geometrical and physical characteristics of bodies: If we set $f = 1$, the result will be the volume V of the body $\mathcal{T}$. If we set $f = \rho$ (bulk mass density), we get $\rho\,\mathrm{d}V = \mathrm{d}m$ hence the mass of the body element $\mathcal{T}$, and the integration will result in total mass M of the body,

$$M = \iiint_{\mathcal{T}} \mathrm{d}m = \iiint_V \rho\,\mathrm{d}V. \tag{7.26}$$

If we set, for example, $f = z\rho$, we get the so-called static moment S_z of the body with respect to the axis z, by dividing it by its mass, we get the z-coordinate of the center of mass z_T of the body (similarly for other coordinate directions), that is,

$$x_T = \frac{1}{M}\iiint_{\mathcal{T}} x\,\mathrm{d}m = \frac{1}{M}\iiint_V x\rho\,\mathrm{d}V, \quad y_T = \frac{1}{M}\iiint_{\mathcal{T}} y\,\mathrm{d}m, \quad z_T = \frac{1}{M}\iiint_{\mathcal{T}} z\,\mathrm{d}m. \tag{7.27}$$

If we set $f = r^2\rho$, where r is the distance of the general point of the body from the selected line in space (from the general axis o), we get a moment of inertia J_o of the body $\mathcal{T}$ with respect to this axis. The moments of inertia of the body $\mathcal{T}$, for example, relative to particular Cartesian coordinate axes, will then be

$$J_x = \iiint_{\mathcal{T}} (y^2 + z^2)\,\mathrm{d}m = \iiint_V (y^2 + z^2)\,\rho\,\mathrm{d}V,\ J_y = \iiint_{\mathcal{T}} (z^2 + x^2)\,\mathrm{d}m,\ J_z = \iiint_{\mathcal{T}} (x^2 + y^2)\,\mathrm{d}m. \tag{7.28}$$

Examples that cover the problematics of the volume integral are part of the following Section 7.4.

7.4 Geometric and physical characteristics of structures

- **Calculate the volume:**

7.51 of an ellipsoid with half-axes a, b, c, $V = \frac{4}{3}\pi abc$

7.52 of the cone with base radius R and height H, $V = \frac{\pi R^2 H}{3}$

7.53 of a body $\mathcal{A} = \{(x,y,z) \,|\, z \in \langle 0,\, H - x^2 - y^2\rangle\}$ where $H = R^2$, $V = \frac{\pi R^2 H}{2}$

7.54 of a body $\mathcal{A} = \{(x,y,z) \,|\, z \in \langle 0,\, H - x^2 - y^2\rangle\}$, $x^2 + y^2 \leq R^2$, $H > R^2$, $V = \pi R^2 \left(H - \frac{R^2}{2}\right)$

7.55 of an annuloid (toroid) with torus radius R and tube radius a,[1] $V = 2\pi^2 R a^2$

7.56 of a body $\mathcal{A} = \left\{(x,y,z) \,|\, z \in \left\langle \sqrt{\frac{x^2+y^2}{3}},\, \sqrt{R^2 - x^2 - y^2}\right\rangle\right\}$, $V = \frac{\pi R^3}{3}$

7.57 of a body $\mathcal{A} = \left\{(x,y,z) \,|\, z \in \left\langle \frac{R}{2},\, \sqrt{R^2 - x^2 - y^2}\right\rangle\right\}$, $V = \frac{5}{24}\pi R^3$

7.58 of a body $\mathcal{A}$ whose surface is created by rotation of the astroid from Example 6.7 around the axis y,

$V = \frac{32}{105}\pi a^3$

7.59 of a body $\mathcal{A}$ whose surface is created by rotation of the cardioid from Example 6.16 around the axis y.

$V = \frac{8}{3}\pi a^3$

- **Calculate the surface area:**

7.60 of a spherical shell with radius R, $S = 4\pi R^2$

7.61 of a cone shell with the cone base radius R and height H, $S = \pi R\sqrt{R^2 + H^2}$

7.62 of a shell of the body from Example 7.53, $S = \frac{\pi}{6}\left[(1 + 4R^2)^{\frac{3}{2}} - 1\right]$

7.63 of an entire surface of the body from Example 7.54,

$S = \frac{\pi}{6}\left[(1 + 4R^2)^{\frac{3}{2}} - 1\right] + 2\pi R(H - R^2) + \pi R^2$

7.64 of a shell of the body from Example 7.56, $S = \left(\frac{\sqrt{3}}{2} + 1\right)\pi R^2$

[1] For a detailed description of the torus, see Section B.6 in Appendix B.

7.65 of the entire surface of the body from Example 7.57, $S = \frac{7}{4}\pi R^2$

7.66 of a torus surface with the torus axis radius R and tube radius a,[1]

$S = 4\pi^2 Ra$

7.67 bounded by the astroid from Example 6.7, $S = \frac{3}{8}\pi a^2$

7.68 that is created by rotation of the astroid from Example 6.7 around the axis y, $S = \frac{12}{5}\pi a^2$

7.69 bounded by the cardioid from Example 6.16, $S = \frac{3}{2}\pi a^2$

7.70 that is created by rotation of the cardioid from Example 6.16 around the axis y, $S = \frac{32}{5}\pi a^2$

7.71 of a hyperbolic paraboloid given by the prescription $z = x^2 - y^2$, $x^2 + y^2 \leq 4$,

$S = \frac{\pi}{6}\left(17^{\frac{3}{2}} - 1\right) \approx 36.18$

7.72 of a hyperbolic paraboloid given by the prescription $z = xy$, $x^2 + y^2 \leq 4$. What would be the radius ρ of the cylinder by whose shell is the hyperbolic paraboloid bounded, to be its area the same as in Example 7.71 ?

$S = \frac{2\pi}{3}\left(5^{\frac{3}{2}} - 1\right) \approx 21.32$, $\rho = \left[\left(\frac{17^{\frac{3}{2}} + 3}{4}\right)^{\frac{2}{3}} - 1\right]^{\frac{1}{2}} \approx 2.44$

- **Calculate the position of the center of mass using an appropriately selected coordinate system:**

7.73 of a homogeneous hemisphere with a radius R, $z_T = \frac{3}{8}R$

7.74 of a homogeneous cone with the base radius R and height H, $z_T = \frac{H}{4}$

7.75 of a homogeneous symmetric pyramid with base edge A and height H,

$z_T = \frac{H}{4}$

7.76 of the homogeneous body from Example 7.53, $z_T = \frac{H}{3}$

7.77 of the homogeneous body from Example 7.54, $z_T = \frac{3H^2 - 3HR^2 + R^4}{3\,(2H - R^2)}$

7.78 of the homogeneous body from Example 7.56, $z_T = \frac{9}{16}R$

7.79 of the homogeneous surface from Example 7.70 and the homogeneous body from Example 7.59,

$$y_T = -\frac{25}{32}\,a, \quad y_T = -\frac{4}{5}\,a$$

7.80 of a homogeneous body bounded from the “top” by the surface $x^2 + y^2 + z^2 = R^2$ and from the “bottom” by the surface $z = \sqrt{x^2 + y^2}$,

$$z_T = \frac{3R}{8\,(2 - \sqrt{2})} \approx 0.64\,R$$

7.81 of the body from Example 7.57, $z_T = \dfrac{27}{40}R$

7.82 of half of a homogeneous ellipsoid with half-axes a, b, c, with the base plane delimited by half-axes a, b.

$$z_T = \frac{3}{8}c$$

- **Calculate the moment of inertia with respect to the axis of symmetry:**

7.83 of a homogeneous sphere of mass M and radius R, $J = \dfrac{2}{5}MR^2$

7.84 of a homogeneous cylinder of mass M and radius R, $J = \dfrac{MR^2}{2}$

7.85 of a homogeneous cone of mass M, the base radius R, and height H,

$$J = \frac{3}{10}MR^2$$

7.86 of the homogeneous body from Example 7.53, $J = \dfrac{MR^2}{3}$

7.87 of the homogeneous body from Example 7.54, $J = \dfrac{3H - 2R^2}{6H - 3R^2}MR^2$

7.88 of the homogeneous body from Example 7.56, $J = \dfrac{MR^2}{4}$

7.89 of the body from Example 7.57, $J = \dfrac{53}{200}MR^2$

7.90 of a homogeneous ellipsoid of mass M and half-axes a, b, c, rotating around the half-axis c,

$$J = \frac{M}{5}(a^2 + b^2)$$

7.91 of a homogeneous body whose surface is created by rotation of the astroid from Example 6.7 around the axis y,

$J = \frac{64}{143} M a^2$

7.92 of a homogeneous body whose surface is created by rotation of the cardioid from Example 6.16 around the axis y,

$J = \frac{24}{35} M a^2$

7.93 of a homogeneous body bounded from the "top" by the surface $z = H - 2\left(x^2 + y^2\right)$ and from the "bottom" by the surface $z = 0$. Express the result as a function of body mass and the length $R = \sqrt{x^2 + y^2} = \sqrt{H/2}$ in the plane $z = 0$,

$J = \frac{MR^2}{3}$

7.94 of an empty closed cylindrical tank, i.e., consisting of a shell and both bases, made of material of negligible thickness with constant surface density σ, with radius R and height $H = R$; express the result as a function of entire mass M of the tank and its radius R,

$J = \frac{3}{4} M R^2$

7.95 of an empty closed conical tank, i.e., consisting of a shell and a base, made of material of negligible thickness with constant surface density σ with radius R and height H; express the result as a function of entire mass M of the tank and its radius R,

$J = \frac{MR^2}{2}$

7.96 of an empty closed tank created by the entire surface of the body (i.e., consisting of its shell and the base) from Example 7.53, made of material of negligible thickness with constant surface density σ; express the result as a function of entire mass M of the tank and its radius R,

$$J = M \frac{\left(1 + 4R^2\right)^{3/2} \left(\frac{3}{5} R^2 - \frac{1}{10}\right) + \frac{1}{10} + 3R^4}{\left(1 + 4R^2\right)^{3/2} - 1 + 6R^2}$$

7.97 of an empty closed tank created by the entire surface of the body (i.e., consisting of its shell and the base) from Example 7.56, made of material of negligible thickness with constant surface density σ; express the result as a function of entire mass M of the tank and its radius R.

$$J = \frac{\left(9\sqrt{3} + 20\right) M R^2}{\left(\sqrt{3} + 2\right) 24}$$

7.98 Derive the moment of inertia of a homogeneous semicircular plate of negligible thickness with radius R, rotating

(a) around the axis passing through its center, perpendicular to the plane of the plate,

(b) around the axis lying in the plane of the plate, passing through its base (diameter),

(c) around the axis lying in the plane of the plate, passing through its center of mass, parallel to its base.

Express the result as a function of mass M of the plate and its radius R.

(a) $J = \dfrac{MR^2}{2}$

(b) $J = \dfrac{MR^2}{4}$

(c) using the Steiner's (parallel axis) theorem: $z_T = \dfrac{4}{3\pi}R$, $J = \dfrac{MR^2}{4} - \left(\dfrac{4}{3\pi}\right)^2 MR^2 \approx \dfrac{7}{100}MR^2$

7.99 Derive the moment of inertia of a homogeneous plate of negligible thickness whose edge is shaped as the astroid from Example 6.7, rotating around the axis passing through its center, perpendicular to its plane. Express the result as a function of mass M of the plate and the length of half-axis a.

$J = \dfrac{7}{32}Ma^2$

7.100 Derive the moment of inertia J_k of a hollow sphere with radius R with the spherical concentric cavity of radius H with constant density ρ. Express the result in units of mass M of the hollow sphere, its radius R, and cavity radius H. Using the limit transition (or otherwise) subsequently derive the moment of inertia J_s of a homogeneous spherical shell with radius R.

$J_k = \dfrac{2}{5}M\dfrac{R^5 - H^5}{R^3 - H^3}$, $J_s = \dfrac{2}{3}MR^2$

7.101 Derive the moment of inertia of a homogeneous cube of edge A, rotating

(a) around the axis, passing through its center and the midpoints of two opposite sides,

(b) around the axis, passing through its center and the midpoints of two opposite edges,

(c) around the axis, passing the edge of the cube (calculate by direct integration and verify by the parallel axis (Steiner's) theorem).

Express the result as a function of the mass M of the cube and length of its edge A.

(a) $J = \dfrac{MA^2}{6}$

(b) $J = \dfrac{MA^2}{6}$

(c) $J = \dfrac{2}{3}MA^2$

Chapter 8

Integral theorems[1] [2]

8.1 Green's theorem

The theorem, named after the mathematician and physicist George Green (1793 - 1841), correlates the integral over the region $D \in \mathbb{R}^2$ and the integral along the closed curve $\mathcal{C}$ bounding the region D. For a vector field $\vec{F} = [F_1(x,y), F_2(x,y)]$, continuously differentiable in $D(x,y)$, the following formulation of the Green's theorem applies;

$$\iint_D \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} \right) \mathrm{d}x\, \mathrm{d}y = \oint_{\partial \vec{D}} \left(F_1\, \mathrm{d}x + F_2\, \mathrm{d}y \right), \tag{8.1}$$

where $\partial \vec{D}$ denotes a mathematically positively oriented closed boundary of the region D (the curve $\mathcal{C}$). Stokes' theorem (see Section 8.2) is the generalization of the Green's theorem for $\mathbb{R}^3$.

- **Examples:**

8.1 Using the Green's theorem calculate the line integral $\oint_{\mathcal{C}} \mathrm{e}^x \left[(1 - \cos y)\, \mathrm{d}x - (y - \sin y)\, \mathrm{d}y \right]$, where $\mathcal{C}$ is a positively oriented closed boundary curve of the region D: $0 < x < \pi$, $0 < y < \sin x$.

$\frac{1}{5}\left(1 - \mathrm{e}^{\pi}\right)$

8.2 Using the Green's theorem calculate the line integral $\oint_{\mathcal{C}} y^2\, \mathrm{d}x + x^2\, \mathrm{d}y$, where $\mathcal{C}$ is a positively oriented closed boundary curve of the region D: $0 < x < 3$, $0 < y < 2 - \frac{2}{3}x$.

2

8.3 Use the Green's theorem to calculate the radius circle's radius R of a circle.

Using the identity $S = \iint_S \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} \right) \mathrm{d}S = \left\{ \frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} = 1 \right\} = \oint_{\partial \vec{S}} \vec{F} \cdot \mathrm{d}\vec{s}$, $S = \pi R^2$

[1] We do not give the corresponding physical units in the results of the examples with geometric or physical quantities.

[2] Recommended literature for this chapter: Dĕmidovič (2003), Kvasnica (2004), Arfken & Weber (2005), Bartsch (2008), Rektorys (2009).

8.4 Calculate the area of the ellipse with half-axes a, b using surface integral and the Green's theorem.

In the same way as in the previous Example, $S = \pi ab$

8.5 Using the surface integral and the Green's theorem, calculate the area of a triangle with vertices at the points $[0, 0]$, $[2, 1]$, and $[1, 2]$.

$S = \frac{3}{2}$

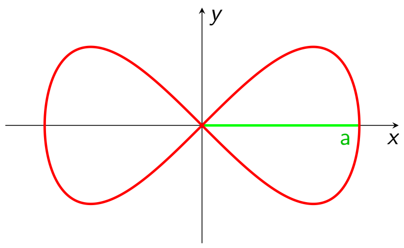

Figure 8.1: Lemniscate of Gerono (lemniscate of Huygens), the geometric meaning of the constant a is highlighted by green color.

8.6 Using the surface integral and the Green's theorem, calculate the area of the surface of the lemniscate of Gerono, enclosed by a curve given by the general equation $x^4 - a^2\left(x^2 - y^2\right) = 0$, where a is a constant (see Figure 8.1, see also Example 8.42).

$S = \frac{4a^2}{3}$

8.7 Using the surface integral and the Green's theorem, calculate the area of the astroid-enclosed surface from Example 6.7.

$S = \frac{3\pi}{8} a^2$

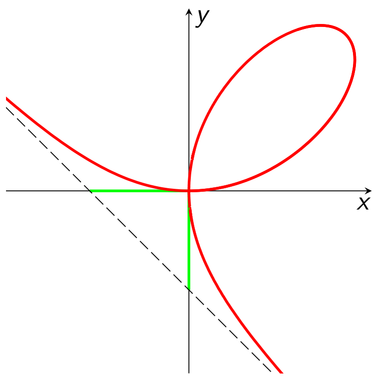

Figure 8.2: Folium of Descartes. The geometric meaning of the constant a is highlighted by green color.

8.8 Using the surface integral and the Green's theorem, calculate the area of a surface, enclosed by the loop of the curve, given by the general equation $x^3 + y^3 = 3\,axy$ (the so-called folium of Descartes, see Figure 8.2). The appropriate parameterization, for example, is $x = x(t)$, $y = tx(t)$, where $t = \tan\phi$.

$S = \frac{3}{2}a^2$

8.2 Stokes' theorem (Stokes-Kelvin theorem)

The Stokes theorem identifies the flux of a vector field $\vec{F}$ through a surface S, defined in $\mathbb{R}^3$ with an integral of this field along the closed curve s, which bounds this surface. Mathematical notation of the Stokes' theorem has the form

$$\iint_S \left(\vec{\nabla} \times \vec{F}\right) \cdot \vec{n}\,\mathrm{d}S = \oint_{\partial\vec{S}} \vec{F} \cdot \mathrm{d}\vec{s}, \tag{8.2}$$

where $\vec{F}$ is the given vector field, $\vec{n}$ is a normal unit vector of the surface S, and $\partial\vec{S}$ is a closed boundary of the surface S (smooth or by parts smooth boundary curve s oriented by a tangent vector $\mathrm{d}\vec{s}$ of its length element $\mathrm{d}s$).

- **Examples:**

8.9 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (x^2 - y, x, 0)$ that acts along a whole circle with radius R with the center at the point $[0, 0, 0]$ in the mathematically positive direction whose start and end points are at the point $[R, 0, 0]$. Will the amount of work change if the force acts in the mathematically negative direction?

$W = 2\pi R^2$, changes: $W = -2\pi R^2$

8.10 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (x^2 - y, x, 0)$ that acts along the circumference of a square, successively from the point $[0, 0, 3]$ to the points $[1, 0, 3]$, $[1, 1, 3]$, $[0, 1, 3]$, and back to the starting point. Will the amount of work change if the force acts in the opposite direction?

$W = 2$, changes: $W = -2$

8.11 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (x^3 - x^2, x - 1, 0)$ that acts along the circumference of a triangle, successively from the point $[0, 0, 1]$ to the points $[2, 0, 1]$, $[0, 1, 1]$, and back to the starting point. Will the amount of work change if the force acts in the opposite direction?

$W = 1$, changes: $W = -1$

8.12 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (x^3 - x^2, x - 1, 0)$ that acts along the circumference of a triangle, successively from the point $[0, 0, 0]$ to the points $[2, 0, 0]$, $[0, 1, 0]$, and back to the starting point. Will the amount of work change if the force acts in the opposite direction?

$W = 1$, changes: $W = -1$

8.13 Use the Stokes' theorem to verify the calculation of the work done by the force from Example 6.38.

$$W = \oint_{\partial V} \operatorname{rot} \vec{F} \cdot \vec{n} \, \mathrm{d}S, \ \operatorname{rot} \vec{F} = (0, 0, 2), \ \vec{n} = (0, 0, -1), \ S = \frac{\pi}{4}, \ W = -\frac{\pi}{2}$$

8.14 Use the Stokes' theorem to verify the calculation of the work done by the force from Example 6.39.

$$W = \oint_{\partial V} \operatorname{rot} \vec{F} \cdot \vec{n} \, \mathrm{d}S, \ \operatorname{rot} \vec{F} = (0, 0, 2), \ \vec{n} = (0, 0, 1), \ S = \pi - 1, \ W = 2(\pi - 1)$$

8.15 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = [y^2, \ (x + y)^2, 0]$ that acts along the circumference of a triangle in the direction of its vertices at the points $[3, 0, 0]$, $[0, 3, 0]$, $[3, 3, 0]$.

$W = -18$

8.16 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = [y, \ (x + y)^2, 0]$ that acts in the mathematically negative direction along the curve $x^2 + y^2 = 1, z = 0$.

$W = \pi$

8.17 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y, -x, z)$ that acts initially along the curve $y^2 = R^2 - x^2$ from the point $[R, 0, 0]$ to the point $[0, R, 0]$, then along the curve $z^2 = R^2 - y^2$ from the point $[0, R, 0]$ to the point $[0, 0, R]$, and finally along the curve $x^2 = R^2 - z^2$ from the point $[0, 0, R]$ back to the starting point.

$$W = -\frac{\pi R^2}{2}$$

8.18 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y^2, z^2, x^2)$ that acts initially along the curve $y^2 = R^2 - x^2$ from the point $[R, 0, 0]$ to the point $[0, R, 0]$, then along the curve $z^2 = R^2 - y^2$ from the point $[0, R, 0]$ to the point $[0, 0, R]$, and finally along the curve $x^2 = R^2 - z^2$ from the point $[0, 0, R]$ back to the starting point.

$W = -2R^3$

8.19 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y, z, x)$, acting on the surface of the body from Example 7.53

(a) initially along the curve $y^2 = R^2 - x^2$ from the point $[0, -R, 0]$ in the mathematically positive direction to the point $[R, 0, 0]$, then along the curve $z = H - x^2$ from the point $[R, 0, 0]$ to the point $[0, 0, H]$, and finally along the curve $z = H - y^2$ from the point $[0, 0, H]$ back to the starting point,

(b) initially along the curve $y^2 = R^2 - x^2$ from the point $[R, 0, 0]$ in the mathematically positive direction to the point $[0, R, 0]$, then along the curve $z = H - y^2$ from the point $[0, R, 0]$ to the point $[0, 0, H]$, and finally along the curve $z = H - x^2$ from the point $[0, 0, H]$ back to the starting point,

(c) initially along the curve $y^2 = R^2 - x^2$ from the point $[0, -R, 0]$ in the mathematically positive direction to the point $[0, R, 0]$, then along the curve $z = H - y^2$ from the point $[0, R, 0]$ to the point $[0, 0, H]$, and finally along the curve $z = H - y^2$ from the point $[0, 0, H]$ back to the starting point.

(a) $W = -\dfrac{\pi R^2}{4}$

(b) $W = -\dfrac{\pi R^2}{4} - \dfrac{4}{3}R^3$

(c) $W = -\dfrac{\pi R^2}{2} - \dfrac{4}{3}R^3$

8.20 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y^2, z^2, x^2)$, acting on the surface of the body from Example 7.13

(a) initially along the curve $y^2 = R^2 - x^2$ from the point $[R, 0, 0]$ in the mathematically positive direction to the point $[0, R, 0]$, then in the shortest possible way from the point $[0, R, 0]$ to the point $[0, 0, H]$, and then again in the shortest possible way from the point $[0, 0, H]$ back to the starting point,

(b) initially along the curve $y^2 = R^2 - x^2$ from the point $[0, -R, 0]$ in the mathematically positive direction to the point $[0, R, 0]$, then in the shortest possible way from the point $[0, R, 0]$ to the point $[0, 0, H]$, and finally again in the shortest possible way from the point $[0, 0, H]$ back to the starting point.

(a) $W = -\dfrac{R}{3}\left(2R^2 + HR + H^2\right)$

(b) $W = -\dfrac{2}{3}H^2R$

8.21 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y^2, -z^2, x^2)$, acting on the surface of the body from Example 7.53

(a) initially along the curve $y^2 = R^2 - x^2$ from the point $[0, -R, 0]$ in the mathematically positive direction to the point $[R, 0, 0]$, then along the curve $z = H - x^2$ from the point $[R, 0, 0]$ to the point $[0, 0, H]$, and finally along the curve $z = H - y^2$ from the point $[0, 0, H]$ back to the starting point,

(b) initially along the curve $y^2 = R^2 - x^2$ from the point $[R, 0, 0]$ in the mathematically positive direction to the point $[0, R, 0]$, then along the curve $z = H - y^2$ from the point $[0, R, 0]$ to the point $[0, 0, H]$, and finally along the curve $z = H - x^2$ from the point $[0, 0, H]$ back to the starting point.

(a) $W = \dfrac{2}{3}R^3(2H + 1) + \dfrac{R^4}{2} - \dfrac{4}{5}R^5 = \dfrac{8}{15}R^5 + \dfrac{R^4}{2} + \dfrac{2}{3}R^3$

(b) $W = \dfrac{2}{3}R^3(2H - 1) - \dfrac{R^4}{2} - \dfrac{4}{5}R^5 = \dfrac{8}{15}R^5 - \dfrac{R^4}{2} - \dfrac{2}{3}R^3$

8.22 Using line integral and the Stokes theorem, prove that the work done by the force $\vec{F}(x, y, z) = (z^2, x^2, y^2)$ acting in the mathematically positive direction along the curve given by the intersection of the surfaces $S_1 = \{x^2 + y^2 + z^2 = R^2\}$ and $S_2 = \{x - z = 0\}$ is zero.

The problem can be solved both in spherical and in a rotated cylindrical coordinate system (transformation of bases).

8.23 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (z^3, x^2, y)$ acting on the circumference of a parallelogram from the starting point $[0, 0, 0]$ in the direction of the points $[A, 0, A]$, $[A, A, A]$, $[0, A, 0]$, and back to the starting point.

$W = A^3 - A^2$

8.24 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (z^3, x^2, y)$ acting on the circumference of a triangle from the starting point $[0, 0, 0]$ in the direction of the points $[A, 0, 0]$, $[0, B, C]$, and back to the starting point.

$$W = \frac{A^2B}{3} - \frac{AC^3}{4}$$

8.25 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (y^2, xz, y^2)$ acting on the circumference of a plane given by the prescription $S = \big\{(x, y, z)\big|x^2 + y^2 \le R^2,\ z = 6\big\}$, after performing one circuit from the point $[R, 0, 6]$ to the same point, in the mathematically negative direction.

$-6\pi R^2$

8.26 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (z^2, x^2, y^2)$ acting on the circumference of a plane given by the prescription $S = \big\{(x, y, z)\big|x^2 + y^2 + (z - R)^2 = R^2,\ x, y, z \in \langle 0, R\rangle\big\}$, in the direction of the points $[0, 0, 0]$, $[R, 0, R]$, $[0, R, R]$, and back to the point $[0, 0, 0]$.

$$W = 2R^3\left(\frac{1}{3} - \frac{\pi}{4}\right)$$

8.27 Using line integral and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (z^2, x^2, y^2)$ acting on the circumference of a plane given by the prescription $S = \big\{(x, y, z)\big|x^2 + (y - R)^2 + z^2 = R^2,\ x \in \langle -R, 0\rangle,\ y, z \in \langle 0, R\rangle\big\}$, in the direction of the points $[-R, R, 0]$, $[0, R, R]$, $[0, 0, 0]$, and back to the point $[-R, R, 0]$.

$$W = 2R^3\left(\frac{1}{3} + \frac{\pi}{4}\right)$$

8.28 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x, y, z) = (z^2, x^2, y^2)$ acting on the circumference of a plane given by the prescription $S = \big\{(x, y, z)\big|x^2 + (y + R)^2 + z^2 = R^2,\ x \in \langle -R, 0\rangle,\ y \in \langle -R, 0\rangle, z \in \langle 0, R\rangle\big\}$, in the direction of the points $[-R, -R, 0]$, $[0, -R, R]$, $[0, 0, 0]$, and back to the point $[-R, -R, 0]$.

$$W = 2R^3\left(\frac{\pi}{4} - \frac{1}{3}\right)$$

8.29 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x,y,z) = (xz, -yz, 0)$ acting on the shell of a cylinder of radius R whose axis intersects the point $[-R, 0, 0]$ and coalesces with the vector $(0, 0, z)$. The force acts along a closed trajectory from the starting point $[0, 0, 0]$ in the direction of the points $[-R, R, 0]$, $[-R, R, H]$, $[0, 0, H]$, and back to the point $[0, 0, 0]$.

$W = 0$

8.30 Using line integral of type II and the Stokes' theorem, calculate the work done by the force $\vec{F}(x,y,z) = (xz^2, xz^2, yz^2)$ acting on the surface of a cylinder of radius R whose axis intersects the point $[R, 0, 0]$ and coalesces with the vector $(0, 0, z)$, $z \in \langle 0, H\rangle$. The force acts along a closed trajectory from the starting point $[R, R, H]$ along the edge of a cylinder shell to the point $[0, 0, H]$, then along a straight line to the point $[2R, 0, H]$, and again along the edge of a cylinder shell back to the point $[R, R, H]$.

$W = \dfrac{\pi R^2 H^2}{2}$

8.3 Gauss's (Gauss-Ostrogradsky) theorem[1]

The Gauss theorem (also called the divergence theorem) says that the flux of a vector field through a closed surface S is equal to the integral of the divergence of this field over the volume V that is bounded by this surface defined in $\mathbb{R}^3$ (generally in $\mathbb{R}^n$). Mathematical notation of the Gauss's theorem has the form

$$\iiint_V \vec{\nabla} \cdot \vec{F}\, \mathrm{d}V = \oiint_{\partial V} \vec{F} \cdot \vec{n}\, \mathrm{d}S, \tag{8.3}$$

where $\vec{F}$ is a common vector field, $\vec{n}$ is a unit vector of the outer normal of the surface S, and ∂V denotes boundary region of the volume V (boundary surface S).

- **Examples:**

8.31 Using the Gauss's theorem, derive the formula for calculating the volume of a cylinder of a radius R and a height H.

Using the identity $V = \displaystyle\int_V \operatorname{div} \vec{F}\, \mathrm{d}V\ (\operatorname{div} \vec{F} = 1) = \oint_{\partial V} \vec{F} \cdot \vec{n}\, \mathrm{d}S$, $V = \pi R^2 H$

8.32 Using the Gauss's theorem, derive the formula for calculating the volume of a sphere of a radius R.

In the same way as in the previous example, $V = \dfrac{4}{3}\pi R^3$

8.33 Using the Gauss's theorem, derive the formula for calculating the volume of a cone of radius R and height H.

$V = \dfrac{\pi R^2 H}{3}$

[1] Unless stated otherwise, the flux in the direction of outer normal to a given closed surface is always regarded.

8.34 Using the Gauss's theorem, derive the relation for the calculation of the volume of an annuloid (torus) with the radius of the axis of torus R and the radius of tube a (see Example 7.55).

$V = 2\pi^2 R a^2$

8.35 Use the Gauss's theorem to calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through a closed surface given by the formula $S = \{(x, y, z) \,|\, x \in \langle A,\, 2A\rangle,\ y \in \langle B,\, 2B\rangle,\ z \in \langle C,\, 2C\rangle\}$.

$\Phi_F = 3ABC(A + B + C)$

8.36 Use the Gauss's theorem to calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through a closed surface given by the formula $S = \left\{(x, y, z) \,|\, x^2 + y^2 = R^2,\ z \in \langle 0,\ H\rangle\right\}$.

$\Phi_F = \pi R^2 H^2$

8.37 Use the Gauss's theorem to calculate the flux of the vector field $\vec{F} = \left[(x-1)^2, (y-1)^2, z^2\right]$ through the surface of a body given by the formula $\mathcal{V} = \left\{(x, y, z) \,|\, x^2 + y^2 \leq R^2,\ y \geq 0,\ z \in \langle 0, H\rangle\right\}$.

$\dfrac{4}{3} R^3 H + \dfrac{\pi R^2 H^2}{2} - 2\pi R^2 H$

8.38 Use the Gauss's theorem to calculate the flux of the vector field $\vec{F} = \left(x^2, y^2, z^2\right)$ through a closed surface formed by the surface of the body from Example 7.53.

$\Phi_F = \dfrac{\pi R^2 H^2}{3}$

8.39 Using the Gauss's theorem, calculate the flux of the vector field $\vec{F} = \left(x^3 - y^3, x^3 + y^3, z\right)$ through a closed surface formed by the surface of the body $\mathcal{V} = \left\{(x, y, z) \,|\, z \in \langle 0,\ H\rangle,\ x^2 + y^2 \leq \dfrac{R^2}{H^2}(H - z)^2\right.$

$\Phi_F = \dfrac{\pi R^2 H}{30}\left(9R^2 + 10\right)$

8.40 Use the Gauss's theorem to calculate the flux of the vector field $\vec{F} = (x^3, y^3, z^3)$ through a surface given by the formula $S = \left\{(x, y, z) \,|\, x^2 + y^2 + z^2 = R^2\right\}$.

$\Phi_F = \dfrac{12}{5} \pi R^5$

8.41 The force field $\vec{F} = (x^3 - x^2,\ y^3 - y^2,\ z^3 - z^2)$ is given. Use the Gauss's theorem to calculate its flux through the surface of a body specified by the formula $\mathcal{V} = \left\{(x, y, z) \,|\, x, y, z \in \langle 0, R\rangle,\ x^2 + y^2 + z^2 \leq \right.$

$\Phi_F = \dfrac{3\pi R^4}{40}\,(4R - 5)$

8.42 Use the Gauss's theorem to derive the formula for calculating the volume of an axisymmetric body $\mathcal{M}$ with axis $(0, 0, z)$, $\mathcal{M} = \{(x, y, z) \,|\, \sqrt{x^2 + y^2} \leq a \sin\theta,\ z \leq a \sin\theta \cos\theta,\ \theta \in \langle 0, \pi\rangle\}$. The surface of the body is created by the rotation of a plane curve, the so-called lemniscate of Gerono (Huygens), around an axis lying in the plane of the curve and passing through its center - see Figure 8.1 (where the axis y will now become the axis z), see also Example 8.6.

$$V = \frac{\pi^2 a^3}{4}$$

8.43 Use the Gauss's theorem to verify the calculation of the volume of the body from Example 7.58.

$$V = \frac{32}{105}\pi a^3$$

8.44 Using the Gauss's theorem, derive the relation for the calculation of the volume of the axially symmetrical body $\mathcal{M}$ created by the rotation of the closed loop of the folium of Descartes from Example 8.8 around the axis y, shown in Figure 8.2. Specify also the maximum length L of the loop, that is, the length along the straight line, cutting the first quadrant in the illustration into two halves, and coordinates of the horizontal and vertical maximum, everything as a function of the constant a.

$$V = \frac{4\pi^2 a^3}{3\sqrt{3}},\ L = \frac{3}{\sqrt{2}}a,\ (2^{\frac{2}{3}}a, 2^{\frac{1}{3}}a),\ (2^{\frac{1}{3}}a, 2^{\frac{2}{3}}a)$$

8.45 Use the Gauss's theorem to determine the position of the center of mass of a homogeneous body from Example 8.44 in the direction of the vertical axis shown in Figure 8.2.

$$z_T = \frac{27\sqrt{3}}{16\pi}a$$

8.46 Use the Gauss's theorem to determine the moment of inertia of a homogeneous body $\mathcal{M}$ from Example 8.42, rotating around the axis $(0, 0, z)$. Express the result in units of total mass M of the body and the radius a.

$$J = \frac{Ma^2}{2}$$

8.47 Use the Gauss's theorem to determine the moment of inertia of a homogeneous body $\mathcal{A}$ from Example 7.58, rotating around the same axis y. Express the result in units of total mass M of the body and the half-axis a.

$$J = \frac{32}{143}Ma^2$$

8.48 Use the Gauss's theorem to determine the moment of inertia of a homogeneous body from Example 8.44, rotating around the vertical axis, denoted in Figure 8.2. Express the result in units of total mass M of the body and the maximum dimension R of the loop in the horizontal direction.

$$J = \frac{81\sqrt{3}}{40\pi}\frac{MR^2}{2^{4/3}}$$

8.49 Use the Gauss's theorem to calculate the flux of a vector field $\vec{F} = (x, y, z)$ through the closed surface of the body from Example 8.42. Why is the resulting value three times the result from the example mentioned above?

$$\Phi_F = \frac{3\pi^2 a^3}{4}$$

8.50 Use the Gauss's theorem to calculate the flux of a vector field $\vec{F} = (x^3, y^3, z^3)$ through the closed surface of the body from Example 8.42.

$$\Phi_F = \frac{27}{64}\pi^2 a^5 = \left(\frac{3}{4}\right)^3 \pi^2 a^5$$

8.51 Use the Gauss's theorem to calculate the flux Φ of a vector field $\vec{F}(x, y, z) = (0, 0, z^2)$ through the closed surface of the body $\mathcal{V} = \big\{(x, y, z) \,\big|\, x^2 + y^2 \leq 4,\ x \leq 0,\ y \geq 0,\ z \in \langle 0, |x| \rangle \big\}$.

$$\Phi_F = \pi$$

8.52 Use the Gauss's theorem to calculate the flux Φ of a vector field $\vec{F}(x, y, z) = (0, 0, z^2)$ through the closed surface of the body $\mathcal{V} = \big\{(x, y, z) \,\big|\, x^2 + y^2 + z^2 \leq 4,\ x \geq 0,\ y \leq 0,\ z \geq 0,\ \dfrac{z^2}{x^2 + y^2 + z^2} \leq \dfrac{1}{2} \big\}$.

$$\Phi_F = \pi$$

8.53 Using the surface integral of type II and also the Gauss's theorem, calculate the flux Φ of a vector field $\vec{F}(x, y, z) = (0, 0, z^2)$ through the closed surface of the body $\mathcal{V} = \big\{(x, y, z) \,\big|\, x^2 + y^2 + z \leq 9 \wedge z - 3x^2 - 3y^2 \geq 0 \big\}$.

$$\Phi_F = 21\pi \left(\frac{9}{4}\right)^2$$

8.54 Using the surface integral of type II and also the Gauss's theorem, calculate the flux Φ of a vector field $\vec{F}(x, y, z) = (x^2, 0, 0)$ through the closed surface of the body $\mathcal{V} = \big\{(x, y, z) \,\big|\, x^2 + y^2 + z \leq 5,\ x \geq 0,\ y \leq 0,\ z \geq 1 \big\}$.

$$\Phi_F = \frac{128}{15}$$

8.55 Calculate the capacity of a cylindrical capacitor, which consists of two concentric conductive cylindrical shells (electrodes) with radii R_1 and R_2, and length H, where $R_1 < R_2$. A charge $+Q$ is brought to the inner electrode, a charge $-Q$ to the outer electrode. Neglect the electric field irregularities at both ends of the electrodes.

$$C = \frac{2\pi\epsilon_0 H}{\ln(R_2/R_1)}$$

8.56 Calculate the capacity of a spherical capacitor, which consists of two concentric conductive spherical shells (electrodes) with radii R_1 and R_2, where $R_1 < R_2$. A charge $+Q$ is brought to the inner electrode, a charge $-Q$ to the outer electrode.

$$C = 4\pi\epsilon_0 \frac{R_1 R_2}{R_2 - R_1}$$

Chapter 9

Taylor expansion[1]

The possibility of substituting any mathematical function by a polynomial was formulated in the early 18th century by the mathematicians James Gregory and Brook Taylor. In case of an infinitely differentiable function, it will be an infinite power series obeying certain, precisely defined conditions. The expansion of a function into series is one of the most commonly used tools for expressing the approximate value of functions, which forms the basis of many principles of numerical mathematics, etc.

9.1 Expansion of function of a single variable

Infinite series

$$f(x) = f(x_0) + \left.\frac{\partial f}{\partial x}\right|_{x_0}(x-x_0) + \frac{1}{2!}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x_0}(x-x_0)^2 + \frac{1}{3!}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x_0}(x-x_0)^3$$
$$+\frac{1}{4!}\left.\frac{\partial^4 f}{\partial x^4}\right|_{x_0}(x-x_0)^4 + \ldots = \sum_{n=0}^{\infty}\frac{1}{n!}\left.\frac{\partial^n f}{\partial x^n}\right|_{x_0}(x-x_0)^n \qquad (9.1)$$

express the general notation of the Taylor expansion of an infinitely differentiable function of a single variable with all derivatives at the general point x_0 being finite and continuous. The order of derivative characterizes the Taylor expansion order, the degree of power determines the degree of the term of the Taylor polynomial (in case of a function of a single variable, both coincide). Putting $x_0 = 0$ gives the so-called Maclaurin series (expansion) as a particular case of Taylor expansion.

- **Examples:**

9.1 Write Taylor expansion of the following functions at the given points x_0:

(a) $f(x) = \mathrm{e}^x$, $x_0 = 0$, $\quad 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120} + \ldots$

(b) $f(x) = \mathrm{e}^x$, $x_0 = 1$, $\quad \mathrm{e} + \mathrm{e}(x-1) + \frac{1}{2}\mathrm{e}(x-1)^2 + \frac{1}{6}\mathrm{e}(x-1)^3 + \ldots$

(c) $f(x) = \sin x$, $x_0 = 0$, $\quad x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \ldots$

[1] Recommended literature for this chapter: Dĕmidovič (2003), Kvasnica (2004), Rektorys (2009), Zemánek & Hasil (2012).

(d) $f(x)=\cos x,\ x_0=0,$ $\quad 1-\dfrac{x^2}{2}+\dfrac{x^4}{24}-\dfrac{x^6}{720}+\ldots$

(e) $f(x)=\ln x,\ x_0=1,$ $\quad x-1-\dfrac{1}{2}(x-1)^2+\dfrac{1}{3}(x-1)^3-\dfrac{1}{4}(x-1)^4+\ldots$

(f) $f(x)=\sin x\cos x,\ x_0=0,$ $\quad x-\dfrac{2x^3}{3}+\dfrac{2x^5}{15}-\dfrac{4x^7}{315}+\ldots$

(g) $f(x)=\tan x,\ x_0=0,$ $\quad x+\dfrac{x^3}{3}+\dfrac{2x^5}{15}+\dfrac{17x^7}{315}+\ldots$

(h) $f(x)=\tan^2 x,\ x_0=\dfrac{\pi}{4},$ $\quad 1+4\left(x-\dfrac{\pi}{4}\right)+8\left(x-\dfrac{\pi}{4}\right)^2+\dfrac{40}{3}\left(x-\dfrac{\pi}{4}\right)^3+\ldots$

9.2 Write Taylor expansion of the following functions at the given points x_0:

(a) $f(x)=\dfrac{1}{x},\ x_0=1,$ $\quad 1-(x-1)+(x-1)^2-(x-1)^3+(x-1)^4+\ldots$

(b) $f(x)=\dfrac{1}{x^2},\ x_0=1,$ $\quad 1-2(x-1)+3(x-1)^2-4(x-1)^3+5(x-1)^4+\ldots$

(c) $f(x)=\mathrm{e}^{-x^2},\ x_0=0,$ $\quad 1-x^2+\dfrac{x^4}{2}-\dfrac{x^6}{6}+\dfrac{x^8}{24}-\dfrac{x^{10}}{120}+\ldots$

(d) $f(x)=\mathrm{e}^x\sin x,\ x_0=0,$ $\quad x+x^2+\dfrac{x^3}{3}-\dfrac{x^5}{30}-\dfrac{x^6}{90}-\dfrac{x^7}{630}+\ldots$

(e) $f(x)=\sin^2 x\cos^2 x,\ x_0=\dfrac{\pi}{2},$ $\quad \left(x-\dfrac{\pi}{2}\right)^2-\dfrac{4}{3}\left(x-\dfrac{\pi}{2}\right)^4+\dfrac{32}{45}\left(x-\dfrac{\pi}{2}\right)^6+\ldots$

9.3 Write expansion of the following functions up to 4th degree at the given point $x_0=0$ (Maclaurin expansion):

(a) $f(x)=\mathrm{e}^{3x},$ $\quad 1+3x+\dfrac{9}{2}(x^2+x^3)+\dfrac{27}{8}x^4+\ldots$

(b) $f(x)=\dfrac{x^2-x+1}{2x+1},$ $\quad 1-3x+7x^2-14x^3+28x^4+\ldots$

(c) $f(x)=\ln\left(1-\sin^2 x\right),$ $\quad -x^2-\dfrac{x^4}{6}+\ldots$

(d) $f(x)=\dfrac{\mathrm{e}^{-x^3}}{(x-1)^3},$ $\quad -1-3x-6x^2-9x^3-12x^4+\ldots$

(e) $f(x)=\dfrac{\sinh\left(x^2+2\sin^4 x\right)}{1+x^{10}},$ $\quad x^2+2x^4+\ldots$

(f) $f(x)=\sqrt{\cos\left(3x+x^3\right)}.$ $\quad 1-\dfrac{9}{4}x^2-\dfrac{75}{32}x^4+\ldots$

9.4 Solve the following indefinite integrals using an appropriate expansion of the integrand into Taylor series at the point $x_0=0$ (Maclaurin expansion):

(a) $\displaystyle\int\frac{\mathrm{e}^{x^2}}{x}\,\mathrm{d}x,$ $\quad \displaystyle\ln x+\sum_{k=1}^{\infty}\frac{x^{2k}}{k!\,2k}+C$

(b) $\displaystyle\int \frac{\sin x}{x}\,\mathrm{d}x$, $\displaystyle\sum_{k=0}^{\infty}(-1)^k\frac{x^{2k+1}}{(2k+1)!\,(2k+1)}+C$

(c) $\displaystyle\int \frac{\cos x}{x}\,\mathrm{d}x$, $\displaystyle\ln x+\sum_{k=1}^{\infty}(-1)^k\frac{x^{2k}}{(2k)!\,2k}+C$

(d) $\displaystyle\int \frac{\sin x\cos x}{x}\,\mathrm{d}x$. $\displaystyle\sum_{k=0}^{\infty}\left[(-1)^k\frac{x^{2k+1}}{2k+1}\sum_{m=0}^{k}\frac{1}{m!\,(2k-m+1)!}\right]+C$

9.5 Using Taylor expansion, calculate values of the given limits of the following functions:

(a) $\displaystyle\lim_{x\to 0}\frac{\mathrm{e}^x-1-x}{x^2}$, $\frac{1}{2}$

(b) $\displaystyle\lim_{x\to 0}\frac{\mathrm{e}^x-\sin x-\cos x}{\mathrm{e}^{x^2}-\mathrm{e}^{x^3}}$, 1

(c) $\displaystyle\lim_{x\to 0}\sqrt{\frac{1-\mathrm{e}^x}{\ln(x+1)}}$, i

(d) $\displaystyle\lim_{x\to 0}\frac{\sqrt[5]{1-5x^2+x^4}-1+x^2}{x^4}$, $-\frac{9}{5}$

(e) $\displaystyle\lim_{x\to 0}\frac{\sin\sqrt[3]{x^2}-\sqrt[3]{x^2}-\ln\cos x}{x\sin x}$, $\frac{1}{3}$

(f) $\displaystyle\lim_{x\to 0}\frac{\ln(1+x\arctan x)+1-\mathrm{e}^{x^2}}{\sqrt{1+2x^4}-1}$, $-\frac{4}{3}$

(g) $\displaystyle\lim_{x\to 0}\frac{\cos x-1+\frac{1}{2}x\sin x}{[\ln(1+x)]^4}$, $-\frac{1}{24}$

(h) $\displaystyle\lim_{x\to 0}\left[\frac{1}{\ln(1+x)}-\frac{1}{\tan x}\right]$, $\frac{1}{2}$

(i) $\displaystyle\lim_{x\to 0}\frac{1}{\sin x}\sqrt{3\left(1-\frac{x}{\tan x}\right)}$. $\displaystyle\lim_{x\to 0^+}=1,\ \lim_{x\to 0^-}=-1$

9.6 Calculate the approximate value of the following integrals with an error not exceeding 10^{-3}:

(a) the so-called error function $\operatorname{erf} x=\dfrac{2}{\sqrt{\pi}}\displaystyle\int_0^x \mathrm{e}^{-t^2}\,\mathrm{d}t$ for the upper limit $x=1$, $0.842\,714\,222$

(b) the so-called sine integral (sinc function) $\operatorname{Si} x=\displaystyle\int_0^x\frac{\sin t}{t}\,\mathrm{d}t$ for the upper limit $x=1$, $0.946\,082\,766$

(c) the so-called cosine integral $\operatorname{Ci} x=-\displaystyle\int_x^{\infty}\frac{\cos t}{t}\,\mathrm{d}t$ $(x>0)$ for the lower limit $x=1$. This integral can be rewritten into the form $\operatorname{Ci} x=\gamma+\ln x+\displaystyle\int_0^x\frac{\cos t-1}{t}\,\mathrm{d}t$, where the so-called Euler (Euler-Mascheroni) constant $\gamma = \lim\limits_{n\to\infty}\left(\sum\limits_{k=1}^{n}\frac{1}{k} - \ln n\right) \approx 0.577\,215\,665$,

$0.337\,400\,849$

(d) the so-called exponential integral $\operatorname{Ei} x = -\int_{-x}^{\infty}\frac{\mathrm{e}^{-t}}{t}\,\mathrm{d}t = \int_{-\infty}^{x}\frac{\mathrm{e}^{t}}{t}\,\mathrm{d}t$ for $x=-1$. This integral can be rewritten into the form $\operatorname{Ei} x = \gamma + \ln|x| + \int_{0}^{-x}\frac{\mathrm{e}^{-t}-1}{t}\,\mathrm{d}t$, where γ is the same Euler constanta as in Example 9.6c,

$-0.219\,386\,753$

(e) exponential integral $\operatorname{Ei} x$ described in Example 9.6d, where the upper limit value $x=1$ (this case has a finite solution because integrating a function with a singularity can be done under certain conditions by assigning the so-called principal value of a definite integral - see Section 1.3),

$1.894\,854\,554$

(f) the so-called logarithmic integral $\operatorname{li} x = \int_{x_1}^{x_2}\frac{\mathrm{d}t}{\ln t}$ for $x_1 = 2$ and $x_2 = 10$ (the integrated function can be expanded into an appropriate series by substitution $t = \mathrm{e}^{u}$).

$5.073\,622\,569$

9.7 Using Taylor expansion, prove the Euler's identity for $y(x)$: $C_1\,\mathrm{e}^{\mathrm{i}x} + C_2\,\mathrm{e}^{-\mathrm{i}x} = A\cos x + B\sin x$. What is the relationship between the particular coefficients and what will be their values if $y(0)=1$, $y'(0)=1$?

$A = C_1 + C_2$, $B = \mathrm{i}(C_1 - C_2)$, $C_1 = \frac{1-\mathrm{i}}{2}$, $C_2 = \frac{1+\mathrm{i}}{2}$, $A=1$, $B=1$

9.8 Verify the validity of the classical kinetic energy relation $T = \frac{1}{2}mv^2$ for small velocities, $v \ll c$. The complete relativistic expression for kinetic energy has the form $T = E - E_0$, where E means the total energy $E = mc^2$, and E_0 is the so-called rest energy, $E_0 = m_0c^2$. The quantities m and m_0, that is, the relativistic and rest mass, are bound by relation $m = \gamma\, m_0$, where the so-called Lorentz factor $\gamma = (1 - v^2/c^2)^{-1/2}$.

Using Taylor expansion of the relativistic expression up to the second-order.

9.9 Write Taylor expansion of the function $f(x) = \frac{Ax}{(B+x^2)^{3/2}}$, where A, B are constants, up to the third-order. Write also:

(a) Taylor polynomial of the third degree of the function $f(x)$ in the neighborhood of the point $x_0 = 0$,

(b) Third-degree of this polynomial in the neighborhood of the point $x_0 = 1$.

(a) $T_3(x)\big|_{x_0=0} = \frac{A}{B^{\frac{3}{2}}}x - \frac{3A}{2B^{\frac{5}{2}}}x^3$

(b) $T_3^{\mathrm{III}}(x)\big|_{x_0=1} = -\frac{A\left(3B^2 - 24B + 8\right)}{2\,(B+1)^{\frac{9}{2}}}(x-1)^3$

9.10 Prove that

(a) Planck's law $B_\nu(T)$ for small frequencies ν transits to the Rayleigh-Jeans law, known in the physics of low frequencies,

(b) Convert Planck's law in the form $B_\nu(T)$ into the form $B_\lambda(T)$ and prove the transition to Rayleigh-Jeans law for large wavelengths λ.

(a) $B_\nu(T) = \dfrac{2h\nu^3}{c^2}\dfrac{1}{\mathrm{e}^{\frac{h\nu}{kT}}-1} \to \dfrac{2\nu^2}{c^2}kT$

(b) $B_\lambda(T) = \dfrac{2hc^2}{\lambda^5}\dfrac{1}{\mathrm{e}^{\frac{hc}{\lambda kT}}-1} \to \dfrac{2c}{\lambda^4}kT$

9.2 Expansion of function of several variables

In case of an infinitely differentiable function of two variables x, y, satisfying the condition of finality and continuity of all derivatives according to both variables at the general point $[x_0, y_0]$, the general form of the Taylor expansion can be written as

$$\begin{aligned} f(x,y) = f(x_0,y_0) &+ \left.\frac{\partial f}{\partial x}\right|_{x_0,y_0}(x-x_0) + \left.\frac{\partial f}{\partial y}\right|_{x_0,y_0}(y-y_0) \\ &+ \frac{1}{2!}\left[\left.\frac{\partial^2 f}{\partial x^2}\right|_{x_0,y_0}(x-x_0)^2 + \left.\frac{2\,\partial^2 f}{\partial x\,\partial y}\right|_{x_0,y_0}(x-x_0)(y-y_0) + \left.\frac{\partial^2 f}{\partial y^2}\right|_{x_0,y_0}(y-y_0)^2\right] \\ &+ \frac{1}{3!}\left[\left.\frac{\partial^3 f}{\partial x^3}\right|_{x_0,y_0}(x-x_0)^3 + \left.\frac{3\,\partial^3 f}{\partial x^2\,\partial y}\right|_{x_0,y_0}(x-x_0)^2(y-y_0)\right. \\ &\qquad\left. + \left.\frac{3\,\partial^3 f}{\partial x\,\partial y^2}\right|_{x_0,y_0}(x-x_0)(y-y_0)^2 + \left.\frac{\partial^3 f}{\partial y^3}\right|_{x_0,y_0}(y-y_0)^3\right] + \dots \end{aligned} \tag{9.2}$$

The order of derivative again characterizes the order of Taylor expansion, and the power degree determines the degree of the particular term of Taylor polynomial. In general, Taylor expansion of a function of several variables can be written as

$$f(x_1,\dots,x_k) = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_k=0}^{\infty}\left.\left(\frac{\partial^{n_1+\dots+n_k} f}{\partial x_1^{n_1}\cdots\partial x_k^{n_k}}\right)\right|_{x_{01},\dots,x_{0k}}\frac{(x_1-x_{01})^{n_1}\cdots(x_k-x_{0k})^{n_k}}{n_1!\cdots n_k!}. \tag{9.3}$$

- **Examples:**

9.11 Calculate all non-zero terms of Taylor expansion of the function $f(x,y) = x^2y$ and always calculate the value of $f\,(2.1,\,2.9)$ for particular orders of expansion. Compare the results with the value given by a calculator.

$T_0 = 12$, $T_1 = 12.8$, $T_2 = 12.79$, $T_3 = 12.789$ (by calculator 12.789)

9.12 Using Taylor expansion of the function $f(x,y) = \sqrt{1+4x^2+y^2}$ up to first, second, and third-order, always calculate the approximate value of $f\,(1.1,\ 2.05)$. Compare the results with the value given by a calculator.

$T_1 = 3.1\overline{66}$, $T_2 = 3.169\,120$, $T_3 = 3.168\,984$ (by calculator 3.168 990...)

9.13 Calculate all non-zero terms of Taylor expansion of the function $f(x,y,z) = x^3+y^3+z^3-3\,xyz$ and particular orders of expansion, and always calculate the value of $f\,(0.95,\ 1.05,\ 1.1)$. Compare the results with the value given by a calculator.

$T_0 = 0$, $T_1 = 0$, $T_2 = 0.0525$, $T_3 = 0.054\,25$ (by calculator 0.054 25)

9.14 Using Taylor expansion of the function $f(x,y,z) = \dfrac{1}{xyz}$ up to first, second, and third-order, always calculate the approximate value of $f\,(0.9,\ 2.1,\ 3.1)$. Compare the results with the value given by a calculator.

$T_1 = 0.169\,\overline{444}$, $T_2 = 0.170\,602...$, $T_3 = 0.170\,634...$, $T_4 = 0.170\,648...$, (by calculator 0.170 678...)

9.15 Calculate the second degree Taylor polynomial of the function $f(x,y) = \mathrm{e}^{-(x^2+y^2)}$ at the points

(a) $P_1 = [0,0]$,

(b) $P_2 = [1,2]$.

(a) $T_1(0,0) = 1 - x^2 - y^2$

(b) $T_2(1,2) = \mathrm{e}^{-5}\left[x(x+8y-20) + y(7y-40) + 56\right]$

9.16 Calculate Taylor polynomial of the function from Example 9.12

(a) of the third degree at the point $[0,0]$,

(b) of the second degree at the point $[1,2]$.

(a) $T_3(0,0) = 1 + 2x^2 + \dfrac{y^2}{2}$

(b) $T_2(1,2) = \dfrac{1}{3}\left[4x + y - 8(x-1)(y-2) - 5\right] + \dfrac{5}{27}\left[2(x-1)^2 + \dfrac{1}{2}(y-2)^2\right]$

9.17 Calculate the third degree Taylor polynomial of the function from Example 9.14 at the point $[1,1,1]$.

$T_3(1,1,1) = -x^3 - y^3 - z^3 - x^2y - x^2z - xy^2 - xz^2 - y^2z - yz^2 - xyz + 6(x^2+y^2+z^2+xy+xz+yz) - 15(x+y+z) + 20$

9.18 Write the second degree Taylor polynomial of the function $f(x,y) = \sqrt{x^2-y^2-2}$ at the point $[2,1]$.

$2x - y - 2 + \dfrac{1}{2}\left[-3(x-2)^2 + 4(x-2)(y-1) - 2(y-1)^2\right]$

9.19 Write the second degree Taylor polynomial of the function $f(x,y) = \sqrt{e^{2x} - y^2 + 1}$ at the point $[0,1]$.

$2 + x - y + \frac{1}{2}\left[x^2 + 2x(y-1) - 2(y-1)^2\right]$

9.20 Write the second degree Taylor polynomial of the function $f(x,y) = \sqrt{\frac{x}{y} - 1}$ at the point $[2,1]$.

$1 + \frac{x}{2} - y + \frac{1}{2}\left[-\frac{1}{4}(x-2)^2 + (y-1)^2\right]$

9.21 Write the second degree Taylor polynomial of the function $f(x,y) = \frac{y^2}{\sqrt{x^2+1}}$ at the point $[0,1]$.

$1 + 2(y-1) + \frac{1}{2}\left[-x^2 + 2(y-1)^2\right]$

9.22 Write the third degree Taylor polynomial of the function $f(x,y,z) = \frac{1}{x^2yz}$ at the point $[1,1,1]$.

$T_3(1,1,1) = -4x^3 - y^3 - z^3 - 3x^2y - 3x^2z - 2xy^2 - 2xz^2 - 2y^2z - yz^2 - 2xyz + 7(3x^2 + z^2 + 2xy + 2xz) + 8y^2 + 9yz - 2(21x + 11z) - 23y + 36$

Chapter 10

Fourier series[1]

The method of decomposing general periodic functions into the sum of the infinite number of sine and cosine waves was named after French mathematician Jean-Baptiste Joseph Fourier (1768–1830). Fourier series are applied to various degrees in most fields of physics, e.g., in acoustics, optics, quantum physics, etc. The principle formulated first for Fourier series was later generalized in the so-called Fourier analysis. Any periodic function $f(x)$ with a period T, integrable within the interval $\langle x_0, x_0 + T)$, can be expressed as the following infinite sum (Fourier series)

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(k\omega x) + b_k \sin(k\omega x), \tag{10.1}$$

where $\omega = 2\pi/T$. The Fourier coefficients a_k, b_k, can be determined as follows

$$a_0 = \frac{2}{T}\int_{x_0}^{x_0+T} f(x)\,\mathrm{d}x, \tag{10.2}$$

$$a_k = \frac{2}{T}\int_{x_0}^{x_0+T} f(x)\cos(k\omega x)\,\mathrm{d}x, \tag{10.3}$$

$$b_k = \frac{2}{T}\int_{x_0}^{x_0+T} f(x)\sin(k\omega x)\,\mathrm{d}x. \tag{10.4}$$

In principle, it is possible to decompose as a Fourier series also a function which contains a singularity within the period T (for example the function $1/x$, $x \in \langle -1, 1)$), with use of Equation (1.57) in Section 1.3. However, such functions usually lead to the integrals of type $\mathrm{Si}\,x$, $\mathrm{Ci}\,x$, $\mathrm{Ei}\,x$, and so on (see Example 9.6 in Section 9.1), solvable only numerically, the Fourier series itself then also contain a singularity at the singular point; Fourier coefficients can be complex terms and, moreover, the Fourier expansion of such a function has no physical meaning in principle.

For clarity, Figure 10.1 shows composite graphs of Fourier series of odd function $f(x) = x - 1$ for $x \in \langle -1, 0)$, $f(x) = x + 1$ for $x \in \langle 0, 1)$, even function $f(x) = 0$ for $x \in \langle -1, -\frac{1}{2}) \cup \langle \frac{1}{2}, 1)$, $f(x) = 1$ for $x \in \langle -\frac{1}{2}, \frac{1}{2})$, and common function $f(x) = \mathrm{e}^x$, where for all the functions the basic interval is $x \in \langle -1, 1)$, for different n, distinguished by different colors. Each n thus denotes here the highest $n_{\max}$, which forms the upper limit of the summation in Equation (10.1), instead of the ideal ∞. However, the individual n correspond only to those k in Equation (10.1), for which the Fourier coefficients a_k and/or b_k are nonzero, thus $n = k$ in the graphs in top and

[1] Recommended literature for this chapter: Dĕmidovič (2003), Kvasnica (2004), Arfken & Weber (2005).

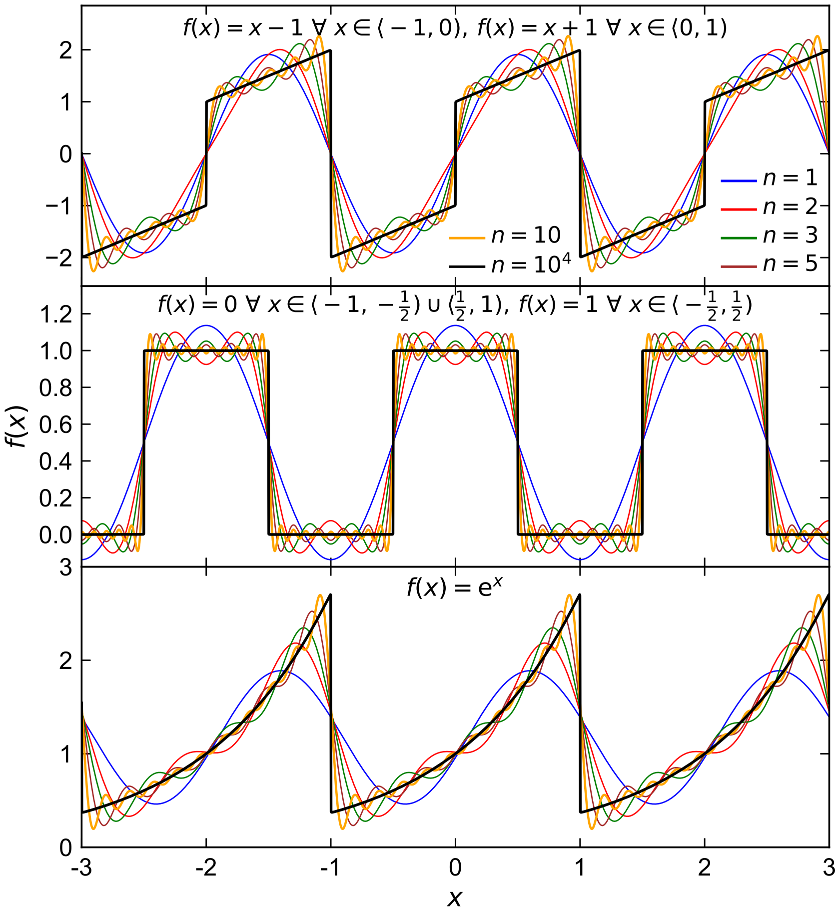

Figure 10.1: Graphs of Fourier series of functions $f(x) = x-1$ for $x \in \langle -1, 0)$, $f(x) = x+1$ for $x \in \langle 0, 1)$ (top panel), $f(x) = 0$ for $x \in \langle -1, -\frac{1}{2}) \cup \langle \frac{1}{2}, 1)$, $f(x) = 1$ for $x \in \langle -\frac{1}{2}, \frac{1}{2})$ (middle panel), and $f(x) = \mathrm{e}^x$ (bottom panel), where for all functions the basic interval is $x \in \langle -1, 1)$. Individual colors (see the legend in the top panel) denote the highest n, up to which are the particular series summed (the meaning of index n is explained in text).

bottom panels of Fig. 10.1, while $n = 2k - 1$ in the graph in middle panel. The graphs clearly illustrate how for higher n the Fourier series more and more resemble the original function with a given periodicity, when for $n \sim 10^4$ it is practically impossible to distinguish them.

The Fourier transform is a generalization of the continuous Fourier series. If we replace the discrete Fourier coefficients a_k, b_k by a continuous function $F(\xi)\,\mathrm{d}\xi$, then, assuming $1/T \to \xi$ (frequency), the discrete Fourier series transforms (by substituting sum for the integral) into a continuous form

$$F(\xi) = \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-2\pi\mathrm{i}\xi x}\,\mathrm{d}x, \qquad f(x) = \int_{-\infty}^{\infty} F(\xi)\,\mathrm{e}^{2\pi\mathrm{i}\xi x}\,\mathrm{d}\xi. \tag{10.5}$$

In physics and engineering applications, Fourier transform is written more often using *angular frequency* $\omega = 2\pi\xi$. Fourier transform $\mathcal{F}(f) = \widehat{f}$ (where $\widehat{f}$ is the so-called *Fourier image* of a function f, i.e., of the pattern) and the inverse Fourier transform $\mathcal{F}^{-1}(\widehat{f}) = f$ are then (with some loss of symmetry) defined as

$$\widehat{f}(\omega) = \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-\mathrm{i}\omega x}\,\mathrm{d}x, \qquad f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{f}(\omega)\,\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}\omega. \tag{10.6}$$

Next, we introduce the concept of the *convolution* of two functions $f(x), g(x)$ (see Figure 10.2), which is defined as

$$(f * g)(x) = \int_{-\infty}^{\infty} f(y)\, g(x-y)\, \mathrm{d}y, \tag{10.7}$$

where, however, x and y do not mean two different coordinate directions, but merely two different variables. The Fourier image of the convolution of the functions $f(x), g(x)$, will then be:

$$\widehat{(f * g)}(\omega) = \int_{-\infty}^{\infty} (f*g)(x)\, \mathrm{e}^{-\mathrm{i}\omega x}\, \mathrm{d}x = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(y)\, g(x-y)\, \mathrm{e}^{-\mathrm{i}\omega x}\, \mathrm{d}x\, \mathrm{d}y. \tag{10.8}$$

Using the transformation $\left\{\begin{matrix} x-y=z \\ y=y \end{matrix}\right\}$, whose Jacobian $\det\begin{vmatrix} \frac{\partial z}{\partial x} & \frac{\partial z}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{vmatrix} = \det\begin{vmatrix} 1 & -1 \\ 0 & 1 \end{vmatrix} = 1$, we get

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(y)\, g(z)\, \mathrm{e}^{-\mathrm{i}\,\omega(y+z)}\, \mathrm{d}y\, \mathrm{d}z = \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{-\mathrm{i}\omega y}\, \mathrm{d}y \int_{-\infty}^{\infty} g(z)\, \mathrm{e}^{-\mathrm{i}\omega z}\, \mathrm{d}z = \widehat{f}(\omega)\, \widehat{g}(\omega). \tag{10.9}$$

The resulting relation can thus be written in a simple way,

$$\widehat{(f * g)} = \widehat{f}\,\widehat{g}, \tag{10.10}$$

The Fourier image of the convolution of two functions $f(x), g(x)$, is equal to the product of their Fourier images.

An example of the convolution of two functions $f * g$, which were originally given in the form

$$f(x) = \left\{\begin{array}{cl} 0 & x \in (-\infty, 0) \\ 3\,\mathrm{e}^{-x} & x \in \langle 0, \infty), \end{array}\right. \tag{10.11}$$

$$g(x) = \left\{\begin{array}{ll} 0 & x \in (-\infty, 0) \\ 1 & x \in \langle 0, 2\rangle \\ 0 & x \in (2, \infty), \end{array}\right. \tag{10.12}$$

is shown in Figure 10.2. We transform the functions f, g according to Equation (10.7) as follows:

$$f(x) = 3\,\mathrm{e}^{-x} \quad \to \quad f(y) = 3\,\mathrm{e}^{-y}, \tag{10.13}$$

$$g(x) \quad \to \quad g\,(x-y) \quad = \quad g\,(z)\,, \tag{10.14}$$

where then for the function $g\,(z)$ (convolution kernel) holds $g(z) = 1$ for $z \in \langle 0, 2\rangle$ (and so $y \in \langle x, x-2\rangle$) and $g(z) = 0$ for $z \notin \langle 0, 2\rangle$ (and so $y \notin \langle x, x-2\rangle$). Simultaneously there also applies $\mathrm{d}z = -\mathrm{d}y$. Since $f(y) = 0$ for $y < 0$, we get thus three regions of integration of Equation (10.7),

$$x-2 < 0 \wedge x < 0 \qquad \text{(Figure 10.2a)}, \tag{10.15}$$

$$x-2 < 0 \wedge x \geq 0 \qquad \text{(Figure 10.2b)}, \tag{10.16}$$

$$x-2 \geq 0 \wedge x > 0 \qquad \text{(Figure 10.2c)}. \tag{10.17}$$

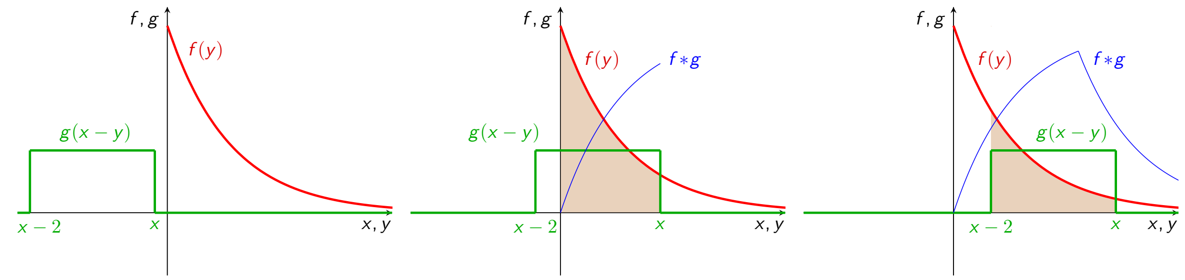

Figure 10.2a Figure 10.2b Figure 10.2c

Figure 10.2: Scheme of convolution $f * g$ of functions $f(x)$, $g(x)$, initially described by Equations (10.11) and (10.12). Figure 10.2a shows the case $x \in (-\infty, 0)$ in Equations (10.13) and (10.14); in Figure 10.2b, there is $x \in \langle 0, 2\rangle$; in Figure 10.2c, there is $x \in (2, \infty)$. The profile of the resulting function $(f * g)(x)$ is highlighted by blue color; the function is described in Equation (10.18), and its value will be for each x equal to the size of the highlighted area.

Integration of Equation (10.7) will for these three regions take the form

$$(f * g)(x) = \begin{cases} 0 & \text{for } x \in (-\infty, 0) \\ 3\displaystyle\int_0^x \mathrm{e}^{-y}\,\mathrm{d}y = 3\left(1 - \mathrm{e}^{-x}\right) & \text{for } x \in \langle 0, 2\rangle, \\ 3\displaystyle\int_{x-2}^x \mathrm{e}^{-y}\,\mathrm{d}y = 3\,\mathrm{e}^{-x}\left(\mathrm{e}^2 - 1\right) & \text{for } x \in (2, \infty). \end{cases} \tag{10.18}$$

Convolution of two functions $f(x)$ and $g(x)$ will thus become the function $(f * g)(x)$, whose value for each $x \in (-\infty, \infty)$ will be equal to the size of the highlighted area in Figure 10.2.

10.1 Fourier series

- **Examples:**

Write the Fourier series for the following periodic functions with a period T:

10.1 $f(x) = \dfrac{x^2}{\pi}$, $x \in \langle -\pi, \pi)$, $T = 2\pi$ $\qquad \dfrac{\pi}{3} + \dfrac{4}{\pi}\displaystyle\sum_{k=1}^{\infty} \frac{(-1)^k}{k^2}\cos(kx)$

10.2 $f(x) = \dfrac{x^2}{\pi}$, $x \in \langle 0, 2\pi)$, $T = 2\pi$ $\qquad \dfrac{4\pi}{3} + 4\displaystyle\sum_{k=1}^{\infty}\left[\frac{1}{k^2\pi}\cos(kx) - \frac{1}{k}\sin(kx)\right]$

10.3 $f(x) = |x|$, $x \in \langle -\pi, \pi)$, $T = 2\pi$ $\qquad \dfrac{\pi}{2} + \dfrac{2}{\pi}\displaystyle\sum_{k=1}^{\infty} \frac{(-1)^k - 1}{k^2}\cos(kx)$

10.4 $f(x) = x|x|$, $x \in \langle -L, L)$, $T = 2L$ $\qquad \dfrac{2L^2}{\pi^3}\displaystyle\sum_{k=1}^{\infty} \frac{(2 - \pi^2 k^2)(-1)^k - 2}{k^3}\sin\left(\frac{k\pi}{L}x\right)$

10.5 $f(x) = \dfrac{|x^3|}{x}$, $x \in \langle -1, 1)$, $T = 2$ $\qquad \dfrac{2}{\pi^3}\displaystyle\sum_{k=1}^{\infty} \frac{(2 - \pi^2 k^2)(-1)^k - 2}{k^3}\sin(k\pi x)$

10.6 $f(x) = \begin{cases} 0 & x \in \langle 0, 1) \\ x-1 & x \in \langle 1, 2) \end{cases}$, $T = 2$ $\quad \dfrac{1}{4} + \sum_{k=1}^{\infty} \left[\dfrac{1-(-1)^k}{k^2\pi^2} \cos(k\pi x) - \dfrac{1}{k\pi} \sin(k\pi x) \right]$

10.7 $f(x) = \mathrm{e}^{ax}$, $x \in \langle -\pi, \pi)$, constant $a \neq 0$, $T = 2\pi$

$$\frac{2}{\pi} \sinh(a\pi) \left\{ \frac{1}{2a} + \sum_{k=1}^{\infty} \left[\frac{(-1)^k}{a^2+k^2} \left[a\cos(kx) - k\sin(kx) \right] \right] \right\}$$

10.8 $f(x) = (x-1)(x-3)$, $x \in \langle 1, 3)$, $T = 2$ $\quad -\dfrac{2}{3} + \dfrac{4}{\pi^2} \sum_{k=1}^{\infty} \dfrac{(-1)^k}{k^2} \cos(k\pi x)$

10.9 $f(x) = \dfrac{x}{2L}$, $x \in \langle 0, 2L)$, $T = 2L$ $\quad \dfrac{1}{2} - \dfrac{1}{\pi} \sum_{k=1}^{\infty} \dfrac{1}{k} \sin\left(\dfrac{k\pi}{L} x\right)$

10.10 $f(x) = x^4$, $x \in \langle -1, 1)$, $T = 2$ $\quad \dfrac{1}{5} + \dfrac{8}{\pi^4} \sum_{k=1}^{\infty} (-1)^k \dfrac{k^2\pi^2 - 6}{k^4} \cos(k\pi x)$

10.11 $f(x) = \operatorname{sgn}\left[\sin\left(\dfrac{\pi x}{L}\right)\right]$, $x \in \langle 0, 2L)$, $T = 2L$

$$\frac{4}{\pi} \sum_{k=0}^{\infty} \frac{1}{2k+1} \sin\left[\frac{(2k+1)\pi}{L} x\right]$$

10.12 $f(x) = \begin{cases} -x & x \in \langle -1, 0) \\ x & x \in \langle 0, 1) \end{cases}$, $T = 2$ $\quad \dfrac{1}{2} - \dfrac{4}{\pi^2} \sum_{k=0}^{\infty} \dfrac{1}{(2k+1)^2} \cos\left[(2k+1)\pi x\right]$

10.13 $f(x) = \begin{cases} 1 & x \in \left\langle 0, \dfrac{\pi}{2}\right) \\ -1 & x \in \left\langle -\dfrac{\pi}{2}, 0\right) \\ 0 & |x| \in \left\langle \dfrac{\pi}{2}, \pi\right) \end{cases}$, $T = 2\pi$ $\quad \dfrac{2}{\pi} \sum_{k=1}^{\infty} \dfrac{1}{4k-2} \left\{ 1 - \cos\left[(4k-2)\dfrac{\pi}{2}\right] \right\} \sin\left[(4k-2)x\right]$

10.14 $f(x) = \begin{cases} 0 & x \in \left\langle -1, -\dfrac{1}{2}\right) \\ \cos 3\pi x & x \in \left\langle -\dfrac{1}{2}, \dfrac{1}{2}\right) \\ 0 & x \in \left\langle \dfrac{1}{2}, 1\right) \end{cases}$, $T = 2$

$$-\frac{1}{3\pi} + \frac{6\cos(2\pi x)}{5\pi} + \frac{\cos(3\pi x)}{2} + \frac{6}{\pi} \sum_{k=4}^{\infty} \frac{1}{\widetilde{k}^2 - 9} \cos\left(\frac{\widetilde{k}\pi}{2}\right) \cos(\widetilde{k}\pi x), \quad \text{where} \quad \widetilde{k} = 2k-4$$

10.15 $f(x) = \begin{cases} 1 & x \in \langle -1, 0) \\ \dfrac{1}{2} & x = 0 \\ x & x \in (0, 1) \end{cases}$, $T = 2$ $\quad \dfrac{3}{4} + \sum_{k=1}^{\infty} \left[\dfrac{(-1)^k - 1}{k^2\pi^2} \cos(k\pi x) - \dfrac{1}{k\pi} \sin(k\pi x) \right]$

10.16 $f(x) = \begin{cases} \dfrac{4}{\pi} x & x \in \left\langle 0, \dfrac{\pi}{2}\right) \\ -\dfrac{4}{\pi} x & x \in \left\langle -\dfrac{\pi}{2}, 0\right) \end{cases}$, $T = \pi$ $\quad 1 - \dfrac{8}{\pi^2} \sum_{k=1}^{\infty} \dfrac{\cos\left[2\left(2k-1\right)x\right]}{(2k-1)^2}$

10.17 $f(x)=\begin{cases} x\,(1-x) & x\in\langle 0,1)\\ 0 & x\in\langle -1,0)\end{cases}$, $T=2$

$$\frac{1}{12}-\frac{1}{\pi^2}\sum_{k=1}^{\infty}\left\{\frac{1}{k^2}\left[1+(-1)^k\right]\cos(k\pi x)-\frac{2}{k^3\pi}\left[1-(-1)^k\right]\sin(k\pi x)\right\}$$

10.18 $f(x)=|\sin x|,\ x\in\langle -\pi,\pi),\ T=2\pi$ $\quad \frac{2}{\pi}-\frac{4}{\pi}\sum_{k=1}^{\infty}\frac{1}{(4k^2-1)}\cos(2kx)$

10.19 $f(x)=|\cos x|,\ x\in\langle -\pi,\pi),\ T=2\pi$ $\quad \frac{2}{\pi}-\frac{4}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k}{(4k^2-1)}\cos(2kx)$

10.20 $f(x)=\sin x\cos x,\ x\in\langle -1,1)$ $\quad \pi\sin(2)\sum_{k=1}^{\infty}\frac{k(-1)^k}{4-k^2\pi^2}\sin(k\pi x)$

10.21 $f(x)=|x|+a,\ x\in\langle -L,L)$, where a is a constant.

$$a+\frac{L}{2}-\frac{4L}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2}\cos\left[\frac{(2k-1)\pi}{L}x\right]$$

10.22 $f(x)=\begin{cases} x-a & x\in\langle -L,0)\\ x+a & x\in\langle 0,L)\end{cases}$, where a is a constant.

$$\frac{2}{\pi}\sum_{k=1}^{\infty}\frac{a-(a+L)(-1)^k}{k}\sin\left(\frac{k\pi}{L}x\right)$$

10.23 (a) $f(x)=x,\ x\in\langle 2,3)$ $\quad \frac{5}{2}-\frac{1}{\pi}\sum_{k=1}^{\infty}\frac{1}{k}\sin\left(2k\pi x\right)$

(b) $f(x)=\begin{cases} x,\ x\in\langle -3,-2)\\ 0,\ x\in\langle -2,2)\\ x,\ x\in\langle 2,3)\end{cases}$

$$-\frac{6}{\pi}\sum_{k=1}^{\infty}\left[\frac{(-1)^k}{k}-\frac{2}{3k}\cos\left(\frac{2k\pi}{3}\right)+\frac{1}{k^2\pi}\sin\left(\frac{2k\pi}{3}\right)\right]\sin\left(\frac{k\pi}{3}x\right)$$

10.2 Fourier analysis ★

We are interested in all "signals" defined for all t (here, the time independent variable): The Fourier transform of the signal f is defined by the function

$$\widehat{f}(\omega)=\int_{-\infty}^{\infty}f(t)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t. \tag{10.19}$$

The value of the function $\widehat{f}(\omega)$ (often referred to as $F(\omega)$) is, in general, a complex number

$$\widehat{f}(\omega)=\int_{-\infty}^{\infty}f(t)\cos\omega t\,\mathrm{d}t-\mathrm{i}\int_{-\infty}^{\infty}f(t)\sin\omega t\,\mathrm{d}t, \tag{10.20}$$

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

where $|\widehat{f}(\omega)|$ is the *amplitude spectrum* of the function f and $\angle\widehat{f}(\omega)$ is often referred to as the *phase spectrum* of the function f.

Fourier and Laplace transforms (see Appendix A) of the function f are defined very similarly, with two differences:

- the integration range of the Laplace transform is $0 \le t < \infty$; the integration range of the Fourier transform is $-\infty < t < \infty$,
- Laplace transform: s can be any complex number in *region of convergence* (ROC); Fourier transform: $\mathrm{i}\omega$ lies on *imaginary axis*,

so,

- if $f(t) = 0\ \forall\ t < 0$:
  - if the imaginary axis lies inside the ROC of Laplace transform, then $\widehat{f}(\omega) = F(\mathrm{i}\omega)$ (where F denotes the Laplace image - see Appendix A), i.e. the Fourier transform is identical to the Laplace transform restricted to the imaginary axis,
  - if the imaginary axis does not lie inside the ROC of the Laplace transform, then the Fourier transform does not exist (but the Laplace transform does, at least for all s inside the ROC)
- if $f(t) \neq 0\ \forall\ t < 0$, then the Fourier and Laplace images can be very different.

Properties of the Fourier transform:

- linearity: $$a f(t) + b g(t) \quad\to\quad a\widehat{f}(\omega) + b\widehat{g}(\omega) \tag{10.21}$$
- time scale: $$f(at) \quad\to\quad \frac{1}{|a|}\widehat{f}\left(\frac{\omega}{a}\right) \tag{10.22}$$
- time shift: $$f(t-T) \quad\to\quad \mathrm{e}^{-\mathrm{i}\omega T}\widehat{f}(\omega) \tag{10.23}$$
- differentiation: $$\frac{\mathrm{d}^k f(t)}{\mathrm{d}t^k} \quad\to\quad (\mathrm{i}\omega)^k \widehat{f}(\omega) \tag{10.24}$$
- integration: $$\int_{-\infty}^{t} f(\tau)\,\mathrm{d}\tau \quad\to\quad \frac{\widehat{f}(\omega)}{\mathrm{i}\omega} + \pi\widehat{f}(0)\delta(\omega) \tag{10.25}$$
- multiplication by t: $$t^k f(t) \quad\to\quad \mathrm{i}^k \frac{\mathrm{d}^k \widehat{f}(\omega)}{\mathrm{d}\omega^k} \tag{10.26}$$
- convolution: $$\int_{-\infty}^{\infty} f(\tau)g(t-\tau)\,\mathrm{d}\tau \quad\to\quad \widehat{f}(\omega)\,\widehat{g}(\omega) \tag{10.27}$$
- multiplication: $$f(t)\,g(t) \quad\to\quad \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{f}(\widetilde{\omega})\,\widehat{g}(\omega-\widetilde{\omega})\,\mathrm{d}\widetilde{\omega}. \tag{10.28}$$

- **Illustrating solved examples of the Fourier transform:** ★
  - "Single-sided" decreasing exponential $f(t) = \begin{cases} 0 & t < 0 \\ \mathrm{e}^{-t} & t \ge 0 \end{cases}$. The Laplace image in this case is $F(s) = 1/(s+1)$ and thus the ROC $\{s \,|\, \mathrm{Re}\, s > -1\}$, the imaginary axis lies inside the ROC of the Laplace transform and the Fourier transform therefore exists:
  $$\widehat{f}(\omega) = \int_{-\infty}^{\infty} f(t)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = \int_{0}^{\infty} \mathrm{e}^{-(1+\mathrm{i}\omega)t}\,\mathrm{d}t = \frac{1}{1+\mathrm{i}\omega} = F(\mathrm{i}\omega). \tag{10.29}$$

- "Single-sided" rising exponential $f(t) = \begin{cases} 0 & t < 0 \\ \mathrm{e}^t & t \geq 0 \end{cases}$. The Laplace image in this case is $F(s) = 1/(s-1)$ and thus the ROC $\{s \,|\, \mathrm{Re}\, s > 1\}$, the imaginary axis lies outside the ROC of the Laplace transform, the Fourier transform does not exist in this case.

- A bilaterally "decreasing" exponential of the form $f(t) = \mathrm{e}^{-\alpha|t|}$ (constant $\alpha > 0$),

$$\widehat{f}(\omega) = \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha|t|}\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = \int_{-\infty}^{0} \mathrm{e}^{(\alpha-\mathrm{i}\omega)t}\,\mathrm{d}t + \int_{0}^{\infty} \mathrm{e}^{-(\alpha+\mathrm{i}\omega)t}\,\mathrm{d}t = \frac{2\alpha}{\alpha^2+\omega^2}. \tag{10.30}$$

- Rectangular pulse $f(t) = \begin{cases} 1 & -T \leq t \leq T \\ 0 & |t| > T \end{cases}$,

$$\widehat{f}(\omega) = \int_{-T}^{T} \mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = \frac{-1}{\mathrm{i}\omega}\left(\mathrm{e}^{-\mathrm{i}\omega T} - \mathrm{e}^{\mathrm{i}\omega T}\right) = \frac{2\sin\omega T}{\omega}. \tag{10.31}$$

- Offset rectangular pulse $f(t) = \begin{cases} 1 & 1-T \leq t \leq 1+T \\ 0 & t < 1-T \text{ nebo } t > 1+T \end{cases}$,

$$\widehat{f}(\omega) = \int_{1-T}^{1+T} \mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = \frac{-1}{\mathrm{i}\omega}\left[\mathrm{e}^{-\mathrm{i}\omega(1+T)} - \mathrm{e}^{-\mathrm{i}\omega(1-T)}\right] = \frac{2\sin\omega T}{\omega}\,\mathrm{e}^{-\mathrm{i}\omega}. \tag{10.32}$$

- Pulse in the form of δ function: $f(t) = \delta(t)$,

$$\widehat{f}(\omega) = \int_{-\infty}^{\infty} \delta(t)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = 1. \tag{10.33}$$

- Constant signals: $f(t) = C$,

$$\widehat{f}(\omega) = C\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t. \tag{10.34}$$

The given integral does not converge in the upper or lower bound (be careful not to confuse with the real exponent function, which would converge to zero in the upper bound and diverge in the lower bound), but the solution can easily be found using the inverse Fourier transform,

$$C = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{f}(\omega)\,\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}\omega \quad \text{and so} \quad \widehat{f}(\omega) = 2\pi C\delta(\omega). \tag{10.35}$$

- The function $\mathrm{sgn}(t)$: $f(t) = \begin{cases} -1 & t < 0 \\ 1 & t > 0 \end{cases}$. The imaginary axis in this case does not lie inside the ROC of Laplace transform, but it is "infinitesimally" close, so a solution can be found using the limit $f(t) = \lim\limits_{\alpha\to 0} \mathrm{e}^{-\alpha|t|}\,\mathrm{sgn}(t)$:

$$\widehat{f}(\omega) = \lim_{\alpha\to 0}\left[-\int_{-\infty}^{0} \mathrm{e}^{(\alpha-\mathrm{i}\omega)t}\,\mathrm{d}t + \int_{0}^{\infty} \mathrm{e}^{-(\alpha+\mathrm{i}\omega)t}\,\mathrm{d}t\right] = \tag{10.36}$$

$$= \lim_{\alpha\to 0}\left[-\int_{0}^{\infty} \mathrm{e}^{-(\alpha-\mathrm{i}\omega)t}\,\mathrm{d}t + \int_{0}^{\infty} \mathrm{e}^{-(\alpha+\mathrm{i}\omega)t}\,\mathrm{d}t\right] = \tag{10.37}$$

$$= \lim_{\alpha\to 0}\left[\frac{-1}{\alpha-\mathrm{i}\omega} + \frac{1}{\alpha+\mathrm{i}\omega}\right] = \frac{2}{\mathrm{i}\omega}. \tag{10.38}$$

- Heaviside function: $f(t) = \begin{cases} 0 & t < 0 \\ 1 & t > 0 \end{cases}$. The imaginary axis in this case again does not lie inside the ROC of Laplace transform, but is "infinitesimally" close; the solution can be found by combining the constant signal $C = 1$ and the function $\mathrm{sgn}(t)$: $f(t) = \frac{1}{2}\left[1 + \mathrm{sgn}(t)\right)$,

$$\widehat{f}(\omega) = \pi\delta(\omega) + \frac{1}{\mathrm{i}\omega}. \tag{10.39}$$

- Sinusoidal signal with constant frequency: $f(t) = \sin(\omega_0 t) = \left(\mathrm{e}^{\mathrm{i}\omega_0 t} - \mathrm{e}^{-\mathrm{i}\omega_0 t}\right)/(2\mathrm{i})$. Similar to some of the previous cases, we can find the Fourier image using the inverse transform, where

$$\mathrm{e}^{\mathrm{i}\omega_0 t} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{f}_+(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}\omega \quad \text{and so} \quad \widehat{f}_+(\omega) = 2\pi\delta(\omega - \omega_0), \tag{10.40}$$

$$\mathrm{e}^{-\mathrm{i}\omega_0 t} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{f}_-(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}\omega \quad \text{and so} \quad \widehat{f}_-(\omega) = 2\pi\delta(\omega + \omega_0). \tag{10.41}$$

  The entire Fourier image will be

$$\widehat{f}(\omega) = \frac{1}{2\mathrm{i}}\left(\widehat{f}_+(\omega) - \widehat{f}_-(\omega)\right) = -\mathrm{i}\pi\delta(\omega - \omega_0) + \mathrm{i}\pi\delta(\omega + \omega_0). \tag{10.42}$$

- Cosinusoidal signal with constant frequency: $f(t) = \cos(\omega_0 t) = \left(\mathrm{e}^{\mathrm{i}\omega_0 t} + \mathrm{e}^{-\mathrm{i}\omega_0 t}\right)/2$. In the same way as in the case of the previous sinusoidal signal, we arrive at the Fourier image

$$\widehat{f}(\omega) = \frac{1}{2}\left(\widehat{f}_+(\omega) + \widehat{f}_-(\omega)\right) = \pi\delta(\omega - \omega_0) + \pi\delta(\omega + \omega_0). \tag{10.43}$$

- **Examples:** ★

Determine the convolution of the functions $(f * g)(x)$:

10.24 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ 2 & x \in \langle 0, \infty) \end{cases}$ $g(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 & x \in \langle 0, \infty) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ 2x & x \in \langle 0, \infty) \end{cases}$

10.25 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \mathrm{e}^{-2x} & x \in \langle 0, \infty) \end{cases}$ $g(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \mathrm{e}^{-x} & x \in \langle 0, \infty) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ \mathrm{e}^{-x}\left(1 - \mathrm{e}^{-x}\right) & x \in \langle 0, \infty) \end{cases}$

10.26 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \mathrm{e}^{-x} & x \in \langle 0, \infty) \end{cases}$ $g(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \sin x & x \in \langle 0, \infty) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ \frac{1}{2}\left(\mathrm{e}^{-x} + \sin x - \cos x\right) & x \in \langle 0, \infty) \end{cases}$

10.27 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \sin x & x \in \langle 0, \infty) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 - \cos x & x \in \langle 0, \infty) \end{cases}$

$g(x) = 1$

10.28 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \sin x & x \in \langle 0, \infty) \end{cases}$

$g(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 & x \in \left\langle 0, \frac{\pi}{2} \right\rangle \\ 0 & x \in \left(\frac{\pi}{2}, \infty \right) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 - \cos x & x \in \left\langle 0, \frac{\pi}{2} \right\rangle \\ \sin x - \cos x & x \in \left(\frac{\pi}{2}, \infty \right) \end{cases}$

10.29 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \sin x & x \in \langle 0, \infty) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ \frac{1}{a^2 - 1} [a \sin x - \sin(ax)] & x \in \langle 0, \infty) \end{cases}$

$g(x) = \sin(ax)$, $a > 0$

10.30 $f(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ \sin x & x \in \langle 0, \infty) \end{cases}$

$g(x) = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 - \frac{2}{\pi} x & x \in \left\langle 0, \frac{\pi}{2} \right\rangle \\ 0 & x \in \left(\frac{\pi}{2}, \infty \right) \end{cases}$ $\qquad f * g = \begin{cases} 0 & x \in (-\infty, 0) \\ 1 - \frac{2}{\pi} x + \frac{2}{\pi} \sin x - \cos x & x \in \left\langle 0, \frac{\pi}{2} \right\rangle \\ \frac{2}{\pi} (\sin x + \cos x) - \cos x & x \in \left(\frac{\pi}{2}, \infty \right) \end{cases}$

10.31 Find the Fourier image of the functions:

(a) $f(x) = 1$ for $x \in \left\langle -\frac{1}{2}, \frac{1}{2} \right\rangle$, $f(x) = 0$ for $x \notin \left\langle -\frac{1}{2}, \frac{1}{2} \right\rangle$,

(b) $f(x) = \mathrm{e}^{-bx}$ for $x \in \langle 0, \infty)$, $f(x) = 0$ for $x \in (-\infty, 0)$, $\quad b > 0 = \text{const.}$,

(c) $f(x) = \mathrm{e}^{-b|x|}$ for $x \in (-\infty, \infty)$,

(d) $f(x) = \mathrm{e}^{-bx^2}$ for $x \in (-\infty, \infty)$,

(e) $f(x) = 1 + x$ for $x \in \langle -1, 0)$, $f(x) = 1 - x$ for $x \in \langle 0, 1)$, $f(x) = 0$ for $|x| > 1$,

(f) $f(x) = x^2$ for $x \in \langle -1, 1 \rangle$, $f(x) = 0$ for $|x| > 1$.

(a) $\widehat{f}(\omega) = \frac{2}{\omega} \sin\left(\frac{\omega}{2}\right)$

(b) $\widehat{f}(\omega) = \frac{1}{b + \mathrm{i}\omega}$

(c) $\widehat{f}(\omega) = \frac{2b}{b^2 + \omega^2}$

(d) $\widehat{f}(\omega) = \sqrt{\frac{\pi}{b}}\, \mathrm{e}^{-\frac{\omega^2}{4b}}$

(e) $\widehat{f}(\omega) = \frac{2}{\omega^2} (1 - \cos\omega)$

(f) $\widehat{f}(\omega) = \dfrac{2}{\omega^3}\left[(\omega^2 - 2)\sin\omega + 2\omega\cos\omega\right]$

10.32 Find the Fourier image of the functions:

(a) $f(x) = \sin x$ for $x \in \langle 0, 2\pi\rangle$, $f(x) = 0$ for $x \notin \langle 0, 2\pi\rangle$, $\widehat{f}(\omega) = \dfrac{\mathrm{i}\omega\left(1 - \mathrm{e}^{-2\pi\mathrm{i}\omega}\right)}{1-\omega^2}$

(b) $f(x) = \cos x$ for $x \in \langle 0, 2\pi\rangle$, $f(x) = 0$ for $x \notin \langle 0, 2\pi\rangle$, $\widehat{f}(\omega) = -\dfrac{1 - \mathrm{e}^{-2\pi\mathrm{i}\omega}}{\omega^2 - 1}$

(c) $f(x) = \sin x\cos x$ for $x \in \langle 0, 2\pi\rangle$, $f(x) = 0$ for $x \notin \langle 0, 2\pi\rangle$, $\widehat{f}(\omega) = -\dfrac{1 - \mathrm{e}^{-2\pi\mathrm{i}\omega}}{\omega^2 - 4}$

(d) $f(x) = \sin^2 x\cos^2 x$ for $x \in \langle 0, 2\pi\rangle$, $f(x) = 0$ for $x \notin \langle 0, 2\pi\rangle$, $\widehat{f}(\omega) = -\dfrac{2\mathrm{i}\left(1 - \mathrm{e}^{-2\pi\mathrm{i}\omega}\right)}{\omega\left(\omega^2 - 16\right)}$

(e) $f(x) = A^{Bx}$ for $x \in \langle 0, 1\rangle$, $f(x) = 0$ for $x \notin \langle 0, 1\rangle$. $\widehat{f}(\omega) = \dfrac{1 - \mathrm{e}^{-\mathrm{i}\omega}A^B}{\mathrm{i}\omega - B\ln A}$

10.33 Verify Equation (10.10) using Examples 10.24, 10.25, 10.26, and 10.27:

(a) (10.24): $\widehat{f}(\omega) = -\dfrac{2\mathrm{i}}{\omega}$, $\widehat{g}(\omega) = -\dfrac{\mathrm{i}}{\omega}$, $\widehat{(f*g)}(\omega) = -\dfrac{2}{\omega^2}$

(b) (10.25): $\widehat{f}(\omega) = \dfrac{1}{2+\mathrm{i}\omega}$, $\widehat{g}(\omega) = \dfrac{1}{1+\mathrm{i}\omega}$, $\widehat{(f*g)}(\omega) = \dfrac{1}{2-\omega^2+3\mathrm{i}\omega}$

(c) (10.26): $\widehat{f}(\omega) = \dfrac{1}{1+\mathrm{i}\omega}$, $\widehat{g}(\omega) = \dfrac{1}{1-\omega^2}$, $\widehat{(f*g)}(\omega) = \dfrac{1}{(1+\mathrm{i}\omega)(1-\omega^2)}$

(d) (10.27): $\widehat{f}(\omega) = \dfrac{1}{1-\omega^2}$, $\widehat{g}(\omega) = \dfrac{1}{\mathrm{i}\omega}$, $\widehat{(f*g)}(\omega) = \dfrac{1}{\mathrm{i}\omega(1-\omega^2)}$

Chapter 11

Introduction to complex analysis[1]

11.1 Complex numbers

Algebraic notation of a complex number (complex variable) $z \in \mathbb{C}$ takes the form

$$z = x + \mathrm{i}y, \tag{11.1}$$

where $x = \mathrm{Re}\, z$ is the *real* part of a complex number and $y = \mathrm{Im}\, z$ is the *imaginary* part of a complex number. The so-called *imaginary (complex) unit* i is defined as

$$\mathrm{i} \equiv \sqrt{-1}. \tag{11.2}$$

Thus, for any $k \in \mathbb{Z}$, the following periodically repeating identities,

$$\mathrm{i}^{4k} = 1, \quad \mathrm{i}^{4k+1} = \mathrm{i}, \quad \mathrm{i}^{4k+2} = -1, \quad \mathrm{i}^{4k+3} = -\mathrm{i}, \tag{11.3}$$

hold. A number z^* (also denoted $\bar{z}$) is called the *complex conjugate* to a number z, where $z^* = x - \mathrm{i}y$. For the sum, product, and ratio of two complex numbers $z_1 = x_1 + \mathrm{i}y_1$, $z_2 = x_2 + \mathrm{i}y_2$, the following (easily derivable) rules apply

$$z_1 + z_2 = (x_1 + x_2) + \mathrm{i}(y_1 + y_2), \tag{11.4}$$

$$z_1 z_2 = (x_1 x_2 - y_1 y_2) + \mathrm{i}(x_1 y_2 + x_2 y_1), \tag{11.5}$$

$$\frac{z_1}{z_2} = \frac{z_1}{z_2}\frac{z_2^*}{z_2^*} = \left(\frac{x_1 x_2 + y_1 y_2}{x_2^2 + y_2^2}\right) + \mathrm{i}\left(\frac{x_2 y_1 - x_1 y_2}{x_2^2 + y_2^2}\right), \tag{11.6}$$

where the first bracket represents the real part and the second bracket represents the imaginary part of the resulting complex number. Other operations (inverse value, powers, etc.) can be derived analogously.

Complex numbers can be written in *goniometric* or *exponential* form,

$$z = r(\cos\varphi + \mathrm{i}\sin\varphi) = r\,\mathrm{e}^{\mathrm{i}\varphi}, \tag{11.7}$$

where $r = |z| = \sqrt{x^2 + y^2}$ is the *absolute value of a complex number* (norm, module) and the oriented angle $\varphi = \arccos(x/r) = \arcsin(y/r) = \arctan(y/x)$ is the *argument* (phase) of a *complex number* (the denominator of Equation (11.6) demonstrates the relation $zz^* = |z|^2$). Exponential or trigonometric form of the complex number also allows for easy multiplication,

[1]Recommended literature for this chapter: Jefgafrov et al. (1976), Kvasnica (2004), Arfken & Weber (2005).

division, and exponentiation (see Euler's identity in Example 9.7) in particular. If we write two different complex numbers as $z_1 = r_1\,\mathrm{e}^{\mathrm{i}\varphi_1}$, $z_2 = r_2\,\mathrm{e}^{\mathrm{i}\varphi_2}$, their product and ratio will be

$$z_1 z_2 = r_1 r_2\,\mathrm{e}^{\mathrm{i}(\varphi_1+\varphi_2)} = r_1 r_2\left[\cos(\varphi_1+\varphi_2) + \mathrm{i}\sin(\varphi_1+\varphi_2)\right], \tag{11.8}$$

$$\frac{z_1}{z_2} = \frac{r_1}{r_2}\,\mathrm{e}^{\mathrm{i}(\varphi_1-\varphi_2)} = \frac{r_1}{r_2}\left[\cos(\varphi_1-\varphi_2) + \mathrm{i}\sin(\varphi_1-\varphi_2)\right]. \tag{11.9}$$

These rules can be easily generalized to any number of complex numbers. For any rational power of a complex number $z^{m/n}$, where $m \in \mathbb{Z}$, $n \in \mathbb{N}$, $n \neq 0$, the relation (the so-called *generalized de Moivre's formula*)

$$(x+\mathrm{i}y)^{m/n} = r^{m/n}\,\mathrm{e}^{\mathrm{i}(m\varphi+2k\pi)/n} = \tag{11.10}$$

$$= r^{m/n}\left[\cos\left(\frac{m\varphi+2k\pi}{n}\right) + \mathrm{i}\sin\left(\frac{m\varphi+2k\pi}{n}\right)\right], \tag{11.11}$$

where $k = 0, 1, \ldots, n-1$, also holds.

- **Examples:**

11.1 Write the given complex numbers always in the other forms (algebraic, trigonometric or exponential):

(a) $5\sqrt{3} + 5\mathrm{i}$ $\quad 10\left(\cos\frac{\pi}{6} + \mathrm{i}\sin\frac{\pi}{6}\right)$ $\quad 10\,\mathrm{e}^{\frac{\pi\mathrm{i}}{6}}$

(b) $3\sqrt{2} + 3\sqrt{2}\mathrm{i}$ $\quad 6\left(\cos\frac{\pi}{4} + \mathrm{i}\sin\frac{\pi}{4}\right)$ $\quad 6\,\mathrm{e}^{\frac{\pi\mathrm{i}}{4}}$

(c) $-12\left(1 - \frac{\mathrm{i}}{\sqrt{3}}\right)$ $\quad 8\sqrt{3}\left(\cos\frac{5\pi}{6} + \mathrm{i}\sin\frac{5\pi}{6}\right)$ $\quad 8\sqrt{3}\,\mathrm{e}^{\frac{5\pi\mathrm{i}}{6}}$

(d) $-6 + \frac{6\,\mathrm{i}}{\sqrt{3}}$ $\quad \frac{12}{\sqrt{3}}\left(\cos\frac{5\pi}{6} + \mathrm{i}\sin\frac{5\pi}{6}\right)$ $\quad \frac{12}{\sqrt{3}}\,\mathrm{e}^{\frac{5\pi\mathrm{i}}{6}}$

(e) $-2\left(1 + \sqrt{3}\mathrm{i}\right)$ $\quad 4\left(\cos\frac{4\pi}{3} + \mathrm{i}\sin\frac{4\pi}{3}\right)$ $\quad 4\,\mathrm{e}^{\frac{4\pi\mathrm{i}}{3}}$

(f) $3\left(\cos\frac{5\pi}{4} + \mathrm{i}\sin\frac{5\pi}{4}\right)$ $\quad -\frac{3}{\sqrt{2}}(1+\mathrm{i})$ $\quad 3\,\mathrm{e}^{\frac{5\pi\mathrm{i}}{4}}$

(g) $12\left(\cos\frac{\pi}{6} - \mathrm{i}\sin\frac{\pi}{6}\right)$ $\quad 6\sqrt{3} - 6\mathrm{i}$ $\quad 12\,\mathrm{e}^{-\frac{\pi\mathrm{i}}{6}}$

(h) $-2\left(\cos\frac{\pi}{6} + \mathrm{i}\sin\frac{\pi}{6}\right)$ $\quad -\left(\sqrt{3} + \mathrm{i}\right)$ $\quad 2\,\mathrm{e}^{\frac{7\pi\mathrm{i}}{6}}$

(i) $3\left(\cos\frac{\pi}{3} + \mathrm{i}\cos\frac{5\pi}{6}\right)$ $\quad \frac{3}{2}\left(1 - \sqrt{3}\mathrm{i}\right)$ $\quad 2\,\mathrm{e}^{\frac{5\pi\mathrm{i}}{3}}$

(j) $2^{7/10}\left(\sin\frac{3\pi}{20} + \mathrm{i}\cos\frac{3\pi}{20}\right)$ $\quad (1+\mathrm{i})^{7/5}$ $\quad 2^{7/10}\,\mathrm{e}^{\frac{7\pi\mathrm{i}}{20}}$

(k) $3\,\mathrm{e}^{-\frac{2\pi\mathrm{i}}{3}}$ $\quad -\frac{3}{2}\left(1 + \sqrt{3}\mathrm{i}\right)$ $\quad 3\left(\cos\frac{4\pi}{3} + \mathrm{i}\sin\frac{4\pi}{3}\right)$

(l) $\sqrt{2}\,\mathrm{e}^{\frac{7\pi\mathrm{i}}{12}}$ $\quad (1+\mathrm{i})^{7/3} \quad \sqrt{2}\left(\cos\frac{\pi}{4}+\mathrm{i}\sin\frac{\pi}{4}\right)^{7/3}$

11.2 Write the sum, product, and ratio of the following complex numbers:

(a) $z_1 = 2+3\mathrm{i},\ z_2 = 7-\mathrm{i}$ $\quad z_1+z_2 = 9+2\mathrm{i} \quad z_1z_2 = 17+19\mathrm{i} \quad \dfrac{z_1}{z_2} = \dfrac{11+23\mathrm{i}}{50}$

(b) $z_1 = 12+\mathrm{i},\ z_2 = 6-3\mathrm{i}$ $\quad z_1+z_2 = 18-2\mathrm{i} \quad z_1z_2 = 75-30\mathrm{i} \quad \dfrac{z_1}{z_2} = \dfrac{23+14\mathrm{i}}{15}$

(c) $z_1 = 7+3\mathrm{i},\ z_2 = 3-3\mathrm{i}$ $\quad z_1+z_2 = 10 \quad z_1z_2 = 30-12\mathrm{i} \quad \dfrac{z_1}{z_2} = \dfrac{2+5\mathrm{i}}{3}$

(d) $z_1 = 2+12\mathrm{i},\ z_2 = 5-\mathrm{i}$ $\quad z_1+z_2 = 7+11\mathrm{i} \quad z_1z_2 = 22+58\mathrm{i} \quad \dfrac{z_1}{z_2} = \dfrac{-1+31\mathrm{i}}{13}$

(e) $z_1 = 1-\mathrm{i},\ z_2^* = 11+5\mathrm{i}$ $\quad z_1+z_2 = 12-6\mathrm{i} \quad z_1z_2 = 6-16\mathrm{i} \quad \dfrac{z_1}{z_2} = \dfrac{8-3\mathrm{i}}{73}$

(f) $z_1 = 2\left(\cos\dfrac{\pi}{3}+\mathrm{i}\sin\dfrac{\pi}{3}\right),\ z_2 = 3\left(\cos\dfrac{2\pi}{3}+\mathrm{i}\sin\dfrac{2\pi}{3}\right)$

$z_1+z_2 = \dfrac{-1+5\sqrt{3}\mathrm{i}}{2} \quad z_1z_2 = -6 \quad \dfrac{z_1}{z_2} = \dfrac{1-\sqrt{3}\mathrm{i}}{3}$

(g) $z_1 = 3\left(\cos\dfrac{\pi}{6}-\mathrm{i}\sin\dfrac{\pi}{6}\right),\ z_2 = 2\left(\cos\dfrac{5\pi}{3}-\mathrm{i}\sin\dfrac{5\pi}{3}\right)$

$z_1+z_2 = \dfrac{3\sqrt{3}}{2}+1+\left(\sqrt{3}-\dfrac{3}{2}\right)\mathrm{i} \quad z_1z_2 = 3(\sqrt{3}+\mathrm{i}) \quad \dfrac{z_1}{z_2} = \dfrac{\sqrt{3}-(2+3\sqrt{3})\mathrm{i}}{8}$

11.3 Write the following powers (roots) of complex numbers:

(a) $(1+\mathrm{i})^7$ $\quad 8(1-\mathrm{i})$

(b) $(-\sqrt{3}+\mathrm{i})^8$ $\quad 128(-1+\sqrt{3}\mathrm{i})$

(c) $\sqrt[3]{1}$ $\quad 1,\ -\dfrac{1}{2}(1\pm\sqrt{3}\mathrm{i})$

(d) $\sqrt[6]{729}$ $\quad \pm3,\ \pm\dfrac{3}{2}(1\pm\sqrt{3}\mathrm{i})$

(e) $\sqrt{-2+2\mathrm{i}}$ $\quad \sqrt[4]{8}\left[\cos\left(\dfrac{3\pi}{8}+k\pi\right)+\mathrm{i}\sin\left(\dfrac{3\pi}{8}+k\pi\right)\right],\ k=0,1$

(f) $\sqrt[5]{1+\sqrt{3}\mathrm{i}}$ $\quad \sqrt[5]{2}\left[\cos\left(\dfrac{\pi}{15}+\dfrac{2}{5}k\pi\right)+\mathrm{i}\sin\left(\dfrac{\pi}{15}+\dfrac{2}{5}k\pi\right)\right],\ k=0,1,2,3,4$

(g) $\sqrt[3]{5-\dfrac{15\,\mathrm{i}}{\sqrt{3}}}$ $\quad \sqrt[3]{10}\left[\cos\left(\dfrac{5\pi}{9}+\dfrac{2}{3}k\pi\right)+\mathrm{i}\sin\left(\dfrac{5\pi}{9}+\dfrac{2}{3}k\pi\right)\right],\ k=0,1,2$

(h) $\sqrt[3]{-5+\dfrac{5\,\mathrm{i}}{\sqrt{3}}}$ $\quad \sqrt[6]{\dfrac{100}{3}}\left[\cos\left(\dfrac{5\pi}{18}+\dfrac{2}{3}k\pi\right)+\mathrm{i}\sin\left(\dfrac{5\pi}{18}+\dfrac{2}{3}k\pi\right)\right],\ k=0,1,2$

(i) $\sqrt{-6+\dfrac{6\,\mathrm{i}}{\sqrt{3}}}$ $\qquad$ $\left(\dfrac{12}{\sqrt{3}}\right)^{1/2}\left[\cos\left(\dfrac{5\pi}{12}+k\pi\right)+\mathrm{i}\sin\left(\dfrac{5\pi}{12}+k\pi\right)\right],\ k=0,1$

11.2 Function of a complex variable

Assume a function of *a single* complex variable $f(z) = u(x,y) + \mathrm{i}v(x,y)$ defined on an area $G : x_1 \le x \le x_2,\ y_1 \le y \le y_2$, alternatively in polar coordinates $f(z) = u(r,\varphi) + \mathrm{i}v(r,\varphi)$, where $G : r_1 \le r \le r_2,\ \varphi_1 \le \varphi \le \varphi_2$. The derivative of a function of a single complex variable $f'(z)$ is then defined in this area as a limit

$$
\begin{aligned}
f'(z) = \frac{\mathrm{d}f(z)}{\mathrm{d}z} &= \lim_{\Delta z\to 0}\frac{f(z+\Delta z)-f(z)}{\Delta z} \\
&= \lim_{\substack{\Delta x\to 0\\ \Delta y\to 0}}\frac{u(x+\Delta x,y+\Delta y)+\mathrm{i}v(x+\Delta x,y+\Delta y)-u(x,y)-\mathrm{i}v(x,y)}{\Delta x+\mathrm{i}\Delta y}.
\end{aligned} \tag{11.12}
$$

If we expand this expression for both variables x, y separately (assuming the function $f(z)$ is differentiable in direction of real and imaginary axes, we separately set $\Delta y = 0$ and $\Delta x = 0$) in the way described in Equations (1.1) and (5.4), we get

$$\frac{\mathrm{d}f}{\mathrm{d}z} = \frac{\partial u}{\partial x} + \mathrm{i}\,\frac{\partial v}{\partial x}, \qquad \frac{\mathrm{d}f}{\mathrm{d}z} = -\mathrm{i}\,\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \tag{11.13}$$

By comparing real and imaginary parts of both equations, we get the so-called *Cauchy-Riemann* conditions of existence of derivative of a complex function $f(z)$,

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}. \tag{11.14}$$

The function $f(z)$ of a complex variable defined on the area G has thus a derivative at the point $z = x + \mathrm{i}y$ if for real differentiable functions $u(x,y)$ and $v(x,y)$ the condition (11.14) applies. We call this function *regular* at the point z. We call the function $f(z)$, which has the derivative in the area G *everywhere*, *analytic*, or *holomorphic* in the area G. Points inside the area G, where the bijective function $f(z)$ (i.e., such that for *every* $z \in D_f$ will $f(z)$ be a unit set) is not regular, we call *singular points* or *singularities* of the function $f(z)$. If we also calculate second derivatives of Equations (11.14), we get for both functions u, v, the so-called *Laplace* equation (see Equations (5.21) for two variables) $\Delta u = \Delta v = 0$.

Using Equations (11.13) and (11.14), the so-called *Cauchy theorem* can be derived for an arbitrary by parts smooth closed curve $\mathcal{C}$ and a holomorphic function $f(z)$ in the area G,

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = 0 \tag{11.15}$$

(for proof and other details, see, for example, Kvasnica (2004)). We can also derive the so-called *Cauchy formula*, again for any by parts smooth closed curve $\mathcal{C}$ and a function $f(z)$, holomorphic inside this curve loop and on this curve, where ζ is an arbitrary point *inside* this curve loop,

$$f(\zeta) = \frac{1}{2\pi\mathrm{i}}\oint_{\mathcal{C}}\frac{f(z)\,\mathrm{d}z}{z-\zeta}. \tag{11.16}$$

The Cauchy formula thus expresses the value of a function $f(z)$ (holomorphic inside and on a closed curve $\mathcal{C}$) at an arbitrary point ζ inside the curve $\mathcal{C}$, with the use of integral dependent *only* on values of $f(z)$ at points lying on the curve $\mathcal{C}$. It can be shown that derivatives of any order of a function $f(z)$ holomorphic in the region G also form the holomorphic functions in this region. Therefore, if a function of a complex variable has the first derivative at all points of the region G, then this function also has all derivatives of *any* order in all points of this region. There is no corresponding property in functions of a real variable (Kvasnica, 2004).

The function $f(z)$ has the so-called isolated singularity (isolated pole) at the point $z = \zeta$ if the function $f(z)$ is not holomorphic at the point ζ if it is not holomorphic at this point while it is holomorphic everywhere in a "complex" neighborhood of the point ζ (i.e., at all points of the complex plane that "surround" the point ζ). An isolated pole is of mth-order if the function $f(z)$ in the neighborhood of the point $z = \zeta$ can be expressed in the form

$$f(z) = \frac{a_{-m}}{(z-\zeta)^m} + \ldots + \frac{a_{-1}}{z-\zeta} + g(z), \tag{11.17}$$

where a_{-m}, ..., a_{-1} are coefficients, and $g(z)$ is a bijective holomorphic function in the neighborhood of the point $z = \zeta$ and also at the point ζ. The coefficient $a_{-1} \equiv \mathrm{Res}$ is the so-called *residue* of the function $f(z)$ at the point $z = \zeta$. Function $f(z)$ can have different isolated poles at points ζ_1, ζ_2, ..., ζ_p, in which case we can write the function $f(z)$ in the form

$$f(z) = g(z) + \frac{\mathrm{Res}_1}{z-\zeta_1} + \frac{\mathrm{Res}_2}{z-\zeta_2} + \ldots + \frac{\mathrm{Res}_p}{z-\zeta_p} + \ldots, \tag{11.18}$$

where Res_i is the residue of the function $f(z)$ at the point ζ_i and $g(z)$ is a bijective holomorphic function inside the closed curve $\mathcal{C}$ and on it.

These relations imply an important the so-called *residual theorem*: if we have a closed curve $\mathcal{C}$ in the area where $f(z)$ is a bijective holomorphic function except for the isolated poles of this function, then the integral of the function $f(z)$ along such a curve is equal to

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = 2\pi\mathrm{i} \sum_i \mathrm{Res}_i. \tag{11.19}$$

The value of the integral is thus entirely determined by oefficients at the first-order isolated pole of the function $f(z)$. The calculation of the residue for the mth-order isolated pole at the point $z = \zeta$ is given by the relation

$$\mathrm{Res} = \frac{1}{(m-1)!} \lim_{z\to\zeta} \left\{ \frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}} \left[(z-\zeta)^m f(z)\right] \right\}. \tag{11.20}$$

If the function $f(z)$ is a ratio of two complex polynomials, $f(z) = P(z)/Q(z)$, where $P(z)$ is a holomorphic function at all points inside or on the curve $\mathcal{C}$ and $Q(z)$ has a simple root at the point $z = \zeta$, the relation (11.20) transforms to a much simpler form,

$$\mathrm{Res} = \frac{P(\zeta)}{Q'(\zeta)}. \tag{11.21}$$

- The elementary use of the residual theorem can be seen in a simple example,

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = \oint_{\mathcal{C}} \frac{\sin z}{z^4}\mathrm{d}z, \tag{11.22}$$

where $\mathcal{C}$ is a closed curve containing all singularities (poles) of a given function $f(z)$. However, the function has a single pole at zero point of the complex plane, whose order (see Equation (11.17)) is proved by expansion of the function $f(z)$ into the so-called *Laurent series* (extension of Taylor series for complex numbers), whose general formula has the form

$$\sum_{n=-\infty}^{\infty} a_n (z-z_0)^n = \\ = \ldots + \frac{a_{-2}}{(z-z_0)^2} + \frac{a_{-1}}{(z-z_0)} + a_0 + a_1 (z-z_0) + a_2 (z-z_0)^2 + \ldots \,, \tag{11.23}$$

where a_n, $z_0 \in \mathbb{C}$ (both the coefficients can thus be zero!). The part of Laurent series, where $n \geq 0$, corresponds to a holomorphic (analytical) function $g(z)$ in Equation (11.17). Laurent series of the function $f(z)$ will be

$$\frac{1}{z^4}\left(0 + z + 0 - \frac{z^3}{3!} + 0 + \frac{z^5}{5!} - \ldots\right) = \frac{0}{z^4} + \frac{1}{z^3} + \frac{0}{z^2} - \frac{1}{6z} + 0 + \frac{z}{120} - \ldots \,, \tag{11.24}$$

the singularity of the given function is therefore of the 4th order. From this expansion can be directly read the residue of the function $f(z)$ at zero point, given by the coefficient $a_{-1} = -1/6$.

The same result would be obtained using Equation (11.20), that is

$$\mathrm{Res} = \frac{1}{6} \lim_{z \to 0} \frac{\mathrm{d}^3 (\sin z)}{\mathrm{d}z^3} = -\frac{1}{6}, \tag{11.25}$$

we thus get from Equation (11.19) the result

$$\oint_{\mathcal{C}} \frac{\sin z}{z^4} \mathrm{d}z = -\frac{\pi \mathrm{i}}{3}. \tag{11.26}$$

- As an example of the application of the residual theorem, we can give, for example, the following simple integral of the real function $f(x)$, which has no singularities (isolated poles) on the real axis:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(1+x^2)^3} \quad \longrightarrow \quad \oint_{\mathcal{C}_+} \frac{\mathrm{d}z}{(1+z^2)^3} \quad \text{where} \quad \zeta_1, \zeta_2 = \pm \mathrm{i}. \tag{11.27}$$

Integrating along the closed curve $\mathcal{C}_+$ that coincides with a part of the real axis and, e.g., a positive isolated pole (in this case, it is a third-order pole due to its third power), its residue will, according to the relation (11.20), be

$$\mathrm{Res} = \frac{1}{2} \lim_{z \to \mathrm{i}} \left\{ \frac{\mathrm{d}^2}{\mathrm{d}z^2} \left[\frac{z-\mathrm{i}}{(z-\mathrm{i})(z+\mathrm{i})} \right]^3 \right\} = \frac{1}{2} \lim_{z \to \mathrm{i}} \frac{12}{(z+\mathrm{i})^5} = -\frac{3\mathrm{i}}{16}. \tag{11.28}$$

By substituting this into Equation (11.19), we get

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(1+x^2)^3} = \frac{3\pi}{8}. \tag{11.29}$$

★ Example of calculating the integral of the holomorphic (analytical) function of a complex variable (*contour integral*)

$$\oint_{\mathcal{C}} \frac{z^2 \, \mathrm{d}z}{\mathrm{e}^z - 1} = 0 \tag{11.30}$$

along a closed, by parts smooth curve $\mathcal{C}$ (the so-called *Jordan curve*), without the use of a residual theorem (see the Cauchy's theorem, Equation (11.15)); there are no singularities within the closed curve. Obviously, the given function will have singularities at points (x, y), where $\mathrm{e}^z = \mathrm{e}^{x+\mathrm{i}y} = 1$, which satisfy all points $(0, 2k\pi)$, where $k \in \mathbb{Z}$ (see Euler's identity in Example 9.7). To solve this integral, consider a rectangle with vertices (written in the form of complex numbers in algebraic form) 0, R, $R + 2\pi\mathrm{i}$, and $2\pi\mathrm{i}$. Since there are singularities of the given function in the first and the last of these vertices, we have to indent these points by using a quarter circle with "small" radius ϵ for each one (see Figure 11.1). This radius ϵ can be regarded as the absolute value of the complex function elements (numbers) on these circles (with respect to the center of each circle).

Noting that the complex function in this case can be specified as $z = x + \mathrm{i}y$ on the straight lines and $z = \epsilon\,\mathrm{e}^{\mathrm{i}\phi} + x_0 + \mathrm{i}y_0$ on the quarter circles (where $x_0 + \mathrm{i}y_0$ is the center of each quarter circle), and so $\mathrm{d}z = \mathrm{d}x + \mathrm{i}\,\mathrm{d}y$, $\mathrm{d}z = \mathrm{i}\epsilon\,\mathrm{e}^{\mathrm{i}\phi}\,\mathrm{d}\phi$, we can spread the entire Equation (11.30) for the closed curve as

$$\begin{aligned}
&\int_\epsilon^R \frac{x^2}{\mathrm{e}^x - 1}\,\mathrm{d}x + \int_0^{2\pi} \frac{(R + \mathrm{i}y)^2}{\mathrm{e}^{R+\mathrm{i}y} - 1}\,\mathrm{i}\,\mathrm{d}y + \int_R^\epsilon \frac{(x + 2\pi\mathrm{i})^2}{\mathrm{e}^{x+2\pi\mathrm{i}} - 1}\,\mathrm{d}x + \qquad (11.31)\\
&+ \int_0^{-\pi/2} \frac{(\epsilon\,\mathrm{e}^{\mathrm{i}\phi} + 2\pi\mathrm{i})^2}{\mathrm{e}^{\epsilon\,\mathrm{e}^{\mathrm{i}\phi}+2\pi\mathrm{i}} - 1}\,\mathrm{i}\epsilon\,\mathrm{e}^{\mathrm{i}\phi}\,\mathrm{d}\phi + \int_{2\pi-\epsilon}^\epsilon \frac{(\mathrm{i}y)^2}{\mathrm{e}^{\mathrm{i}y} - 1}\,\mathrm{i}\,\mathrm{d}y + \int_{\pi/2}^0 \frac{(\epsilon\,\mathrm{e}^{\mathrm{i}\phi})^2}{\mathrm{e}^{\epsilon\,\mathrm{e}^{\mathrm{i}\phi}} - 1}\,\mathrm{i}\epsilon\,\mathrm{e}^{\mathrm{i}\phi}\,\mathrm{d}\phi = 0.
\end{aligned}$$

Next, we implement for R and ϵ the limit values $R \to +\infty$ and $\epsilon \to 0^+$, the second and the last integral in Equation (11.31) thus cancel and the fourth integral will be $2\mathrm{i}\pi^3$. We thus obtain

$$\int_0^\infty \frac{x^2}{\mathrm{e}^x - 1}\,\mathrm{d}x - \int_0^\infty \frac{x^2 + 4\pi\mathrm{i}x - 4\pi^2}{\mathrm{e}^x - 1}\,\mathrm{d}x + 2\mathrm{i}\pi^3 + \int_0^{2\pi} \frac{y^2}{\mathrm{e}^{\mathrm{i}y} - 1}\,\mathrm{i}\,\mathrm{d}y = 0. \qquad (11.32)$$

We split the last integral in Equation (11.32) into its real and imaginary part, by converting it to a trigonometric form and expanding it by complex conjugate expression to its denominator,

$$\int_0^{2\pi} \frac{y^2}{\mathrm{e}^{\mathrm{i}y} - 1}\,\mathrm{i}\,\mathrm{d}y = \frac{1}{2}\int_0^{2\pi} \frac{y^2 \sin y}{1 - \cos y}\,\mathrm{d}y - \frac{\mathrm{i}}{2}\int_0^{2\pi} y^2\,\mathrm{d}y. \qquad (11.33)$$

Since the first integral in Equation (11.32) also cancels with the first term in the second integral, we can rewrite Equation (11.32), after substituting Equation (11.33), into the form

$$\begin{aligned}
&4\pi^2 \int_0^\infty \frac{\mathrm{d}x}{\mathrm{e}^x - 1} + \frac{1}{2}\int_0^{2\pi} \frac{y^2 \sin y}{1 - \cos y}\,\mathrm{d}y + \\
&+ \mathrm{i}\left(2\pi^3 - 4\pi \int_0^\infty \frac{x}{\mathrm{e}^x - 1}\,\mathrm{d}x - \frac{1}{2}\int_0^{2\pi} y^2\,\mathrm{d}y\right) = 0. \qquad (11.34)
\end{aligned}$$

To satisfy Equation (11.30), both its real and imaginary part must be equal to zero. From this condition for the imaginary part of Equation (11.34), we can thus, for example, easily find the value of the integral

$$\int_0^\infty \frac{x}{\mathrm{e}^x - 1}\,\mathrm{d}x = \frac{\pi^2}{6}. \qquad (11.35)$$

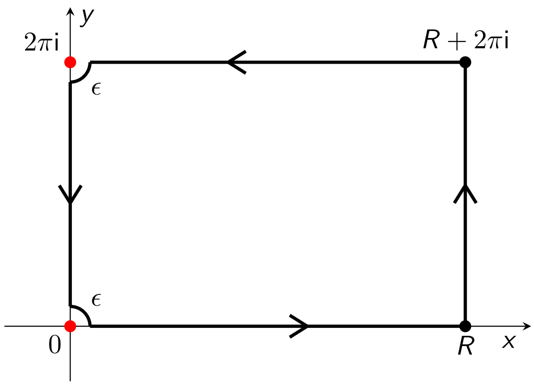

Figure 11.1: Schematic picture of the closed curve $\mathcal{C}$ for solution of Equation (11.30). The first two singularities ($k = 0$, $k = 1$) are denoted by red points.

We can use in an analogous way, for example, the integral of the function of the complex variable

$$\oint_{\mathcal{C}} \frac{z^4 \,\mathrm{d}z}{\mathrm{e}^z - 1} = 0, \tag{11.36}$$

where we substitute the already obtained solution of the integral in Equation (11.35), to find the value of the integral

$$\int_0^{\infty} \frac{x^3}{\mathrm{e}^x - 1} \,\mathrm{d}x = \frac{\pi^4}{15}. \tag{11.37}$$

Integrals of this type are of particular importance in thermodynamics and statistical physics, for example, in solving the Planck function, calculating thermodynamic potentials, etc.

The problem of the function of a complex variable is, of course, a vast field, here we only give its very brief and elementary "outline". I recommend the literature and corresponding courses related to this topic for further study.

- **Examples:**

11.4 Verify if the following complex functions $f(z) = f(x + \mathrm{i}y)$ can be holomorphic on open subsets of the complex plane:

(a) $3y - 3x\mathrm{i}$ yes

(b) $3x^2 + 3y + 6xy\mathrm{i}$ no

(c) $z^2 + \ln z + 1$ yes

(d) $z^3 + 5z - \sin z$ yes

(e) $|z^2 + y|$ no

(f) $\dfrac{z-1}{z+1}$ yes

(g) $\sqrt{z+1+\mathrm{i}}$ yes

(h) $\exp\left(-\mathrm{i}z^2\right)$ yes

(i) $\exp\left[\frac{(z+1)^2}{\mathrm{i}}\right]$ yes

(j) $\ln\left(\frac{z+1}{\mathrm{i}}\right)$ yes

11.5 Find the holomorphic functions of a complex variable $f(z)$ if only $\operatorname{Re} f(z) = u(x,y)$ or $\operatorname{Im} f(z) = v(x,y)$ is specified:

(a) $u = x\,\mathrm{e}^{3y}$ holomorphic function $f(z)$ does not exist

(b) $u = x^2 + 3x - y^2 + 5y$ $f(z) = z^2 + 3z - 5\mathrm{i}z + C$

(c) $u = \mathrm{e}^x(\cos y + 2\sin y)$ $f(z) = (1-2\mathrm{i})\,\mathrm{e}^z + C$

(d) $u = \sin(2x)\cosh(2y)$ $f(z) = \sin 2z + C$

(e) $u = x^2 - y^2 + \sin(x)\cosh(y)$ $f(z) = z^2 + \sin z + C$

(f) $u = x^3 - 3xy^2 + \ln|z|$ $f(z) = z^3 + \ln z + C,\ z \neq 0$

(g) $u = x - \frac{x}{x^2+y^2}$ $f(z) = z - \frac{1}{z} + C,\ z \neq 0$

(h) $v = y - \sin(x)\sinh(y)$ $f(z) = z + \cos z + C$

(i) $v = x + \sinh(x)\sin(y)$ $f(z) = \mathrm{i}z + \cos(\mathrm{i}z) + C$

11.6 Use the residual theorem to calculate the following integrals (where $\mathcal{C}$ denotes a closed curve enclosing all singularities of a given function $f(z)$ while $\mathcal{C}_+$ denotes a closed curve enclosing only one arbitrary singularity of a given function):

(a) $\oint_{\mathcal{C}} \frac{z}{z^2-1}\,\mathrm{d}z$ $2\pi\mathrm{i}$

(b) $\oint_{\mathcal{C}_+} \frac{z}{z^2-1}\,\mathrm{d}z$ $\pi\mathrm{i}$

(c) $\oint_{\mathcal{C}} \frac{\sin z}{z^2+5}\,\mathrm{d}z$ $2\pi\mathrm{i}\,\frac{\sinh\sqrt{5}}{\sqrt{5}}$

(d) $\oint_{\mathcal{C}} \frac{\mathrm{e}^z}{z^2+1}\,\mathrm{d}z$ $2\pi\mathrm{i}\sin(1)$

(e) $\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{x^2+1}$ π

(f) $\int_{-\infty}^{\infty} \frac{\sin x}{x^2+2x+2}\,\mathrm{d}x$ $-\frac{\pi}{\mathrm{e}}\sin(1)$

(g) $\displaystyle\int_{-\infty}^{\infty} \frac{\cos x}{6x^2+6x+3}\,\mathrm{d}x$ $\qquad \displaystyle\frac{\pi}{3\sqrt{\mathrm{e}}}\cos\left(\frac{1}{2}\right)$

(h) $\displaystyle\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{x^2+3x+3}$ (see Example 1.69) $\qquad \displaystyle\frac{2\pi}{\sqrt{3}}$

(i) $\displaystyle\int_{-\infty}^{\infty} \frac{4\,\mathrm{d}x}{(x^2+4)^4}$ $\qquad \displaystyle\frac{5\pi}{512}$

11.7 ★ Using the residual theorem or the contour integral, calculate the following complex or real integrals ($\mathcal{C}$ is the counter-clockwise unit circle centered at the origin of the complex plane, while $\mathcal{C}_+$ is the counter-clockwise unit half-circle in the positive half-plane where $\varphi \in \langle 0, \pi\rangle$, also centered at the origin of the complex plane):

(a) $\displaystyle\oint_{\mathcal{C}} z^2\,\mathrm{d}z$ $\qquad 0$

(b) $\displaystyle\oint_{\mathcal{C}} \frac{1}{z}\,\mathrm{d}z$ $\qquad 2\pi\mathrm{i}$

(c) $\displaystyle\oint_{\mathcal{C}} \frac{1}{z^5}\,\mathrm{d}z$ $\qquad 0$

(d) $\displaystyle\oint_{\mathcal{C}_+} \frac{1}{|z|}\,\mathrm{d}z$ $\qquad -2$

(e) $\displaystyle\oint_{\mathcal{C}_+} \frac{z}{z^*}\,\mathrm{d}z$ $\qquad \displaystyle-\frac{2}{3}$

(f) $\displaystyle\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2z^2-7\mathrm{i}z-3}$ $\qquad \displaystyle-\frac{2\pi}{5}$

(g) $\displaystyle\int_0^{2\pi} \frac{\mathrm{d}\theta}{a+\cos\theta}$, $\quad a>1$ is a constant $\qquad \displaystyle\frac{2\pi}{\sqrt{a^2-1}}$

(h) $\displaystyle\int_{-\infty}^{\infty} \frac{x^2}{x^4+1}\,\mathrm{d}x$ $\qquad \displaystyle\frac{\pi}{\sqrt{2}}$

(i) $\displaystyle\int_{-\infty}^{\infty} \frac{\cos(ax)}{x^2+1}\,\mathrm{d}x$, $\quad a\in\mathbb{R}$ is a constant $\qquad \pi\,\mathrm{e}^{-|a|}$

(j) $\displaystyle\int_{-\infty}^{\infty} \frac{\sin x}{x}\,\mathrm{d}x$ $\qquad \pi$

(k) $\displaystyle\int_0^{\infty} \frac{x^2\cos x}{(x^2+9)^2}\,\mathrm{d}x$ $\qquad \displaystyle-\frac{\pi}{6}\,\mathrm{e}^{-3}$

Chapter 12

Combinatorics, probability calculus, and basics of statistics[1]

12.1 Combinatorics

Combinatorics is one of the oldest mathematical disciplines dealing with the internal structure of so-called discrete element configurations (such as numbers or other objects), their existence, searching for the number of different types of such elements depending on conditions, etc. Typical examples of such configurations are *combinations*, *permutations*, and *variations* (k-permutations of n). Combinatorial principles form the mathematical basis for the definition of the so-called statistical distributions used to describe the behavior of physical systems, for example, in quantum mechanics, statistical physics, etc.

- **Combination without repetition:**

The number of k-element combinations (combinations of the kth class) without repetition of a set of n elements ($k, n \in \mathbb{N} \cup 0$), i.e., each element can occur only once in a given combination, is given by the relation

$$C(k,n) = \frac{n!}{k!\,(n-k)!} = \binom{n}{k}, \tag{12.1}$$

where the last term in the bracket, the so-called *binomial coefficient*, we read as "n over k". The binomial coefficient is also a determining factor in the so-called *binomial theorem*,

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k, \tag{12.2}$$

using which the binomial $x+y$ of the nth power can be decomposed into a sum of $n+1$ terms.

Combination without repetition is a mathematical basis of the so-called *Fermi-Dirac statistics*, describing systems composed of the so-called *fermions*, that is, from mutually indistinguishable quantum particles with *antisymmetric wave function* and *half-integer spin* (such as protons, neutrons, electrons, neutrinos, etc.). A typical simple example would be the number of different pairs that can be grouped of totally 30 people, where the "no repetition" condition stems from the fact that each particular individual can occur only once in each pair. At the same time, the combination can be regarded as a variation where the *order of the elements does not matter*, i.e., the pair A-B is identical to the pair B-A. The result is 435.

[1]Recommended literature for this chapter: Kvasnica (2004), Musilová & Musilová (2006).

- **Combination with repetition:**

The number of k-element combinations with repetition of a set of n elements, i.e., a given element can in a given combination occur multiple times (regardless of the order of the elements) is given by the relation

$$C'(k,n) = \frac{(n+k-1)!}{k!\,(n-1)!} = \binom{n+k-1}{k}. \tag{12.3}$$

Combination with repetition is the mathematical basis of the so-called *Bose-Einstein statistics*, describing systems composed of the so-called *bosons*, that is, of mutually indistinguishable quantum particles with *symmetric wave function* and *integer spin* (such as photons, mesons, gluons, ^{4} He nuclei, etc.).

A typical example could be the number of different ways in which a set of eight lettuce seedlings can be purchased if they have (in sufficient quantity) six different types of seedlings in store (in each set, any of the six types of seedlings can occur in any number from 1 to 8). The result is 1287.

- **Permutation without repetition:**

Generally, we define a permutation as an ordered n-element, where the total number of elements of the selection set is also n. If these elements in each such ordered n-element cannot repeat, the number of such different n-elements (permutations without repetition) is given by

$$P(n) = n!. \tag{12.4}$$

Example: how many different arrangements, each containing all letters, exist for the five letters a, b, c, d, e? The number of such ordered pentads ($n = 5$) without repetition is given by the relation $P(5) = 5!$, the total number of such arrangements (permutations) is thus 120.

- **Permutation with repetition:**

If between n elements of a selection set, there are k groups that have successively n_1, n_2, $\ldots$, n_k of the same elements, then the number of the so-called permutations with repetition is given by the relation

$$P'_{n_1,n_2,\ldots,n_k}(n) = \frac{n!}{n_1!\cdot n_2!\cdot\;\ldots\;\cdot n_k!}, \qquad \text{where} \qquad n = \sum_{i=1}^{k} n_i. \tag{12.5}$$

Example: how many different permutations exist for a seven-element set of four letters with a possible repetition of a, a, a, b, b, c, d, where the first letter occurs three times and second letter twice? The total number of such permutations will be $7!/(3!\cdot 2!\cdot 1!\cdot 1!) = 420$.

The expression (12.5) also forms the mathematical basis of the generalized binomial theorem (12.2) for an arbitrary number of terms $x_1 + x_2 + \ldots + x_m$, where for the so-called *multinomial coefficient*,

$$\binom{n}{k_1, k_2, \ldots, k_m} = \frac{n!}{k_1!\,k_2!\ldots k_m!}, \tag{12.6}$$

must for all $m \in \mathbb{N}$ and $k_i, n \in \mathbb{N}\cup 0$ again hold $k_1 + k_2 + \ldots + k_m = n$. This extended binomial theorem (12.2) is then written as a so-called *multinomial theorem* in the form

$$(x_1 + x_2 + \ldots + x_m)^n = \sum_{k_1+k_2+\ldots+k_m=n} \binom{n}{k_1, k_2, \ldots, k_m} x_1^{k_1} x_2^{k_2} \ldots x_m^{k_m}, \tag{12.7}$$

where the product of m elements $x_1^{k_1} x_2^{k_2} \dots x_m^{k_m}$ can be written using the multiplication symbol as $\prod_{i=1}^{m} x_i^{k_i}$.

- **Variations without repetition:**

We generally define a variation (k-permutation of n elements) as an ordered k-element (i.e., a k-element in which the so-called *order of the elements plays a role*), selected from the set containing n elements. If these elements in each such ordered k-element cannot repeat, the number of such different k-elements ($k \leq n$) is given by the relation

$$V(k, n) = \frac{n!}{(n-k)!}. \tag{12.8}$$

A typical example can be the following: How many colored tricolors can be made of a total of six colors? The variation without repetition, in this case, follows from the definition of the tricolor (if any of the three colors repeats, it will not be a tricolor). At the same time, it depends on the order of the particular elements, i.e., the tricolor with the ordering of colors *red-blue-green* is a different tricolor than the tricolor with the sequence of colors *green-blue-red*. So the total number of tricolor will be $6!/3! = 120$.

- **Variations with repetition:**

The number of ordered k-elements (when it again depends on the order of the elements) with repetition of n elements, i.e., when a given element can appear multiple times in a given k-element, is given by the relation

$$V'(k, n) = n^k. \tag{12.9}$$

A typical example: how many two-digit numbers can be created from the digits 1, 2, 3, 4, 5? Again, it depends on the ordering of particular elements, i.e., for example, the number 21 is different than the number 12, but at the same time, we must include the numbers 11, 22, etc., where the digits repeat. The total number of such two-digit numbers will be $5^2 = 25$.

- **Examples:**

12.1 How many circles are defined by 12 points lying on the same plane if no 3 points lie in one straight line?

220

12.2 Determine the number of ways in which one can choose a six-member group with exactly two women from seven men and four women.

210

12.3 There are 54 products in the box, of which 21 are first quality, 27 are second quality, and the rest are defective. In how many ways can a group of six products being selected to include three first quality products, two products of the second quality, and one defective product?

147 420

12.4 The hockey team has a total number of 24 players: 13 attackers, eight defenders, and three goalkeepers. How many different lineups can a coach build if one lineup is to have three attackers, two defenders, and one goalkeeper?

6 552

12.5 How many elements will we need to create six times more fourth-class combinations (without repeating elements) than second class combinations?

11

12.6 The curling coach has seven players available: Aleš, Bedřich, Cyril, David, Emil, Filip, and Gustav. He is to form a team of four.

(a) How many teams can he build?

(b) How many teams can he build if from the three players, Aleš, Bedřich, and Cyril, plays only one?

(c) How many teams can he build if from the three players, Aleš, Bedřich, and Cyril, play no more than two, and one of the pair David and Emil does not play?

(d) How many teams can he build if from the three players, Aleš, Bedřich, and Cyril, play no more than two, and Filip and Gustav do not play at the same time?

(a) 35

(b) 12

(c) 18

(d) 21

12.7 How many five-digit numbers are there?

90 000

12.8 How many numbers can be created from a set of the non-repeating digits 7, 3, 5, 2, 4, 8, 1, 9, to include the year of discovery of America?

1 680

12.9 In Cyprus, vehicle registration plates consist of a block of 3 letters followed by a four-digit number. The first part is selected only from the fourteen letters A, B, E, H, I, J, K, M, N, P, T, X, Y, Z.

(a) How many such registration plates exist?

(b) How many do such registration plates have each letter different?

(c) In how many of such registration plates is the vowel first?

(d) In how many of such registration plates are vowels only in 1st and 3rd position?

(a) $14^3 \cdot 9 \cdot 10^3 = 24\,696\,000$

(b) $14 \cdot 13 \cdot 12 \cdot 9 \cdot 10^3 = 19\,656\,000$

(c) $4 \cdot 14^2 \cdot 9 \cdot 10^3 = 7\,056\,000$

(d) $4^2 \cdot 10 \cdot 9 \cdot 10^3 = 1\,440\,000$

12.10 In how many ways can we build an arbitrarily large working group of 15 people? There can be 1 to 15 people in the group.

32 767

12.11 There are 10^5 ideal gas particles in the container. What is the probability that all completely randomly moving particles will find themselves in the left half of the container if the particles will be

(a) molecules of NH_3?

(b) ^{4}He nuclei?

(a) 2^{-10^5}

(b) $(10^5 + 1)^{-1}$

12.12 Consider $k = 3$ coins, each of which can have two "values", i.e., *virgin* or *eagle*. Obviously, if we toss all the coins at the same time, there may be a total of $n = 8$ possible results: PPP, PPO, POP, OPP, OOP, OPO, POO, OOO. We call each particular result a *microstate*, which takes into account the state of each coin (or particle, if it is a physical system in general). If we take into account only the number of virgins or eagles tossed, we specify the so-called *macrostate* (we denote it, for example, E_i) in this case; we thus have four possible macrostates: 3P, 2P+1O, 1P+2O, 3O. The number of microstates that create one macrostate is called *statistical weight* (multiplicity of a microstate within a macrostate) $W(E_i)$. In this case, for four macrostates, we get $W_0 = 1$, $W_1 = 3$, $W_2 = 3$, $W_3 = 1$, where the serial numbers of individual macrostates correspond to the number of, e.g., virgins in the given macrostate. The ratio of its statistical weight $W(E_i)$ to the total number of microstates n gives the probability of occurrence of a particular macrostate $P(E_i)$. The entropy S of a particular macrostate E_i will be $S = \ln W$. Specify the number of possible microstates and the probabilities of each macrostate if we toss

(a) by four coins,

(b) by twenty coins, which macrostate is most probable?

(c) What is the probability of a macrostate with 12 virgins and 8 eagles?

(d) By one hundred coins, which macrostate is most probable?

(e) Write entropy of the macrostates E_0, E_1, $E_{\max}$.

(a) $n = 16$, $P_0 = 1/16$, $P_1 = 1/4$, $P_2 = 3/8$, $P_3 = 1/4$, $P_4 = 1/16$

(b) $n = 2^{20}$, $P_0 = 1/2^{20}$, $P_1 = 20/2^{20}$, $P_2 = 190/2^{20}$, $\ldots$, $P(E_i) = \dfrac{20!}{i!(20-i)!\,2^{20}}$, $\ldots$, $P_{20} = 1/2^{20}$, $P_{\max} = P_{10}$

(c) approximately 0.12

(d) $n = 2^{100}$, $P_0 = 1/2^{100}$, $P_1 = 100/2^{100}$, $P_2 = 4950/2^{100}$, $\ldots$, $P(E_i) = \dfrac{100!}{i!(100-i)!\,2^{100}}$, $\ldots$, $P_{100} = 1/2^{100}$, $P_{\max} = P_{50}$

(e) 0, $\ln 100 \approx 4.6$, $\ln 100! - 2\ln 50! \approx 66.78$ - the most probable macrostate thus has the highest entropy, the least probable the lowest (zero).

12.13 Let's have *three* ideal gas particles and *five* "bins" - quantum "boxes", we denote them, for example, a, b, c, d, and e. The particles may be distributed in the individual bins (compartments) in any manner appropriate to their type (for example, multiple fermions cannot be in one compartment). Let us call each particular variation or combination of a particle system a microstate. Let us call "macrostate" a set of microstates where all three particles are in one bin (we call it "macrostate" "3"), or there are two particles in one compartment and a third in another (we call it "macrostate" "2/1"), or each particle is in one separate compartment (we call it "macrostate" "1/1/1"). Thus, there may be a maximum of 3 "macrostates" in the system.

(a) How many "microstates" can occur for molecules NH_3, ^4He nuclei, and protons, respectively?

(b) How many "macrostates" can occur for molecules NH_3, ^4He nuclei, and protons, respectively?

(c) What is the probability of a particular "microstate" occurrence if all three particles will be in one particular compartment (a, for example) for molecules NH_3, ^4He nuclei, and protons, respectively?

(d) What is the probability of a particular "microstate" occurrence if each of the three particles will be distributed separately in compartments a, c, e, for molecules NH_3, ^4He nuclei, and protons, respectively?

(e) What is the probability of occurrence of particular "macrostates" for molecules NH_3, ^4He nuclei, and protons, respectively?

(a) 125, 35, 10

(b) 3, 3, 1

(c) 1/125, 1/35, 0

(d) 6/125, 1/35, 1/10

(e) "macrostate" "3": 1/25, 1/7, 0
"macrostate" "2/1": 12/25, 4/7, 0
"macrostate" "1/1/1": 12/25, 2/7, 1

12.2 Probability calculus and basics of statistics[2]

The probability distribution of a *discrete* random quantity X is expressed by the so-called probability function $P(X)$ with probability values $p(x_i) = p_i$, where $\sum_i p_i = 1$. The distribution of

[2]In this chapter, examples from the book Musilová & Musilová (2006) are used.

the probability of a *continuous* random quantity X gives the probability of density distribution of probability (probability density) $f(x)$, for which holds $\int_\Omega f(x)\,\mathrm{d}x = 1$, where Ω is the domain of the quantity X. For values of $x \notin \Omega$ holds $f(x) = 0$. Important probability distributions are:

- *Uniform* probability distribution of *discrete* or *continuous* random quantity X, which assigns the same probability to all its values. Uniform distribution has constant probability density at all points of the given interval $\langle a, b\rangle$,

$$f(x) = \begin{cases} \frac{1}{b-a} & \text{for } x \in \langle a, b\rangle \\ 0 & \text{for } x \notin \langle a, b\rangle \end{cases}. \tag{12.10}$$

- The *Poisson* probability distribution of a *discrete* random quantity X, which can be expressed using the selected parameter $\lambda > 0$ as

$$p_i = \frac{\lambda^{x_i}}{x_i!}\,\mathrm{e}^{-\lambda}. \tag{12.11}$$

- *Normal* (Gaussian) probability distribution of a *continuous* random quantity X, which is defined by the probability density in the form of the so-called Gaussian function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\,\mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{12.12}$$

  where the parameter μ represents the mean value of the quantity X, parameter σ its standard deviation (see below).

In statistical physics, the mean number of distinguishable particles (e.g., molecules) in the state with energy E is also determined by the so-called *Maxwell-Boltzmann* distribution function. For indistinguishable particles, the so-called *Fermi-Dirac* distribution for fermions (electrons, protons, neutrinos, etc.) and the *Bose-Einstein* distribution for bosons (e.g., photons) apply. In mathematical statistics, there is often used the so-called *Student's t-distribution* (see, e.g., Pánek, 2001), etc. Following the probability distribution, we can identify a number of *statistical tools* to analyze a random quantity X (representing, for example, a set of measured values). The most important of them are:

- *Statistical weight* - in case of a *discrete* random quantity X with particular values x_i, we introduce the so-called (statistical) weight w_i, which can usually be determined by the so-called *internal uncertainties* (errors) δx_i of the values x_i (e.g., measurement errors, etc.). It follows the relation

$$w_i \sim \frac{1}{\delta {x_i}^2}. \tag{12.13}$$

  Next, we introduce the so-called sum of weights S_w and the so-called mean weight w_s,

$$S_w = \sum_{i=1}^{N} w_i, \quad w_s = \frac{1}{N}\sum_{i=1}^{N} w_i = \frac{S_w}{N}, \tag{12.14}$$

  where N is the total number of discrete values x_i. So there is a free relation between weights and probability values - if the sum of the weights $S_w = 1$, then $w_i = p_i$. Similarly, in the case of a continuous random variable, we can introduce the so-called weight function $w(x)$, whose "sum" will be given as $\int_\Omega w(x)\,\mathrm{d}x$. It is again apparent that if this integral is normalized (equal to one), $w(x) = f(x)$ holds, and the weight function thus becomes the probability density.

- The *mean value* (arithmetic mean), which is usually denoted $\bar{x}$, $\langle x \rangle$, or also μ. For a discrete random variable X, the mean value will be defined as the sum of all x_i values of a quantity$X$ divided by their number or the sum of products of all values of variable X with the corresponding values of the probability function that is

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} x_i p_i. \tag{12.15}$$

When using the other relation, we also speak about the so-called expected value, denoted by $E(X)$, or about the weighted arithmetic mean. The subtle difference between these terms depends on the definition of the element x_i of the quantity X, or on how we choose the so-called statistical weight. We determine the so-called weighted mean value (weighted arithmetic mean) as

$$\langle x \rangle = \frac{1}{S_w} \sum_{i=1}^{N} x_i w_i. \tag{12.16}$$

The mean value (unweighted and weighted) of a *continuous* random variable X is determined as

$$\langle x \rangle = E(X) = \int_{\Omega} x\, f(x)\, \mathrm{d}x, \quad \langle x \rangle = \frac{\int_{\Omega} x\, w(x)\, \mathrm{d}x}{\int_{\Omega} w(x)\, \mathrm{d}x}. \tag{12.17}$$

In the case of the following statistical tools, the determination of their weighted forms is quite similar.

- The *variance* and the *standard deviation* are mostly denoted as $D(X)$, $\mathrm{var}(X)$, optionally $\sigma^2(X)$ (variance) and $\sigma(X)$ (standard deviation). The variance (dispersion) is defined as the mean value of squares of deviations from the mean value (arithmetic mean) of the quantity X; the standard deviation is the square root of the variance. For a *discrete* random variable X with the same weight (probability) of all values x_i, the variance is defined as

$$D(X) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \langle x \rangle)^2 = \langle x^2 \rangle - \langle x \rangle^2 . \tag{12.18}$$

For different probabilities of discrete values of the random variable X, the variance will be determined by the relation

$$D(X) = \sum_{i=1}^{N} p_i \cdot (x_i - \langle x \rangle)^2 = -\langle x \rangle^2 + \sum_{i=1}^{N} x_i^2 \cdot p_i. \tag{12.19}$$

For *continuous* random variable X, the variance is defined by the relation

$$D(X) = \int_{\Omega} (x - \langle x \rangle)^2\, f(x)\, \mathrm{d}x = -\langle x \rangle^2 + \int_{\Omega} x^2 f(x)\, \mathrm{d}x. \tag{12.20}$$

In general, $\sigma(X) = \sqrt{D(X)}$ applies to the standard deviation.

- We determine the *most probable value* $P_{\max}(X)$ for a *discrete* random variable X as a value x_i with the highest value of the probability function p_i, i.e., $P_{\max}(X) = (x_i, \max(p_i))$. In the case of a *continuous* random variable X, we determine the most probable value $P_{\max}(X)$ as the maximum of the probability density function $f(x)$ in the domain Ω of the variable X, hence $P_{\max}(X) = \max(f(x))$ for $x \in \Omega$.

- *Median* ($\tilde{x}_{0.5}$) and *quartiles* ($\tilde{x}_{0.25}$, $\tilde{x}_{0.75}$, also called lower and upper quartiles) are the values x_i, in which the monotonically organized statistical set is divided into a corresponding number of equally numerous parts. Median, therefore, divides the statistical set into two equally numerous halves. The advantage of the median over the mean value is that extremely deviated values can not influence it. For example, for a set $\{1, 2, 2, 3, 27\}$, the median $\tilde{x}_{0.5} = 2$, while the mean value $\langle x \rangle = 7$. In the case of a *continuous* random variable X, we determine the median and the quartiles (or any quantiles defined in any other way) from the integral equations

$$\int_{-\infty}^{\tilde{x}_{0.5}} f(x)\,\mathrm{d}x = \frac{1}{2}, \quad \int_{-\infty}^{\tilde{x}_{0.25}} f(x)\,\mathrm{d}x = \frac{1}{4}, \quad \int_{-\infty}^{\tilde{x}_{0.75}} f(x)\,\mathrm{d}x = \frac{3}{4}. \tag{12.21}$$

- The *distribution function* $F(x)$ expresses the probability that the value of a random variable X with a given probability distribution will be less than or equal to x. In the case of a *discrete* random variable X, the distribution function $F(x)$ will be given by the formula

$$F(x) = P(X \leq x) = \sum_{x_i \leq x} p_i\,, \tag{12.22}$$

it will be thus discontinuous at the points x_i and constant between the points x_i. For a *continuous* random variable X, the distribution function $F(x)$ can be written as an integral of the probability density function,

$$F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t. \tag{12.23}$$

Each distribution function $F(x)$ is non-decreasing and right-continuous, its asymptotic properties can be expressed as $\lim_{x\to+\infty} F(x) = 1$, $\lim_{x\to-\infty} F(x) = 0$, for an arbitrary pair x_1, x_2 holds $P(x_1 < x \leq x_2) = F(x_2) - F(x_1)$.

★ *Maxwell-Boltzmann distribution of velocities*: Assume a *normal distribution* of velocities $v_x \equiv v$ of individual particles (molecules), in the sense of Equation (12.12), in the form

$$f(v) = a\,\mathrm{e}^{-bv^2}, \tag{12.24}$$

with so far unknown constants a and b, wherefrom the symmetry of the Gaussian function for positive and negative velocities we can assume the mean velocity μ according to Equation (12.12) as zero. Therefore, in a three-dimensional case, it must apply

$$\int_\Omega f(v) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A\,\mathrm{e}^{-Bv^2}\,\mathrm{d}v_x\,\mathrm{d}v_y\,\mathrm{d}v_z = 1, \tag{12.25}$$

where $v^2 = v_x^2 + v_y^2 + v_z^2$. Since the velocity distribution (if the substance as a whole is at rest) is isotropic in every location in the velocity vector space (the same in each direction), we can switch with advantage to a spherical system (spherical velocity space) where

$$\mathrm{d}v_x\,\mathrm{d}v_y\,\mathrm{d}v_z = v^2 \sin\theta\,\mathrm{d}v\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{12.26}$$

(see analogy with coordinate transformation in Chapter 4). Thus, Equation (12.25) can be rewritten into a one-dimensional form

$$P(v) = \int_\Omega f(v)\,\mathrm{d}v = 4\pi A \int_0^{\infty} v^2\,\mathrm{e}^{-Bv^2}\,\mathrm{d}v = 1, \tag{12.27}$$

where v is the radial component of the velocity vector in the spherical velocity space, that is, the magnitude of the velocity, actually. Integration of Equation (12.27) is best done using the substitution $Bv^2 = x$,

$$1 = \frac{4\pi A}{2B^{3/2}} \int_0^\infty \mathrm{e}^{-x} \sqrt{x}\, \mathrm{d}x. \tag{12.28}$$

The integral in Equation (12.28) is the so-called *Gamma function* (generalized factorial, see, for example, Arfken & Weber (2005)), defined as

$$\Gamma(x) = \int_0^\infty \mathrm{e}^{-t} t^{x-1}\, \mathrm{d}t, \tag{12.29}$$

Therefore, it is a *functional* $\Gamma(\frac{3}{2})$, which is defined in mathematical analysis as a mapping that assigns a real or complex number to the *function space* elements. Obviously, $\Gamma(x+1) = x\,\Gamma(x)$ holds for the Γ function, so it can be determined as $\Gamma(\frac{3}{2}) = \frac{1}{2}\Gamma(\frac{1}{2}) = \sqrt{\pi}/2$, whereas finding the value of the functional $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ can be done in a similar way to finding the values of the integrals in Example 1.97. So we get from Equation (12.28),

$$A = \left(\frac{B}{\pi}\right)^{3/2}. \tag{12.30}$$

Because the mean kinetic energy of a particle moving with a velocity v is $\langle E_k \rangle = \frac{1}{2}m\langle v^2 \rangle = \frac{3}{2}kT$ (see, e.g., Halliday et al. (2001), Chapter 20.5), we can write Equation

$$\frac{3}{2}kT = \frac{1}{2}m \int_\Omega v^2 f(v)\, \mathrm{d}v = 2\pi m \left(\frac{B}{\pi}\right)^{3/2} \int_0^\infty v^4\, \mathrm{e}^{-Bv^2}\, \mathrm{d}v \tag{12.31}$$

whose solution (similarly to Equation (12.28) but using the functional $\Gamma(\frac{5}{2})$) gives the constant B,

$$B = \frac{m}{2kT}. \tag{12.32}$$

Thus, the explicit form of the Maxwell-Boltzmann velocity distribution in the sense of Equation (12.27) will be

$$f(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2\, \mathrm{e}^{-\frac{mv^2}{2kT}}. \tag{12.33}$$

- **Examples:**

12.14 The shooter made $N = 150$ shots on the target, which consists of a system of $n = 5$ annular rings MK_i, $i = 1, \ldots, 5$. Ring MK_i he hit N_i times, where $N_1 = 15$, $N_2 = 20$, $N_3 = 35$, $N_4 = 45$, $N_5 = 35$. He received i points for the MK_i annulus hit. We define a random variable X with a discrete distribution as the number of points obtained for one random shot. Calculate:

(a) distribution $\{(x_i, p_i)\}$ of the variable X,

(b) probability that the shooter gets at least I points for a random shot, $I = 1, 2, 3, 4, 5$,

(c) mean value of the quantity X,

(d) standard deviation of the quantity X,

(e) probability that the shooter will score points in the interval $i \in \langle 2, 4 \rangle$.

(a) $\left\{ \left(1, \frac{1}{10}\right), \left(2, \frac{2}{15}\right), \left(3, \frac{7}{30}\right), \left(4, \frac{3}{10}\right), \left(5, \frac{7}{30}\right) \right\}$

(b) $P_1 = 1,\ P_2 = \frac{9}{10},\ P_3 = \frac{23}{30},\ P_4 = \frac{8}{15},\ P_5 = \frac{7}{30}$

(c) $3.4\bar{3}$

(d) 1.26

(e) $\frac{2}{3}$

12.15 There are four cabins at the airport toilets. The distribution function of cabin occupancy is given as $F(0) = 0.1$, $F(1) = 0.35$, $F(2) = 0.6$, $F(3) = 0.95$, $F(4) = 1$. Calculate:

(a) distribution of random variable X, corresponding to the number of occupied cabins,

(b) mean value of the variable X and its variance,

(c) probability that at least two cabins will be occupied.

(a) $\{(0,\ 0.1), (1,\ 0.25), (2,\ 0.25), (3,\ 0.35), (4,\ 0.05)\}$

(b) $2,\ 1.2$

(c) 0.65

12.16 The function $f(x) = k \cdot x$ is given for $0 \leq x \leq 2$ and $f(x) = 0$ otherwise. Calculate:

(a) a constant k so that the function is the probability density,

(b) mean value and variance,

(c) most probable value,

(d) median and quartiles $\tilde{x}_{0.25}, \tilde{x}_{0.75}$,

(e) distribution function.

(a) $k = \frac{1}{2}$

(b) $\frac{4}{3},\ \frac{2}{9}$

(c) 2

(d) $\tilde{x}_{0.5} = \sqrt{2},\ \tilde{x}_{0.25} = 1,\ \tilde{x}_{0.75} = \sqrt{3}$

(e) $F(x) = 0\ \forall\ x < 0,\ F(x) = \frac{1}{4}x^2\ \forall\ 0 \leq x \leq 2,\ F(x) = 1\ \forall\ x > 2$

12.17 The function $f(x) = \dfrac{k}{(x+1)^2}$ is given for $x \geq 0$ and $f(x) = 0$ for $x < 0$. Calculate:

(a) a constant k so that the function is the probability density,

(b) distribution function,

(c) most probable value, median, and quartiles $\tilde{x}_{0.25}, \tilde{x}_{0.75}$.

(a) $k = 1$

(b) $F(x) = 0 \ \forall\ x \le 0,\ F(x) = \dfrac{x}{x+1} \ \forall\ x > 0$

(c) $0,\ \tilde{x}_{0.5} = 1,\ \tilde{x}_{0.25} = \dfrac{1}{3},\ \tilde{x}_{0.75} = 3$

12.18 The function $f(x) = \dfrac{k}{x^2}$ is given for $1 \le x \le 2$ while $f(x) = 0$ otherwise, and the function $g(x) = c\big(x - x^2\big)$ is given for $0 \le x \le 1$ while $g(x) = 0$ otherwise. Calculate:

(a) constants k and c so that the functions are the probability densities,

(b) corresponding distribution functions,

(c) most probable value, mean value, variance, and median for each distribution.

(a) $k = 2,\ c = 6$

(b) $F_1(x) = 0 \ \forall\ x < 1,\ F_1(x) = 2\dfrac{x-1}{x} \ \forall\ 1 \le x \le 2,\ F_1(x) = 1 \ \forall\ x > 2,\ F_2(x) = 0 \ \forall\ x < 0,\ F_2(x) = 3x^2 - 2x^3 \ \forall\ 0 \le x \le 1,\ F_2(x) = 1 \ \forall\ x > 1$

(c) $f:\ 1,\ 2\ln 2,\ 2 - 4\ln^2 2,\ \dfrac{4}{3},\ g:\ \dfrac{1}{2}, \dfrac{1}{2}, \dfrac{1}{20}, \dfrac{1}{2}$

12.19 We roll two dice. Let us assign the random quantity X to the sum of points on both dice within one roll. Calculate:

(a) distribution of quantity X,

(b) distribution functions,

(c) mean value, variance, and the most probable value,

(d) the probability that the sum of the points on the dice will lie in the interval $\langle 5, 7\rangle$.

(a) $\Big\{(1,0), \Big(2, \dfrac{1}{36}\Big), \Big(3, \dfrac{1}{18}\Big), \Big(4, \dfrac{1}{12}\Big), \Big(5, \dfrac{1}{9}\Big), \Big(6, \dfrac{5}{36}\Big), \Big(7, \dfrac{1}{6}\Big), \Big(8, \dfrac{5}{36}\Big), \Big(9, \dfrac{1}{9}\Big), \Big(10, \dfrac{1}{12}\Big), \Big(11, \dfrac{1}{18}\Big), \Big(12, \dfrac{1}{36}\Big)\Big\}$

(b) $F(x) = 0 \ \forall\ x < 2,\ F(x) = \dfrac{1}{36} \ \forall\ x \in \langle 2, 3),\ F(x) = \dfrac{1}{12} \ \forall\ x \in \langle 3, 4),\ F(x) = \dfrac{1}{6} \ \forall\ x \in \langle 4, 5),\ F(x) = \dfrac{5}{18} \ \forall\ x \in \langle 5, 6),\ F(x) = \dfrac{5}{12} \ \forall\ x \in \langle 6, 7),\ F(x) = \dfrac{7}{12} \ \forall\ x \in \langle 7, 8),\ F(x) = \dfrac{13}{18} \ \forall\ x \in \langle 8, 9),\ F(x) = \dfrac{5}{6} \ \forall\ x \in \langle 9, 10),\ F(x) = \dfrac{11}{12} \ \forall\ x \in \langle 10, 11),\ F(x) = \dfrac{35}{36} \ \forall\ x \in \langle 11, 12),\ F(x) = 1 \ \forall\ x \ge 12$

(c) $7,\ 5.83,\ 7$

(d) $\dfrac{5}{12}$

12.20 Prove that

(a) a quantity μ in Equation (12.12) is both the most probable value $P_{\max}(x)$ and the mean value $\langle x \rangle$,

(b) a quantity σ in Equation (12.12) is equal to the standard deviation of the quantity x.

(a) Using the relation (12.17)

(b) Using the relation (12.20) and the definition of standard deviation

12.21 Using Maxwell-Boltzmann velocity (speed) distribution (Equation (12.33)), calculate:

(a) most probable speed $P_{\max}(v)$,

(b) mean velocity $\langle v \rangle$,

(c) root mean square velocity $\sqrt{\langle v^2 \rangle}$.

(a) $P_{\max}(v) = \sqrt{\dfrac{2kT}{m}}$

(b) $\langle v \rangle = \sqrt{\dfrac{8kT}{\pi m}}$

(c) $\sqrt{\langle v^2 \rangle} = \sqrt{\dfrac{3kT}{m}}$

Appendix A

Laplace transform ★

The Laplace transform is one of the basic integral transforms that assigns a function of a real variable (usually representing time t) to a function of a complex variable (complex frequency parameter) $s = \sigma + \mathrm{i}\omega$, where σ and ω are real numbers. It is particularly useful in areas of mathematics related to oscillations and waves.

A.1 Definitions and overview of elementary transformations

If we consider a continuous or piecewise continuous function $f(t)$ of the real variable $t \geq 0$ (the "pattern" or "original"), then its Laplace image $F(s)$, often denoted as $\mathcal{L}\{f(t)\}$, is defined as

$$F(s) = \int_0^\infty f(t)\,\mathrm{e}^{-st}\,\mathrm{d}t. \tag{A.1}$$

The inverse Laplace transform is then given by the following complex integral

$$f(t) = \mathcal{L}^{-1}\{F(s)\} = \frac{1}{2\pi\mathrm{i}} \lim_{T\to\infty} \int_{\gamma-\mathrm{i}T}^{\gamma+\mathrm{i}T} F(s)\,\mathrm{e}^{st}\,\mathrm{d}s, \tag{A.2}$$

where $\gamma$is a real number, so that the contour (Jordan) curve of integration is in the region of convergence of the function $F(s)$, and in the vast majority of cases the residue theorem can be used (see section 11.2).

In addition to the above "one-sided" Laplace transform, a "two-sided" Laplace transform is also defined. If $f(t)$ is a real or complex function of the real variable $t \in \mathbb{R}$, then the two-sided Laplace transform is defined as the integral of

$$\mathcal{B}\{f\}(s) = F(s) = \int_{-\infty}^{\infty} \mathrm{e}^{-st} f(t)\,\mathrm{d}t, \tag{A.3}$$

where the usual notation $\mathcal{B}$ comes from "bilateral". It is a non-proper integral that converges only if the following partial integrals exist:

$$\int_0^\infty \mathrm{e}^{-st} f(t)\,\mathrm{d}t, \quad \int_{-\infty}^{0} \mathrm{e}^{-st} f(t)\,\mathrm{d}t. \tag{A.4}$$

We do not discuss the two-sided Laplace transform in detail here. I refer the interested reader to the literature, e.g., Arfken & Weber (2005), Bracewell (2000), etc.

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

- The following list summarizes the Laplace transforms derived from the definition of (A.1), but is not a complete list of Laplace transforms and contains only some of the most commonly used formulas. Some functions that are explained in more detail later, such as the Heaviside or Dirac delta functions, are also listed.

$$\mathcal{L}\{C\} = \frac{C}{s}, \text{ where } C \in \mathbb{C} \text{ is a constant,} \tag{A.5}$$

$$\mathcal{L}\{t^n\} = \frac{n!}{s^{n+1}}, \text{ where } n \in \mathbb{N}^+ \text{ is a constant,} \tag{A.6}$$

$$\mathcal{L}\{t^p\} = \frac{\Gamma(p+1)}{s^{p+1}}, \text{ where } p \in \mathbb{R},\ p > -1, \text{ is a constant,} \tag{A.7}$$

$$\mathcal{L}\left\{\mathrm{e}^{at}\right\} = \frac{1}{s-a}, \text{ where } a \in \mathbb{R} \text{ is a constant,} \tag{A.8}$$

$$\mathcal{L}\left\{t^n \mathrm{e}^{at}\right\} = \frac{n!}{(s-a)^{n+1}}, \tag{A.9}$$

$$\mathcal{L}\{\sin at\} = \frac{a}{s^2+a^2}, \tag{A.10}$$

$$\mathcal{L}\{\cos at\} = \frac{s}{s^2+a^2}, \tag{A.11}$$

$$\mathcal{L}\{t \sin at\} = \frac{2as}{(s^2+a^2)^2}, \tag{A.12}$$

$$\mathcal{L}\{t \cos at\} = \frac{s^2-a^2}{(s^2+a^2)^2}, \tag{A.13}$$

$$\mathcal{L}\{\sin at - t \cos at\} = \frac{2a^3}{(s^2+a^2)^2}, \tag{A.14}$$

$$\mathcal{L}\{\sin at + t \cos at\} = \frac{2as^2}{(s^2+a^2)^2}, \tag{A.15}$$

$$\mathcal{L}\{\cos at - t \sin at\} = \frac{s(s^2-a^2)}{(s^2+a^2)^2}, \tag{A.16}$$

$$\mathcal{L}\{\cos at + t \sin at\} = \frac{s(s^2+3a^2)}{(s^2+a^2)^2}, \tag{A.17}$$

$$\mathcal{L}\{\sin(at+b)\} = \frac{s \sin b + a \cos b}{s^2+a^2}, \text{ where } a,\ b \in \mathbb{R} \text{ are constants,} \tag{A.18}$$

$$\mathcal{L}\{\cos(at+b)\} = \frac{s \cos b - a \sin b}{s^2+a^2}, \tag{A.19}$$

$$\mathcal{L}\{\sinh at\} = \frac{a}{s^2-a^2}, \tag{A.20}$$

$$\mathcal{L}\{\cosh at\} = \frac{s}{s^2-a^2}, \tag{A.21}$$

$$\mathcal{L}\left\{\mathrm{e}^{at} \sin bt\right\} = \frac{b}{(s-a)^2+b^2}, \tag{A.22}$$

$$\mathcal{L}\left\{\mathrm{e}^{at} \cos bt\right\} = \frac{s-a}{(s-a)^2+b^2}, \tag{A.23}$$

$$\mathcal{L}\left\{\mathrm{e}^{at} \sinh bt\right\} = \frac{b}{(s-a)^2-b^2}, \tag{A.24}$$

$$\mathcal{L}\left\{\mathrm{e}^{at} \cosh bt\right\} = \frac{s-a}{(s-a)^2-b^2}, \tag{A.25}$$

$$\mathcal{L}\left\{f(Ct)\right\} = \frac{1}{C}F\left(\frac{s}{C}\right), \tag{A.26}$$

$$\mathcal{L}\left\{\theta_c(t) \equiv \theta(t-c)\right\} = \frac{\mathrm{e}^{-cs}}{s}, \text{ where } \theta_c(t) \text{ is the Heaviside function,} \tag{A.27}$$

$$\mathcal{L}\left\{\delta(t-c)\right\} = \mathrm{e}^{-cs}, \text{ where } \delta \text{ is the Dirac delta function,} \tag{A.28}$$

$$\mathcal{L}\left\{\theta_c(t)f(t-c)\right\} = \mathrm{e}^{-cs}F(s), \tag{A.29}$$

$$\mathcal{L}\left\{\mathrm{e}^{ct}f(t)\right\} = F(s-c), \tag{A.30}$$

$$\mathcal{L}\left\{t^n f(t)\right\} = (-1)^n F^{(n)}(s), \tag{A.31}$$

$$\mathcal{L}\left\{\frac{1}{t}f(t)\right\} = \int_s^\infty F(u)\,\mathrm{d}u, \tag{A.32}$$

$$\mathcal{L}\left\{\int_0^t f(u)\,\mathrm{d}u\right\} = \frac{F(s)}{s}, \tag{A.33}$$

$$\mathcal{L}\left\{(f*g)(t)\right\} = F(s)G(s), \text{ where } (f*g)(t) \text{ denotes a convolution,} \tag{A.34}$$

$$\mathcal{L}\left\{f'(t)\right\} = sF(s) - f(0), \tag{A.35}$$

$$\mathcal{L}\left\{f''(t)\right\} = s^2F(s) - sf(0) - f'(0), \tag{A.36}$$

$$\begin{aligned}\mathcal{L}\left\{f^{(n)}\right\} &= s^nF(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \dots \\ &\dots - sf^{(n-2)}(0) - f^{(n-1)}(0),\end{aligned} \tag{A.37}$$

$$\mathcal{L}\left\{tf^{(n)}\right\} = -\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{L}\left\{f^{(n)}\right\}. \tag{A.38}$$

A closer look shows that the equation (A.5) is a special case of the equation (A.6) where $n = 0$, while the equation (A.6) is a special case of the equation (A.7) with a positive integer p, where in the equation (A.7) itself, Γ means Gamma function (see equation (12.29) and further explanation within the example 12.2), and the condition for real $p > -1$ means that we consider only the "properly behaving", i.e., positive Gamma function.

A.2 Step function

In this section, we will focus on the so-called step functions, where the Laplace transform will greatly facilitate the solution of differential equations containing this function. The elementary step (sometimes also "unit step") function is called the Heaviside function, and is usually denoted by H or θ, sometimes also by u or 1 (here we use the notation θ or θ_c, since the other symbols used are reserved for other types of functions) and is defined as

$$\theta_c(t) = \begin{cases} 0 & \text{if } t < c, \\ 1 & \text{if } t \geq c. \end{cases} \tag{A.39}$$

More complicated functions can be defined using the Heaviside function, for example $6\theta_c(t)$ means a function that is zero if $t < c$ and equal to 6 if $t \geq c$. Another function, $6 - \theta_c(t)$, is equal to 6 if $t < c$ and to 5 if $t \geq c$. Even more complicated cases can be defined, for example, for the case of an arbitrary function $f(t)$ for $t > 0$ where we want the new function $g(t)$ to have the same behavior as $f(t)$ but only above some chosen value $c > 0$ (the function $g(t)$ is thus a "horizontally shifted" function $f(t-c)$ for $t>c$ and has zero value for $t<c$). The function $g(t)$ can thus be written as

$$g(t)=\theta_c(t)f(t-c). \tag{A.40}$$

If we now insert the function (A.40) into the definition of the Laplace transform (A.1), we get

$$\mathcal{L}\{g(t)\}=\int_0^{\infty}\mathrm{e}^{-st}\theta_c(t)f(t-c)\,\mathrm{d}t. \tag{A.41}$$

Next, by substituting $u=t-c$, the integral (A.41) takes the form

$$\mathcal{L}\{g(t)\}=\mathrm{e}^{-cs}\int_0^{\infty}\mathrm{e}^{-su}f(u)\,\mathrm{d}u=\mathrm{e}^{-cs}F(s). \tag{A.42}$$

Therefore, we can also formulate the inverse Laplace transform of the step function (or the function containing the Heaviside function),

$$\mathcal{L}^{-1}\left\{\mathrm{e}^{-cs}F(s)\right\}=\theta_c(t)f(t-c). \tag{A.43}$$

Using the equation (A.42), we can define the Laplace transform of the Heaviside function itself by setting the function $f=1$, i.e.,

$$\mathcal{L}\{\theta_c(t)\}=\mathrm{e}^{-cs}\mathcal{L}\{1\}=\frac{\mathrm{e}^{-cs}}{s}. \tag{A.44}$$

The inverse transformation therefore gives

$$\mathcal{L}^{-1}\left\{\frac{\mathrm{e}^{-cs}}{s}\right\}=\theta_c(t). \tag{A.45}$$

Example: Solve the inverse transform of the function (Laplace image)

$$F(s)=\frac{3s+8\mathrm{e}^{-20s}-2s\,\mathrm{e}^{-3s}+6\mathrm{e}^{-7s}}{s^2(s+3)} \tag{A.46}$$

We modify the function to the form corresponding to the left-hand side of the equation (A.43),

$$F(s)=\left(3-2\mathrm{e}^{-3s}\right)G(s)+\left(8\mathrm{e}^{-20s}+6\mathrm{e}^{-7s}\right)H(s), \tag{A.47}$$

where

$$G(s)=\frac{1}{s(s+3)},\quad H(s)=\frac{1}{s^2(s+3)}. \tag{A.48}$$

By decomposition into partial fractions and by inverse transformation of functions (images) $G(s)$ and $H(s)$, we get

$$g(t)=\frac{1}{3}\left(1-\mathrm{e}^{-3t}\right),\quad h(t)=\frac{1}{3}t+\frac{1}{9}\left(-1+\mathrm{e}^{-3t}\right). \tag{A.49}$$

Since the inverse transformation by (A.43) gives the formula

$$f(t)=3g(t)-2\theta_3(t)\,g(t-3)+8\theta_{20}(t)\,h(t-20)+6\theta_7(t)\,h(t-7), \tag{A.50}$$

Thus, the final form of the Laplace pattern we are looking for will be

$$f(t)=1-\mathrm{e}^{-3t}-2\theta_3(t)\left(1-\mathrm{e}^{9}\,\mathrm{e}^{-3t}\right)+8\theta_{20}(t)\left[\frac{t-20}{3}+\frac{1}{9}\left(-1+\mathrm{e}^{60}\,\mathrm{e}^{-3t}\right)\right]+$$
$$+6\theta_7(t)\left[\frac{t-7}{3}+\frac{1}{9}\left(-1+\mathrm{e}^{21}\,\mathrm{e}^{-3t}\right)\right], \tag{A.51}$$

where, for example, $\theta_7(t)$ means that $\theta=0$ if $t<7$, and $\theta=1$ if $t\geq 7$.

A.3 Dirac delta function

Although there are various definitions of the Dirac delta function, the following three properties of the function are defining:

$$\delta(t-a) = 0 \;\; \forall \;\; t \neq a, \tag{A.52}$$

$$\int_{a-\epsilon}^{a+\epsilon} \delta(t-a)\,\mathrm{d}t = 1 \;\; \forall \;\; \epsilon > 0, \tag{A.53}$$

$$\int_{a-\epsilon}^{a+\epsilon} f(t)\,\delta(t-a)\,\mathrm{d}t = f(a) \;\; \forall \;\; \epsilon > 0. \tag{A.54}$$

Thus, the Dirac delta function is zero everywhere except at the single point $t = a$, where its value can be considered "infinite". The integrals (A.53) and (A.54) are valid for any interval containing the point a (unless this is its endpoint). Despite its "strangeness", this "function" is very useful in modeling, for example, shock waves or the action of very strong, extremely short-lived forces.

It follows from the above that the Laplace transform of the Dirac delta function takes the form

$$\mathcal{L}\left\{\delta(t-a)\right\} = \int_0^{\infty} \mathrm{e}^{-st}\delta(t-a)\,\mathrm{d}t = \mathrm{e}^{-as} \;\; \forall \;\; a > 0. \tag{A.55}$$

Furthermore, we can also define the connection between the Dirac delta function and the Heaviside function by noting that the following integral

$$\int_{-\infty}^{t} \delta(u-a)\,\mathrm{d}u = \begin{cases} 0 & \text{if } t < a, \\ 1 & \text{if } t > a, \end{cases} \tag{A.56}$$

where, unlike the equation (A.39), is a sharp inequality for $t > a$, since a must not be the endpoint of the interval. However, this is also the definition of the Heaviside function, that is,

$$\int_{-\infty}^{t} \delta(u-a)\,\mathrm{d}u = \theta_a(t). \tag{A.57}$$

Since u is actually a similar independent variable to t, $\mathrm{d}u/\mathrm{d}t = 1$, and hence

$$\theta_a'(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{t} \delta(u-a)\,\mathrm{d}u = \delta(t-a), \tag{A.58}$$

The Dirac delta function can thus be considered as a derivative of the Heaviside function.

A.4 Ordinary second order differential equations with constant coefficients, with boundary conditions

Since we want to use the Laplace transform to solve ordinary differential equations as well, we recall here again the Laplace transforms of the derivatives. In the case of the general n-th derivative, this will be (see (A.37))

$$\mathcal{L}\left\{f^{(n)}\right\} = s^n F(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \ldots - sf^{(n-2)}(0) - f^{(n-1)}(0), \tag{A.59}$$

where the nonbracketted exponents of the variable s denote the n-th power. Since we are overwhelmingly concerned with differential equations of at most second order, we will again give explicitly the Laplace transform of the first and second derivatives (see (A.35) and (A.36)),

$$\mathcal{L}\left\{y'\right\} = sY(s) - y(0) \tag{A.60}$$
$$\mathcal{L}\left\{y''\right\} = s^2Y(s) - sy(0) - y'(0). \tag{A.61}$$

At the same time, it can be seen that the values of the functions that appear here, $y(0)$ and $y'(0)$, are often also the values of the initial or boundary conditions in the differential equations. This means that if we are to use the above relations to solve equations with such conditions, we will need the initial or boundary conditions at $x = 0$ (for greater consistency with the previous discussion of ordinary differential equations, we will formally denote the independent variable here by x instead of t).

In the following, we will give some typical simple examples to show how this procedure is applied.

Example: Solve the equation

$$y'' - 10y' + 9y = 5x, \quad y(0) = -1, \quad y'(0) = 2. \tag{A.62}$$

Using the appropriate formulas for the Laplace transform, we can give the following transformed equation,

$$s^2Y(s) - sy(0) - y'(0) - 10\left[sY(s) - y(0)\right] + 9Y(s) = \frac{5}{s^2}. \tag{A.63}$$

After inserting the boundary conditions and adjusting, we get the equation

$$Y(s) = \frac{5 + 12s^2 - s^3}{s^2(s-9)(s-1)}, \tag{A.64}$$

and, after its decomposition into partial fractions,

$$Y(s) = \frac{50}{81s} + \frac{5}{9s^2} + \frac{31}{81(s-9)} - \frac{2}{s-1}. \tag{A.65}$$

By inverse Laplace transformation, according to the given principles (in practice, the best way is to use the tabulated formulas), we get the resulting solution,

$$y(x) = \frac{50}{81} + \frac{5}{9}x + \frac{31}{81}\,\mathrm{e}^{9x} - 2\mathrm{e}^{x}. \tag{A.66}$$

Example: Solve the equation

$$2y'' + 3y' - 2y = x\,\mathrm{e}^{-2x}, \quad y(0) = 0, \quad y'(0) = -2. \tag{A.67}$$

As in the previous example, using the appropriate formulas for the Laplace transform, we can give the following transformed equation,

$$2\left[s^2Y(s) - sy(0) - y'(0)\right] + 3\left[sY(s) - y(0)\right] - 2Y(s) = \frac{1}{(s+2)^2}. \tag{A.68}$$

After inserting the boundary conditions and adjusting, we get the equation

$$Y(s) = -\frac{4s^2 + 16s + 15}{(2s-1)(s+2)^3}, \tag{A.69}$$

and, after its decomposition into partial fractions,

$$Y(s) = \frac{1}{125}\left[\frac{-192}{2\left(s-\frac{1}{2}\right)} + \frac{96}{s+2} - \frac{10}{(s+2)^2} - \frac{25\frac{2!}{2!}}{(s+2)^3}\right], \tag{A.70}$$

where, for better illustration of accordance with the principles of inverse transformation, we have also included the expansion by the two's in the denominator of the first term in the outer square bracket and the expansion by the number 2! in the numerator of the last term. By inverse Laplace transformation according to the above (tabulated) principles, we obtain the resulting solution,

$$y(x) = \frac{1}{125}\,\mathrm{e}^{-2x}\left(96 - 10x - \frac{25}{2}x^2 - 96\,\mathrm{e}^{5x/2}\right). \tag{A.71}$$

Example: Solve the equation

$$y'' - 6y' + 15y = 2\sin 3x, \quad y(0) = -1, \quad y'(0) = -4. \tag{A.72}$$

In a similar way to the previous examples, we can derive the following transformed equation,

$$s^2Y(s) - sy(0) - y'(0) - 6\left[sY(s) - y(0)\right] + 15Y(s) = 2\frac{3}{s^2+9}. \tag{A.73}$$

After inserting the boundary conditions and adjusting, we get the equation

$$Y(s) = -\frac{s^3 - 2s^2 + 9s - 24}{(s^2 - 6s + 15)(s^2+9)}, \tag{A.74}$$

and, after its decomposition into partial fractions,

$$Y(s) = \frac{1}{10}\left[\frac{s}{s^2+9} + \frac{1\frac{3}{3}}{s^2+9} - \frac{11(s-3)}{(s-3)^2+6} - \frac{8\frac{\sqrt{6}}{\sqrt{6}}}{(s-3)^2+6}\right], \tag{A.75}$$

where, for better illustration of accordance with the inverse transformation principles, we have shown the expansion of the fractions in the numerators of the second and last terms in the outer square bracket. By inverse Laplace transformation according to the above principles, we obtain the resulting solution,

$$y(x) = \frac{1}{10}\left(\cos 3x + \frac{1}{3}\sin 3x - 11\,\mathrm{e}^{3x}\cos\sqrt{6}x - \frac{8}{\sqrt{6}}\,\mathrm{e}^{3x}\sin\sqrt{6}x\right). \tag{A.76}$$

Example: Solve the equation

$$y'' + 4y' = \cos(x-3) + 4x, \quad y(3) = 0, \quad y'(3) = 7. \tag{A.77}$$

First, we must reformulate the equation in such a way as to obtain the boundary conditions for $x = 0$. This is best done by changing the variables,

$$\eta = x - 3, \quad \text{and thus} \quad x = \eta + 3. \tag{A.78}$$

The original equation (A.77), where $y = y(x)$, can be rewritten as

$$y'' + 4y' = \cos\eta + 4(\eta + 3), \tag{A.79}$$

where $y = y(\eta + 3)$. We now rewrite the function $y(\eta + 3)$ as a new function $z(\eta)$, using the "chain rule" for derivatives, we easily derive that $y'(\eta + 3) = z'(\eta)$ and $y''(\eta + 3) = z''(\eta)$. We can also transform the boundary conditions as $y(3) = z(0) = 0$ and $y'(3) = z'(0) = 7$. The original equation (A.77) will have the following form $z(\eta)$ for the new function,

$$z'' + 4z' = \cos\eta + 4\eta + 12, \quad z(0) = 0, \quad z'(0) = 7. \tag{A.80}$$

Again, in a similar way as in the previous examples, we can derive the following transformed equation,

$$s^2 Z(s) - sz(0) - z'(0) + 4\left[sZ(s) - z(0)\right] = \frac{s}{s^2+1} + \frac{4}{s^2} + \frac{12}{s}. \tag{A.81}$$

After inserting the boundary conditions and adjusting, we get the equation

$$Z(s) = \frac{7s^4 + 13s^3 + 11s^2 + 12s + 4}{s^3(s^2+1)(s+4)}, \tag{A.82}$$

and, after its decomposition into partial fractions, with a similar emphasizing of the terms important for illustrating the inverse transformation,

$$Z(s) = \frac{17}{16s} + \frac{11}{4s^2} + \frac{1\frac{2!}{2!}}{s^3} - \frac{273}{272(s+4)} + \frac{1}{17}\left(\frac{-s}{s^2+1} + \frac{4}{s^2+1}\right). \tag{A.83}$$

By inverse Laplace transformation, we get the resulting solution first for $z(\eta)$,

$$z(\eta) = \frac{17}{16} + \frac{11}{4}\eta + \frac{1}{2}\eta^2 - \frac{273}{272}\,\mathrm{e}^{-4\eta} + \frac{1}{17}\left(4\sin\eta - \cos\eta\right), \tag{A.84}$$

and, after substituting $y(x) = z(\eta) = z(x - 3)$ and modifications, we get the solution of the equation (A.77) in the resulting form

$$y(x) = \frac{1}{2}x^2 - \frac{1}{4}x - \frac{43}{16} - \frac{273}{272}\,\mathrm{e}^{-4(x-3)} + \frac{1}{17}\left[4\sin(x-3) - \cos(x-3)\right]. \tag{A.85}$$

Example: Solve the equation with the Heaviside and Dirac delta functions on the right-hand side:

$$2y'' + 10y = 3\theta_{12}(t) - 5\,\delta(t-4), \quad y(0) = -1, \quad y'(0) = -2. \tag{A.86}$$

We derive the transformed equation,

$$2\left[s^2 Y(s) - sy(0) - y'(0)\right] + 10Y(s) = \frac{3\mathrm{e}^{-12s}}{s} - 5\mathrm{e}^{-4s}, \tag{A.87}$$

after inserting the boundary conditions and adjusting, we get

$$Y(s) = \frac{3\mathrm{e}^{-12s}}{s(2s^2+10)} - \frac{5\mathrm{e}^{-4s}}{2s^2+10} - \frac{2s+4}{2s^2+10} = 3\mathrm{e}^{-12s}F(s) - 5\mathrm{e}^{-4s}G(s) - H(s). \tag{A.88}$$

After decomposing the individual terms of the first right-hand side, we get the individual functions $f(t)$, $g(t)$, and $h(t)$,

$$f(t) = \frac{1}{10}\left(1 - \cos\sqrt{5}t\right), \quad g(t) = \frac{1}{2\sqrt{5}}\sin\sqrt{5}t, \quad h(t) = \cos\sqrt{5}t + \frac{2}{\sqrt{5}}\sin\sqrt{5}t. \tag{A.89}$$

The final solution will be

$$y(t) = 3\theta_{12}(t)\, f(t-12) - 5\theta_4(t)\, g(t-4) - h(t), \tag{A.90}$$

where $f(t)$, $g(t)$ and $h(t)$ are defined above, for a better understanding of the individual symbols, see also the solved example in the paragraph “step function”.

The results of the examples in this paragraph can be easily verified by the standard procedure for solving second-order ordinary differential equations with constant coefficients given in Section 3.2.1.

A.5 Ordinary second order differential equations with non-constant coefficients, with boundary conditions

Let us also introduce here the following identity: if $f(t)$ is a piecewise continuous function in the interval $\langle 0, \infty)$ of a general the so-called *exponential order*, and if there exist positive constants T and M such that $|f(t)| \le M\mathrm{e}^{\alpha t}$ for all $t \ge T$, then

$$\lim_{s\to\infty} F(s) = 0. \tag{A.91}$$

In other words, a function of general *exponential order* does not grow more steeply than $M\mathrm{e}^{\alpha t}$ for any M and α, and for all sufficiently large t. Whether or not a function is a function of the general exponential order α can be determined by computing the following limit $\lim_{t\to\infty} |f(t)|\,\mathrm{e}^{-\alpha t}$: if this limit is finite for some α, then the function $f(t)$ is a function of the *exponential order* of α; if the limit diverges to infinity, the function is not a function of any general *exponential order*. Almost all the functions we will encounter in this chapter when solving differential equations are functions of some particular exponential order. A good example of a function that is not a function of exponential order is $f(t) = \exp(t^3)$, where we can easily verify that $\lim_{t\to\infty} \exp\left[t(t^2-\alpha)\right] = \infty$, which under the given conditions is true for any α.

Example: Solve the equation

$$y'' + 3xy' - 6y = 2, \quad y(0) = 0, \quad y'(0) = 0. \tag{A.92}$$

From the partial relations derived earlier (the equation (A.38), in addition to the relations mentioned earlier in the examples of equations with constant coefficients), we know that

$$\mathcal{L}\left\{tf'(t)\right\} = \mathcal{L}\left\{xy'\right\} = -\frac{\mathrm{d}}{\mathrm{d}s}(\mathcal{L}\{y'\}) = -\frac{\mathrm{d}}{\mathrm{d}s}\left[sY(s) - y(0)\right] = -sY'(s) - Y(s). \tag{A.93}$$

If we plug all these already known identities into the given equation, we get

$$s^2Y(s) - sy(0) - y'(0) + 3\left[-sY'(s) - Y(s)\right] - 6Y(s) = \frac{2}{s}. \tag{A.94}$$

After inserting the boundary conditions and a small adjustment, we get a first order differential equation,

$$Y'(s) + \left(\frac{3}{s} - \frac{s}{3}\right) Y(s) = -\frac{2}{3s^2}. \tag{A.95}$$

Unlike the examples in the previous section for second-order differential equations with constant coefficients, where we got the transformed solutions straight away, here we get a linear ordinary differential equation of first order that needs to be solved to get the final transformed solution. The solution of the equation (A.95) for $Y(s)$ will be

$$Y(s) = \frac{1}{s^3}\left(2 + C\mathrm{e}^{\frac{s^2}{6}}\right). \tag{A.96}$$

Since the second term (exponential) in parentheses in the transformed solution (A.96) does not resemble any of the elementary (tabulated) solutions of the Laplace transforms, let us assume that it is a function of general *exponential order* and use the above rule for its limit. This means

$$\lim_{s\to\infty} \frac{1}{s^3}\left(2 + C\mathrm{e}^{\frac{s^2}{6}}\right) = 0, \tag{A.97}$$

where the first term always converges to zero, while the second term converges to zero only if $C = 0$. Thus, the transformed solution represents only the first term of the equation (A.96), the resulting solution of the equation (A.92) will be

$$y(x) = x^2, \tag{A.98}$$

which is easy to verify.

Example: Solve the equation

$$xy'' - xy' + y = 2, \quad y(0) = 2, \quad y'(0) = -4. \tag{A.99}$$

From the previous example, we know that $\mathcal{L}\{xy'\} = -sY'(s) - Y(s)$. Here we will also need an analogous identity containing the second derivative,

$$\mathcal{L}\{xy''\} = -\frac{\mathrm{d}}{\mathrm{d}s}(\mathcal{L}\{y''\}) = -\frac{\mathrm{d}}{\mathrm{d}s}\left[s^2Y(s) - sy(0) - y'(0)\right] = -s^2Y'(s) - 2sY(s) + y(0). \tag{A.100}$$

If we plug all these already known identities into the given equation, we get

$$-s^2Y'(s) - 2sY(s) + y(0) - \left[-sY'(s) - Y(s)\right] + Y(s) = \frac{2}{s}. \tag{A.101}$$

After inserting the boundary conditions and adjusting, we get the first order differential equation,

$$Y'(s) + \frac{2}{s}Y(s) = \frac{2}{s^2}. \tag{A.102}$$

Again, we have to solve here the first order equation to get the transformed solution,

$$Y(s) = \frac{2}{s} + \frac{C}{s^2}. \tag{A.103}$$

This transformed solution converges to zero for any constant C, so we don't need to use the principle given in equation (A.91) to get rid of any of the terms, as in the previous example. The inverse transformation then gives

$$y(x) = 2 + Cx \tag{A.104}$$

and after inserting the second boundary condition,

$$y(x) = 2 - 4x. \tag{A.105}$$

In the previous examples we have shown how to solve some ordinary differential equations of second order with non-constant coefficients, but we have chosen the coefficients so that the solution can be found in this way. With differently chosen coefficients, finding a solution could be quite difficult; in general, such equations with non-constant coefficients are usually very difficult to solve.

A.6 Use of convolution in the Laplace transform

Let us now consider the transformed equation in the form

$$H(s) = F(s)G(s), \tag{A.106}$$

which is not solvable by decomposition into partial fractions. One way of its inverse transformation is to use convolution. If $f(t)$ and $g(t)$ are piecewise continuous functions in the interval $\langle 0, \infty)$, then the convolution of the functions $f(t)$ and $g(t)$ will be (see the explanation of convolution above in the section 10)

$$(f * g)(t) = \int_0^t f(\tau)g(t-\tau)\,\mathrm{d}\tau, \tag{A.107}$$

where, in contrast to the general definition of the convolution (10.7), the limits are defined only in the range $\langle 0, t\rangle$, which corresponds to the lower limit for the Laplace transform and the "practical" upper limit for the convolution variable - see the examples on convolutions in chapter 10.

The following identity allows us to solve the inverse Laplace transform of the product of two transformed functions (Laplace images),

$$\mathcal{L}\left\{(f*g)(t)\right\} = F(s)G(s), \quad \mathcal{L}^{-1}\left\{F(s)G(s)\right\} = (f*g)(t). \tag{A.108}$$

In the following two examples, we show how the use of convolution to solve the Laplace transform can look like in practice.

Example: Use convolution to find the inverse transform of the following Laplace image:

$$H(s) = \frac{1}{(s^2+a^2)^2}. \tag{A.109}$$

Let us first decompose the function (A.109) as a product of two functions,

$$H(s) = \frac{1}{s^2+a^2}\frac{1}{s^2+a^2} = F(s)G(s), \tag{A.110}$$

so,

$$f(t) = g(t) = \frac{1}{a} \sin at. \tag{A.111}$$

Using the convolution of these functions, we perform the inverse transformation (only the result is given here),

$$h(t) = (f * g)(t) = \frac{1}{a^2} \int_0^t \sin a\tau \sin(at - a\tau)\, \mathrm{d}\tau = \frac{1}{2a^3} (\sin at - at \cos at)\,. \tag{A.112}$$

Example: Solve the following differential equation with general right-hand side and boundary conditions,

$$4y'' + y = g(t), \quad y(0) = 3, \quad y'(0) = -7. \tag{A.113}$$

As in the previous examples, we find the transformed function

$$4\left[s^2 Y(s) - sy(0) - y\prime(0)\right] + Y(s) = G(s), \tag{A.114}$$

after decomposing it into partial fractions and modifying it with the usual "accents for the inverse transformation", we get

$$Y(s) = \frac{3s}{s^2 + \frac{1}{4}} - \frac{7\frac{2}{2}}{s^2 + \frac{1}{4}} + \frac{1}{4} G(s) \frac{\frac{2}{2}}{s^2 + \frac{1}{4}}. \tag{A.115}$$

The first two terms on the right-hand side of the equation (A.115) can be solved easily, the third term can be solved as a convolution of two functions, the first of the specified "pattern" function and the second as a general one,

$$f(t) = 2 \sin\left(\frac{t}{2}\right), \quad g(t). \tag{A.116}$$

The resulting form of the inverse transformation in this case will be

$$y(t) = 3 \cos\left(\frac{t}{2}\right) - 14 \sin\left(\frac{t}{2}\right) + \frac{1}{2} \int_0^t \sin\left(\frac{\tau}{2}\right) g(t - \tau)\, \mathrm{d}\tau. \tag{A.117}$$

As this last example shows, using convolution can to a large extent help to solve differential equations with boundary conditions, with a general function on the right-hand side. This can be very useful when we have a number of such right-hand-side functions and need to choose only one (or some), for example. Using convolution, we can "superpose" the equation in this way and then just substitute the specific forms of the function $g(t)$ into the convolution integral.

Appendix B

Curvilinear coordinates ★

The basic principles concerning the main curvilinear coordinate systems and the transformation relations associated with them have already been mentioned in Chapter 4. In addition to the *cylindrical* and *spherical* systems, there are also a number of special curvilinear coordinate systems, e.g., elliptical, parabolic, conical, etc., including non-orthogonal systems, i.e., those where the individual coordinate directions do not form a right angle. Mastering a mathematical apparatus describing curvilinear coordinates, their relations, and mutual conversions, is essential for physical practice. In the following sections, we will show in more detail the practical procedures for calculating in Cartesian, cylindrical, spherical, and some other coordinate systems, including the derivation of metric tensors, differential operators, position, velocity, and acceleration vectors, etc.

B.1 Cartesian system

Although the Cartesian system is not a curvilinear system de facto, we refer to it here as a naturally orthogonal coordinate system, where we illustrate the basic relationships and geometric principles that we merely specify and apply by analogy in the more complex, truly curvilinear coordinate systems. Its fundamental advantage is that the (unit) vectors of the Cartesian basis,

$$\vec{e}_x = \hat{\boldsymbol{x}} = (1,0,0), \quad \vec{e}_y = \hat{\boldsymbol{y}} = (0,1,0), \quad \vec{e}_z = \hat{\boldsymbol{z}} = (0,0,1), \tag{B.1}$$

are constant (they are always of the same magnitude and the same direction), so the derivatives of these vectors are zero. We hereafter implicitly assume that we "live" in $\mathbb{R}^3$ in the whole of Appendix B; we will also use here the bold-faced "hat" notation of the unit basis vectors for the typographical clarity (that is, for example, $\hat{\boldsymbol{x}}$ instead of $\vec{e}_x$, etc.). For the squared distance of two points, in differential form holds

$$\mathrm{d}s^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2, \quad \text{which can be generalized by the so-called } \textit{metric form} \quad \mathrm{d}s^2 = g_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j, \tag{B.2}$$

where indexes i, j denote particular coordinate directions ($i, j = x, y, z$) and at the same time thus determine particular components of 3×3 metric tensor. Thus, the *covariant* metric tensor g_{ij} of the Cartesian system has the elementary form of a unit matrix. The significance of the *contravariant* metric tensor g^{ij} of the Cartesian system is formally determined by the square of

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

the vector magnitude,

$$\left(\frac{\partial}{\partial s}\right)^2 = g^{ij}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} = \left(\frac{\partial}{\partial x}\right)^2 + \left(\frac{\partial}{\partial y}\right)^2 + \left(\frac{\partial}{\partial z}\right)^2 . \tag{B.3}$$

At the same time, to each metric must generally apply $g_{ij}\, g^{ij} = \boldsymbol{E}$, covariant and contravariant metric tensor will thus always form mutually inverse matrices. Therefore, in the Cartesian system, they will have the form

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g^{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{B.4}$$

B.1.1 Differential operators

- *Gradient* of a scalar function $f(x, y, z)$ is defined in the Cartesian system (see Chapter 5.3) as a vector in the form

$$\vec{\nabla} f = \operatorname{grad} f = \hat{\boldsymbol{x}}\frac{\partial f}{\partial x} + \hat{\boldsymbol{y}}\frac{\partial f}{\partial y} + \hat{\boldsymbol{z}}\frac{\partial f}{\partial z} = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right). \tag{B.5}$$

The gradient represents at each point of the scalar field the *direction of largest* (*steepest*) *increase* of this field. *Gradient of a vector* (of a vector field) $\vec{A}(x, y, z)$ is defined as a second-order tensor (see Section 2.3) in the form

$$\vec{\nabla}\vec{A} = \operatorname{grad}\vec{A} = \left(\hat{\boldsymbol{x}}\frac{\partial}{\partial x} + \hat{\boldsymbol{y}}\frac{\partial}{\partial y} + \hat{\boldsymbol{z}}\frac{\partial}{\partial z}\right)\left(A_x\hat{\boldsymbol{x}} + A_y\hat{\boldsymbol{y}} + A_z\hat{\boldsymbol{z}}\right). \tag{B.6}$$

Because it is the so-called *tensor product*, where the particular vectors of the basis are multiplied as matrices, the first of which is a column vector, and the second is a row vector, the ordering of the tensor elements must always be kept. Using matrix formalism, we can write tensor of the vector field gradient as (see, for example, Arfken & Weber (2005))

$$\vec{\nabla}\vec{A} = \begin{array}{c} \\ \hat{\boldsymbol{x}} \\ \hat{\boldsymbol{y}} \\ \hat{\boldsymbol{z}} \end{array} \begin{array}{c} \begin{array}{ccc} \quad\hat{\boldsymbol{x}} & \quad\hat{\boldsymbol{y}} & \quad\hat{\boldsymbol{z}} \end{array} \\ \begin{pmatrix} \dfrac{\partial A_x}{\partial x} & \dfrac{\partial A_y}{\partial x} & \dfrac{\partial A_z}{\partial x} \\ \dfrac{\partial A_x}{\partial y} & \dfrac{\partial A_y}{\partial y} & \dfrac{\partial A_z}{\partial y} \\ \dfrac{\partial A_x}{\partial z} & \dfrac{\partial A_y}{\partial z} & \dfrac{\partial A_z}{\partial z} \end{pmatrix} \end{array}. \tag{B.7}$$

- *Divergence* of a vector (vector field) $\vec{A}(x, y, z)$ is defined as a scalar (scalar field)

$$\vec{\nabla}\cdot\vec{A} = \operatorname{div}\vec{A} = \hat{\boldsymbol{x}}_{\boldsymbol{i}}\cdot\hat{\boldsymbol{x}}_{\boldsymbol{j}}\frac{\partial A_i}{\partial x_j} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}. \tag{B.8}$$

The divergence of a vector in *orthogonal* systems corresponds to the tensor trace of the vector field gradient; thus, it is a contraction of this tensor (see Section 2.3). In general *orthogonal* coordinates, it can be written in the form

$$\vec{\nabla}\cdot\vec{A} = \left[\frac{\partial}{\partial x_j}(h^k A^k) + \Gamma^k_{jl} h^l A^l\right]\delta^k_j = \frac{\partial}{\partial x_j}(h^j A^j) + \Gamma^j_{jl} h^l A^l. \tag{B.9}$$

By using Equation (2.61), this expression can also be rewritten into the form of

$$\vec{\nabla} \cdot \vec{A} = \left[\frac{\partial}{\partial x_j}(h_k A_k) - \Gamma^l_{jk} h_l A_l \right] \delta_{jk} = \frac{\partial}{\partial x_j}(h_j A_j) - \Gamma^l_{jj} h_l A_l. \tag{B.10}$$

The terms h_i are the so-called *Lamé coefficients* (see also Chapter 4), often also called the *scaling factors* (not to be confused with the Lamé coefficients of the same name in mechanics of continua), named after French mathematician Gabriel Lamé. For the corresponding metric tensor, there applies

$$h_i h_i = g_{ii}, \quad h^i h^i = g^{ii} \tag{B.11}$$

(therefore, only the orthogonal systems whose metric tensors have non-zero elements only on the main diagonal are now considered). The expression Γ^l_{jk} is the so-called *Christoffel symbol* (see Section 2.3) named after the German mathematician and physicist Elwin Bruno Christoffel, defining the so-called *curvature terms* in curvilinear coordinate systems,

$$\Gamma^l_{jk} = \frac{1}{2} g^{lm} \left(\frac{\partial g_{km}}{\partial x_j} + \frac{\partial g_{jm}}{\partial x_k} - \frac{\partial g_{jk}}{\partial x_m} \right), \tag{B.12}$$

where indexes l, m are the so-called free indexes that can take any of the values $1, 2, 3$, or x, y, z, at any time. The explicit expression for a vector divergence in a general orthogonal system can be written in the form (where $i \neq j \neq k$)

$$\vec{\nabla} \cdot \vec{A} = \frac{1}{h_i h_j h_k} \left[\frac{\partial}{\partial x_i} (h_j h_k A_i) + \frac{\partial}{\partial x_j} (h_k h_i A_j) + \frac{\partial}{\partial x_k} (h_i h_j A_k) \right]. \tag{B.13}$$

This is fully equivalent to a more compact form of expression,

$$\vec{\nabla} \cdot \vec{A} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_i} (h_j h_k A_i) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_i} \left(\sqrt{g}\, h^i A^i \right). \tag{B.14}$$

Components $h^i A^i$ (in literature, only A^i is usually abbreviated) of a vector $\vec{A}$ correspond to (see Equation (2.61)) $h^i A^i = g^{ij}(h_j A_j)$, where g is the determinant of the metric tensor that is identical to the square of the corresponding Jacobian of the coordinate transformation. So it is

$$\sqrt{|\det g_{ij}|} = J, \quad \sqrt{|\det g^{ij}|} = J^{-1}. \tag{B.15}$$

Generally, the divergence of the *tensor* of nth-order is a tensor of an order $n-1$, so the second-order tensor divergence will be a vector. The compact form of the *second-order tensor* divergence notation will have the form

$$\nabla_j A^{ij} = A_i. \tag{B.16}$$

Explicit notation of a second-order tensor divergence in the Cartesian system (practically it is a matrix multiplication of a vector with a transposed matrix; the scalar product of two vectors is also a matrix multiplication of two vectors where the second one is transposed, i.e., column; see Section 2.3) will take the form (see Arfken & Weber (2005))

$$\vec{\nabla} \cdot A_{ij} = \left(\hat{\boldsymbol{x}} \frac{\partial}{\partial x} + \hat{\boldsymbol{y}} \frac{\partial}{\partial y} + \hat{\boldsymbol{z}} \frac{\partial}{\partial z} \right) \begin{array}{c|ccc} & \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \hat{\boldsymbol{x}} & & & \\ \hat{\boldsymbol{y}} & & \left(\begin{matrix} A_{xx} & A_{xy} & A_{xz} \\ A_{yx} & A_{yy} & A_{yz} \\ A_{zx} & A_{zy} & A_{zz} \end{matrix} \right)^T & \\ \hat{\boldsymbol{z}} & & & \end{array} = \tag{B.17}$$

$$\hat{\boldsymbol{x}} \left(\frac{\partial A_{xx}}{\partial x} + \frac{\partial A_{xy}}{\partial y} + \frac{\partial A_{xz}}{\partial z} \right) + \hat{\boldsymbol{y}} \left(\frac{\partial A_{yx}}{\partial x} + \frac{\partial A_{yy}}{\partial y} + \frac{\partial A_{yz}}{\partial z} \right) + \hat{\boldsymbol{z}} \left(\frac{\partial A_{zx}}{\partial x} + \frac{\partial A_{zy}}{\partial y} + \frac{\partial A_{zz}}{\partial z} \right).$$

- *Curl* of a vector (vector field) $\vec{A}(x,y,z)$ in the Cartesian system is called a vector

$$\vec{\nabla}\times\vec{A} = \hat{\boldsymbol{x}}\left(\frac{\partial A_z}{\partial y}-\frac{\partial A_y}{\partial z}\right)+\hat{\boldsymbol{y}}\left(\frac{\partial A_x}{\partial z}-\frac{\partial A_z}{\partial x}\right)+\hat{\boldsymbol{z}}\left(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right). \tag{B.18}$$

General expression for curl $\vec{\nabla}\times\vec{A}$ of a vector $\vec{A}$ in an arbitrary *orthogonal* coordinate system can be defined in the following way,

$$\vec{\nabla}\times\vec{A} = \epsilon_{ijk}\frac{1}{h_jh_k}\left[\nabla_j(h_kA_k)\right]\hat{\boldsymbol{x}}_{\boldsymbol{i}} = \epsilon_{ijk}\frac{1}{h_jh_k}\left[\frac{\partial}{\partial x_j}(h_kA_k)-\Gamma^l_{jk}h_lA_l\right]\hat{\boldsymbol{x}}_{\boldsymbol{i}}. \tag{B.19}$$

In Equation (B.19), the expression ϵ_{ijk} (where all three indexes i,j,k can successively correspond to all three coordinate directions) corresponds to the antisymmetric (the so-called *Levi-Civita*, see Equation (2.50)) symbol, which is $+1$ for even index permutations, -1 for odd index permutations, and 0 if two or more indexes repeat.

Due to the symmetry of the indexes in the components of the curl vector and the complete anti-symmetry of the Levi-Civita ϵ-symbol, the expressions $\Gamma^l_{jk}A_l$ in Equation (B.19) are canceled; this simplifies the expression into the form

$$\vec{\nabla}\times\vec{A} = \epsilon_{ijk}\frac{1}{h_jh_k}\left[\frac{\partial}{\partial x_j}(h_kA_k)\right]\hat{\boldsymbol{x}}_{\boldsymbol{i}}. \tag{B.20}$$

In the Cartesian system where $h_1,h_2,h_3=1$, Equation (B.20) will correspond to Equation (B.18). If we write the curl vector again by components, we get

$$\vec{\nabla}\times\vec{A} = \left(\frac{\partial A_z}{\partial y}-\frac{\partial A_y}{\partial z},\frac{\partial A_x}{\partial z}-\frac{\partial A_z}{\partial x},\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right). \tag{B.21}$$

- *Laplacian* (Laplace operator) is defined as a divergence of a gradient, i.e., $\vec{\nabla}\cdot\vec{\nabla}$ (we usually denote it by the symbol Δ). It is thus a scalar operator, which can act on scalar functions, vectors (by individual components), tensors (by individual elements) without changing their *tensor order* (i.e., a scalar remains a scalar, a vector remains a vector, etc.). In the Cartesian system, the Laplacian has a quite simple form. Analogously to Equation (B.8), where the components of the gradient vector replace the components of the vector $\vec{A}$, we can write

$$\Delta = \vec{\nabla}\cdot\vec{\nabla} = \operatorname{div}\operatorname{grad} = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}. \tag{B.22}$$

B.1.2 Surfaces, volumes

Let's denote S_k the coordinate surface (see Chapter 4) with a constant value of the coordinate x_k, bounded by the coordinate curves $x_i, x_i+\Delta x_i, x_j, x_j+\Delta x_j$, $i\neq j\neq k$. For example, in the Cartesian system, it will be a surface with a constant value of $z=z_0$, bounded by lines $x=x_0, x=x_0+\Delta x, y=y_0, y=y_0+\Delta y$. The calculation of the area of such surface is, of course, quite trivial; it will be a rectangle (square) with the area $\Delta x\Delta y$. The general relation for calculating the area of such surface will have the form

$$S_k = \int\limits_{x_{0i}}^{x_{0i}+\Delta x_i}\int\limits_{x_{0j}}^{x_{0j}+\Delta x_j} J'_{ij}\,\mathrm{d}x_i\,\mathrm{d}x_j, \tag{B.23}$$

where J'_{ij} is the square root of the absolute value of the determinant (minor) of the relevant submatrix of the metric tensor. In this case, it would be the determinant $J'_{ij} = \sqrt{|g_{ii}g_{jj} - g_{ij}g_{ji}|}$. We define the integrand of Equation (B.23) as a *surface element* $\mathrm{d}S_k = J'_{ij}\,\mathrm{d}x_i\,\mathrm{d}x_j$. In the Cartesian system, the determinants of all three submatrices $J'_{ij} = 1$. Next, if we denote V the volume, defined by coordinate surfaces with constant coordinates $x_i, x_i + \Delta x_i, x_j, x_j + \Delta x_j, x_k, x_k + \Delta x_k$, $i \neq j \neq k$, the general relation for calculating the magnitude of such a volume will have the form

$$V = \int\limits_{x_{0i}}^{x_{0i}+\Delta x_i} \int\limits_{x_{0j}}^{x_{0j}+\Delta x_j} \int\limits_{x_{0k}}^{x_{0k}+\Delta x_k} J\,\mathrm{d}x_i\,\mathrm{d}x_j\,\mathrm{d}x_k, \tag{B.24}$$

where J is the square root of the absolute value of the determinant of the metric tensor (Jacobian, see Equation (B.15)). The integrand of Equation (B.24) expresses the *volume element* $\mathrm{d}V = J\,\mathrm{d}x_i\,\mathrm{d}x_j\,\mathrm{d}x_k$. In the Cartesian system again $J = 1$, and the volume element will have the shape of a rectangular cuboid of volume $\Delta x \Delta y \Delta z$.

B.1.3 Vectors of position, velocity and acceleration

In the Cartesian system, the vector notation is very simple, a position vector $\vec{r}$, a velocity vector $\vec{v}$, and an acceleration vector $\vec{a}$ will take the form

$$\vec{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}} = (x, y, z), \tag{B.25}$$

$$\vec{v} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \dot{x}\hat{\boldsymbol{x}} + \dot{y}\hat{\boldsymbol{y}} + \dot{z}\hat{\boldsymbol{z}} = v_x\hat{\boldsymbol{x}} + v_y\hat{\boldsymbol{y}} + v_z\hat{\boldsymbol{z}} = (v_x, v_y, v_z), \tag{B.26}$$

$$\vec{a} = \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \ddot{x}\hat{\boldsymbol{x}} + \ddot{y}\hat{\boldsymbol{y}} + \ddot{z}\hat{\boldsymbol{z}} = a_x\hat{\boldsymbol{x}} + a_y\hat{\boldsymbol{y}} + a_z\hat{\boldsymbol{z}} = (a_x, a_y, a_z), \tag{B.27}$$

where $\dot{x} = \mathrm{d}x/\mathrm{d}t$, $\dot{y} = \mathrm{d}y/\mathrm{d}t$, and $\dot{z} = \mathrm{d}z/\mathrm{d}t$, respectively.

B.2 Cylindrical system

The cylindrical system may be useful for describing a variety of axially symmetric and rotational phenomena, e.g., electric and magnetic fields around direct conductors, fluid vortices, galaxies, stellar disks, etc. Coordinate directions are (see Section 4.2): ρ - distance from the axis of cylindrical symmetry, ϕ - azimuthal angle, z - height. The transformation from cylindrical to the Cartesian system is given by relations[1]

$$x = \rho\cos\phi, \quad y = \rho\sin\phi, \quad z = z. \tag{B.28}$$

For the reverse transformation from Cartesian to cylindrical system applies

$$\rho = \sqrt{x^2 + y^2}, \quad \phi = \arccos\frac{x}{\sqrt{x^2 + y^2}}, \quad \phi = \arcsin\frac{y}{\sqrt{x^2 + y^2}}, \quad \phi = \arctan\frac{y}{x}. \tag{B.29}$$

Unit vectors of the cylindrical basis will in the Cartesian system (see Figure 4.1) have a form

$$\hat{\boldsymbol{\rho}} = \hat{\boldsymbol{x}}\cos\phi + \hat{\boldsymbol{y}}\sin\phi = (\cos\phi, \sin\phi, 0), \quad \hat{\boldsymbol{\phi}} = -\hat{\boldsymbol{x}}\sin\phi + \hat{\boldsymbol{y}}\cos\phi = (-\sin\phi, \cos\phi, 0),$$
$$\hat{\boldsymbol{z}} = (0, 0, 1). \tag{B.30}$$

[1] In the following description, we will distinguish ρ for a radial cylindrical coordinate, r for a radial spherical coordinate.

Thus, the only constant basis vector will be $\hat{\boldsymbol{z}}$; the other basis vectors will change direction depending on the angle ϕ. Nonzero derivatives of the basis vectors in the direction of the coordinate axes and nonzero time derivatives of the basis vectors will be (from Equation (B.30))

$$\begin{aligned} \frac{\partial \hat{\boldsymbol{\rho}}}{\partial \phi} &= (-\sin\phi, \cos\phi, 0) = \hat{\boldsymbol{\phi}}, & \frac{\partial \hat{\boldsymbol{\rho}}}{\partial t} &= \frac{\partial \hat{\boldsymbol{\rho}}}{\partial \phi}\frac{\partial \phi}{\partial t} = \hat{\boldsymbol{\phi}}\dot{\phi}, \\ \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} &= (-\cos\phi, -\sin\phi, 0) = -\hat{\boldsymbol{\rho}}, & \frac{\partial \hat{\boldsymbol{\phi}}}{\partial t} &= \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi}\frac{\partial \phi}{\partial t} = -\hat{\boldsymbol{\rho}}\dot{\phi}. \end{aligned} \tag{B.31}$$

If we derive unit vectors of the cylindrical basis in the direction of Cartesian coordinate axes, then, for example, in the direction of the x-axis, we get

$$\begin{aligned} \frac{\partial \hat{\boldsymbol{\rho}}}{\partial x} &= \frac{\partial}{\partial x}(\cos\phi, \sin\phi,\ 0) = \frac{\partial}{\partial x}\left(\frac{x}{\sqrt{x^2+y^2}}, \frac{y}{\sqrt{x^2+y^2}}, 0\right) = -\hat{\boldsymbol{\phi}}\,\frac{\sin\phi}{\rho}, \\ \frac{\partial \hat{\boldsymbol{\phi}}}{\partial x} &= \frac{\partial}{\partial x}(-\sin\phi, \cos\phi,\ 0) = \hat{\boldsymbol{\rho}}\,\frac{\sin\phi}{\rho}. \end{aligned} \tag{B.32}$$

Similarly, we get derivatives in all other directions. Reverse transformation of unit basis vectors (see Equation (B.30)) will be

$$\hat{\boldsymbol{x}} = \hat{\boldsymbol{\rho}}\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi, \quad \hat{\boldsymbol{y}} = \hat{\boldsymbol{\rho}}\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi, \quad \hat{\boldsymbol{z}} = \hat{\boldsymbol{z}}. \tag{B.33}$$

The metric form of the cylindrical system can be easily derived from the fact that the distance of two points in space must be independent of the choice of the coordinate system, i.e., $\mathrm{d}s^2$ from Equation (B.2) must be identical for all coordinate systems. From Equation (B.28) we get

$$\mathrm{d}x = \cos\phi\,\mathrm{d}\rho - \rho\sin\phi\,\mathrm{d}\phi, \quad \mathrm{d}y = \sin\phi\,\mathrm{d}\rho + \rho\cos\phi\,\mathrm{d}\phi, \quad \mathrm{d}z = \mathrm{d}z. \tag{B.34}$$

Substituting this into Equation (B.2), we get the metric form of the cylindrical coordinate system,

$$\mathrm{d}s^2 = \mathrm{d}\rho^2 + \rho^2\,\mathrm{d}\phi^2 + \mathrm{d}z^2. \tag{B.35}$$

So we can write covariant (g_{ij}) and contravariant (g^{ij}) metric tensor and also (see Equation (B.11)) the corresponding *Lamé coefficients* of the cylindrical coordinate system,

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \rho^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g^{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{1}{\rho^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad h_\rho = 1,\ h_\phi = \rho,\ h_z = 1. \tag{B.36}$$

From Equation (B.12), the nonzero *Christoffel symbols* of the cylindrical metric will be

$$\Gamma^{\rho}_{\phi\phi} = -\rho,\ \Gamma^{\phi}_{\phi\rho}\,(\Gamma^{\phi}_{\rho\phi}) = \frac{1}{\rho}. \tag{B.37}$$

B.2.1 Differential operators

- *Gradient* of a scalar function $f(\rho, \phi, z)$ in the cylindrical system is derived from Equation (B.5), where we substitute the expressions from Equation (B.33) for unit basis vectors and expand the particular components of the gradient by a chain rule for derivatives of composite functions. After more detailed rewriting, we get

$$\vec{\nabla} f = \left(\hat{\boldsymbol{\rho}} \cos\phi - \hat{\boldsymbol{\phi}} \sin\phi\right) \left(\frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial x}\right) + \\ + \left(\hat{\boldsymbol{\rho}} \sin\phi + \hat{\boldsymbol{\phi}} \cos\phi\right) \left(\frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial y} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial y} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial y}\right) + \hat{\boldsymbol{z}}\frac{\partial f}{\partial z}. \tag{B.38}$$

Particular non-zero partial derivatives are calculated from Equation (B.29),

$$\frac{\partial \rho}{\partial x} = \frac{x}{\sqrt{x^2+y^2}} = \cos\phi, \; \frac{\partial \phi}{\partial x} = -\frac{y}{x^2+y^2} = -\frac{\sin\phi}{\rho}, \\ \frac{\partial \rho}{\partial y} = \frac{y}{\sqrt{x^2+y^2}} = \sin\phi, \; \frac{\partial \phi}{\partial y} = \frac{x}{x^2+y^2} = \frac{\cos\phi}{\rho}. \tag{B.39}$$

After substitution and adjustment, we get the final form gradient of a scalar function,

$$\vec{\nabla} f = \hat{\boldsymbol{\rho}}\frac{\partial f}{\partial \rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial f}{\partial \phi} + \hat{\boldsymbol{z}}\frac{\partial f}{\partial z} = \left(\frac{\partial f}{\partial \rho}, \frac{1}{\rho}\frac{\partial f}{\partial \phi}, \frac{\partial f}{\partial z}\right). \tag{B.40}$$

Now, the unit vectors of the cylindrical basis are no longer represented by their components from Equation (B.30), where we have "seen" them from Cartesian system. Analogously to Equation (B.6) (tensor product) and using Equation (B.40), the *gradient of a vector field* $\vec{A}(\rho, \phi, z)$ in the cylindrical system is then defined as a second-order tensor in the form

$$\vec{\nabla}\vec{A} = \left(\hat{\boldsymbol{\rho}}\frac{\partial}{\partial \rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial}{\partial \phi} + \hat{\boldsymbol{z}}\frac{\partial}{\partial z}\right)\left(A_\rho\hat{\boldsymbol{\rho}} + A_\phi\hat{\boldsymbol{\phi}} + A_z\hat{\boldsymbol{z}}\right). \tag{B.41}$$

Unlike the Cartesian system, the unit basis vectors $\hat{\boldsymbol{\rho}}$ and $\hat{\boldsymbol{\phi}}$ are no longer constant here, so the gradient operator acts on them also (their derivatives are described in Equation (B.31)). Using matrix formalism, we can write tensor of a vector field gradient in the cylindrical system,

$$\vec{\nabla}\vec{A} = \begin{array}{c c} & \begin{array}{ccc} \hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\phi}} & \hat{\boldsymbol{z}} \end{array} \\ \begin{array}{c} \hat{\boldsymbol{\rho}} \\ \hat{\boldsymbol{\phi}} \\ \hat{\boldsymbol{z}} \end{array} & \begin{pmatrix} \dfrac{\partial A_\rho}{\partial \rho} & \dfrac{\partial A_\phi}{\partial \rho} & \dfrac{\partial A_z}{\partial \rho} \\ \dfrac{1}{\rho}\dfrac{\partial A_\rho}{\partial \phi} - \dfrac{A_\phi}{\rho} & \dfrac{1}{\rho}\dfrac{\partial A_\phi}{\partial \phi} + \dfrac{A_\rho}{\rho} & \dfrac{1}{\rho}\dfrac{\partial A_z}{\partial \phi} \\ \dfrac{\partial A_\rho}{\partial z} & \dfrac{\partial A_\phi}{\partial z} & \dfrac{\partial A_z}{\partial z} \end{pmatrix} \end{array}. \tag{B.42}$$

The same result can be achieved by another procedure, e.g., using the *Christoffel symbols* (see Equation (B.37)), where, unlike in Equation (B.19), we write

$$\vec{\nabla}\vec{A} = \frac{1}{h_j h_k}\left[\nabla_j(h_k A_k)\right]\hat{\boldsymbol{x}}_{\boldsymbol{j}}\hat{\boldsymbol{x}}_{\boldsymbol{k}} = \frac{1}{h_j h_k}\left[\frac{\partial}{\partial x_j}(h_k A_k) - \Gamma^l_{jk} h_l A_l\right]\hat{\boldsymbol{x}}_{\boldsymbol{j}}\hat{\boldsymbol{x}}_{\boldsymbol{k}}. \tag{B.43}$$

However, the procedure given by Equation (B.43) can only be used for orthogonal coordinate systems, while the procedure given by Equation (B.41) is quite general.

- *Divergence* of a vector (vector field) $\vec{A}(\rho, \phi, z)$ is defined in cylindrical coordinates in the sense of Equation (B.41), analogously to Equation (B.8), as a scalar (scalar field)

$$\vec{\nabla} \cdot \vec{A} = \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho A_\rho) + \frac{1}{\rho} \frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}. \tag{B.44}$$

  By comparing with Equation (B.42) again, we see that divergence is a trace of a gradient tensor of the vector field. Divergence of the *second-order tensor*, described by a matrix 3×3, will be a vector (first-order tensor). We will not mention here the explicit form of notation of divergence of a second-order tensor in cylindrical coordinates (cf. Equation (B.17)), for those interested, I refer to the corresponding literature, e.g., Abramowitz & Stegun (1972), Young (1993), Arfken & Weber (2005), etc.

- *Curl* of a vector (vector field) $\vec{A}(\rho, \phi, z)$ in the cylindrical system, where $h_\rho = 1$, $h_\phi = \rho$, $h_z = 1$, is derived according to the already mentioned relation (B.20). We get

$$\vec{\nabla} \times \vec{A} = \left(\frac{1}{\rho} \frac{\partial A_z}{\partial \phi} - \frac{\partial A_\phi}{\partial z} \right) \hat{\boldsymbol{\rho}} + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial \rho} \right) \hat{\boldsymbol{\phi}} + \frac{1}{\rho} \left[\frac{\partial}{\partial \rho} (\rho A_\phi) - \frac{\partial A_\rho}{\partial \phi} \right] \hat{\boldsymbol{z}}. \tag{B.45}$$

- We derive the *Laplacian* (see Equation (B.22)) by replacing the components of the vector $\vec{A}$ in the equation of divergence (B.44) by the corresponding components of the gradient vector from Equation (B.40). We get

$$\Delta = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}. \tag{B.46}$$

B.2.2 Surfaces, volumes

As in the Cartesian system, let S_k denote the coordinate surface with a constant value of the x_k coordinate bounded by coordinate curves $x_i, x_i + \Delta x_i, x_j, x_j + \Delta x_j$, $i \neq j \neq k$. In the cylindrical system, for example, it will be a surface with a constant value of $z = z_0$, bounded by half-lines $\phi = \phi_1, \phi = \phi_2$, and curves (circles) $\rho = \rho_1, \rho = \rho_2$. Calculating the area of such a surface is no longer as trivial as in the Cartesian system, it will be the intersection of a circular sector with an annulus (surface between two concentric circles). If we consider another surface, e.g., with a constant coordinate $\rho = \rho_0$, bounded by coordinate surfaces $\phi = \phi_1, \phi = \phi_2, z = z_1, z = z_2$, it will be a part of the cylindrical surface. When calculating the areas of these surfaces, we start from Equations (B.23) and (B.36),

$$\begin{aligned}
S_\rho &= \int_{\phi_1}^{\phi_2} \int_{z_1}^{z_2} \sqrt{g_{\phi\phi}\, g_{zz}}\, \mathrm{d}\phi\, \mathrm{d}z = \int_{\phi_1}^{\phi_2} \int_{z_1}^{z_2} \rho\, \mathrm{d}\phi\, \mathrm{d}z = \rho \Delta\phi \Delta z, \\
S_\phi &= \int_{z_1}^{z_2} \int_{\rho_1}^{\rho_2} \sqrt{g_{zz}\, g_{\rho\rho}}\, \mathrm{d}z\, \mathrm{d}\rho = \int_{z_1}^{z_2} \int_{\rho_1}^{\rho_2} \mathrm{d}z\, \mathrm{d}\rho = \Delta z \Delta \rho, \\
S_z &= \int_{\rho_1}^{\rho_2} \int_{\phi_1}^{\phi_2} \sqrt{g_{\rho\rho}\, g_{\phi\phi}}\, \mathrm{d}\rho\, \mathrm{d}\phi = \int_{\rho_1}^{\rho_2} \int_{\phi_1}^{\phi_2} \rho\, \mathrm{d}\rho\, \mathrm{d}\phi = \frac{\rho_2^2 - \rho_1^2}{2} \Delta\phi.
\end{aligned} \tag{B.47}$$

In the cylindrical coordinate system, the non-diagonal terms of submatrices J'_{ij} (see Equation (B.23)) will be zero. If V is a volume defined by coordinate surfaces with constant coordinates

$\rho_1, \rho_2, \phi_1, \phi_2, z_1, z_2$, magnitude of this volume, according to Equation (B.24), will be

$$V = \int_{\rho_1}^{\rho_2} \int_{\phi_1}^{\phi_2} \int_{z_1}^{z_2} \rho \,\mathrm{d}\rho \,\mathrm{d}\phi \,\mathrm{d}z = \frac{\rho_2^2 - \rho_1^2}{2} \Delta\phi \Delta z. \tag{B.48}$$

We can calculate the size of any other more complicated structure similarly by determining the integration limits in a given coordinate system.

B.2.3 Vectors of position, velocity, and acceleration

When describing vectors in the cylindrical system, we start from their description in the Cartesian system and substitute all equations for the derivation of unit vectors and vector components (Equations (B.28) - (B.33)). The position and velocity vectors in the cylindrical system will be

$$\vec{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}} = \rho\hat{\boldsymbol{\rho}} + z\hat{\boldsymbol{z}}, \quad \vec{v} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \dot{\rho}\hat{\boldsymbol{\rho}} + \rho\dot{\phi}\hat{\boldsymbol{\phi}} + \dot{z}\hat{\boldsymbol{z}}, \tag{B.49}$$

respectively. This form can be expected since the position vector always starts from the origin of the coordinates. The velocity and acceleration vectors are also defined as

$$\vec{v} = v_\rho\hat{\boldsymbol{\rho}} + v_\phi\hat{\boldsymbol{\phi}} + v_z\hat{\boldsymbol{z}}, \quad \vec{a} = \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = a_\rho\hat{\boldsymbol{\rho}} + a_\phi\hat{\boldsymbol{\phi}} + a_z\hat{\boldsymbol{z}}. \tag{B.50}$$

By differentiating Equation (B.49) by time, we get the particular components of the acceleration vector,

$$a_\rho = \ddot{\rho} - \rho\dot{\phi}^2 = \frac{\mathrm{d}v_\rho}{\mathrm{d}t} - \rho\dot{\phi}^2, \quad a_\phi = \rho\ddot{\phi} + 2\dot{\rho}\dot{\phi} = \frac{\mathrm{d}v_\phi}{\mathrm{d}t} + \dot{\rho}\dot{\phi}, \quad a_z = \ddot{z} = \frac{\mathrm{d}v_z}{\mathrm{d}t}. \tag{B.51}$$

Because there is $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \vec{v}\cdot\vec{\nabla}$ (the chain rule for differentiation, in this case for partial derivatives of $\vec{v} = \vec{v}(t, \rho, \phi, z)$), then the acceleration expressed by the components of the velocity vector will be

$$a_\rho = \frac{\partial v_\rho}{\partial t} + \underbrace{v_\rho\frac{\partial v_\rho}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_\rho}{\partial \phi} + v_z\frac{\partial v_\rho}{\partial z}}_{(\vec{v}\cdot\vec{\nabla})v_\rho} - \frac{v_\phi^2}{\rho}, \tag{B.52}$$

$$a_\phi = \frac{\partial v_\phi}{\partial t} + \underbrace{v_\rho\frac{\partial v_\phi}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_\phi}{\partial \phi} + v_z\frac{\partial v_\phi}{\partial z}}_{(\vec{v}\cdot\vec{\nabla})v_\phi} + \frac{v_\rho v_\phi}{\rho}, \tag{B.53}$$

$$a_z = \frac{\partial v_z}{\partial t} + \underbrace{v_\rho\frac{\partial v_z}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_z}{\partial \phi} + v_z\frac{\partial v_z}{\partial z}}_{(\vec{v}\cdot\vec{\nabla})v_z}. \tag{B.54}$$

B.3 Spherical system

The spherical system is appropriate for describing phenomena with central symmetry, such as physical fields, formed by mass points, astronomical bodies, etc. Its basic description can be found in Section 4.3. Among other things, it is implicitly used also in cartography, where the system of meridians and parallels is de facto a system of azimuthal and elevation angular coordinates (see below). However, the elevation angle is calculated here differently. In the "mathematical convention", it increases from 0 to π (polar angle), while in the "cartographic convention" it increases from $-\pi/2$ to $\pi/2$ (elevation angle), moreover, in the opposite sense to the azimuthal coordinate direction.

Coordinate directions are r - distance from the center of spherical symmetry, θ - polar angle, ϕ - azimuthal angle. The transfer from spherical to the Cartesian system is given by the relations

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta. \tag{B.55}$$

For the reverse transformation from Cartesian to spherical system applies

$$\begin{gathered} r = \sqrt{x^2+y^2+z^2}, \\ \theta = \arccos\frac{z}{\sqrt{x^2+y^2+z^2}}, \quad \theta = \arcsin\sqrt{\frac{x^2+y^2}{x^2+y^2+z^2}}, \\ \phi = \arccos\frac{x}{\sqrt{x^2+y^2}}, \quad \phi = \arcsin\frac{y}{\sqrt{x^2+y^2}}, \quad \phi = \arctan\frac{y}{x}. \end{gathered} \tag{B.56}$$

Analogous to Equation (B.30), unit vectors of the spherical basis will have in the Cartesian system the form (see Figure 4.2)

$$\begin{aligned} \hat{\boldsymbol{r}} &= \hat{\boldsymbol{x}}\sin\theta\cos\phi + \hat{\boldsymbol{y}}\sin\theta\sin\phi + \hat{\boldsymbol{z}}\cos\theta = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \\ \hat{\boldsymbol{\theta}} &= \hat{\boldsymbol{x}}\cos\theta\cos\phi + \hat{\boldsymbol{y}}\cos\theta\sin\phi - \hat{\boldsymbol{z}}\sin\theta = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta), \\ \hat{\boldsymbol{\phi}} &= -\hat{\boldsymbol{x}}\sin\phi + \hat{\boldsymbol{y}}\cos\phi = (-\sin\phi, \cos\phi, 0). \end{aligned} \tag{B.57}$$

In the spherical system, none of the basis vectors is constant. Derivatives of the basis vectors in the direction of particular coordinate axes will be (from Equation (B.57)),

$$\begin{aligned} \frac{\partial\hat{\boldsymbol{r}}}{\partial r} &= 0, & \frac{\partial\hat{\boldsymbol{r}}}{\partial\theta} &= \hat{\boldsymbol{\theta}}, & \frac{\partial\hat{\boldsymbol{r}}}{\partial\phi} &= \hat{\boldsymbol{\phi}}\sin\theta, \\ \frac{\partial\hat{\boldsymbol{\theta}}}{\partial r} &= 0, & \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta} &= -\hat{\boldsymbol{r}}, & \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi} &= \hat{\boldsymbol{\phi}}\cos\theta, \\ \frac{\partial\hat{\boldsymbol{\phi}}}{\partial r} &= 0, & \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\theta} &= 0, & \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi} &= -\hat{\boldsymbol{r}}\sin\theta - \hat{\boldsymbol{\theta}}\cos\theta. \end{aligned} \tag{B.58}$$

Time derivatives of the basis vectors will be

$$\begin{aligned} \frac{\partial\hat{\boldsymbol{r}}}{\partial t} &= \frac{\partial\hat{\boldsymbol{r}}}{\partial\theta}\frac{\partial\theta}{\partial t} + \frac{\partial\hat{\boldsymbol{r}}}{\partial\phi}\frac{\partial\phi}{\partial t} = \hat{\boldsymbol{\theta}}\dot{\theta} + \hat{\boldsymbol{\phi}}\dot{\phi}\sin\theta, \\ \frac{\partial\hat{\boldsymbol{\theta}}}{\partial t} &= \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta}\frac{\partial\theta}{\partial t} + \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi}\frac{\partial\phi}{\partial t} = -\hat{\boldsymbol{r}}\dot{\theta} + \hat{\boldsymbol{\phi}}\dot{\phi}\cos\theta, \\ \frac{\partial\hat{\boldsymbol{\phi}}}{\partial t} &= \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi}\frac{\partial\phi}{\partial t} = -\hat{\boldsymbol{r}}\dot{\phi}\sin\theta - \hat{\boldsymbol{\theta}}\dot{\phi}\cos\theta. \end{aligned} \tag{B.59}$$

By reverse transforming the unit basis vectors (see Equation (B.57)), we get

$$\begin{aligned} \hat{\boldsymbol{x}} &= \hat{\boldsymbol{r}}\sin\theta\cos\phi + \hat{\boldsymbol{\theta}}\cos\theta\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi, \\ \hat{\boldsymbol{y}} &= \hat{\boldsymbol{r}}\sin\theta\sin\phi + \hat{\boldsymbol{\theta}}\cos\theta\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi, \\ \hat{\boldsymbol{z}} &= \hat{\boldsymbol{r}}\cos\theta - \hat{\boldsymbol{\theta}}\sin\theta. \end{aligned} \tag{B.60}$$

We obtain the metric form for the spherical system by differentiating Equation (B.55),

$$\begin{aligned} \mathrm{d}x &= \sin\theta\cos\phi\,\mathrm{d}r + r\cos\theta\cos\phi\,\mathrm{d}\theta - r\sin\theta\sin\phi\,\mathrm{d}\phi, \\ \mathrm{d}y &= \sin\theta\sin\phi\,\mathrm{d}r + r\cos\theta\sin\phi\,\mathrm{d}\theta + r\sin\theta\cos\phi\,\mathrm{d}\phi, \\ \mathrm{d}z &= \cos\theta\,\mathrm{d}r - r\sin\theta\,\mathrm{d}\theta, \end{aligned} \tag{B.61}$$

substituting this into Equation (B.2) gives the spherical metric form

$$\mathrm{d}s^2 = \mathrm{d}r^2 + r^2\,\mathrm{d}\theta^2 + r^2\sin^2\theta\,\mathrm{d}\phi^2. \tag{B.62}$$

Covariant (g_{ij}) and contravariant (g^{ij}) metric tensor, as well as (see Equation (B.11)) the corresponding *Lamé coefficients* of the spherical coordinate system, will be

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2\sin^2\theta \end{pmatrix}, \quad g^{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{1}{r^2} & 0 \\ 0 & 0 & \dfrac{1}{r^2\sin^2\theta} \end{pmatrix}, \quad h_r = 1,\ h_\theta = r,\ h_\phi = r\sin\theta. \tag{B.63}$$

Using Equation (B.12), we derive the nonzero *Christoffel symbols* of the spherical metrics,

$$\Gamma^r_{\theta\theta} = -r,\ \Gamma^\theta_{\theta r}\,(\Gamma^\theta_{r\theta}) = \Gamma^\phi_{\phi r}\,(\Gamma^\phi_{r\phi}) = \frac{1}{r},\ \Gamma^r_{\phi\phi} = -r\sin^2\theta,\ \Gamma^\theta_{\phi\phi} = -\sin\theta\cos\theta,\ \Gamma^\phi_{\phi\theta}\,(\Gamma^\phi_{\theta\phi}) = \cot\theta. \tag{B.64}$$

B.3.1 Differential operators

- *Gradient* of a scalar function $f(r,\theta,\phi)$ in the spherical system is derived from Equation (B.5), where we substitute the expressions from Equation (B.60) for unit basis vectors and expand the particular components of the gradient by a chain rule for derivatives of composite functions. After more detailed rewriting, we get

$$\begin{aligned} \vec{\nabla} f = {} & \left(\hat{\boldsymbol{r}}\sin\theta\cos\phi + \hat{\boldsymbol{\theta}}\cos\theta\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi\right)\left(\frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}\right) + \\ & + \left(\hat{\boldsymbol{r}}\sin\theta\sin\phi + \hat{\boldsymbol{\theta}}\cos\theta\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi\right)\left(\frac{\partial f}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial y}\right) + \\ & + \left(\hat{\boldsymbol{r}}\cos\theta - \hat{\boldsymbol{\theta}}\sin\theta\right)\left(\frac{\partial f}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial z}\right). \end{aligned} \tag{B.65}$$

Individual partial derivatives are calculated from Equation (B.56),

$$\begin{aligned} \frac{\partial r}{\partial x} &= \frac{x}{\sqrt{x^2+y^2+z^2}} = \sin\theta\cos\phi, & \frac{\partial \theta}{\partial x} &= \frac{xz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = \frac{\cos\theta\cos\phi}{r}, \\ \frac{\partial r}{\partial y} &= \frac{y}{\sqrt{x^2+y^2+z^2}} = \sin\theta\sin\phi, & \frac{\partial \theta}{\partial y} &= \frac{yz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = \frac{\cos\theta\sin\phi}{r}, \\ \frac{\partial r}{\partial z} &= \frac{z}{\sqrt{x^2+y^2+z^2}} = \cos\theta, & \frac{\partial \theta}{\partial z} &= -\frac{\sqrt{x^2+y^2}}{x^2+y^2+z^2} = -\frac{\sin\theta}{r}, \\ \frac{\partial \phi}{\partial x} &= -\frac{y}{x^2+y^2} = -\frac{\sin\phi}{r\sin\theta}, \\ \frac{\partial \phi}{\partial y} &= \frac{x}{x^2+y^2} = \frac{\cos\phi}{r\sin\theta}. \end{aligned} \tag{B.66}$$

After substitution and adjustment, we get the final form of the gradient,

$$\vec{\nabla} f = \hat{\boldsymbol{r}}\frac{\partial f}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial f}{\partial \theta} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi} = \left(\frac{\partial f}{\partial r}, \frac{1}{r}\frac{\partial f}{\partial \theta}, \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\right). \tag{B.67}$$

Again, we do not substitute for the spherical basis unit vectors their components from Equation (B.57), where we "saw" them from the Cartesian system. Analogously to Equation (B.6) (tensor product), using Equation (B.67) is then the *gradient of a vector field* $\vec{A}(r,\theta,\phi)$ in the spherical system defined as a second-order tensor in the form

$$\vec{\nabla}\vec{A} = \left(\hat{\boldsymbol{r}}\frac{\partial}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\right)\left(A_r\hat{\boldsymbol{r}} + A_\theta\hat{\boldsymbol{\theta}} + A_\phi\hat{\boldsymbol{\phi}}\right). \tag{B.68}$$

Unlike the cylindrical system, the gradient operator here already acts on all unit basis vectors (their derivatives - see Equation (B.58)). Employing the matrix formalism, we can write the tensor of a vector field gradient in the spherical system as (Arfken & Weber, 2005)

$$\vec{\nabla}\vec{A} = \begin{array}{c} \\ \hat{\boldsymbol{r}} \\ \hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{\phi}} \end{array} \begin{array}{c} \begin{array}{ccc} \hat{\boldsymbol{r}} & \hat{\boldsymbol{\theta}} & \hat{\boldsymbol{\phi}} \end{array} \\ \begin{pmatrix} \dfrac{\partial A_r}{\partial r} & \dfrac{\partial A_\theta}{\partial r} & \dfrac{\partial A_\phi}{\partial r} \\ \dfrac{1}{r}\dfrac{\partial A_r}{\partial \theta} - \dfrac{A_\theta}{r} & \dfrac{1}{r}\dfrac{\partial A_\theta}{\partial \theta} + \dfrac{A_r}{r} & \dfrac{1}{r}\dfrac{\partial A_\phi}{\partial \theta} \\ \dfrac{1}{r\sin\theta}\dfrac{\partial A_r}{\partial \phi} - \dfrac{A_\phi}{r} & \dfrac{1}{r\sin\theta}\dfrac{\partial A_\theta}{\partial \phi} - \dfrac{A_\phi}{r}\cot\theta & \dfrac{1}{r\sin\theta}\dfrac{\partial A_\phi}{\partial \phi} + \dfrac{A_r}{r} + \dfrac{A_\theta}{r}\cot\theta \end{pmatrix} \end{array}. \tag{B.69}$$

We achieve the same result in this case, for example, by using the formalism of *Christoffel symbols* (see Equation (B.37)) according to the general relation (B.43). However, this procedure can be used only for orthogonal coordinate systems, whereas the method of Equation (B.68) is quite general.

- *Divergence* of a vector (vector field) $\vec{A}(r,\theta,\phi)$ is in the spherical coordinates defined by Equation (B.68). Analogously to Equation (B.8), it is defined as a scalar (scalar field)

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 A_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta A_\theta\right) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}. \tag{B.70}$$

By comparison with Equation (B.69), we again see that divergence is the trace of the gradient tensor of a vector field.

- *Curl* of a vector (vector field) $\vec{A}(r,\theta,\phi)$ in the spherical system, where $h_r = 1$, $h_\theta = r$, $h_\phi = r\sin\theta$, we derive from Equation (B.20). We get in this case,

$$\vec{\nabla}\times\vec{A} = \frac{1}{r\sin\theta}\left[\frac{\partial}{\partial \theta}\left(\sin\theta\, A_\phi\right) - \frac{\partial A_\theta}{\partial \phi}\right]\hat{\boldsymbol{r}} + \frac{1}{r}\left[\frac{1}{\sin\theta}\frac{\partial A_r}{\partial \phi} - \frac{\partial}{\partial r}\left(rA_\phi\right)\right]\hat{\boldsymbol{\theta}} + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(rA_\theta\right) - \frac{\partial A_r}{\partial \theta}\right]\hat{\boldsymbol{\phi}}. \tag{B.71}$$

- We derive the *Laplacian* (see Equation (B.22)) by replacing components of the vector $\vec{A}$ in the divergence equation (B.70) by the corresponding components of the gradient vector from Equation (B.67). The resulting compactly written form is

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}. \tag{B.72}$$

B.3.2 Surfaces, volumes

As in the previous systems, let S_k be a coordinate surface with a constant value of x_k coordinate bounded by coordinate curves $x_i, x_i + \Delta x_i, x_j, x_j + \Delta x_j$, $i \neq j \neq k$. In the spherical system, for example, it will be a surface with constant value $r = r_0$, bounded by pairs of curves (circles) with coordinates $\theta = \theta_1, \theta = \theta_2$, and $\phi = \phi_1, \phi = \phi_2$. Calculating the area of such a surface is here not trivial at all, it will be a part of a surface with double curvature bounded by two diverging coordinate surfaces (in which the curves with the coordinates $\phi = \phi_1$, $\phi = \phi_2$ lie) and two circles with centers on a common axis but lying in different planes perpendicular to this axis (curves with the coordinates $\theta = \theta_1, \theta = \theta_2$). If we consider another surface, e.g., with a constant coordinate $\phi = \phi_0$, bounded by the coordinate surfaces $\theta = \theta_1, \theta = \theta_2, r = r_1, r = r_2$, it will be part of a circular sector limited by two concentric circles. When calculating the sizes of these surfaces, we start again from Equation (B.23) and Equation (B.63), so

$$\begin{aligned}
S_r &= \int_{\theta_1}^{\theta_2}\int_{\phi_1}^{\phi_2} \sqrt{g_{\theta\theta}\, g_{\phi\phi}}\, \mathrm{d}\theta\, \mathrm{d}\phi = \int_{\theta_1}^{\theta_2}\int_{\phi_1}^{\phi_2} r^2 \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi = r^2 \left(\cos\theta_1 - \cos\theta_2\right) \Delta\phi, \\
S_\theta &= \int_{\phi_1}^{\phi_2}\int_{r_1}^{r_2} \sqrt{g_{\phi\phi}\, g_{rr}}\, \mathrm{d}\phi\, \mathrm{d}r = \int_{\phi_1}^{\phi_2}\int_{r_1}^{r_2} r \sin\theta\, \mathrm{d}\phi\, \mathrm{d}r = \frac{r_2^2 - r_1^2}{2} \sin\theta \Delta\phi, \\
S_\phi &= \int_{r_1}^{r_2}\int_{\theta_1}^{\theta_2} \sqrt{g_{rr}\, g_{\theta\theta}}\, \mathrm{d}r\, \mathrm{d}\theta = \int_{r_1}^{r_2}\int_{\theta_1}^{\theta_2} r\, \mathrm{d}r\, \mathrm{d}\theta = \frac{r_2^2 - r_1^2}{2} \Delta\theta.
\end{aligned} \tag{B.73}$$

In the spherical, thus again orthogonal coordinate system, all non-diagonal terms of submatrix J'_{ij} (see Equation (B.23)) will be zero. Let us traditionally denote V the volume defined by coordinate surfaces with constant coordinates $r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2$, in this case, the shape of such a structure corresponds to the intersection of a pyramid with a concentric spherical intermediate layer (spherical annulus). The formula for calculating the magnitude of such a volume will have, according to Equation (B.24), the form

$$V = \int_{r_1}^{r_2}\int_{\theta_1}^{\theta_2}\int_{\phi_1}^{\phi_2} r^2 \sin\theta\, \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\phi = \frac{r_2^3 - r_1^3}{3} \left(\cos\theta_1 - \cos\theta_2\right) \Delta\phi. \tag{B.74}$$

In the orthogonal spherical coordinate system, as in the cylindrical system, Jacobian J can be determined as $\sqrt{g_{rr}\, g_{\theta\theta}\, g_{\phi\phi}} = r^2 \sin\theta$. This method makes it possible to calculate the size of any more complex structures in the spherical coordinate system by appropriately determining the integration limits.

B.3.3 Vectors of position, velocity, and acceleration

When describing vectors in the spherical system, we start from their basic description in the Cartesian system, including all equations for the derivation of unit vectors and vector components (Equations (B.55)-(B.60)). The position and velocity vectors in the spherical system will be

$$\vec{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}} = r\hat{\boldsymbol{r}}, \quad \vec{v} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \frac{\mathrm{d}\left(r\hat{\boldsymbol{r}}\right)}{\mathrm{d}t} = \dot{r}\hat{\boldsymbol{r}} + r\left(\dot{\theta}\hat{\boldsymbol{\theta}} + \dot{\phi}\hat{\boldsymbol{\phi}}\sin\theta\right). \tag{B.75}$$

Again, this conclusion can be expected, given that the position vector starts from the origin of the coordinates. The velocity and acceleration vectors are defined as

$$\vec{v} = v_r \hat{\boldsymbol{r}} + v_\theta \hat{\boldsymbol{\theta}} + v_\phi \hat{\boldsymbol{\phi}}, \quad \vec{a} = \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = a_r \hat{\boldsymbol{r}} + a_\theta \hat{\boldsymbol{\theta}} + a_\phi \hat{\boldsymbol{\phi}}. \tag{B.76}$$

By differentiating Equation (B.75) by time, we obtain the particular components of the acceleration vector in the spherical coordinate system,

$$a_r = \ddot{r} - r\dot{\theta}^2 - r\dot{\phi}^2 \sin^2\theta = \frac{\mathrm{d}v_r}{\mathrm{d}t} - r\dot{\theta}^2 - r\dot{\phi}^2 \sin^2\theta, \tag{B.77}$$

$$a_\theta = r\ddot{\theta} + 2\dot{r}\dot{\theta} - r\dot{\phi}^2 \sin\theta\cos\theta = \frac{\mathrm{d}v_\theta}{\mathrm{d}t} + \dot{r}\dot{\theta} - r\dot{\phi}^2 \sin\theta\cos\theta, \tag{B.78}$$

$$a_\phi = r\ddot{\phi}\sin\theta + 2\dot{r}\dot{\phi}\sin\theta + 2r\dot{\theta}\dot{\phi}\cos\theta = \frac{\mathrm{d}v_\phi}{\mathrm{d}t} + \dot{r}\dot{\phi}\sin\theta + r\dot{\theta}\dot{\phi}\cos\theta. \tag{B.79}$$

Because there is $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \vec{v} \cdot \vec{\nabla}$ (the chain rule for differentiation, in this case for partial derivative $\vec{v} = \vec{v}(t, r, \theta, \phi)$), then the acceleration, expressed in the spherical coordinate system using the components of the velocity vector, will be

$$a_r = \frac{\partial v_r}{\partial t} + \underbrace{v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial v_r}{\partial \phi}}_{(\vec{v}\cdot\vec{\nabla})v_r} - \frac{v_\theta^2 + v_\phi^2}{r}, \tag{B.80}$$

$$a_\theta = \frac{\partial v_\theta}{\partial t} + \underbrace{v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial v_\theta}{\partial \phi}}_{(\vec{v}\cdot\vec{\nabla})v_\theta} + \frac{v_r v_\theta}{r} - \frac{v_\phi^2 \cot\theta}{r}, \tag{B.81}$$

$$a_\phi = \frac{\partial v_\phi}{\partial t} + \underbrace{v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}}_{(\vec{v}\cdot\vec{\nabla})v_\phi} + \frac{v_r v_\phi}{r} + \frac{v_\theta v_\phi \cot\theta}{r}. \tag{B.82}$$

It would certainly be possible to describe this stuff in much more detail, e.g., operations with vectors and tensors within the systems, etc. Anyway, at least some of the procedures are shown here from a practical point of view. In the following sections, we will briefly present at least one non-orthogonal coordinate system whose description was, to some extent, enforced by the creation of a numerical computational grid for hydrodynamic modeling of a particular physical phenomenon.

B.4 Elliptical system

We will briefly mention three specific orthogonal systems, which may be related to the previous topic or to the given examples (or they may have interesting physical applications) - elliptic, parabolic, and "annuloid" (toroidal). The two-dimensional *elliptical* coordinate system (see Figure B.1) is defined by two classes of coordinate curves with constant $\sigma \in \langle 0, \infty)$ and $\tau \in \langle 0, 2\pi)$ (this notation is not completely fixed, it may vary in different literature), with two common foci at points $[-a,\, 0], [a,\, 0]$. In three-dimensional version (the system is then called *elliptic cylindrical*), the azimuthal angular parameter ϕ is added (cylindrical symmetry with respect to the z-axis).

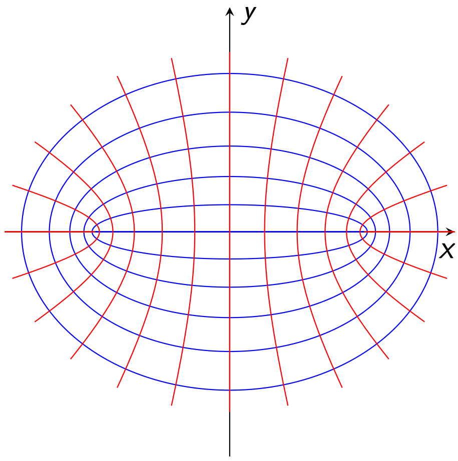

Figure B.1: Scheme of the two-dimensional elliptical system in the x, y plane, common foci are at points $[-a, 0], [a, 0]$. Blue-colored are the elliptic curves with constant parameter σ, with sequence (from the narrowest to the widest) $\sigma = 0, 0.2, 0.4, 0.6, 0.8, 1$, red-colored are the hyperbolic curves with constant parameter τ, with sequence (from right to left) from $\tau = 0$ to $\tau = \pi$ with increment $\pi/12$. In the three-dimensional version (see description), the z direction corresponds to the shown y direction.

Transformation equations from the Cartesian to the elliptical system in a three-dimensional case will be

$$x = a\cosh\sigma\cos\tau\cos\phi, \quad y = a\cosh\sigma\cos\tau\sin\phi, \quad z = a\sinh\sigma\sin\tau. \tag{B.83}$$

From the definition of hyperbolic sine and cosine (1.20),(1.21), and from the exponential expression of sine and cosine (see Euler's relations in Example 9.7), we can easily derive reverse transformational relations. These, however (in the clockwise order of variables σ, ϕ, τ), will be complex (the plane ρ-z, where $\rho = \sqrt{x^2 + y^2}$, we can imagine as the Gaussian plane),

$$\begin{aligned} \sigma &= \frac{1}{2}\left[\operatorname{argcosh}\frac{\rho + \mathrm{i}z}{a} + \operatorname{argcosh}\frac{\rho - \mathrm{i}z}{a}\right], \quad \phi = \arctan\frac{y}{x}, \\ \tau &= \frac{1}{2\mathrm{i}}\left[\operatorname{argcosh}\frac{\rho + \mathrm{i}z}{a} - \operatorname{argcosh}\frac{\rho - \mathrm{i}z}{a}\right]. \end{aligned} \tag{B.84}$$

The metric form of such an elliptical system will be

$$\begin{aligned} \mathrm{d}s^2 &= a^2\left[\left(\cosh^2\sigma\sin^2\tau + \sinh^2\sigma\cos^2\tau\right)\left(\mathrm{d}\sigma^2 + \mathrm{d}\tau^2\right) + \cosh^2\sigma\cos^2\tau\,\mathrm{d}\phi^2\right] = \\ &= a^2\left[\left(\sinh^2\sigma + \sin^2\tau\right)\left(\mathrm{d}\sigma^2 + \mathrm{d}\tau^2\right) + \cosh^2\sigma\cos^2\tau\,\mathrm{d}\phi^2\right] = \\ &= a^2\left[\left(\cosh^2\sigma - \cos^2\tau\right)\left(\mathrm{d}\sigma^2 + \mathrm{d}\tau^2\right) + \cosh^2\sigma\cos^2\tau\,\mathrm{d}\phi^2\right]. \end{aligned} \tag{B.85}$$

Covariant metric tensor g_{ij} and the corresponding *Lamé coefficients* of the elliptical coordinate system in the order of directions σ, ϕ, τ will be

$$g_{ij} = \begin{bmatrix} a^2\left(\sinh^2\sigma + \sin^2\tau\right) & 0 & 0 \\ 0 & a^2\cosh^2\sigma\cos^2\tau & 0 \\ 0 & 0 & a^2\left(\sinh^2\sigma + \sin^2\tau\right) \end{bmatrix}, \tag{B.86}$$

$$h_\sigma = a\sqrt{\sinh^2\sigma + \sin^2\tau}, \quad h_\phi = a\cosh\sigma\cos\tau, \quad h_\tau = a\sqrt{\sinh^2\sigma + \sin^2\tau}. \tag{B.87}$$

Contravariant metric tensor g^{ij} of the diagonal metric will be a tensor with inverted element values on the main diagonal. The Jacobian of the coordinate transformation from the Cartesian to the elliptical system will be

$$J = a^3 \left(\sinh^2\sigma + \sin^2\tau\right)\cosh\sigma\cos\tau = a^3\left(\cosh^2\sigma - \cos^2\tau\right)\cosh\sigma\cos\tau, \tag{B.88}$$

while J^{-1} is the Jacobian of the reverse transformation. The nonzero *Christoffel symbols* of the elliptical metric (see Equation (B.12)) will be (where $\mathcal{S} = \cosh 2\sigma - \cos 2\tau$),

$$\begin{aligned}
&\Gamma^{\sigma}_{\sigma\sigma} = -\Gamma^{\sigma}_{\tau\tau} = \Gamma^{\tau}_{\sigma\tau}(\Gamma^{\tau}_{\tau\sigma}) = \frac{\sinh 2\sigma}{\mathcal{S}},\ \Gamma^{\tau}_{\tau\tau} = -\Gamma^{\tau}_{\sigma\sigma} = \Gamma^{\sigma}_{\sigma\tau}(\Gamma^{\sigma}_{\tau\sigma}) = \frac{\sin 2\tau}{\mathcal{S}},\\
&\Gamma^{\sigma}_{\phi\phi} = -\frac{\sinh 2\sigma\cos^2\tau}{\mathcal{S}},\ \Gamma^{\tau}_{\phi\phi} = \frac{\cosh^2\sigma\sin 2\tau}{\mathcal{S}},\ \Gamma^{\phi}_{\sigma\phi}(\Gamma^{\phi}_{\phi\sigma}) = \tanh\sigma,\ \Gamma^{\phi}_{\phi\tau}(\Gamma^{\phi}_{\tau\phi}) = -\tan\tau.
\end{aligned} \tag{B.89}$$

The differential operators of the gradient of a scalar function, divergence and curl of a vector, and the Laplacian will have in this elliptical coordinate system (using the formalization of the Lamé coefficients for orthogonal systems as well as Equations (B.14) and (B.20)) successively the form,

$$\vec{\nabla} f = \left(\frac{\frac{\partial f}{\partial\sigma}}{a\sqrt{\sinh^2\sigma + \sin^2\tau}}, \frac{\frac{\partial f}{\partial\phi}}{a\cosh\sigma\cos\tau}, \frac{\frac{\partial f}{\partial\tau}}{a\sqrt{\sinh^2\sigma + \sin^2\tau}}\right), \tag{B.90}$$

$$\begin{aligned}
\vec{\nabla}\cdot\vec{A} = {} & \frac{\frac{\partial}{\partial\sigma}\left(\sqrt{\sinh^2\sigma + \sin^2\tau}\cosh\sigma\, A_\sigma\right)}{a\left(\sinh^2\sigma + \sin^2\tau\right)\cosh\sigma} + \\
& + \frac{\frac{\partial A_\phi}{\partial\phi}}{a\cosh\sigma\cos\tau} + \frac{\frac{\partial}{\partial\tau}\left(\sqrt{\sinh^2\sigma + \sin^2\tau}\cos\tau\, A_\tau\right)}{a\left(\sinh^2\sigma + \sin^2\tau\right)\cos\tau},
\end{aligned} \tag{B.91}$$

$$\begin{aligned}
\vec{\nabla}\times\vec{A} = {} & \frac{\cosh\sigma\frac{\partial}{\partial\tau}(\cos\tau\, A_\phi) - \sqrt{\sinh^2\sigma + \sin^2\tau}\,\frac{\partial A_\tau}{\partial\phi}}{a\sqrt{\sinh^2\sigma + \sin^2\tau}\cosh\sigma\cos\tau}\,\hat{\boldsymbol{\sigma}} + \\
& + \frac{\frac{\partial}{\partial\sigma}\left(\sqrt{\sinh^2\sigma + \sin^2\tau}\, A_\tau\right) - \frac{\partial}{\partial\tau}\left(\sqrt{\sinh^2\sigma + \sin^2\tau}\, A_\sigma\right)}{a\left(\sinh^2\sigma + \sin^2\tau\right)}\,\hat{\boldsymbol{\phi}} + \\
& + \frac{\sqrt{\sinh^2\sigma + \sin^2\tau}\,\frac{\partial A_\sigma}{\partial\phi} - \cos\tau\frac{\partial}{\partial\sigma}(\cosh\sigma\, A_\phi)}{a\sqrt{\sinh^2\sigma + \sin^2\tau}\cosh\sigma\cos\tau}\,\hat{\boldsymbol{\tau}},
\end{aligned} \tag{B.92}$$

$$\Delta = \frac{\frac{\partial}{\partial\sigma}\left(\cosh\sigma\frac{\partial}{\partial\sigma}\right) + \frac{\partial}{\partial\tau}\left(\cos\tau\frac{\partial}{\partial\tau}\right)}{a^2\left(\sinh^2\sigma + \sin^2\tau\right)\cosh\sigma\cos\tau} + \frac{\frac{\partial^2}{\partial\phi^2}}{a^2\cosh^2\sigma\cos^2\tau}. \tag{B.93}$$

Other operator identities and geometric parameters are derived in a similar way as in the case of the cylindrical or spherical coordinate system.

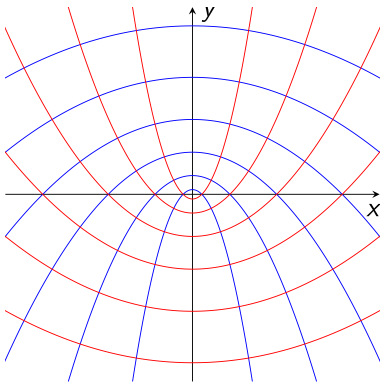

Figure B.2: Scheme of the two-dimensional parabolic system in the plane x, y. Curves with a constant parameter $u = 0.5$ (narrowest), 1, 1.5, 2, 2.5, 3 (widest) are indicated in blue color, curves with the same sequence of constant parameters v are marked in red color. In the three-dimensional case (see description), to the direction y then corresponds the direction z.

B.5 Parabolic system

Parabolic coordinate system is defined in two-dimensional version (see Figure B.2) by two classes of parabolic coordinate curves with constant parameters u and v (this notation is not completely fixed again, it can differ in different literature) and with a common focus at the point $[0, 0]$. In the three-dimensional version (the system is then called *parabolic cylindrical*), the azimuthal angle parameter ϕ will be added (cylindrical symmetry with respect to the z-axis).

The transformation equations in a three-dimensional case will be

$$x = uv\cos\phi, \quad y = uv\sin\phi, \quad z = \frac{u^2 - v^2}{2}. \tag{B.94}$$

Reverse transformations in the clockwise order of the variables u, v, ϕ will have the form

$$u = \sqrt{\sqrt{x^2 + y^2 + z^2} + z}, \quad v = \sqrt{\sqrt{x^2 + y^2 + z^2} - z}, \quad \phi = \arctan\frac{y}{x}. \tag{B.95}$$

The metric form of the parabolic system will have the form

$$\mathrm{d}s^2 = \left(u^2 + v^2\right)\left(\mathrm{d}u^2 + \mathrm{d}v^2\right) + u^2v^2\,\mathrm{d}\phi^2. \tag{B.96}$$

Covariant metric tensor g_{ij} and the corresponding *Lamé coefficients* of the parabolic coordinate system in the order of directions u, v, ϕ will be

$$g_{ij} = \begin{bmatrix} u^2 + v^2 & 0 & 0 \\ 0 & u^2 + v^2 & 0 \\ 0 & 0 & u^2v^2 \end{bmatrix}, \quad h_u = \sqrt{u^2 + v^2},\, h_v = \sqrt{u^2 + v^2},\, h_\phi = uv. \tag{B.97}$$

Contravariant metric tensor g^{ij} of the diagonal metric will be a tensor with inverted element values on the main diagonal. The Jacobian coordinate transformation from the Cartesian to the parabolic system will be

$$J = uv\left(u^2 + v^2\right), \tag{B.98}$$

while J^{-1} is Jacobian of the reverse transformation. Nonzero *Christoffel symbols* of the parabolic metrics (see Equation (B.12)) will be,

$$\Gamma^u_{uu} = \Gamma^v_{uv}\,(\Gamma^v_{vu}) = \frac{u}{u^2+v^2},\ \Gamma^v_{vv} = \Gamma^u_{uv}\,(\Gamma^u_{vu}) = \frac{v}{u^2+v^2},\ \Gamma^v_{uu} = -\frac{v}{u^2+v^2},\ \Gamma^u_{vv} = -\frac{u}{u^2+v^2},$$
$$\Gamma^u_{\phi\phi} = -\frac{uv^2}{u^2+v^2},\ \Gamma^v_{\phi\phi} = -\frac{u^2v}{u^2+v^2},\ \Gamma^\phi_{u\phi}\,(\Gamma^\phi_{\phi u}) = \frac{1}{u},\ \Gamma^\phi_{v\phi}\,(\Gamma^\phi_{\phi v}) = \frac{1}{v}. \tag{B.99}$$

Differential operators of the gradient of a scalar function, divergence, and rotation of the vector, and the Laplacian (using the Lamé coefficient formalism for orthogonal systems as well as Equations (B.14) and (B.20)) will in the parabolic coordinate system be

$$\vec{\nabla} f = \left(\frac{\frac{\partial f}{\partial u}}{\sqrt{u^2+v^2}}, \frac{\frac{\partial f}{\partial v}}{\sqrt{u^2+v^2}}, \frac{1}{uv}\frac{\partial f}{\partial \phi} \right), \tag{B.100}$$

$$\vec{\nabla}\cdot\vec{A} = \frac{\frac{\partial}{\partial u}\left(u\sqrt{u^2+v^2}\,A_u\right)}{u(u^2+v^2)} + \frac{\frac{\partial}{\partial v}\left(v\sqrt{u^2+v^2}\,A_v\right)}{v(u^2+v^2)} + \frac{1}{uv}\frac{\partial A_\phi}{\partial \phi}, \tag{B.101}$$

$$\vec{\nabla}\times\vec{A} = \frac{\frac{\partial}{\partial v}(uvA_\phi) - \sqrt{u^2+v^2}\,\frac{\partial A_v}{\partial \phi}}{uv\sqrt{u^2+v^2}}\,\hat{\boldsymbol{u}} + \frac{\sqrt{u^2+v^2}\,\frac{\partial A_u}{\partial \phi} - \frac{\partial}{\partial u}(uvA_\phi)}{uv\sqrt{u^2+v^2}}\,\hat{\boldsymbol{v}} +$$
$$+\frac{\frac{\partial}{\partial u}\left(\sqrt{u^2+v^2}\,A_v\right) - \frac{\partial}{\partial v}\left(\sqrt{u^2+v^2}\,A_u\right)}{u^2+v^2}\,\hat{\boldsymbol{\phi}}, \tag{B.102}$$

$$\Delta = \frac{\frac{1}{u}\frac{\partial}{\partial u}\left(u\frac{\partial}{\partial u}\right) + \frac{1}{v}\frac{\partial}{\partial v}\left(v\frac{\partial}{\partial v}\right)}{(u^2+v^2)} + \frac{1}{u^2v^2}\frac{\partial^2}{\partial \phi^2}, \tag{B.103}$$

respectively.

Other operator identities and geometric parameters are derived in a similar way as in the case of the cylindrical or spherical coordinate system.

B.6 "Annuloid" (toroidal) system

We will not give a complete description of all relations and operators in this case since the system is too specific; it only concerns one type of a geometric body, the so-called toroid (see Figure B.3, the description of the system also refers to Examples 7.55 and 7.66). We will only show how it is possible to flexibly adapt the principles derived for previous, more universal geometric systems to (basically any) special case. We call an annuloid a body that is created by the rotation of a circle around an axis that lies in the plane of this circle and has no common point with it (a cylindrical symmetrical tube - a torus resembling a tire) is created.

We denote R the radius of the toroidal axis, a the radius of the tube (torus), r the radial distance inside the tube relative to the axis of the tube, and t the angular coordinate of the tube interior. The other directions will correspond to the standard cylindrical notation of the torus, that is, ρ will correspond to the radial distance from the axis of the whole torus, ϕ will be the azimuthal angle of the torus, and z the vertical coordinate (all shown in Figure B.3). We can thus consider r, ϕ, t (in the clockwise sense) as toroidal coordinates. Transformation relations can be written as follows,

$$x = (R + r\cos t)\cos\phi, \quad y = (R + r\cos t)\sin\phi, \quad z = r\sin t. \tag{B.104}$$

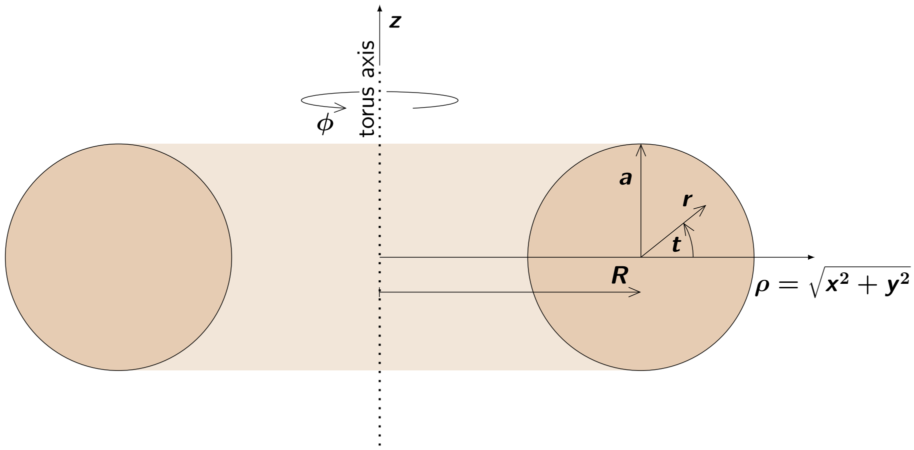

Figure B.3: Transverse slice of the torus in the plane ρ-z, particular directions correspond to the cylindrical system.

In this case, the reverse transformation relations will have a form

$$r = \sqrt{\left(\sqrt{x^2+y^2}-R\right)^2+z^2}, \quad \phi = \arctan\frac{y}{x}, \quad t = \arcsin\frac{z}{\sqrt{\left(\sqrt{x^2+y^2}-R\right)^2+z^2}}. \tag{B.105}$$

Covariant metric tensor g_{ij} and corresponding *Lamé coefficients* of the toroidal coordinate systems will be

$$g_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & (R+r\cos t)^2 & 0 \\ 0 & 0 & r^2 \end{bmatrix}, \quad h_r = 1,\ h_\phi = R + r\cos t,\ h_t = r. \tag{B.106}$$

Since it is a diagonal metric, the contravariant metric tensor g^{ij} of the reverse transformation will also be the tensor of the inverse elements on the main diagonal. Thus, the Jacobian of the coordinate transformation from the Cartesian to the toroidal system will be

$$J = r(R + r\cos t), \tag{B.107}$$

The J^{-1} expression will again be the Jacobian of the reverse transformation. Other parameters can be easily derived in a similar way as in the previous systems.

B.7 Examples of non-orthogonal system

B.7.1 “Conical” system

A natural example of a non-orthogonal coordinate system can be the “conical” system (I intentionally put the name in quotes here, because the regular so-called conic system has a different meaning, it is orthogonal and is constructed in a different way, which I do not introduce here). The coordinate directions of this conical system are: $z \in \langle 0, H)$ - vertical coordinates, $\phi \in \langle 0, 2\pi)$ - azimuthal angle, $\theta \in \langle 0, \pi/2)$ - polar angle and is defined as follows (see Fig. B.4): The transformation equations from this *cone* to the Cartesian coordinate system are

$$x = z\tan\theta\cos\phi, \quad y = z\tan\theta\sin\phi, \quad z = z. \tag{B.108}$$

For the reverse transformation from the Cartesian to the *conical* system we get[2]

$$z = z, \quad \phi = \arctan\frac{y}{x}, \quad \theta = \arctan\frac{\sqrt{x^2+y^2}}{z}. \tag{B.109}$$

Unit basis vectors can be chosen in two ways: as tangent vectors to coordinate curves or as normal vectors to coordinate surfaces. In the case of orthogonal systems, this is the same; in non-orthogonal systems, the two methods are different. In this and the following section, which deals with the "astrophysical disk" system, we will choose the second option for simplicity; the first option gives in our case inadequately extensive and complicated expressions. In case of choosing tangent vectors to coordinate curves, we can obtain the general unit basis vector $\hat{\boldsymbol{v}}$ in an arbitrary coordinate system from the Cartesian expression using the identity

$$\hat{\boldsymbol{v}} = \frac{1}{\|\hat{\boldsymbol{v}}\|}\left(\frac{\partial x}{\partial v}\hat{\boldsymbol{x}} + \frac{\partial y}{\partial v}\hat{\boldsymbol{y}} + \frac{\partial z}{\partial v}\hat{\boldsymbol{z}}\right), \tag{B.110}$$

or solving geometrically using vector addition rules. If the general unit basis vector $\hat{\boldsymbol{v}}$ is chosen as the normal vector to the coordinate surfaces, it is obtained in the same way as the unit normal vector $\hat{\boldsymbol{n}}$ in paragraph 7.1 or again geometrically using the vector addition rules.

Analogously to Eqs. (B.30) and (B.57), the thus chosen unit vectors $\hat{\boldsymbol{z}}$, $\hat{\boldsymbol{\phi}}$, $\hat{\boldsymbol{\theta}}$ of the *conical* basis in the Cartesian system will have the form

$$\hat{\boldsymbol{z}} = \hat{\boldsymbol{z}}, \quad \hat{\boldsymbol{\phi}} = -\hat{\boldsymbol{x}}\sin\phi + \hat{\boldsymbol{y}}\cos\phi, \quad \hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{x}}\cos\phi + \hat{\boldsymbol{y}}\sin\phi)\cos\theta - \hat{\boldsymbol{z}}\sin\theta. \tag{B.111}$$

where none of the basis vectors is constant. The vector $\hat{\boldsymbol{w}}$ is de facto identical to the spherical $\hat{\boldsymbol{r}}$, the vector $\hat{\boldsymbol{\phi}}$ to the cylindrical (also spherical) $\hat{\boldsymbol{\phi}}$, and the vector $\hat{\boldsymbol{\theta}}$ to the cylindrical $\hat{\boldsymbol{r}}$. By backtransforming the unit basis vectors (see equation (B.111)) we obtain

$$\hat{\boldsymbol{x}} = \frac{\hat{\boldsymbol{z}}\sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi, \quad \hat{\boldsymbol{y}} = \frac{\hat{\boldsymbol{z}}\sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi, \quad \hat{\boldsymbol{z}} = \hat{\boldsymbol{z}}. \tag{B.112}$$

In the thus defined *conical* system, there is only one constant basis vector $\hat{\boldsymbol{z}}$ (analogous to Cartesian or cylindrical system), the other basis vectors are non-constant (the basis vector $\hat{\boldsymbol{\phi}}$ corresponds to the same vector of cylindrical or spherical system, the basis vector $\hat{\boldsymbol{\theta}}$ is analogous to spherical system). Figure B.4 schematically shows this system in the vertical plane z-θ ($\phi = \text{const.}$). The free parameters are the maximum vertical dimension (height) $z = z_{\max} \equiv H$ and the maximum polar angle $\lim\limits_{\theta\to\pi/2}\theta_{\max}$, i.e. excluding the extreme angular range.

The derivatives of the basis vectors in the direction of each coordinate axis will be (from the equation (B.111))

$$\begin{aligned}
&\frac{\partial\hat{\boldsymbol{z}}}{\partial z} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{z}}}{\partial\phi} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{z}}}{\partial\theta} = \mathbf{0},\\
&\frac{\partial\hat{\boldsymbol{\phi}}}{\partial z} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi} = -\frac{\hat{\boldsymbol{z}}\sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}, && \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\theta} = \mathbf{0},\\
&\frac{\partial\hat{\boldsymbol{\theta}}}{\partial z} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi} = \hat{\boldsymbol{\phi}}\cos\theta, && \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta} = -\frac{\hat{\boldsymbol{z}} + \hat{\boldsymbol{\theta}}\sin\theta}{\cos\theta}.
\end{aligned} \tag{B.113}$$

[2] In this system the same transformation equations apply for the azimuthal coordinate ϕ as in the case of cylindrical coordinates.

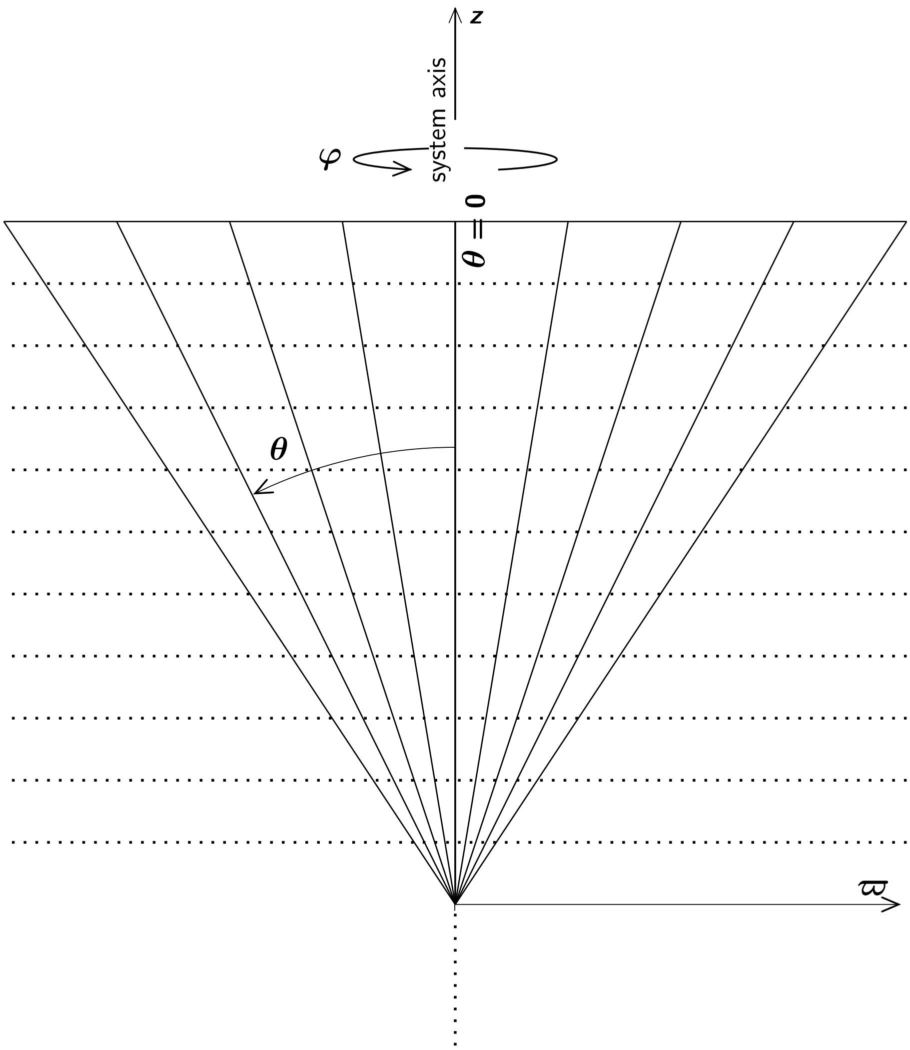

Figure B.4: Representation of a "conical" coordinate system, defined by the coordinates z, φ, and θ, where z is the vertical distance from the origin, φ is the azimuth angle and θ is the angular deviation from the z axis. The given coordinate ϖ denotes the distance from the z axis, thus corresponding to a cylindrical radial coordinate.

The time derivatives of the basis vectors will be

$$\frac{\partial \hat{\boldsymbol{z}}}{\partial t} = \mathbf{0}, \quad \frac{\partial \hat{\boldsymbol{\phi}}}{\partial t} = \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi}\frac{\partial \phi}{\partial t} = -\frac{\hat{\boldsymbol{z}}\sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}\,\dot{\phi},$$
$$\frac{\partial \hat{\boldsymbol{\theta}}}{\partial t} = \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi}\frac{\partial \phi}{\partial t} + \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \theta}\frac{\partial \theta}{\partial t} = \hat{\boldsymbol{\phi}}\dot{\phi}\cos\theta - \frac{\hat{\boldsymbol{z}} + \hat{\boldsymbol{\theta}}\sin\theta}{\cos\theta}\,\dot{\theta}. \tag{B.114}$$

We derive the metric form for the *conic* system by differentiating the equation (B.108),

$$\mathrm{d}x = \tan\theta\cos\phi\,\mathrm{d}z - z\tan\theta\sin\phi\,\mathrm{d}\phi + \frac{z\cos\phi}{\cos^2\theta}\,\mathrm{d}\theta,$$
$$\mathrm{d}y = \tan\theta\sin\phi\,\mathrm{d}z + z\tan\theta\cos\phi\,\mathrm{d}\phi + \frac{z\sin\phi}{\cos^2\theta}\,\mathrm{d}\theta, \quad \mathrm{d}z = \mathrm{d}z, \tag{B.115}$$

by substituting into the equation (B.2) we obtain the non-diagonal *conical* metric form in the form

$$\mathrm{d}s^2 = \frac{\mathrm{d}z^2}{\cos^2\theta} + \frac{2z\sin\theta}{\cos^3\theta}\,\mathrm{d}z\,\mathrm{d}\theta + z^2\left(\tan^2\theta\,\mathrm{d}\phi^2 + \frac{\mathrm{d}\theta^2}{\cos^4\theta}\right). \tag{B.116}$$

The covariant and contravariant metric tensors of the system with coordinates in the order z, ϕ, θ will be

$$g_{ij} = \begin{pmatrix} \frac{1}{\cos^2\theta} & 0 & \frac{z\sin\theta}{\cos^3\theta} \\ 0 & z^2\tan^2\theta & 0 \\ \frac{z\sin\theta}{\cos^3\theta} & 0 & \frac{z^2}{\cos^4\theta} \end{pmatrix}, \quad g^{ij} = \begin{pmatrix} 1 & 0 & -\frac{\sin\theta\cos\theta}{z} \\ 0 & \frac{1}{z^2\tan^2\theta} & 0 \\ -\frac{\sin\theta\cos\theta}{z} & 0 & \frac{\cos^2\theta}{z^2} \end{pmatrix}. \tag{B.117}$$

The Jacobi matrix of the Cartesian transformation and the inverse transformation matrix will be

$$J_{ij} = \begin{pmatrix} \tan\theta\cos\phi & -z\tan\theta\sin\phi & \frac{z\cos\phi}{\cos^2\theta} \\ \tan\theta\sin\phi & z\tan\theta\cos\phi & \frac{z\sin\phi}{\cos^2\theta} \\ 1 & 0 & 0 \end{pmatrix}, \quad J^{-1}_{ij} = \begin{pmatrix} 0 & 0 & 1 \\ -\frac{\sin\phi}{z\tan\theta} & \frac{\cos\phi}{z\tan\theta} & 0 \\ \frac{\cos\phi\cos^2\theta}{z} & \frac{\sin\phi\cos^2\theta}{z} & -\frac{\sin\theta\cos\theta}{z} \end{pmatrix}, \tag{B.118}$$

the corresponding Jacobians will therefore be,

$$J = |\det J_{ij}| = \sqrt{|\det g_{ij}|} = \frac{z^2\sin\theta}{\cos^3\theta}, \quad J^{-1} = \left|\det J^{-1}_{ij}\right| = \sqrt{|\det g^{ij}|} = \frac{\cos^3\theta}{z^2\sin\theta}. \tag{B.119}$$

The nonzero Christoffel symbols of the *conical* metric are

$$\Gamma^{\phi}_{z\phi}\,(\Gamma^{\phi}_{\phi z}) = \Gamma^{\theta}_{z\theta}\,(\Gamma^{\theta}_{\theta z}) = \frac{1}{z},\ \Gamma^{\phi}_{\phi\theta}\,(\Gamma^{\phi}_{\theta\phi}) = \frac{1}{\sin\theta\cos\theta},\ \Gamma^{\theta}_{\phi\phi} = -\sin\theta\cos\theta,\ \Gamma^{\theta}_{\theta\theta} = 2\tan\theta. \tag{B.120}$$

Since this is not an orthogonal metric (expressed by a diagonal metric tensor), we do not define any *Lamé* coefficients here.

Differential operators

- *Gradient* of the scalar function $f(z, \phi, \theta)$ in the *conical* system is derived in the same way as in the previous systems. The individual non-zero partial derivatives for the *conical* system from the equation (B.109) will be

$$\frac{\partial z}{\partial z} = 1, \quad \frac{\partial\phi}{\partial x} = -\frac{y}{x^2+y^2} = -\frac{\sin\phi}{z\tan\theta}, \quad \frac{\partial\phi}{\partial y} = \frac{x}{x^2+y^2} = \frac{\cos\phi}{z\tan\theta},$$
$$\frac{\partial\theta}{\partial x} = \frac{xz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = \frac{\cos\phi\cos^2\theta}{z},$$
$$\frac{\partial\theta}{\partial y} = \frac{yz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = \frac{\sin\phi\cos^2\theta}{z},$$
$$\frac{\partial\theta}{\partial z} = -\frac{\sqrt{x^2+y^2}}{x^2+y^2+z^2} = -\frac{\sin\theta\cos\theta}{z}.$$

As in the previous coordinate systems, we get the gradient of the scalar function,

$$\vec{\nabla} f = \hat{\boldsymbol{z}}\frac{\partial f}{\partial z} + \hat{\boldsymbol{\phi}}\frac{1}{z\tan\theta}\frac{\partial f}{\partial \phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{z}\frac{\partial f}{\partial \theta} = \left(\frac{\partial f}{\partial z}, \frac{1}{z\tan\theta}\frac{\partial f}{\partial \phi}, \frac{\cos\theta}{z}\frac{\partial f}{\partial \theta}\right). \tag{B.121}$$

Using the same procedure as in the previous coordinate systems, we can also obtain the gradient tensor of the *vector field*, which we can write using the matrix formalism in the *conical* system,

$$\vec{\nabla}\vec{A} = \begin{array}{c c} & \begin{array}{ccc} \hat{\boldsymbol{z}} & \hat{\boldsymbol{\phi}} & \hat{\boldsymbol{\theta}} \end{array} \\ \begin{array}{c} \hat{\boldsymbol{z}} \\ \hat{\boldsymbol{\phi}} \\ \hat{\boldsymbol{\theta}} \end{array} & \begin{pmatrix} \dfrac{\partial A_z}{\partial z} & \dfrac{\partial A_\phi}{\partial z} & \dfrac{\partial A_\theta}{\partial z} \\ \dfrac{1}{z\tan\theta}\dfrac{\partial A_z}{\partial \phi} - \dfrac{A_\phi}{z} & \dfrac{1}{z\tan\theta}\dfrac{\partial A_\phi}{\partial \phi} + \dfrac{A_\theta\cos\theta}{z\tan\theta} & \dfrac{1}{z\tan\theta}\dfrac{\partial A_\theta}{\partial \phi} - \dfrac{A_\phi}{z\sin\theta} \\ \dfrac{\cos\theta}{z}\dfrac{\partial A_z}{\partial \theta} - \dfrac{A_\theta}{z} & \dfrac{\cos\theta}{z}\dfrac{\partial A_\phi}{\partial \theta} & \dfrac{\cos\theta}{z}\dfrac{\partial A_\theta}{\partial \theta} - \dfrac{A_\theta\sin\theta}{z} \end{pmatrix} \end{array}. \tag{B.122}$$

- *Divergence* of the vector (vector field) $\vec{A}(z,\phi,\theta)$ is again defined in *conical* coordinates as the scalar product of the gradient vector with the general vector, i.e.

$$\vec{\nabla}\cdot\vec{A} = \left(\hat{\boldsymbol{z}}\frac{\partial}{\partial z} + \hat{\boldsymbol{\phi}}\frac{1}{z\tan\theta}\frac{\partial}{\partial \phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{z}\frac{\partial}{\partial \theta}\right)\cdot\left(A_z\hat{\boldsymbol{z}} + A_\phi\hat{\boldsymbol{\phi}} + A_\theta\hat{\boldsymbol{\theta}}\right), \tag{B.123}$$

where, however, unlike orthogonal systems, the scalar products of different basis vectors are generally not zero, so it may not hold that $e_i e^j = \delta_i^j$. Namely, in this system the non-zero product will be

$$\underset{i\neq j}{e_i e^j} = \hat{\boldsymbol{z}}\cdot\hat{\boldsymbol{\theta}} = -\sin\theta. \tag{B.124}$$

By direct calculation and after some adjustments we get

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\rho) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial \phi} + \frac{\cos\theta}{\rho}\frac{\partial A_\theta}{\partial \theta} - \frac{\sin\theta}{\rho}\left[\frac{\partial}{\partial\rho}(\rho A_\theta) + \cos\theta\frac{\partial A_\rho}{\partial\theta}\right]. \tag{B.125}$$

Unlike orthogonal systems, in this case the divergence is not a simple trace of the gradient tensor of the vector field (B.122), but rather it is necessary to add the elements on the minor diagonal (or rather those that correspond to the non-zero elements of the metric tensor (B.117)), multiplied by the scalar product of the corresponding unit vectors, in this case the equation (B.124).

- *Curl* of the vector (vector field) $\vec{A}(\rho,\phi,\theta)$ in *disk* coordinates cannot be derived according to the equation (B.20) (the system is not orthogonal), in this case we must perform a direct calculation from the definition of vector curl,

$$\vec{\nabla}\times\vec{A} = \left(\hat{\boldsymbol{\rho}}\frac{\partial}{\partial\rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial}{\partial\phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{\rho}\frac{\partial}{\partial\theta}\right)\times\left(A_\rho\hat{\boldsymbol{\rho}} + A_\phi\hat{\boldsymbol{\phi}} + A_\theta\hat{\boldsymbol{\theta}}\right), \tag{B.126}$$

where we must first perform all (nonzero) derivatives of the unit basis vectors (see equation (B.113)), then the cross products. If we keep only the nonzero components, i.e. if we omit the zero derivatives of the unit basis vectors and also the terms with the same basis vectors and therefore with zero cross product, we get the explicit expression

$$\vec{\nabla} \times \vec{A} = \hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\phi}} \left(\frac{\partial A_\phi}{\partial \rho} + \frac{A_\phi}{\rho} - \frac{1}{\rho} \frac{\partial A_\rho}{\partial \phi} \right) + \hat{\boldsymbol{\phi}} \times \hat{\boldsymbol{\theta}} \left(\frac{1}{\rho} \frac{\partial A_\theta}{\partial \phi} - \frac{\cos\theta}{\rho} \frac{\partial A_\phi}{\partial \theta} \right) + \\ + \hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\rho}} \left(\frac{\cos\theta}{\rho} \frac{\partial A_\rho}{\partial \theta} - \frac{\partial A_\theta}{\partial \rho} - \frac{A_\theta}{\rho} \right). \tag{B.127}$$

However, the vector products of the basis vectors will not be as simple here as in the case of orthogonal systems, based on Eq. (B.111) for even permutations we get

$$\hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\phi}} = \frac{\hat{\boldsymbol{\rho}} \sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}, \quad \hat{\boldsymbol{\phi}} \times \hat{\boldsymbol{\theta}} = \frac{\hat{\boldsymbol{\rho}} + \hat{\boldsymbol{\theta}} \sin\theta}{\cos\theta}, \quad \hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\rho}} = \hat{\boldsymbol{\phi}} \cos\theta. \tag{B.128}$$

After substitution and adjustments, we get the resulting form of the rotation of the vector in the *conical* system,

$$\begin{aligned} \vec{\nabla} \times \vec{A} = & \hat{\boldsymbol{\rho}} \left\{ \frac{\tan\theta}{\rho} \left[\frac{\partial}{\partial \rho} (\rho A_\phi) - \frac{\partial A_\rho}{\partial \phi} \right] + \frac{1}{\rho} \left(\frac{1}{\cos\theta} \frac{\partial A_\theta}{\partial \phi} - \frac{\partial A_\phi}{\partial \theta} \right) \right\} + \\ & \hat{\boldsymbol{\phi}} \left\{ \frac{\cos\theta}{\rho} \left[\cos\theta \frac{\partial A_\rho}{\partial \theta} - \frac{\partial}{\partial \rho} (\rho A_\theta) \right] \right\} + \\ & \hat{\boldsymbol{\theta}} \left\{ \frac{1}{\rho \cos\theta} \left[\frac{\partial}{\partial \rho} (\rho A_\phi) - \frac{\partial A_\rho}{\partial \phi} \right] + \frac{\sin\theta}{\rho} \left(\frac{1}{\cos\theta} \frac{\partial A_\theta}{\partial \phi} - \frac{\partial A_\phi}{\partial \theta} \right) \right\}. \end{aligned} \tag{B.129}$$

- *Laplacian* is derived from the divergence equation (B.123), in which we replace the components of the vector $\vec{A}$ with the corresponding components of the gradient vector from equation (B.121), the resulting form (it is not necessary to repeat the detailed vector notation here, the procedure is completely similar to the previous cases), written in compact form will be

$$\Delta = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\cos\theta}{\rho^2} \frac{\partial}{\partial \theta} \left(\cos\theta \frac{\partial}{\partial \theta} \right) - \frac{\sin 2\theta}{\rho} \frac{\partial^2}{\partial \rho \, \partial \theta}. \tag{B.130}$$

Areas, volumes

As in the previous systems, we derive the sizes of the basic areas and basic volumes of the spatial cell, i.e. the areas and volumes, bounded by individual coordinate surfaces (including the same notation, for other notations see also Fig. B.4). The volume of one cell of the coordinate grid will be

$$V = \int_{z_1}^{z_2} z^2 \, \mathrm{d}z \int_{\phi_1}^{\phi_2} \mathrm{d}\phi \int_{\theta_1}^{\theta_2} \frac{\sin\theta}{\cos^3\theta} \, \mathrm{d}\theta = \frac{z_2^3 - z_1^3}{6} (\phi_2 - \phi_1) \left(\frac{1}{\cos^2\theta_2} - \frac{1}{\cos^2\theta_1} \right). \tag{B.131}$$

The determinants of the submatrices of the metric tensor, corresponding to the individual surfaces of the spatial cell (the notation method is described in the description of the cylindrical and spherical system) will be

$$J'_z = \frac{z^2 \sin\theta}{\cos^3\theta}, \quad J'_\phi = \frac{z}{\cos^2\theta}, \quad J'_\theta = \frac{z \sin\theta}{\cos^2\theta} \tag{B.132}$$

and the areas of individual grid cells will have the size

$$S_z = z^2 \int_{\phi_1}^{\phi_2} \mathrm{d}\phi \int_{\theta_1}^{\theta_2} \frac{\sin\theta}{\cos^3\theta}\,\mathrm{d}\theta = \frac{z^2}{2}(\phi_2 - \phi_1)\left(\frac{1}{\cos^2\theta_2} - \frac{1}{\cos^2\theta_1}\right), \tag{B.133}$$

$$S_\phi = \int_{\theta_1}^{\theta_2} \frac{\mathrm{d}\theta}{\cos^2\theta} \int_{z_1}^{z_2} z\,\mathrm{d}z = \frac{z_2^2 - z_1^2}{2}\,(\tan\theta_2 - \tan\theta_1)\,, \tag{B.134}$$

$$S_\theta = \frac{\sin\theta}{\cos^2\theta} \int_{z_1}^{z_2} z\,\mathrm{d}z \int_{\phi_1}^{\phi_2} \mathrm{d}\phi = \frac{z_2^2 - z_1^2}{2}(\phi_2 - \phi_1)\frac{\sin\theta}{\cos^2\theta}. \tag{B.135}$$

Position, velocity and acceleration vectors

When describing vectors in the *conical* system, we will start as usual from their basic description in the Cartesian system, including all equations for derivation of unit vectors and vector components (equations (B.108) - (B.114)). The position vector in the *conical* system will be

$$\vec{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}} = \frac{\hat{\boldsymbol{z}}z + \hat{\boldsymbol{\theta}}z\sin\theta}{\cos^2\theta}. \tag{B.136}$$

This conclusion is no longer as clear and easy to imagine as in the case of the previous types of coordinates. The velocity vector $\vec{v}$ will be

$$\vec{v} = \hat{\boldsymbol{z}}\left(\frac{\dot{z} - z\dot{\theta}\tan\theta}{\cos^2\theta}\right) + \hat{\boldsymbol{\phi}}z\tan\theta\,\dot{\phi} + \hat{\boldsymbol{\theta}}\left(\frac{\dot{z}\tan\theta}{\cos\theta} + \frac{z\dot{\theta}}{\cos^3\theta}\right). \tag{B.137}$$

The velocity and acceleration vectors must be defined as

$$\vec{v} = v_z\hat{\boldsymbol{z}} + v_\phi\hat{\boldsymbol{\phi}} + v_\theta\hat{\boldsymbol{\theta}}, \quad \vec{a} = \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = a_z\hat{\boldsymbol{z}} + a_\phi\hat{\boldsymbol{\phi}} + a_\theta\hat{\boldsymbol{\theta}}. \tag{B.138}$$

By differentiating Eq. (B.137) with respect to time, we obtain the individual components of the acceleration vector in the *conical* coordinate system

$$\begin{aligned}
a_\rho &= \frac{\ddot{\rho} + \tan\theta[\rho\ddot{\theta} + 2\dot{\theta}(\dot{\rho} + \rho\dot{\theta}\tan\theta)]}{\cos^2\theta} - \rho\dot{\phi}^2 = \frac{\mathrm{d}v_\rho}{\mathrm{d}t} - \rho\dot{\phi}^2 - \frac{\dot{\theta}}{\cos^2\theta}\left(\dot{\rho}\tan\theta + \frac{\rho\dot{\theta}}{\cos^2\theta}\right), \\
a_\phi &= \rho\ddot{\phi} + 2\dot{\rho}\dot{\phi} = \frac{\mathrm{d}v_\phi}{\mathrm{d}t} + \dot{\rho}\dot{\phi}, \\
a_\theta &= \frac{1}{\cos\theta}\left[\ddot{\rho}\tan\theta + \frac{\rho\ddot{\theta} + 2\dot{\theta}\,(\dot{\rho} + \rho\dot{\theta}\tan\theta)}{\cos^2\theta}\right] = \frac{\mathrm{d}v_\theta}{\mathrm{d}t} - \frac{\tan\theta\,\dot{\theta}}{\cos\theta}\left(\dot{\rho}\tan\theta + \frac{\rho\dot{\theta}}{\cos^2\theta}\right).
\end{aligned} \tag{B.139}$$

From the above equations we can easily see that for the main terms of the velocity components the following holds

$$\dot{\rho} = v_\rho - v_\theta\sin\theta, \quad \dot{\phi} = \frac{v_\phi}{\rho}, \quad \dot{\theta} = \frac{(v_\theta - v_\rho\sin\theta)\cos\theta}{\rho}. \tag{B.140}$$

Since $\mathrm{d}\vec{v}/\mathrm{d}t = \partial\vec{v}/\partial t + \vec{v}\cdot\vec{\nabla}\vec{v}$, we can write the acceleration, expressed in a *conical* coordinate system, in terms of the components of the velocity vector,

$$a_z = \frac{\partial v_\rho}{\partial t} + \underbrace{v_\rho\frac{\partial v_\rho}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_\rho}{\partial \phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\rho}{\partial \theta}}_{(\vec{v}\cdot\vec{\nabla})v_\rho} - \frac{v_\phi^2 + v_\theta^2}{\rho} + \frac{v_\rho v_\theta\sin\theta}{\rho}, \tag{B.141}$$

$$a_\phi = \frac{\partial v_\phi}{\partial t} + \underbrace{v_\rho\frac{\partial v_\phi}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_\phi}{\partial \phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\phi}{\partial \theta}}_{(\vec{v}\cdot\vec{\nabla})v_\phi} + \frac{v_\rho v_\phi}{\rho} - \frac{v_\phi v_\theta\sin\theta}{\rho}, \tag{B.142}$$

$$a_\theta = \frac{\partial v_\theta}{\partial t} + \underbrace{v_\rho\frac{\partial v_\theta}{\partial \rho} + \frac{v_\phi}{\rho}\frac{\partial v_\theta}{\partial \phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\theta}{\partial \theta}}_{(\vec{v}\cdot\vec{\nabla})v_\theta} - \frac{v_\theta^2\sin\theta}{\rho} + \frac{v_\rho v_\theta\sin^2\theta}{\rho}. \tag{B.143}$$

The terms on the right-hand sides of the equations (B.141) - (B.143), connected by a brace, express (nonlinear) advection, the remaining terms representing the so-called *fictitious* (inertial) forces - centrifugal force, Coriolis force, Euler force.

By comparing equations (B.108) and (B.140), we can write the components of the velocity vector v_ρ, v_ϕ, v_θ in the disk system using the components of the velocity vector $v_{\rho,\,\mathrm{cyl}}$, $v_{\phi,\,\mathrm{cyl}}$, v_z in the standard cylindrical coordinate system (section B.2). We thus obtain the mutual relationship between the magnitudes of the velocity components in both systems,

$$v_\rho = v_{\rho,\,\mathrm{cyl}} + \frac{z}{\rho}\,v_z = v_{\rho,\,\mathrm{cyl}} + v_z\tan\theta, \quad v_\phi = v_{\phi,\,\mathrm{cyl}}, \quad v_\theta = \frac{\sqrt{\rho^2+z^2}}{\rho}\,v_z = \frac{v_z}{\cos\theta}. \tag{B.144}$$

If we further consider the vertical hydrostatic equilibrium in such a cone, $\mathrm{d}P/\mathrm{d}z = -\rho g_z$, where P is the scalar pressure and g_z is the vertical component of the gravitational acceleration, we obtain for the vertical component of the velocity $v_z = 0$. The equations of motion (B.141) - (B.143) will thus be identical to the corresponding equations of motion (B.52) - (B.54) in standard cylindrical geometry.

B.7.2 "Astrophysical disk" system

Let us now explore another possible geometrical case that may require an introduction of a non-orthogonal coordinate system. It is a geometrical description of a large gaseous disk, extending around a very fast rotating and, therefore, heavily oblate star, that is very thin near the star and expands significantly vertically at great distances from the star. At the same time, it is, of course, rotationally (cylindrically) symmetrical. Figure B.5 schematically illustrates this system in the vertical plane ρ-θ ($\phi = \text{const.}$), the coordinate directions are: $\rho \in \langle 0, \infty)$ - radial cylindrical coordinate, $\phi \in \langle 0, 2\pi)$ - azimuthal angle, $\theta \in (-\pi/2, \pi/2)$ - elevation angle that is calculated in the positive and the negative direction from the equatorial plane. Although the elevation angle can be defined within this entire interval (excluding the endpoints), due to the nature of the phenomena described, only the $\theta \in \langle -\pi/4, \pi/4\rangle$ interval is considered. Free parameters (except for the selected stellar equatorial radius R_{eq}) are the maximum cylindrical radial distance $\rho = R_{\max}$ and the maximum elevation angle, denoted as $\theta_{\max}$ (in the mirror position to him is $\theta_{\min}$). The system is cylindrically symmetrical, the axis of symmetry is perpendicular to the plane of the disk ($z = 0 \wedge \theta = 0$) and passes through the center of

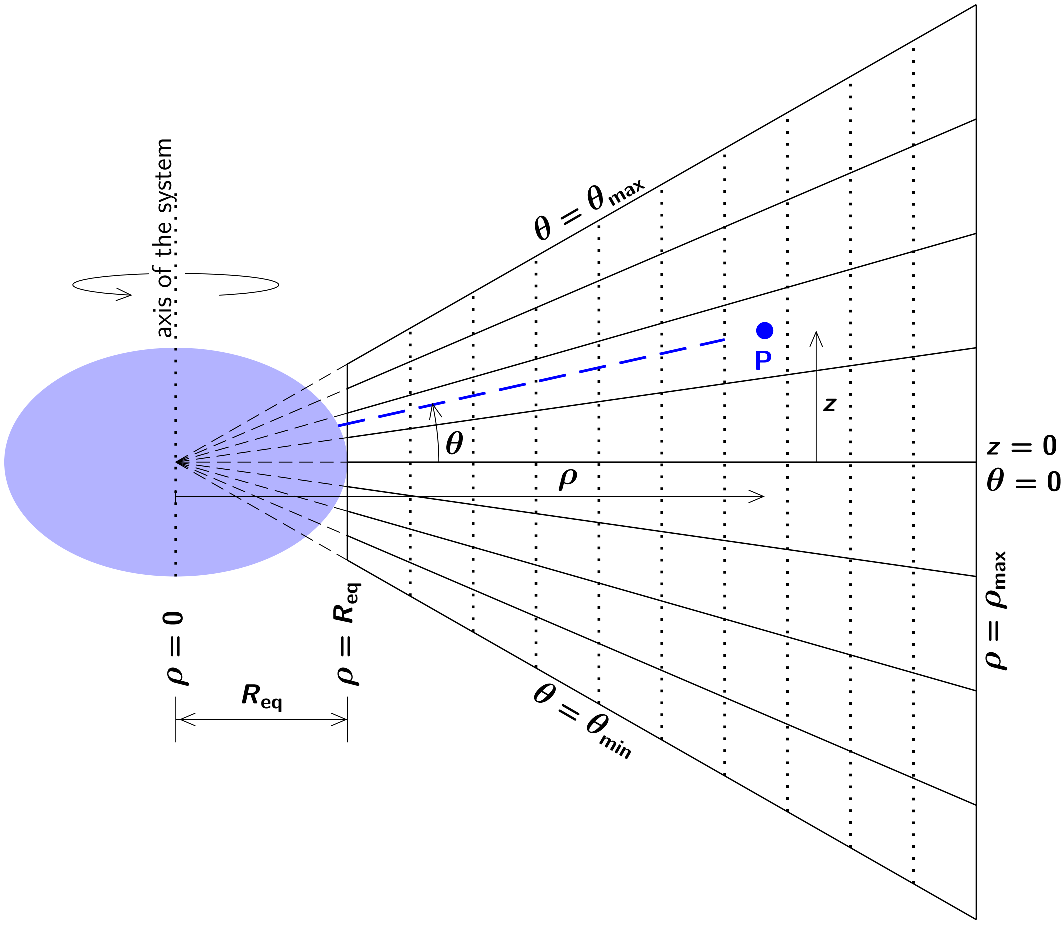

Figure B.5: Schematic illustration of the *cylindrical-conical* coordinate system in the plane ρ-θ ($\phi =$ const.). The blue dashed line passing through the general point P indicates the intersection of the coordinate surfaces S_ϕ and S_θ. The color ellipse highlights the rotationally oblate star.

the star ($\rho = 0$). We can call it, for example, the **cylindrical-conical system**[3] (standard, the so-called *conical* coordinate system means something slightly different - it is an orthogonal system defined by concentric spherical surfaces and two classes of mutually orthogonal generally elliptical conical surfaces with axes x and z, and with vertices at the origin of the coordinate system).

Transformation equations from this *cylindrical-conical* to the Cartesian coordinate system are (for better graphical clarity we will use for a tangent the term tan used in the English-language literature instead of tg used in the Czech literature)

$$x = \rho \cos\phi, \quad y = \rho \sin\phi, \quad z = \rho \tan\theta. \tag{B.145}$$

[3]As an abbreviated working title, we will hereafter use the term *disk-like system*. Radial and azimuthal coordinates are identical to the cylindrical system, so we denote the particular coordinate directions ρ, ϕ, θ and particular unit basis vectors $\hat{\boldsymbol{\rho}}$, $\hat{\boldsymbol{\phi}}$, $\hat{\boldsymbol{\theta}}$.

For the reverse transformation from Cartesian to the *disk-like* system, we get[4]

$$\rho = \sqrt{x^2+y^2}, \quad \phi = \arctan\frac{y}{x}, \quad \theta = \arctan\frac{z}{\sqrt{x^2+y^2}}. \tag{B.146}$$

By analogy to Equations (B.30) and (B.57), the unit vectors of the *disk-like* basis in the Cartesian system will have the form (see the rules for vector summing)

$$\begin{aligned} \hat{\boldsymbol{\rho}} = \hat{\boldsymbol{x}}\cos\phi + \hat{\boldsymbol{y}}\sin\phi, \quad \hat{\boldsymbol{\phi}} = -\hat{\boldsymbol{x}}\sin\phi + \hat{\boldsymbol{y}}\cos\phi,& \\ \hat{\boldsymbol{\theta}} = -(\hat{\boldsymbol{x}}\cos\phi + \hat{\boldsymbol{y}}\sin\phi)\sin\theta + \hat{\boldsymbol{z}}\cos\theta.& \end{aligned} \tag{B.147}$$

By reverse transformation of the unit basis vectors (see Equation (B.147)), we get

$$\hat{\boldsymbol{x}} = \hat{\boldsymbol{\rho}}\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi, \quad \hat{\boldsymbol{y}} = \hat{\boldsymbol{\rho}}\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi, \quad \hat{\boldsymbol{z}} = \frac{\hat{\boldsymbol{\rho}}\sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}. \tag{B.148}$$

In the *disk-like* system, none of the basis vectors is constant. Derivatives of the basis vectors in the direction of individual coordinate axes will be (from Equation (B.147))

$$\begin{aligned} &\frac{\partial\hat{\boldsymbol{\rho}}}{\partial\rho} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{\rho}}}{\partial\phi} = \hat{\boldsymbol{\phi}}, && \frac{\partial\hat{\boldsymbol{\rho}}}{\partial\theta} = \mathbf{0}, \\ &\frac{\partial\hat{\boldsymbol{\phi}}}{\partial\rho} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi} = -\hat{\boldsymbol{\rho}}, && \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\theta} = \mathbf{0}, \\ &\frac{\partial\hat{\boldsymbol{\theta}}}{\partial\rho} = \mathbf{0}, && \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi} = -\hat{\boldsymbol{\phi}}\sin\theta, && \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta} = -\frac{\hat{\boldsymbol{\rho}} + \hat{\boldsymbol{\theta}}\sin\theta}{\cos\theta}. \end{aligned} \tag{B.149}$$

Time derivatives of the basis vectors will be

$$\begin{aligned} &\frac{\partial\hat{\boldsymbol{\rho}}}{\partial t} = \frac{\partial\hat{\boldsymbol{\rho}}}{\partial\phi}\frac{\partial\phi}{\partial t}\hat{\boldsymbol{\phi}}\dot{\phi}, \quad \frac{\partial\hat{\boldsymbol{\phi}}}{\partial t} = \frac{\partial\hat{\boldsymbol{\phi}}}{\partial\phi}\frac{\partial\phi}{\partial t} = -\hat{\boldsymbol{\rho}}\dot{\phi}, \\ &\frac{\partial\hat{\boldsymbol{\theta}}}{\partial t} = \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\phi}\frac{\partial\phi}{\partial t} + \frac{\partial\hat{\boldsymbol{\theta}}}{\partial\theta}\frac{\partial\theta}{\partial t} = -\frac{\hat{\boldsymbol{\rho}}\dot{\theta}}{\cos\theta} - \hat{\boldsymbol{\phi}}\dot{\phi}\sin\theta - \hat{\boldsymbol{\theta}}\dot{\theta}\tan\theta. \end{aligned} \tag{B.150}$$

The metric form of the *disk-like* system is derived by differentiation of Equation (B.145),

$$\mathrm{d}x = \cos\phi\,\mathrm{d}\rho - \rho\sin\phi\,\mathrm{d}\phi, \quad \mathrm{d}y = \sin\phi\,\mathrm{d}\rho + \rho\cos\phi\,\mathrm{d}\phi, \quad \mathrm{d}z = \tan\theta\,\mathrm{d}\rho + \frac{\rho}{\cos^2\theta}\,\mathrm{d}\theta. \tag{B.151}$$

Substituting this into Equation (B.2) gives the non-diagonal *disk-like* metric form as

$$\mathrm{d}s^2 = \frac{\mathrm{d}\rho^2}{\cos^2\theta} + \frac{2\rho\sin\theta}{\cos^3\theta}\,\mathrm{d}\rho\,\mathrm{d}\theta + \rho^2\left(\mathrm{d}\phi^2 + \frac{\mathrm{d}\theta^2}{\cos^4\theta}\right). \tag{B.152}$$

Covariant and contravariant metric tensors of the system with coordinates in the order ρ, ϕ, θ will be

$$g_{ij} = \begin{pmatrix} \dfrac{1}{\cos^2\theta} & 0 & \dfrac{\rho\sin\theta}{\cos^3\theta} \\ 0 & \rho^2 & 0 \\ \dfrac{\rho\sin\theta}{\cos^3\theta} & 0 & \dfrac{\rho^2}{\cos^4\theta} \end{pmatrix}, \quad g^{ij} = \begin{pmatrix} 1 & 0 & -\dfrac{\sin\theta\cos\theta}{\rho} \\ 0 & \dfrac{1}{\rho^2} & 0 \\ -\dfrac{\sin\theta\cos\theta}{\rho} & 0 & \dfrac{\cos^2\theta}{\rho^2} \end{pmatrix}. \tag{B.153}$$

[4] In this system, for the azimuthal coordinate ϕ, the same transformation equations as for cylindrical coordinates apply.

Jacobi transformation matrix from the Cartesian system and the inverse transformation matrix will be

$$J_{ij} = \begin{pmatrix} \cos\phi & -\rho\sin\phi & 0 \\ \sin\phi & \rho\cos\phi & 0 \\ \tan\theta & 0 & \dfrac{\rho}{\cos^2\theta} \end{pmatrix}, \quad J^{-1}_{ij} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\dfrac{\sin\phi}{\rho} & \dfrac{\cos\phi}{\rho} & 0 \\ -\dfrac{\cos\phi\sin\theta\cos\theta}{\rho} & -\dfrac{\sin\phi\sin\theta\cos\theta}{\rho} & \dfrac{\cos^2\theta}{\rho} \end{pmatrix}, \tag{B.154}$$

and the corresponding Jacobians thus will be

$$J = |\det J_{ij}| = \sqrt{|\det g_{ij}|} = \frac{\rho^2}{\cos^2\theta}, \quad J^{-1} = \left|\det J^{-1}_{ij}\right| = \sqrt{|\det g^{ij}|} = \frac{\cos^2\theta}{\rho^2}. \tag{B.155}$$

Nonzero Christoffel symbols of the *disk-like* metrics are

$$\Gamma^{\phi}_{\rho\phi}\,(\Gamma^{\phi}_{\phi\rho}) = \Gamma^{\theta}_{\rho\theta}\,(\Gamma^{\theta}_{\theta\rho}) = \frac{1}{\rho},\ \Gamma^{\rho}_{\phi\phi} = -\rho,\ \Gamma^{\theta}_{\phi\phi} = \sin\theta\cos\theta,\ \Gamma^{\theta}_{\theta\theta} = 2\tan\theta. \tag{B.156}$$

Since it is not an orthogonal metric (that could be expressed by a diagonal metric tensor), we do not define any *Lamé* coefficients here.

B.7.3 Differential operators

- *Gradient* of a scalar function $f(\rho,\phi,\theta)$ in the *disk-like* system can be derived in the same way as in the previous systems. Particular nonzero partial derivatives for the *disk-like* system from Equation (B.146) will be

$$\begin{aligned}
\frac{\partial\rho}{\partial x} &= \frac{x}{\sqrt{x^2+y^2}} = \cos\phi, & \frac{\partial\phi}{\partial x} &= -\frac{y}{x^2+y^2} = -\frac{\sin\phi}{\rho}, \\
\frac{\partial\rho}{\partial y} &= \frac{y}{\sqrt{x^2+y^2}} = \sin\phi, & \frac{\partial\phi}{\partial y} &= \frac{x}{x^2+y^2} = \frac{\cos\phi}{\rho}, \\
\frac{\partial\theta}{\partial x} &= -\frac{xz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = -\frac{\cos\phi\sin\theta\cos\theta}{\rho}, \\
\frac{\partial\theta}{\partial y} &= -\frac{yz}{\sqrt{x^2+y^2}\,(x^2+y^2+z^2)} = -\frac{\sin\phi\sin\theta\cos\theta}{\rho}, \\
\frac{\partial\theta}{\partial z} &= \frac{\sqrt{x^2+y^2}}{x^2+y^2+z^2} = \frac{\cos^2\theta}{\rho}.
\end{aligned}$$

As in the previous coordinate systems, we get the gradient of a scalar function,

$$\vec{\nabla} f = \hat{\boldsymbol{\rho}}\frac{\partial f}{\partial\rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial f}{\partial\phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{\rho}\frac{\partial f}{\partial\theta} = \left(\frac{\partial f}{\partial\rho}, \frac{1}{\rho}\frac{\partial f}{\partial\phi}, \frac{\cos\theta}{\rho}\frac{\partial f}{\partial\theta}\right). \tag{B.157}$$

Using the same procedure as in the previous coordinate systems, we can also obtain the gradient tensor of a *vector field*, which we can write in terms of the matrix formalism in the *disk-like* system as

$$\vec{\nabla}\vec{A} = \begin{array}{c} \\ \hat{\boldsymbol{\rho}} \\ \hat{\boldsymbol{\phi}} \\ \hat{\boldsymbol{\theta}} \end{array} \begin{array}{c} \begin{array}{ccc} \quad\hat{\boldsymbol{\rho}}\quad & \quad\hat{\boldsymbol{\phi}}\quad & \quad\hat{\boldsymbol{\theta}}\quad \end{array} \\ \begin{pmatrix} \dfrac{\partial A_\rho}{\partial \rho} & \dfrac{\partial A_\phi}{\partial \rho} & \dfrac{\partial A_\theta}{\partial \rho} \\ \dfrac{1}{\rho}\dfrac{\partial A_\rho}{\partial \phi} - \dfrac{A_\phi}{\rho} & \dfrac{1}{\rho}\dfrac{\partial A_\phi}{\partial \phi} + \dfrac{A_\rho}{\rho} - \dfrac{A_\theta \sin\theta}{\rho} & \dfrac{1}{\rho}\dfrac{\partial A_\theta}{\partial \phi} \\ \dfrac{\cos\theta}{\rho}\dfrac{\partial A_\rho}{\partial \theta} - \dfrac{A_\theta}{\rho} & \dfrac{\cos\theta}{\rho}\dfrac{\partial A_\phi}{\partial \theta} & \dfrac{\cos\theta}{\rho}\dfrac{\partial A_\theta}{\partial \theta} - \dfrac{A_\theta \sin\theta}{\rho} \end{pmatrix} \end{array} . \tag{B.158}$$

- *Divergence* of a vector (vector field) $\vec{A}(\rho,\phi,\theta)$ is in the *disk-like* coordinates again defined as the scalar product of a gradient vector with a general vector, i.e.,

$$\vec{\nabla}\cdot\vec{A} = \left(\hat{\boldsymbol{\rho}}\frac{\partial}{\partial \rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial}{\partial \phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{\rho}\frac{\partial}{\partial \theta}\right)\cdot\left(A_\rho\hat{\boldsymbol{\rho}} + A_\phi\hat{\boldsymbol{\phi}} + A_\theta\hat{\boldsymbol{\theta}}\right). \tag{B.159}$$

However, unlike in orthogonal systems, the scalar products of different basis vectors are here nonzero in general, so the identity $e_i e^j = \delta_i^j$ may not hold. In particular, there will be the nonzero product

$$\underset{i\neq j}{e_i e^j} = \hat{\boldsymbol{\rho}}\cdot\hat{\boldsymbol{\theta}} = -\sin\theta \tag{B.160}$$

in this system. By direct calculation and after adjustments, we get

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho A_\rho) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial \phi} + \frac{\cos\theta}{\rho}\frac{\partial A_\theta}{\partial \theta} - \frac{\sin\theta}{\rho}\left[\frac{\partial}{\partial \rho}(\rho A_\theta) + \cos\theta\frac{\partial A_\rho}{\partial \theta}\right]. \tag{B.161}$$

Unlike orthogonal systems, divergence is not a simple trace of the tensor of the gradient of the vector field (B.158) in this case; there must also be added the elements on the secondary diagonal (or those corresponding to nonzero elements of the metric tensor (B.153)), multiplied by the scalar product of the unit vectors, respectively; in this case by Equation (B.160).

- *Curl* of a vector (vector field) $\vec{A}(\rho,\phi,\theta)$ in the *disk-like* coordinates cannot be derived from Equation (B.20) (the system is non-orthogonal), we have to do in this case a direct calculation using the definition of a vector curl,

$$\vec{\nabla}\times\vec{A} = \left(\hat{\boldsymbol{\rho}}\frac{\partial}{\partial \rho} + \hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial}{\partial \phi} + \hat{\boldsymbol{\theta}}\frac{\cos\theta}{\rho}\frac{\partial}{\partial \theta}\right)\times\left(A_\rho\hat{\boldsymbol{\rho}} + A_\phi\hat{\boldsymbol{\phi}} + A_\theta\hat{\boldsymbol{\theta}}\right), \tag{B.162}$$

where we first calculate all (nonzero) derivatives of the unit basis vectors (see Equation (B.149)), and then the vector products. If we leave only the nonzero components, i.e., omitting the zero derivatives of unit basis vectors and also the terms with identical basis vectors and thus with zero vector product, we get the explicit expression

$$\begin{aligned}\vec{\nabla}\times\vec{A} = \hat{\boldsymbol{\rho}}\times\hat{\boldsymbol{\phi}}\left(\frac{\partial A_\phi}{\partial \rho} + \frac{A_\phi}{\rho} - \frac{1}{\rho}\frac{\partial A_\rho}{\partial \phi}\right) + \hat{\boldsymbol{\phi}}\times\hat{\boldsymbol{\theta}}\left(\frac{1}{\rho}\frac{\partial A_\theta}{\partial \phi} - \frac{\cos\theta}{\rho}\frac{\partial A_\phi}{\partial \theta}\right) + \\ + \hat{\boldsymbol{\theta}}\times\hat{\boldsymbol{\rho}}\left(\frac{\cos\theta}{\rho}\frac{\partial A_\rho}{\partial \theta} - \frac{\partial A_\theta}{\partial \rho} - \frac{A_\theta}{\rho}\right).\end{aligned} \tag{B.163}$$

However, the vector products of basis vectors will not be as simple here as in orthogonal systems. We get from Eq. (B.147)

$$\hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\phi}} = \frac{\hat{\boldsymbol{\rho}} \sin\theta + \hat{\boldsymbol{\theta}}}{\cos\theta}, \quad \hat{\boldsymbol{\phi}} \times \hat{\boldsymbol{\theta}} = \frac{\hat{\boldsymbol{\rho}} + \hat{\boldsymbol{\theta}} \sin\theta}{\cos\theta}, \quad \hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\rho}} = \hat{\boldsymbol{\phi}} \cos\theta \tag{B.164}$$

for even permutations. After substitution and modification, we get the resulting form of the vector curl in the *disk-like* system,

$$\begin{aligned}\vec{\nabla} \times \vec{A} =& \hat{\boldsymbol{\rho}} \left\{ \frac{\tan\theta}{\rho} \left[\frac{\partial}{\partial\rho} (\rho A_\phi) - \frac{\partial A_\rho}{\partial\phi} \right] + \frac{1}{\rho} \left(\frac{1}{\cos\theta} \frac{\partial A_\theta}{\partial\phi} - \frac{\partial A_\phi}{\partial\theta} \right) \right\} + \\ & \hat{\boldsymbol{\phi}} \left\{ \frac{\cos\theta}{\rho} \left[\cos\theta \frac{\partial A_\rho}{\partial\theta} - \frac{\partial}{\partial\rho} (\rho A_\theta) \right] \right\} + \\ & \hat{\boldsymbol{\theta}} \left\{ \frac{1}{\rho\cos\theta} \left[\frac{\partial}{\partial\rho} (\rho A_\phi) - \frac{\partial A_\rho}{\partial\phi} \right] + \frac{\sin\theta}{\rho} \left(\frac{1}{\cos\theta} \frac{\partial A_\theta}{\partial\phi} - \frac{\partial A_\phi}{\partial\theta} \right) \right\}.\end{aligned} \tag{B.165}$$

- *Laplacian* is derived from Equation (B.159) of divergence, in which we replace the components of vector $\vec{A}$ by the corresponding components of the gradient vector from Equation (B.157). The final form (it is not necessary to repeat a detailed vector notation here, the procedure is quite similar to the previous cases), written in compact notation will be

$$\Delta = \frac{1}{\rho} \frac{\partial}{\partial\rho} \left(\rho \frac{\partial}{\partial\rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial\phi^2} + \frac{\cos\theta}{\rho^2} \frac{\partial}{\partial\theta} \left(\cos\theta \frac{\partial}{\partial\theta} \right) - \frac{\sin 2\theta}{\rho} \frac{\partial^2}{\partial\rho\, \partial\theta}. \tag{B.166}$$

B.7.4 Surfaces, volumes

As in the previous systems, we derive the areas of elementary surfaces and the basic volume of the spatial cell, i.e., the surfaces and the volume, bounded by particular coordinate surfaces (including the same way of notation as before, for additional notation, see also Figure B.5). The volume of one grid cell will be

$$V = \int\limits_{\rho_1}^{\rho_2} \rho^2 \,\mathrm{d}\rho \int\limits_{\phi_1}^{\phi_2} \mathrm{d}\phi \int\limits_{\theta_1}^{\theta_2} \frac{\mathrm{d}\theta}{\cos^2\theta} = \frac{\rho_2^3 - \rho_1^3}{3} (\phi_2 - \phi_1) \big(|\tan\theta_2| - |\tan\theta_1| \big). \tag{B.167}$$

Determinants of submatrices of the metric tensor corresponding to particular surfaces of the spatial grid cell (the method of labeling is shown within the description of the cylindrical and the spherical system) will be

$$J'_\rho = \frac{\rho^2}{\cos^2\theta}, \quad J'_\phi = \frac{\rho}{\cos^2\theta}, \quad J'_\theta = \frac{\rho}{\cos\theta} \tag{B.168}$$

and the areas of each cell surface of the grid will be

$$S_\rho = \rho^2 \int\limits_{\phi_1}^{\phi_2} \mathrm{d}\phi \int\limits_{\theta_1}^{\theta_2} \frac{\mathrm{d}\theta}{\cos^2\theta} = \rho^2 (\phi_2 - \phi_1) \big(|\tan\theta_2| - |\tan\theta_1| \big), \tag{B.169}$$

$$S_\phi = \int\limits_{\theta_1}^{\theta_2} \frac{\mathrm{d}\theta}{\cos^2\theta} \int\limits_{\rho_1}^{\rho_2} \rho \,\mathrm{d}\rho = \frac{\rho_2^2 - \rho_1^2}{2} \big(|\tan\theta_2| - |\tan\theta_1| \big), \tag{B.170}$$

$$S_\theta = \frac{1}{\cos\theta} \int\limits_{\rho_1}^{\rho_2} \rho \,\mathrm{d}\rho \int\limits_{\phi_1}^{\phi_2} \mathrm{d}\phi = \frac{\rho_2^2 - \rho_1^2}{2} \frac{(\phi_2 - \phi_1)}{\cos\theta}. \tag{B.171}$$

B.7.5 Vectors of position, velocity, and acceleration

When describing vectors in the *disk-like* system, we start from their basic description in the Cartesian system as usual, including all equations for derivatives of unit vectors and vector components (Equations (B.145) - (B.150)). The position vector in the *disk-like* system will be

$$\vec{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} = \frac{\hat{\boldsymbol{\rho}}\rho + \hat{\boldsymbol{\theta}}\rho\sin\theta}{\cos^2\theta}. \tag{B.172}$$

This conclusion is no longer as clear and easy to imagine as in the previous types of coordinates. The velocity vector $\vec{v}$ will be

$$\vec{v} = \hat{\boldsymbol{\rho}}\left(\frac{\dot{\rho} + \rho\dot{\theta}\tan\theta}{\cos^2\theta}\right) + \hat{\boldsymbol{\phi}}\rho\dot{\phi} + \hat{\boldsymbol{\theta}}\left(\frac{\dot{\rho}\tan\theta}{\cos\theta} + \frac{\rho\dot{\theta}}{\cos^3\theta}\right). \tag{B.173}$$

The velocity and acceleration vectors must also be defined as

$$\vec{v} = v_\rho\hat{\boldsymbol{\rho}} + v_\phi\hat{\boldsymbol{\phi}} + v_\theta\hat{\boldsymbol{\theta}}, \quad \vec{a} = \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = a_\rho\hat{\boldsymbol{\rho}} + a_\phi\hat{\boldsymbol{\phi}} + a_\theta\hat{\boldsymbol{\theta}}. \tag{B.174}$$

By differentiating Equation (B.173) by time, we get the particular components of the acceleration vector in the *disk-like* coordinate system,

$$\begin{aligned}
a_\rho &= \frac{\ddot{\rho} + \tan\theta[\rho\ddot{\theta} + 2\dot{\theta}(\dot{\rho} + \rho\dot{\theta}\tan\theta)]}{\cos^2\theta} - \rho\dot{\phi}^2 = \frac{\mathrm{d}v_\rho}{\mathrm{d}t} - \rho\dot{\phi}^2 - \frac{\dot{\theta}}{\cos^2\theta}\left(\dot{\rho}\tan\theta + \frac{\rho\dot{\theta}}{\cos^2\theta}\right),\\
a_\phi &= \rho\ddot{\phi} + 2\dot{\rho}\dot{\phi} = \frac{\mathrm{d}v_\phi}{\mathrm{d}t} + \dot{\rho}\dot{\phi},\\
a_\theta &= \frac{1}{\cos\theta}\left[\ddot{\rho}\tan\theta + \frac{\rho\ddot{\theta} + 2\dot{\theta}\,(\dot{\rho} + \rho\dot{\theta}\tan\theta)}{\cos^2\theta}\right] = \frac{\mathrm{d}v_\theta}{\mathrm{d}t} - \frac{\tan\theta\,\dot{\theta}}{\cos\theta}\left(\dot{\rho}\tan\theta + \frac{\rho\dot{\theta}}{\cos^2\theta}\right).
\end{aligned} \tag{B.175}$$

From these equations, we can easily see that

$$\dot{\rho} = v_\rho - v_\theta\sin\theta, \quad \dot{\phi} = \frac{v_\phi}{\rho}, \quad \dot{\theta} = \frac{(v_\theta - v_\rho\sin\theta)\cos\theta}{\rho} \tag{B.176}$$

holds for the main terms of the velocity vector components. Because $\mathrm{d}\vec{v}/\mathrm{d}t = \partial\vec{v}/\partial t + \vec{v}\cdot\vec{\nabla}\vec{v}$ applies, we can write the acceleration, expressed in the *disk-like* coordinate system, using the velocity vector components

$$a_\rho = \frac{\partial v_\rho}{\partial t} + \underbrace{v_\rho\frac{\partial v_\rho}{\partial\rho} + \frac{v_\phi}{\rho}\frac{\partial v_\rho}{\partial\phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\rho}{\partial\theta}}_{(\vec{v}\cdot\vec{\nabla})v_\rho} - \frac{v_\phi^2 + v_\theta^2}{\rho} + \frac{v_\rho v_\theta\sin\theta}{\rho}, \tag{B.177}$$

$$a_\phi = \frac{\partial v_\phi}{\partial t} + \underbrace{v_\rho\frac{\partial v_\phi}{\partial\rho} + \frac{v_\phi}{\rho}\frac{\partial v_\phi}{\partial\phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\phi}{\partial\theta}}_{(\vec{v}\cdot\vec{\nabla})v_\phi} + \frac{v_\rho v_\phi}{\rho} - \frac{v_\phi v_\theta\sin\theta}{\rho}, \tag{B.178}$$

$$a_\theta = \frac{\partial v_\theta}{\partial t} + \underbrace{v_\rho\frac{\partial v_\theta}{\partial\rho} + \frac{v_\phi}{\rho}\frac{\partial v_\theta}{\partial\phi} + v_\theta\frac{\cos\theta}{\rho}\frac{\partial v_\theta}{\partial\theta}}_{(\vec{v}\cdot\vec{\nabla})v_\theta} - \frac{v_\theta^2\sin\theta}{\rho} + \frac{v_\rho v_\theta\sin^2\theta}{\rho}. \tag{B.179}$$

The under-braced terms on the right-hand sides of Equations (B.177)-(B.179) express the (nonlinear) advection; the remaining terms represent the so-called *fictitious* (inertial) forces - centrifugal force, Coriolis force, Euler force.

By comparing Equations (B.145) and (B.176), we can write components of the velocity vector v_ρ, v_ϕ, v_θ in the disk-like system using the velocity vector components $v_{\rho,\,\mathrm{cyl}}$, $v_{\phi,\,\mathrm{cyl}}$, v_z in the standard cylindrical coordinate system (Section B.2). This gives us a correlation between the magnitudes of the velocity vector component in both systems,

$$v_\rho = v_{\rho,\,\mathrm{cyl}} + \frac{z}{\rho}\, v_z = v_{\rho,\,\mathrm{cyl}} + v_z \tan\theta, \quad v_\phi = v_{\phi,\,\mathrm{cyl}}, \quad v_\theta = \frac{\sqrt{\rho^2 + z^2}}{\rho}\, v_z = \frac{v_z}{\cos\theta}. \tag{B.180}$$

Taking further into account the vertical hydrostatic equilibrium in such a disk, $\mathrm{d}P/\mathrm{d}z = -\rho g_z$, where P is the scalar pressure and g_z is the vertical component of the gravitational acceleration, we get for the vertical component of the velocity $v_z = 0$. Thus, the equations of motion (B.177)-(B.179) will be identical to the corresponding equations of motion (B.52)-(B.54) in the standard cylindrical geometry.

Appendix C

Cylindrical and spherical harmonic functions ★

In this chapter, we will attempt to illustrate and justify the use of these functions for the purposes of mathematical physics.

C.1 Bessel functions

In paragraph D.2.4, we meet Bessel functions, which represent the standard form of the solution of the so-called *Bessel differential equation*,

$$x^2 y'' + xy' + \left(x^2 - n^2\right) y = 0, \tag{C.1}$$

where n represents the *order* of this equation. Bessel functions often appear when solving parabolic or hyperbolic equations in cylindrical (or even spherical) coordinates. Bessel functions are therefore classified as cylindrical (or spherical) *harmonic functions*, where n is an integer or semi-integer parameter. Since the Bessel equation is a 2nd order differential equation, it has two linearly independent solutions, $J_n(x)$ and $Y_n(x)$, classified as Bessel functions of type 1 and type 2.

C.1.1 Bessel functions of the 1st kind

Assume a solution of Bessel's differential equation in the form of an infinite power series

$$y(x) = x^n \sum_{k=0}^{\infty} b_k x^k. \tag{C.2}$$

The first and second derivatives of this series will be

$$y'(x) = nx^{n-1} \sum_{k=0}^{\infty} b_k x^k + x^n \sum_{k=0}^{\infty} k b_k x^{k-1} \tag{C.3}$$

and

$$y''(x) = n\,(n-1)\,x^{n-2} \sum_{k=0}^{\infty} b_k x^k + 2nx^{n-1} \sum_{k=0}^{\infty} k b_k x^{k-1} + x^n \sum_{k=0}^{\infty} k\,(k-1)\,b_k x^{k-2}. \tag{C.4}$$

★ are marked paragraphs and examples, intended primarily for students of higher years of bachelor studies.

The complete equation (C.1) will have the form

$$n\,(n-1)\,x^n\sum_{k=0}^{\infty} b_k x^k + 2nx^n\sum_{k=0}^{\infty} kb_k x^k + x^n\sum_{k=0}^{\infty} k\,(k-1)\,b_k x^k + nx^n\sum_{k=0}^{\infty} b_k x^k + \\ + x^n\sum_{k=0}^{\infty} kb_k x^k + x^n\sum_{k=0}^{\infty} b_k x^{k+2} - n^2x^n\sum_{k=0}^{\infty} b_k x^k = 0. \tag{C.5}$$

Since we are solving the equation with terms b_k for the corresponding non-negative k, we may set $b_{-1} = b_{-2} = 0$. The penultimate term on the left-hand side of Eq. (C.5) can then be converted into the form of

$$x^n\sum_{k=0}^{\infty} b_k x^{k+2} = x^n\sum_{k=2}^{\infty} b_{k-2} x^k = x^n\sum_{k=0}^{\infty} b_{k-2} x^k. \tag{C.6}$$

When substituted into the complete Bessel differential equation, it simplifies to Eq.

$$x^n\sum_{k=0}^{\infty}\left(k^2 b_k + 2nkb_k + b_{k-2}\right)x^k = 0, \tag{C.7}$$

from which, if we put the expression in brackets equal to zero, we get

$$b_k = -\frac{b_{k-2}}{k(k+2n)}. \tag{C.8}$$

Since we have $b_{-1} = 0$, we can also deduce $b_1 = 0$ and in fact every other odd $b_{2k-1} = 0$ from Eq. (C.8). For even k we must first determine the value of b_0, since Eq. (C.8) is not defined for $k = 0$ (it gives the type of the $0/0$ limit). For even k, Eq. (C.8) generally implies

$$b_{2k} = -\frac{b_{2k-2}}{4k(k+n)}, \tag{C.9}$$

Thus, for the lowest values $k = 1$ and $k = 2$ we get

$$b_2 = b_{2(1)} = \frac{(-1)b_0}{4(1)(1+n)}, \qquad b_4 = b_{2(2)} = \frac{(-1)\frac{(-1)b_0}{4(1)(1+n)}}{4(2)(2+n)} = \frac{(-1)^2 b_0}{4^2(2\cdot 1)(1+n)(2+n)}. \tag{C.10}$$

Let us now use the method of mathematical induction. Suppose that the above holds for any positive integer ℓ, i.e.

$$b_{2\ell} = \frac{(-1)^\ell b_0}{4^\ell \ell!(1+n)(2+n)...\,(\ell+n)} = \frac{(-1)^\ell b_0}{4^\ell \ell!\,\prod_{1+n}^{\ell+n} m}, \tag{C.11}$$

where the positive integer m symbolizes the individual brackets $(1+n)(2+n)...\,(\ell+n)$ in the denominator. It can easily be shown that the same holds for $\ell + 1$, where

$$b_{2(\ell+1)} = \frac{(-1)\frac{(-1)^\ell b_0}{4^\ell \ell!\,\prod_{1+n}^{\ell+n} m}}{4(\ell+1)(\ell+1+n)} = \frac{(-1)^{\ell+1} b_0}{4^{\ell+1}(\ell+1)!\,\prod_{1+n}^{\ell+1+n} m}, \tag{C.12}$$

we see that Eq. (C.11) holds in general for all natural ℓ.

Before inserting Eq. (C.11) back to the original power series (C.2), we have to determine the appropriate value of b_0. We see that the sum in the power series equation must converge to be a solution of the Bessel equation (C.1). In addition, it will be more convenient to use the factorial $(n+k)!$ in the denominator b_k instead of closing the product on the value $(n+1)$ that we used in the inductive proof. For these reasons, if we introduce

$$b_0 = \frac{1}{2^n n!}, \tag{C.13}$$

so after inserting into Eq. (C.11) we get

$$b_{2k} = \frac{(-1)^k}{2^n 4^k k!(n+k)!}. \tag{C.14}$$

Now we can insert the expression (C.14) for b_{2k} into the full power series (C.2). We get

$$y(x) = x^n \sum_{k=0}^{\infty} \frac{(-1)^k}{2^n 4^k k!(n+k)!} x^{2k} = \left(\frac{x}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(n+k)!} \left(\frac{x}{2}\right)^{2k}, \tag{C.15}$$

where we show that the power series converges, for example, by calculating $\lim_{k\to\infty} b_{k+1}/b_k = 0$.

However, we want to formulate a solution for the general real or complex index ν, not only for the natural index $n \in \mathbb{N}$. The most common way to extend the factorial to real or complex numbers is the Gamma function (see Eq. (12.29) and further explanation in the solved example in Sect. 12.2). The inverse (reciprocal) of the Gamma function is also holomorphic, which means that it is infinitely complex differentiable and expandable into a Taylor series. Since we are applying the Gamma function to the denominators of Eq. (C.15), this property of its reciprocal series will be particularly useful. The gamma function is defined as $\Gamma(n) = (n-1)!$ only for natural n, while for the remaining integers, real and complex numbers it corresponds to the so-called *Mellin* transform $\{\mathcal{M}\}$ of the negative exponential function,

$$\Gamma(z) = \{\mathcal{M}\, \mathrm{e}^{-x}\}(z), \quad \text{where generally} \quad \{Mf\} = \int_0^{\infty} x^{s-1} f(x)\, \mathrm{d}x. \tag{C.16}$$

By modifying Eq. (C.15) in this sense we get

$$J_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma(\nu+k+1)} \left(\frac{x}{2}\right)^{2k}, \tag{C.17}$$

where $\Gamma(k+1)$ in the denominator can equivalently be written as $k!$. However, this equation should not hold for negative integers, $\nu = -n \in \mathbb{N}$, where the Gamma function is not defined. In that case, let's start summing only at $k = n$ to skip (bypass) any undefined terms of the Gamma function (since $k = n$ corresponds to $\Gamma(-n+n+1)$),

$$J_{-n}(x) = \left(\frac{x}{2}\right)^{-n} \sum_{k=n}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma(-n+k+1)} \left(\frac{x}{2}\right)^{2k}. \tag{C.18}$$

If we shift the origin of the sum back to $k = 0$, we can write

$$\begin{aligned} J_{-n}(x) &= \left(\frac{x}{2}\right)^{-n} \sum_{k=0}^{\infty} \frac{(-1)^{k+n}}{\Gamma(k+n+1)\,\Gamma(-n+k+n+1)} \left(\frac{x}{2}\right)^{2(k+n)} = \\ &= (-1)^n \left(\frac{x}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+n+1)\,\Gamma(k+1)} \left(\frac{x}{2}\right)^{2k} = (-1)^n J_n(x). \end{aligned} \tag{C.19}$$

This also represents the solution of the Bessel differential equation (C.1). We have thus found a consistent Bessel function of the first type $J_n(x)$ for $n \in \mathbb{Z}$ and thus we have also completed the last missing link in the very general function $J_\nu(x)$ for $\nu \in \mathbb{C}$.

We now determine the next linearly independent solution. Let's start by examining the behavior of the function $J_\nu(x)$ for $x \to 0$. For further examination, we need to determine whether the complex number $\nu > 0$, $\nu = 0$, or $\nu < 0$. Since 0 is a real number, we need only compare the real parts of $\mathrm{Re}\,(\nu)$ of the complex number ν to make this determination:

- If $\mathrm{Re}\,(\nu) > 0$ (the real part of the complex index ν is positive), then

$$\lim_{x\to 0} J_\nu(x) = \lim_{x\to 0} \left(\frac{x}{2}\right)^{\nu>0} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma(\nu+k+1)} \left(\frac{x}{2}\right)^{2k} = 0, \tag{C.20}$$

  because $\lim\limits_{x\to 0} \left(\frac{x}{2}\right)^{\nu>0} = 0$.

- If $\nu = 0$, then

$$\lim_{x\to 0} J_0(x) = \lim_{x\to 0} \left(\frac{x}{2}\right)^{0} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma(k+1)} \left(\frac{x}{2}\right)^{2k} = 1 + 0 + 0 + \ldots \; = 1, \tag{C.21}$$

  because $\lim\limits_{x\to 0} \left(\frac{x}{2}\right)^{x} = 1$ and at the same time, for $k = 0$, $\lim\limits_{x\to 0} \left(\frac{x}{2}\right)^{2x} = 1$, while for others $k > 0$, $\lim\limits_{x\to 0} \left(\frac{x}{2}\right)^{2k} = 0$.

- If $\mathrm{Re}\,(\nu) < 0$ (the real part of the complex index ν is negative and at the same time for $\nu < 0$ $\nu \neq \mathbb{Z}$ must hold because the Gamma function is not defined here), then

$$\lim_{x\to 0} J_\nu(x) = \lim_{x\to 0} \left(\frac{x}{2}\right)^{\nu<0} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma(\nu+k+1)} \left(\frac{x}{2}\right)^{2k} \to \pm\infty, \tag{C.22}$$

  because $\lim\limits_{x\to 0} \left(\frac{x}{2}\right)^{\nu<0} = \lim\limits_{x\to 0} \left(\frac{2}{x}\right)^{\nu>0} \to \pm\infty$.

Thus, the summary results of the first, second and third steps are as follows:

$$\lim_{x\to 0} J_\nu(x) = \begin{cases} 0, & \mathrm{Re}\,(\nu) > 0 \\ 1, & \nu = 0 \\ \pm\infty, & \mathrm{Re}\,(\nu) < 0 \end{cases}. \tag{C.23}$$

We see that $J_\nu(x)$ and $J_{-\nu}(x)$ are two linearly independent solutions (each of them cannot be expressed by mutual linear combinations) if $\nu \neq \mathbb{Z}$. If $\nu \in \mathbb{Z}$, these solutions are linearly dependent (see Eq. (C.19)). Due to this property and the homogeneity of the Bessel differential equation, every linear combination of $J_\nu(x)$ and $J_{-\nu}(x)$ is a linear combination, where $\nu \neq \mathbb{Z}$, is also a solution.

We can further easily verify the following derivative,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[x^n J_n(x)\right] = x^n J_{n-1}(x) \tag{C.24}$$

and, by combination of Eqs. (C.19) and (C.24), we arrive to

$$\frac{\mathrm{d}J_0(x)}{\mathrm{d}x} = -J_1(x), \qquad \frac{\mathrm{d}J_1(x)}{\mathrm{d}x} = J_0(x) - \frac{J_1(x)}{x}, \tag{C.25}$$

which may be also useful for some cylindrically symmetric solutions.

C.1.2 Bessel functions of the 2nd kind

Next, we introduce the equation (Bessel function of the 2nd kind as a linear combination of $J_\nu(x)$ and $J_{-\nu}(x)$)

$$Y_\nu(x) = \frac{\cos(\nu\pi)\, J_\nu(x) - J_{-\nu}(x)}{\sin(\nu\pi)}, \tag{C.26}$$

for $\nu \neq \mathbb{Z}$ (because $\cos(n\pi) = (-1)^n$). Note that in the case of nonnegative integers ν ($\nu \equiv n \in \mathbb{N}_0$), $Y_{n\geq 0}(x) = 0$; for $n > 0$, this follows directly from substitution into Eq. (C.26), and for $n = 0$ we can easily calculate the corresponding limit by the following Eq. (C.27).

For $\nu \in \mathbb{Z}$ is in general

$$Y_n(x) = \lim_{\nu\to n} Y_\nu(x). \tag{C.27}$$

The calculation of this limit can be done using the L'Hôspital rule as

$$\begin{aligned} Y_n(x) &= \lim_{\nu\to n} \frac{\cos(\nu\pi)\, J_\nu(x) - J_{-\nu}(x)}{\sin(\nu\pi)} = \lim_{\nu\to n} \frac{-\pi\sin(\nu\pi)\, J_\nu(x) + \cos(\nu\pi)\, \frac{\mathrm{d}}{\mathrm{d}\nu} J_\nu(x) - \frac{\mathrm{d}}{\mathrm{d}\nu} J_{-\nu}(x)}{\pi\cos(\nu\pi)} \\ &= \lim_{\nu\to n} \frac{1}{\pi}\left[\frac{\mathrm{d}}{\mathrm{d}\nu} J_\nu(x) - \frac{\mathrm{d}}{\mathrm{d}\nu} J_{-\nu}(x)\right]. \end{aligned} \tag{C.28}$$

The detailed calculation is too lengthy, so I do not present it here. Interested readers may refer to the literature, for example, Abramowitz & Stegun (1972); Arfken & Weber (2005). I only point out that its calculation also uses the so-called Digamma function, which gives the following relationship between the Gamma function and its derivative,

$$\psi(z) = \frac{\mathrm{d}}{\mathrm{d}z} \ln\Gamma(z) = \frac{\Gamma'(z)}{\Gamma(z)}. \tag{C.29}$$

C.1.3 Some important values of Bessel functions of the 1st and 2nd kind

By substituting directly into Eq. C.17 (or C.15), we get

$$J_0(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(k!)^2} \left(\frac{x}{2}\right)^{2k}. \tag{C.30}$$

As mentioned in the previous paragraph C.1.2, $Y_n(x) = 0$ for $n \in \mathbb{N}_0$.

Let us now look at the semi-integer values of the Bessel functions and their justification by substituting them into Eq. C.17,

$$J_{\frac{1}{2}}(x) = \sqrt{\frac{x}{2}} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma\left(k+\frac{3}{2}\right)} \left(\frac{x}{2}\right)^{2k}. \tag{C.31}$$

Since $\Gamma\left(k+\frac{3}{2}\right) = \frac{(2k+1)!\sqrt{\pi}}{k!\,2^{2k+1}}$, we get

$$\sqrt{\frac{x}{2}} \sum_{k=0}^{\infty} \frac{2^{2k+1}(-1)^k}{(2k+1)!\sqrt{\pi}} \left(\frac{x}{2}\right)^{2k} = \sqrt{\frac{2}{\pi x}} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} x^{2k+1}. \tag{C.32}$$

Since the sum in the last expression corresponds to the Taylor expansion of the function $\sin x$, it must also hold

$$J_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \sin x. \tag{C.33}$$

By substituting into Eq. (C.26), we easily find that

$$Y_{-\frac{1}{2}}(x) = J_{\frac{1}{2}}(x). \tag{C.34}$$

In a similar way, it can be found that

$$J_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{x}} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\,\Gamma\left(k+\frac{1}{2}\right)} \left(\frac{x}{2}\right)^{2k}, \tag{C.35}$$

where, because $\Gamma\left(k+\frac{1}{2}\right) = \frac{(2k)!\sqrt{\pi}}{k!\,2^{2k}}$, we get

$$\sqrt{\frac{2}{x}} \sum_{k=0}^{\infty} \frac{2^{2k}(-1)^k}{(2k)!\sqrt{\pi}} \left(\frac{x}{2}\right)^{2k} = \sqrt{\frac{2}{\pi x}} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} x^{2k}, \tag{C.36}$$

where, because the sum in the last expression corresponds to the Taylor expansion of the function $\cos x$,

$$J_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cos x. \tag{C.37}$$

By substituting into Eq. (C.26), we again easily find that

$$Y_{\frac{1}{2}}(x) = J_{-\frac{1}{2}}(x). \tag{C.38}$$

By analogy, we can also derive the values of the semi-integer (summed with the common index k) and other real Bessel functions. For those interested in detailed expressions and mathematical procedures, I refer to the literature, e.g., Abramowitz & Stegun (1972); Arfken & Weber (2005), etc.

C.2 Hankel functions, modified and spherical Bessel functions

In this section we give at least a basic overview of the above special functions as modifications or linear combinations of Bessel functions of the 1st and 2nd kind. Those interested in a more detailed description of these functions are referred to the literature, for example, to Abramowitz & Stegun (1972); Arfken & Weber (2005), and others.

An important formulation of the two linearly independent solutions of the Bessel equation are the so-called itHankel functions of the first and second kind, $H_\nu^{(1)}(x)$ and $H_\nu^{(2)}(x)$, defined as (Abramowitz & Stegun, 1972)

$$H_\nu^{(1)}(x) = J_\nu(x) + \mathrm{i}Y_\nu(x), \tag{C.39}$$

$$H_\nu^{(2)}(x) = J_\nu(x) - \mathrm{i}Y_\nu(x), \tag{C.40}$$

where i is an imaginary unit. These linear combinations are also called Bessel functions of the third kind; they are two linearly independent solutions of the Bessel differential equation.

Bessel functions apply also for complex arguments of x, an important special case is the purely imaginary argument. In this case, the corresponding solutions of the Bessel equation are called itmodified Bessel functions (or occasionally hyperbolic Bessel functions) of the first and second kind, $I_\nu(x)$ and $K_\nu(x)$, and are defined as (Abramowitz & Stegun, 1972)

$$I_\nu(x) = \mathrm{i}^{-\nu} J_\nu(\mathrm{i}x) = \sum_{k=0}^{\infty} \frac{1}{\Gamma(k+1)\,\Gamma(\nu+k+1)} \left(\frac{x}{2}\right)^{2k+\nu}, \tag{C.41}$$

$$K_\nu(x) = \frac{\pi}{2} \frac{I_{-\nu}(x) - I_\nu(x)}{\sin(\pi\nu)}, \tag{C.42}$$

where ν is generally not an integer; if ν is an integer, the limit transform is used. These functions take real values for real and positive arguments x. Thus, the series expansion for $I_\nu(x)$ is similar to that for $J_\nu(x)$, but without the "inverting" factor $(-1)^k$.

When solving an elliptic partial differential (see paragraph D.2.6) so-called *Helmholtz equation*, $\left(\nabla^2 + k^2\right) f$ in spherical coordinates by separation of variables, the radial part of the equation has the form

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + 2x \frac{\mathrm{d}y}{\mathrm{d}x} + \left[x^2 - n(n+1)\right] y = 0, \tag{C.43}$$

where n is an integer. The two linearly independent solutions of this equation are called itspherical Bessel functions j_n and y_n and are related to the "ordinary" Bessel functions J_n and Y_n by the relation (Abramowitz & Stegun, 1972)

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x), \tag{C.44}$$

$$y_n(x) = \sqrt{\frac{\pi}{2x}} Y_{n+\frac{1}{2}}(x) = (-1)^{n+1} \sqrt{\frac{\pi}{2x}} J_{-n-\frac{1}{2}}(x). \tag{C.45}$$

Spherical Bessel functions can also be written as

$$j_n(x) = (-x)^n \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \frac{\sin x}{x}, \tag{C.46}$$

$$y_n(x) = -(-x)^n \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \frac{\cos x}{x}, \tag{C.47}$$

so, for example, the zero spherical Bessel function $j_0(x)$ is also known as the (non-normalized) integral sine function $\mathrm{Si}\, x = \frac{\sin x}{x}$ (see the 9.6 example in the 9.1 paragraph).

C.3 Orthogonal polynomials

We refer to orthogonal polynomials as those types of polynomials in which any two distinct polynomials in a given sequence are mutually orthogonal in some scalar product space. The most commonly used orthogonal polynomials are the classical orthogonal polynomials, which consist of *Hermite polynomials*, *Laguerre polynomials*, and the so-called *Jacobi polynomials*, which include *Chebyshev polynomials* and, particularly important for our purposes, *Legendre polynomials* as special cases. Orthogonal polynomials appear in a number of fields, such as numerical analysis, probability theory, mathematical physics, etc.

C.3.1 Legendre polynomials

The Legendre polynomials $P_\ell(x)$ form an infinite series of functions of a single variable x. Each function in this series is assigned an index ℓ; it is an integer that starts with $\ell = 0$ and ends with $\ell = \infty$. So we have a functions $P_0(x)$, $P_1(x)$, and an infinite number of other functions belonging to this series.

The definition of Legendre polynomials is somewhat specific. First we introduce the function $\Phi(x, h)$ of two variables, known as the *generic function*. The variable x is identical to the argument of Legendre polynomials, the variable h has no specific meaning here yet. The generic function is defined as

$$\Phi(x, h) = \left(1 - 2x\,h + h^2\right)^{-1/2}. \tag{C.48}$$

We will justify this form of the generic function later in Sect. C.3.5, when describing multipole expansion. For now, let us take Eq. (C.48) as given, however arbitrary it may seem now.

Let us fix x in Eq. (C.48) for a moment and consider $\Phi = \Phi(h)$ as a function of a single variable h. The Taylor expansion of the function $\Phi(h)$ can then be written as

$$\Phi(h) = \Phi(0) + \left.\frac{\mathrm{d}\Phi}{\mathrm{d}h}\right|_{h=0} h + \frac{1}{2!}\left.\frac{\mathrm{d}^2\Phi}{\mathrm{d}h^2}\right|_{h=0} h^2 + \frac{1}{3!}\left.\frac{\mathrm{d}^3\Phi}{\mathrm{d}h^3}\right|_{h=0} h^3 + \ldots = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left.\frac{\mathrm{d}^\ell\Phi}{\mathrm{d}h^\ell}\right|_{h=0} h^\ell, \tag{C.49}$$

where we have marked the summation index with ℓ. We now formally recover the dependence of the generating function on the variable x. The general form of the Taylor expansion in Eq. (C.49) remains, only the derivatives according to h will now be written as partial derivatives instead of total derivatives. The compact form of the Taylor series will then be

$$\Phi(x, h) = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left.\frac{\partial^\ell\Phi}{\partial h^\ell}\right|_{h=0} h^\ell. \tag{C.50}$$

In Eq. (C.50), the coefficients of the Taylor expansion are given by the partial derivatives of $\partial\Phi/\partial h$ at $h = 0$. Thus, they depend only on x and are independent of h. The Legendre polynomials of degree ℓ are just equal to these coefficients, so we can write

$$\Phi(x, h) = \sum_{\ell=0}^{\infty} P_\ell(x)\,h^\ell, \qquad \text{so} \qquad P_\ell(x) = \frac{1}{\ell!}\left.\frac{\partial^\ell\Phi}{\partial h^\ell}\right|_{h=0}. \tag{C.51}$$

Since the Taylor expansion generally involves an infinite number of terms, we have an infinite number of coefficients and hence an infinite set of functions of x. Equation (C.51) demonstrates the explicit connection of Legendre polynomials with partial derivatives of $\Phi(x, h)$.

Let's use Eq. (C.51) to calculate the first few polynomials. We get $P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = \frac{1}{2}(3x^2 - 1)$. We can continue in this way and calculate an arbitrarily large number of polynomials. However, the computations get progressively more complicated; more effective methods are available for generating Legendre polynomials over $\ell = 2$, for example, calculating them using a compact, the so-called *Rodrigues' formula*:

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{\mathrm{d}^\ell}{\mathrm{d}x^\ell}(x^2 - 1)^\ell. \tag{C.52}$$

The first few Legendre polynomials have the form

$$P_0 = 1, \tag{C.53}$$
$$P_1 = x, \tag{C.54}$$
$$P_2 = \frac{1}{2}\left(3x^2 - 1\right), \tag{C.55}$$
$$P_3 = \frac{1}{2}\left(5x^3 - 3x\right), \tag{C.56}$$
$$P_4 = \frac{1}{8}\left(35x^4 - 30x^2 + 3\right), \tag{C.57}$$
$$P_5 = \frac{1}{8}\left(63x^5 - 70x^3 + 15x\right), \tag{C.58}$$
$$P_6 = \frac{1}{16}\left(231x^6 - 315x^4 + 105x^2 - 5\right). \tag{C.59}$$

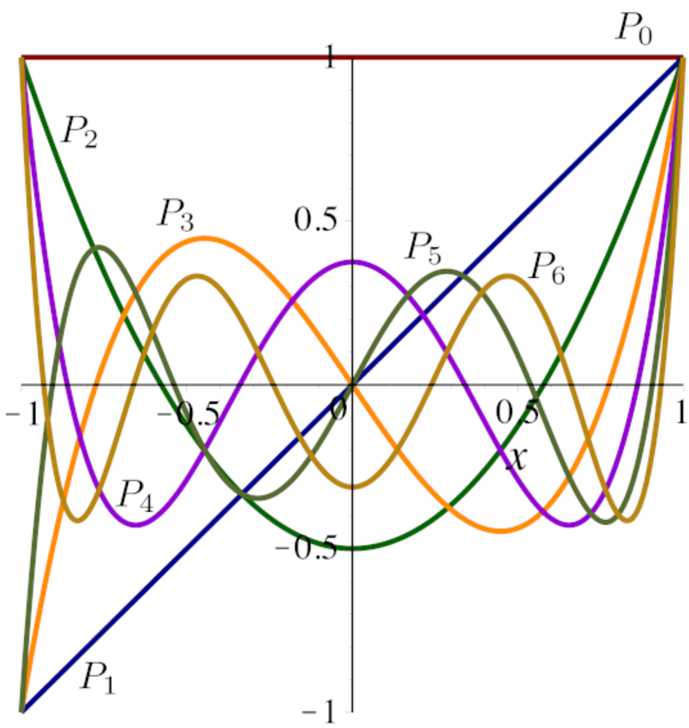

Figure C.1: The first six Legendre polynomials.

C.3.2 Recursive relations and the Legendre equation

Let us now consider the following recursive relation for Legendre polynomials

$$\ell P_\ell(x) = (2\ell - 1)xP_{\ell-1}(x) - (\ell - 1)P_{\ell-2}(x). \tag{C.60}$$

This equation also allows the formation of a sequence of Legendre polynomials. Suppose we have calculated $P_0 = 1$ and $P_1 = x$ from the definition (as we did in the previous section). If we put $\ell = 2$ in Eq. (C.60), we can calculate P_2, P_3, etc. We will use this recursive relation

(C.60) to prove (by induction) that the properties of Legendre polynomials illustrated by the enumeration in Eqs. (C.53) - (C.59) for $\ell \leq 6$ do indeed hold quite generally for all values of ℓ.

The first property that is obvious from Eqs. (C.53) - (C.59) is that the highest power of x that occurs in P_ℓ is x^ℓ. Suppose that this property holds for all values of ℓ up to some limiting value of $\ell_{\max}$, in the list of Eqs. (C.53) - (C.59) $\ell_{\max} = 6$. Using a recursive relation, we can prove that this property holds for higher values of ℓ. In Eq. (C.60) we rename $\ell \to \ell_{\max}+1$, so the right-hand side includes $xP_{\ell_{\max}}$ and $P_{\ell_{\max}-1}$, both multiplied by the appropriate numerical factor. We know that the highest power of x in $P_{\ell_{\max}}$ is $x^{\ell_{\max}}$, multiplying by x this goes to $x^{\ell_{\max}+1} = x^\ell$. The highest power in the second term is $x^{\ell_{\max}-1} = x^{\ell-2}$, which is a lower power than in the first term. Since the recurrent process has no highest finite value, this property will hold for all values of ℓ.

In proving Eq. (C.60), we start from the generic function $\Phi(x,h)$ in Eq. (C.48) and its partial derivatives $\partial\Phi/\partial h$. These relations imply

$$\left(1 - 2xh + h^2\right) \frac{\partial \Phi}{\partial h} = (x-h)\,\Phi, \tag{C.61}$$

whereby we obtain a useful identity by substituting Eq. (C.51) and its derivative by h, which is given by

$$\frac{\partial \Phi}{\partial h} = \sum_{\ell=1}^{\infty} \ell P_\ell(x)\, h^{\ell-1}, \tag{C.62}$$

where, however, the beginning of the sum is only at $\ell = 1$, because the term with $\ell = 0$ obviously drops out. For the left-hand side of Eq. (C.61), we get

$$\left(1 - 2xh + h^2\right) \frac{\partial \Phi}{\partial h} = \sum_{\ell=1}^{\infty} \ell P_\ell\, h^{\ell-1} - 2x \sum_{\ell=1}^{\infty} \ell P_\ell\, h^{\ell} + \sum_{\ell=1}^{\infty} \ell P_\ell\, h^{\ell+1}. \tag{C.63}$$

The three sums on the right-hand side of Eq. (C.63) contain different powers of h, we now shift the lower bounds of the sums by unifying the powers of h, i.e.

$$\left(1 - 2xh + h^2\right) \frac{\partial \Phi}{\partial h} = \sum_{\ell=1}^{\infty} \ell P_\ell\, h^{\ell-1} - 2x \sum_{\ell=2}^{\infty} (\ell-1)\, P_{\ell-1}\, h^{\ell-1} + \sum_{\ell=3}^{\infty} (\ell-2)\, P_{\ell-2}\, h^{\ell-1}. \tag{C.64}$$

Next, we unify the lower bounds of all three sums by expressing the first and second terms on the right side of Eq. (C.64) as

$$\sum_{\ell=1}^{\infty} \ell P_\ell\, h^{\ell-1} = P_1 + 2P_2\, h + \sum_{\ell=3}^{\infty} \ell P_\ell\, h^{\ell-1}, \tag{C.65}$$

$$-2x \sum_{\ell=2}^{\infty} (\ell-1)\, P_{\ell-1}\, h^{\ell-1} = -2xP_1\, h - \sum_{\ell=3}^{\infty} 2\,(\ell-1)\, xP_{\ell-1}\, h^{\ell-1}, \tag{C.66}$$

which adds up to

$$\begin{aligned}\left(1 - 2xh + h^2\right) \frac{\partial \Phi}{\partial h} &= P_1 + (2P_2 - 2xP_1)\, h + \\ &\quad + \sum_{\ell=3}^{\infty} \left[\ell P_\ell - 2\,(\ell-1)\, xP_{\ell-1} + (\ell-2)\, P_{\ell-2}\right] h^{\ell-1}. \end{aligned} \tag{C.67}$$

The right-hand side of Eq. (C.61) is expressed in an analogous way,

$$(x-h)\,\Phi = x\sum_{\ell=0}^{\infty} P_\ell h^\ell - \sum_{\ell=0}^{\infty} P_\ell h^{\ell+1} = xP_0 + (xP_1 - P_0)\,h + \sum_{\ell=3}^{\infty} (xP_{\ell-1} - P_{\ell-2})\,h^{\ell-1}. \quad \text{(C.68)}$$

Since Eqs. (C.67) and (C.68) are equal when substituted into Eq. (C.61), for each power of h the coefficients of expansion on the left-hand side must be equal to the coefficients of expansion on the right-hand side, i.e., for the first and second order $P_1 = xP_0$ and $2P_2 - 2xP_1 = xP_1 - P_0$. For the higher orders must apply

$$\ell P_\ell - 2\,(\ell-1)\,xP_{\ell-1} + (\ell-2)\,P_{\ell-2} = xP_{\ell-1} - P_{\ell-2}, \quad \text{(C.69)}$$

which after simplification reduces to the recursive expression in Eq. (C.60).

Legendre polynomials satisfy a number of other recursive relations which, unlike the original relation in Eq. (C.60), contain derivatives of these polynomials. We establish the first of these using a procedure very similar to that described in Eqs. (C.61) - (C.69). Again, we start with the generic function (C.48), but this time we derive it in terms of x, yielding $\partial\Phi/\partial x = h(1 - 2xh + h^2)^{-3/2}$. This implies the identity

$$\left(1 - 2xh + h^2\right)\frac{\partial\Phi}{\partial x} = h\Phi, \quad \text{(C.70)}$$

which here plays the same role as Eq. (C.61) in the derivative of Eq. (C.60). Inserting the analogue of Eq. (C.51), now differentiated with respect to x, into the left-hand side and making the familiar adjustments, we get

$$\begin{aligned}
\left(1 - 2xh + h^2\right)\frac{\partial\Phi}{\partial x} &= \left(1 - 2xh + h^2\right)\sum_{\ell=0}^{\infty} P'_\ell h^\ell = \\
&= \sum_{\ell=0}^{\infty} P'_\ell h^\ell - 2x\sum_{\ell=0}^{\infty} P'_\ell h^{\ell+1} + \sum_{\ell=0}^{\infty} P'_\ell h^{\ell+2} = \\
&= \sum_{\ell=-1}^{\infty} P'_{\ell+1} h^{\ell+1} - 2x\sum_{\ell=0}^{\infty} P'_\ell h^{\ell+1} + \sum_{\ell=1}^{\infty} P'_{\ell-1} h^{\ell+1} = \\
&= P'_0 + P'_1 h + \sum_{\ell=1}^{\infty} P'_{\ell+1} h^{\ell+1} - 2xP'_0 h - 2x\sum_{\ell=1}^{\infty} P'_\ell h^{\ell+1} + \sum_{\ell=1}^{\infty} P'_{\ell-1} h^{\ell+1} = \\
&= P'_0 + \left(P'_1 - 2xP'_0\right) h + \sum_{\ell=1}^{\infty} \left(P'_{\ell+1} - 2xP'_\ell + P'_{\ell-1}\right) h^{\ell+1},
\end{aligned} \quad \text{(C.71)}$$

where the prime denotes the derivative with respect to x. For the right-hand side we get

$$h\Phi = h\sum_{\ell=0}^{\infty} P_\ell h^\ell = \sum_{\ell=0}^{\infty} P_\ell h^{\ell+1} = P_0 h + \sum_{\ell=1}^{\infty} P_\ell h^{\ell+1}. \quad \text{(C.72)}$$

Comparing the two sides, we find that $P'_0 = 0$ (which we already knew), as well as $P'_1 - 2xP'_0 = P_0$. The higher order terms give the recursive relation

$$P'_{\ell+1} - 2xP'_\ell + P'_{\ell-1} = P_\ell. \quad \text{(C.73)}$$

To determine the next recursive equation, we return to Eq. (C.60), which, if we set $\ell \to \ell+1$, differentiate with respect to x and multiplying by 2, we can rewrite it as

$$2\,(2\ell+1)\,xP'_\ell + 2\,(2\ell+1)\,P_\ell = 2\,(\ell+1)\,P'_{\ell+1} + 2\ell P'_{\ell-1}. \tag{C.74}$$

In the next step, we multiply Eq. (C.73) by $2\ell+1$,

$$2\,(2\ell+1)\,xP'_\ell + (2\ell+1)\,P_\ell = (2\ell+1)\,P'_{\ell+1} + (2\ell+1)\,P'_{\ell-1}, \tag{C.75}$$

and subtract the two equations. This gives us the equation

$$P'_{\ell+1} - P'_{\ell-1} = (2\ell+1)\,P_\ell. \tag{C.76}$$

The next recursive equation results directly from inserting Eq. (C.73) into Eq. (C.76) and dividing by 2,

$$P'_{\ell+1} - xP'_\ell = (\ell+1)\,P_\ell. \tag{C.77}$$

To obtain yet another recursive relation, we subtract Eqs. (C.73) and (C.76),

$$P'_{\ell-1} - xP'_\ell = -\ell P_\ell. \tag{C.78}$$

Finally, to obtain the last such recurrent relation, we replace ℓ with $\ell-1$ in Eq. (C.77), multiply Eq. (C.78) by the variable x and sum the two results,

$$\left(1-x^2\right)P'_\ell = \ell P_{\ell-1} - \ell x P_\ell. \tag{C.79}$$

To arrive at the so-called *Legendre equation*, let us start with the last equation (C.79), which we differentiate with respect to x. This gives us

$$\left(1-x^2\right)P''_\ell - 2xP'_\ell - \ell P'_{\ell-1} + \ell x P'_\ell + \ell P_\ell = 0 \tag{C.80}$$

and then exclude the term involving $P'_{\ell-1}$. using Eq. (C.79). After a little simplification, we get the Legendre equation

$$(1-x^2)P''_\ell - 2xP'_\ell + \ell\,(\ell+1)\,P_\ell = 0, \tag{C.81}$$

which can also be expressed in an alternative form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)\frac{\mathrm{d}P_\ell}{\mathrm{d}x}\right] + \ell\,(\ell+1)\,P_\ell = 0. \tag{C.82}$$

This is a very important equation of mathematical physics with applications in many different fields.

In many textbook descriptions of Legendre polynomials, the Legendre differential equation is first given (with unspecified motivation) and the polynomials $P_\ell(x)$ are then derived as solutions of this differential equation. We will say more about this in Sect. C.3.6. Here, we prefer to first define the polynomials using the generic function and derive the Legendre equation as a consequence.

C.3.3 Orthogonality of Legendre polynomials

As already mentioned, Legendre polynomials form a series of orthogonal functions on the interval $\langle -1, 1\rangle$. It can be shown that

$$\int_{-1}^{1} P_\ell(x) P'_\ell(x)\,\mathrm{d}x = 0, \tag{C.83}$$

if $\ell \neq \ell'$. If $\ell = \ell'$, the integral doesn't vanish, instead we see that

$$N_\ell = N[P_\ell] = \int_{-1}^{1} [P_\ell(x)]^2\,\mathrm{d}x = \frac{2}{2\ell+1}, \tag{C.84}$$

which is the norm of the function $P_\ell(x)$ on the interval $\langle -1.1\rangle$.

In the actual proof of orthogonality according to Eq. (C.83), we start from the Legendre equation of the form (C.82). We multiply the equation by P_ℓ and P'_ℓ, respectively, subtract the first result from the second and express it in compact form as the derivative of the product. We get

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[P_{\ell'}\left(1-x^2\right)\frac{\mathrm{d}P_\ell}{\mathrm{d}x} - P_\ell\left(1-x^2\right)\frac{\mathrm{d}P'_\ell}{\mathrm{d}x}\right] + \left[\ell\left(\ell+1\right) - \ell'\left(\ell'+1\right)\right] P_\ell P_{\ell'} = 0. \tag{C.85}$$

The result expressed in Eq. (C.85) brings us to why the range of the limits must be $\langle -1, 1\rangle$. and not any other interval. So let us first integrate Eq. (C.85) on an arbitrary interval $\langle a, b\rangle$ and see what choice of interval yields something useful. By integration, we get

$$\left[P_{\ell'}\left(1-x^2\right)\frac{\mathrm{d}P_\ell}{\mathrm{d}x} - P_\ell\left(1-x^2\right)\frac{\mathrm{d}P'_\ell}{\mathrm{d}x}\right]\Bigg|_a^b + \left[\ell\left(\ell+1\right) - \ell'\left(\ell'+1\right)\right]\int_a^b P_\ell P_{\ell'}\,\mathrm{d}x = 0 \tag{C.86}$$

and we see that the boundary values in $x = a$ and $x = b$ generally do not vanish; this prevents us from saying anything specific about such an integral. However, we also see how the choice of the interval allows us to eliminate the boundary values: the expression $(1 - x^2)$ vanishes at $x = \pm 1$, so the boundary values vanish when we choose the boundary $\langle -1, 1\rangle$. With this choice of interval, we now get

$$\left[\ell\left(\ell+1\right) - \ell'\left(\ell'+1\right)\right]\int_{-1}^{1} P_\ell P_{\ell'}\,\mathrm{d}x = 0. \tag{C.87}$$

If $\ell = \ell'$, the expression in square brackets disappears and the equation tranforms to the "all-inclusive" identity $0 = 0$. However, when $\ell^{\ell'}$, we get the statement expressed in Eq. (C.83), proving that the various Legendre polynomials are orthogonal on the interval $\langle -1, 1\rangle$.

We can verify the conclusion from Eq. (C.84) by solving the recurrence relation; first we put $\ell = 1$, we get $N_1 = \frac{1}{3}N_0$. If we next choose $\ell = 2$, we get $N_2 = \frac{3}{5}N_1 = \frac{1}{5}N_0$, at $\ell = 3$ we have $N_3 = \frac{5}{7}N_2 = \frac{1}{7}N_0$, so after ℓ iterations we finally get

$$N_\ell = \frac{1}{2\ell+1}N_0 = \frac{2}{2\ell+1}. \tag{C.88}$$

C.3.4 Associated Legendre polynomials

Their simplest definition is based on derivatives of "ordinary" Legendre polynomials ($m \geq 0$),

$$P_\ell^m(x) = (-1)^m(1-x^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}x^m}\left(P_\ell(x)\right). \tag{C.89}$$

The factor $(-1)^m$ is omitted by some authors in this formula. The functions described by this equation satisfy the general so-called *associated Legendre differential equation*

$$\left(1-x^2\right)\frac{\mathrm{d}^2 P_\ell^m}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}P_\ell^m}{\mathrm{d}x} + \left[\ell\left(\ell+1\right) - \frac{m^2}{1-x^2}\right]P_\ell^m = 0, \tag{C.90}$$

with the given values of the parameters ℓ and m. This follows from the m-fold differentiation of the Legendre equation with P_ℓ terms. It is convenient to extend the definition of associated Legendre functions to negative values of m. These are determined by the relation

$$P_\ell^{-m}(x) = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x), \tag{C.91}$$

in which m is considered positive and with this extended definition the parameter m must lie in the interval $-\ell \le m \le \ell$. Using Rodrigues' formula, the associated Legendre polynomial $P_\ell^m(x)$ can be expressed in the form

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!}(1-x^2)^{m/2}\frac{\mathrm{d}^{\ell+m}}{\mathrm{d}x^{\ell+m}}(x^2-1)^\ell. \tag{C.92}$$

From the defining equation (C.89) we can easily form the first few associated Legendre polynomials (we omit the cases with upper zero index, because they form the "classical" Legendre polynomials mentioned above),

$$P_1^1 = \left(1-x^2\right)^{1/2}, \tag{C.93}$$
$$P_2^1 = 3x\left(1-x^2\right)^{1/2}, \tag{C.94}$$
$$P_2^2 = 3\left(1-x^2\right), \tag{C.95}$$
$$P_3^1 = \frac{3}{2}\left(5x^2-1\right)\left(1-x^2\right)^{1/2}, \tag{C.96}$$
$$P_3^2 = 15x\left(1-x^2\right), \tag{C.97}$$
$$P_3^3 = 15\left(1-x^2\right)^{3/2}, \tag{C.98}$$
$$P_4^1 = \frac{5}{2}\left(7x^3-3x\right)\left(1-x2\right)^{1/2}, \tag{C.99}$$
$$P_4^2 = \frac{15}{2}\left(7x^2-1\right)\left(1-x2\right), \tag{C.100}$$
$$P_4^3 = 105x\left(1-x^2\right)^{3/2}, \tag{C.101}$$
$$P_4^4 = 105\left(1-x^2\right)^2. \tag{C.102}$$

Like the classical Legendre polynomials, the associated Legendre polynomials form a series of orthogonal functions on the interval $\langle -1, 1\rangle$ (analogous to Eq. (C.83)),

$$\int_1^{-1} P_\ell^m(x)P_{\ell'}^m(x)\,\mathrm{d}x = 0 \tag{C.103}$$

if $\ell \neq \ell'$. This statement would not hold if the integrand were replaced by $P_\ell^m, P_{\ell'}^{m'}$ with $m \neq m'$. The proof of Eq. (C.103) proceeds in exactly the same way as the proof of orthogonality of the "classical" Legendre polynomials. We will not repeat it here, except to note that the proof begins with Eq. (C.90) multiplied by $P_{\ell'}^m$, which is subtracted from the second copied equation, in which ℓ is replaced by ℓ'. Since m is the same in both copied equations, the terms involving $m^2/(1-x^2)$ cancel after subtraction and the proof proceeds in the same way as in Sect. C.3.3.

We define the norm of the associated Legendre polynomials by putting $\ell' = \ell$ in the integrand. Later we will show that it is given by

$$N_\ell^m = \int_{-1}^{1} \left[P_\ell^m(x)\right]^2 \,\mathrm{d}x = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}. \tag{C.104}$$

The norm obviously reduces to Eq. (C.88) if $m=0$. Equations (C.103) and (C.104) can be combined into a single expression

$$\int_{-1}^{1} P_\ell^m(x) P_{\ell'}^m(x)\,\mathrm{d}x = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\ell'}. \tag{C.105}$$

To derive Eq. (C.90) it will be useful to introduce an auxiliary function

$$U_\ell^m(x) = \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_\ell(x), \tag{C.106}$$

where $m \geq 0$, so we can write $U_\ell^0 \equiv P_\ell$ and write Eq. (C.90) using U_ℓ^0 instead of P_ℓ^m with $m=0$ in the whole equation. By differentiating Eq. (C.90) written in this way, we get

$$\left(1-x^2\right)\frac{\mathrm{d}^2 U_\ell^m}{\mathrm{d}x^2} - 2\,(m+1)\,x\frac{\mathrm{d}U_\ell^m}{\mathrm{d}x} + \left[\ell\,(\ell+1) - m\,(m+1)\right] U_\ell^m = 0. \tag{C.107}$$

To derive Eq. (C.104), we start from Eq. (C.107), which we write in an alternative form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^{m+1} U_\ell^{m+1}\right] + (\ell+m+1)\,(\ell-m)\left(1-x^2\right)^m U_\ell^m = 0. \tag{C.108}$$

In doing so, we transform $m \to m-1$ and get

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^m U_\ell^m\right] = -\,(\ell-m+1)\,(\ell+m)\left(1-x^2\right)^{m-1} U_\ell^{m-1} = 0. \tag{C.109}$$

Equation (C.104) involves $[P_\ell^m]^2 = (1-x^2)^m\,[U_\ell^m]^2$, which we write as

$$\begin{aligned}
\left[P_\ell^m\right]^2 &= \left(1-x^2\right)^m U_\ell^m \frac{\mathrm{d}U_\ell^{m-1}}{\mathrm{d}x} = \\
&= \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^m U_\ell^m U_\ell^{m-1}\right] - U_\ell^{m-1}\frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^m U_\ell^m\right] = \\
&= \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^m U_\ell^m U_\ell^{m-1}\right] + (\ell+m)\,(\ell-m+1)\left(1-x^2\right)^{m-1}\left[U_\ell^{m-1}\right]^2 = \\
&= \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1-x^2\right)^{1/2} P_\ell^m P_\ell^{m-1}\right] + (\ell+m)\,(\ell-m+1)\left[P_\ell^{m-1}\right]^2,
\end{aligned} \tag{C.110}$$

where in the last step we referred to the equation (C.106). Integrating it from $x=-1$ to $x=1$, we see that the limits in the originally derived term disappear, leaving the value

$$N_\ell^m = (\ell+m)(\ell-m+1)N^{m-1}\ell. \tag{C.111}$$

The equation (C.111) is a recurrence relation for the norm of the associated Legendre polynomials.

In many applied solutions, the associated Legendre polynomials are expressed in terms of the cosine of the angle θ instead of the original variable x, i.e. $x = \cos\theta$, $(1-x^2)^{1/2} = \sin\theta$, the polynomials are now written $P_\ell^m(\cos\theta)$ and the interval $\langle -1, 1\rangle$ becomes $-\langle 0, \pi\rangle$. After applying the "chain rule" to change the variable in the derivatives, the differential equation (C.90) goes to

$$\frac{\mathrm{d}^2 P_\ell^m}{\mathrm{d}\theta^2} + \operatorname{cotg}\theta \frac{\mathrm{d}P_\ell^m}{\mathrm{d}\theta} + \left[\ell\,(\ell+1) - \frac{m^2}{\sin^2\theta}\right] P_\ell^m = 0, \tag{C.112}$$

where the first two terms form the polar angle part of the Laplacian on a spherical surface with unit radius (cf. Eq. (B.72)). It is more convenient to write this part in compact form, so that Eq. (C.112) will have the form $\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta \frac{\mathrm{d}P_\ell^m}{\mathrm{d}\theta}\right) + \left[\ell\,(\ell+1) - \frac{m^2}{\sin^2\theta}\right] P_\ell^m = 0$, which we will use with advantage in the spherical Laplacian of spherical functions in paragraph C.4.2.

C.3.5 Multipole expansion

We now consider the electrostatic potential ϕ created by an arbitrary charge distribution associated with the electric field according to the relation $\boldsymbol{E} = -\boldsymbol{\nabla}\phi$. The electrostatic potential is given by

$$\phi\,(\boldsymbol{r}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho\,(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|}\,\mathrm{d}V', \tag{C.113}$$

where $\boldsymbol{r}$ denotes the position vector of the location at which the potential is "measured", ρ is the charge density as a function of the position $\boldsymbol{r'}$ within the space where the charges occur (the charge distribution region), and $\mathrm{d}V' = \mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}z'$ is the volume element associated with the variables contained in the charge distribution region defined by the vector $\boldsymbol{r'}$.

To simplify the notation, we introduce the following notation: $r = |\boldsymbol{r}|$, $r' = |\boldsymbol{r'}|$ and introduce unit vectors $\boldsymbol{n} = \boldsymbol{r}/r$ and $\boldsymbol{n'} = \boldsymbol{r'}/r'$. Let us denote the deviation of the vectors $\boldsymbol{r}$ and $\boldsymbol{r'}$ (the angle between them) by γ and $\boldsymbol{n}\cdot\boldsymbol{n'} = \cos\gamma$. We will further assume that r' is everywhere less than r, so ϕ is "measured" outside the charge distribution region. The quantity $|\boldsymbol{r}-\boldsymbol{r'}|$ in the integral of (C.113) is the distance between the points defined by the vectors $\boldsymbol{r}$ and $\boldsymbol{r'}$. The square of this distance is

$$\begin{aligned}\left|\boldsymbol{r}-\boldsymbol{r'}\right|^2 = \boldsymbol{r}\cdot\boldsymbol{r} - 2\boldsymbol{r}\cdot\boldsymbol{r'} + \boldsymbol{r'}\cdot\boldsymbol{r'} = r^2 - 2rr'\cos\gamma + r'^2 = \\ = r^2\left[1 - 2\cos\gamma\left(\frac{r'}{r}\right) + \left(\frac{r'}{r}\right)^2\right],\end{aligned} \tag{C.114}$$

so this function can be expressed as

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r'}|} = \frac{1}{r}\left[1 - 2\cos\gamma\left(\frac{r'}{r}\right) + \left(\frac{r'}{r}\right)^2\right]^{-1/2}. \tag{C.115}$$

We can formulate this expression using Legendre polynomials. If we compare it with Eq. (C.48), which gives the generic function $\Phi(x,h)$, we see a clear connection. If we denote $x = \cos\gamma$ and $h = r'/r$, then

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r'}|} = \frac{1}{r}\,\Phi(x,h). \tag{C.116}$$

By including Eq. (C.50), defining Legendre polynomials, we get the identity

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{1}{r}\sum_{\ell=0}^{\infty} P_\ell\left(\cos\gamma\right)\left(\frac{r'}{r}\right)^\ell = \sum_{\ell=0}^{\infty}\frac{r'^\ell}{r^{\ell+1}}P_\ell\left(\cos\gamma\right), \tag{C.117}$$

where now instead of x and h we write directly $\cos\gamma$ and r'/r.

The electrostatic potential can then be expressed by substituting Eq. (C.117) into Eq. (C.113).

$$\begin{aligned}\phi\left(\boldsymbol{r}\right) &= \frac{1}{4\pi\epsilon_0}\int\rho\left(\boldsymbol{r}'\right)\left[\sum_{\ell=0}^{\infty}\frac{r'^\ell}{r^{\ell+1}}P_\ell\left(\cos\gamma\right)\right]\mathrm{d}V' = \\ &= \frac{1}{4\pi\epsilon_0}\sum_{\ell=0}^{\infty}\frac{1}{r^{\ell+1}}\int\rho\left(\boldsymbol{r}'\right)r'^\ell P_\ell\left(\cos\gamma\right)\,\mathrm{d}V',\end{aligned} \tag{C.118}$$

If we further define the resulting electrostatic potential ϕ as the infinite sum of all partial potentials ϕ_ℓ,

$$\phi = \sum_{\ell=0}^{\infty}\phi_\ell, \tag{C.119}$$

we write these partial potentials, contained in the relation (C.118) again as

$$\phi_\ell\left(\boldsymbol{r}\right) = \frac{1}{4\pi\epsilon_0}\frac{1}{r^{\ell+1}}\int\rho\left(\boldsymbol{r}'\right)r'^\ell P_\ell\left(\cos\gamma\right)\,\mathrm{d}V'. \tag{C.120}$$

Equation (C.119) is the so-called multipole expansion of the electrostatic potential ϕ and each term ϕ_ℓ in the infinite sum is the electrostatic potential of a particular polarity. A term with $\ell = 0$ is called a monopole term, a term with $\ell = 1$ is a dipole term, a quadrupole term corresponds to $\ell = 2$, an octupole term to $\ell = 3$, etc.

Let's now look at the monopole term in Eq. (C.119). If $\ell = 0$ in Eq. (C.120) (recall that $P_0(\cos\gamma) = 1$), we get

$$V_0 = \frac{1}{4\pi\epsilon_0}\frac{1}{r}\int\rho\left(\boldsymbol{r}'\right)\,\mathrm{d}V', \tag{C.121}$$

where the integral expresses the total charge q. It is therefore the potential of a single point charge q (monopole) located at the origin of the coordinate system. Moving to the dipole term, we put $\ell = 1$ in Eq. (C.120) (recall that $P_1(\cos\gamma) = \cos\gamma$), and we get

$$\phi_1 = \frac{1}{4\pi\epsilon_0}\frac{1}{r^2}\int\rho\left(\boldsymbol{r}'\right)r'\cos\gamma\,\mathrm{d}V', \tag{C.122}$$

If we write $r'\cos\gamma = r'\left(\boldsymbol{n}'\cdot\boldsymbol{n}\right) = \boldsymbol{r}'\cdot\boldsymbol{n}$ and the unit vector $\boldsymbol{n}$ we extract from the integral because it does not depend on the variables contained in the space $\boldsymbol{r}'$, we get

$$\phi_1 = \frac{1}{4\pi\epsilon_0}\frac{1}{r^2}\boldsymbol{n}\cdot\int\rho\left(\boldsymbol{r}'\right)\boldsymbol{r}'\,\mathrm{d}V' = \frac{1}{4\pi\epsilon_0}\frac{\boldsymbol{n}\cdot\boldsymbol{p}}{r^2}, \tag{C.123}$$

where vector $\boldsymbol{p} = \int\rho\left(\boldsymbol{r}'\right)\boldsymbol{r}'\,\mathrm{d}V'$ is the so-called *dipole moment* of the charge distribution, which is given by the product of the positive charge with the position vector relative to the negative charge, in the direction from the negative to the positive charge. Since Eq. (C.123) holds for any charge distribution, the vector $\boldsymbol{p}$ is calculated using an integral.

Let us consider the example of a quadrupole term. Put $\ell = 2$ in Eq. (C.120), so $P_2(\cos\gamma) = \frac{1}{2}(3\cos^2\gamma - 1)$ and we get

$$\phi_2 = \frac{1}{4\pi\epsilon_0}\frac{1}{r^3}\frac{1}{2}\int \rho\, r'^2 \left(3\cos^2\gamma - 1\right)\, \mathrm{d}V'. \tag{C.124}$$

The spatial factor in the integrand of Eq. (C.124) can be rewritten using unit vectors n as

$$r'^2\left[3\left(\boldsymbol{n'}\cdot\boldsymbol{n}\right)^2 - 1\right] = 3\left(\boldsymbol{r'}\cdot\boldsymbol{n}\right)^2 - r'^2 \tag{C.125}$$

and to create the simplest form of the integral, we introduce indexing of the components of the vectors using the notation n_j and r'_j for the vectors $\boldsymbol{n}$ and $\boldsymbol{r'}$ (recall that $n_1 = x/r$, $n_2 = y/r$ and $n_3 = z/r$, while for example $r'_1 = x', r'_2 = y'$ and $r'_3 = z'$). We write $\boldsymbol{n}\cdot\boldsymbol{r'} = \sum_j n_j r'_j$, so

$$\left(\boldsymbol{r'}\cdot\boldsymbol{n}\right)^2 = \left(\sum_{j=1}^{3} n_j r'_j\right)\left(\sum_{k=1}^{3} n_k r'_k\right) = \sum_{j=1}^{3}\sum_{k=1}^{3} n_j n_k r'_j r'_k \tag{C.126}$$

we can then write

$$r'^2 = \boldsymbol{r'}\cdot\boldsymbol{r'} = \sum_{j=1}^{3} r'_j r'_j = \sum_{j=1}^{3}\sum_{k=1}^{3}\delta_{jk} r'_j r'_k, \tag{C.127}$$

so the two terms on the right hand side of Eq. (C.125) can be expressed as a double sum,

$$3\left(\boldsymbol{r'}\cdot\boldsymbol{n}\right)^2 - r'^2 = \sum_{j=1}^{3}\sum_{k=1}^{3}\left(3n_j n_k - \delta_{jk}\right) r'_j r'_k, \tag{C.128}$$

and by substituting into the integral (C.124) we obtain its right-hand side in the form

$$\int \rho\, r'^2\left(3\cos^2\gamma - 1\right) dV' = \sum_{j=1}^{3}\sum_{k=1}^{3}\left(3n_j n_k - \delta_{jk}\right)\int \rho\, r'_j r'_k\, \mathrm{d}V'. \tag{C.129}$$

The quadrupole term of the electrostatic potential can therefore be expressed as

$$\phi_2 = \frac{1}{4\pi\epsilon_0}\frac{1}{r^3}\frac{1}{2}\sum_{j=1}^{3}\sum_{k=1}^{3}\left(3n_j n_k - \delta_{jk}\right) Q_{jk}, \qquad \text{kde} \qquad Q_{jk} = \int \rho\left(\boldsymbol{r'}\right) r'_j r'_k\, \mathrm{d}V'. \tag{C.130}$$

The quantities Q_{jk} in Eq. (C.130) form a tensor and are collectively referred to as the quadrupole moment of the charge distribution.

The multipole expansion, expressed by Eq. (C.119), shows that the potential outside the charge distribution region is the sum of a monopole term, a dipole term, a quadrupole term, an octupole term, etc. To each term ϕ_ℓ we can assign a physical multipole; that is, the overall charge distribution can be represented as a superposition of multipoles. This is not only an important result, but also a practical tool in calculations: note in Eq. (C.120) that the ℓ-pole term in the multipole expansion of the potential is associated with the factor $1/r^{\ell+1}$. Thus, schematically, the expansion has the form

$$\phi = \frac{\text{monopole}}{r} + \frac{\text{dipole}}{r^2} + \frac{\text{qudrupole}}{r^3} + \frac{\text{octupole}}{r^4} + \dots. \tag{C.131}$$

For a completely accurate expression of the potential ϕ we need an infinite number of terms in the multipole expansion (as, for example, in the Taylor expansion and many other similar cases). However, if the distance r is large enough, we can be satisfied with an approximation using only a finite number of terms. Such an approximate potential is computationally much less expensive and the essential details of the charge distribution can be adequately described by a finite number of multipole moments. At the coarsest level, the potential can be approximated by a monopole$/r$ and the only expression of the charge distribution that this description needs is the total charge q, i.e. a single number. For a better approximation, we will also include a dipole$/r^2$ and to express the essential features of the charge distribution, we will also need three components of the dipole moment vector $\boldsymbol{p}$. A suitable approximation may require the inclusion of several additional terms, but the main point is as follows: in any multipole expansion with a finite number of terms, the relevant characteristics of the charge distribution are completely described by a finite number of quantities included in the relevant multipole moments.

C.3.6 Legendre functions

As already mentioned in the paragraph C.3.3, the standard (textbook) description of Legendre polynomials often begins with the Legendre differential equation (C.81) (now rewritten as a function of the dependent variable y),

$$\left(1-x^2\right) y'' - 2xy' + \ell\left(\ell+1\right) y = 0 \tag{C.132}$$

and the polynomial $P_\ell(x)$ is then derived as a solution to this equation. This procedure is analogous to the case where we would define the function $\sin x$ as a solution to the differential equation $y'' + y = 0$. However, this equation also admits a second solution, $y = \cos x$, so let us assume that Eq. (C.81) will also have a second solution, since second-order differential equations generally admit two independent solutions. For each integer ℓ, Eq. (C.81) does indeed admit a second solution $Q_\ell(x)$, called the Legendre function of the second kind. However, these new solutions are not polynomials, the first few are given by the relations

$$Q_0 = \frac{1}{2}\ln\frac{1+x}{1-x}, \tag{C.133}$$

$$Q_1 = \frac{1}{2}x\ln\frac{1+x}{1-x}, \tag{C.134}$$

$$Q_2 = \frac{1}{4}\left(3x^2-1\right)\ln\frac{1+x}{1-x} - \frac{3}{2}x, \tag{C.135}$$

which contain logarithms, so unlike the polynomials $P_\ell(x)$, which are finite everywhere on the interval $\langle -1, 1\rangle$, all functions $Q_\ell(x)$ are singular at the points $x = 1$ and $x = -1$. This is the main difference between the two classes of solutions of Eq. (C.81).

The differential equation (C.81) can be generalized if $\ell \neq \mathbb{Z}$ is not an integer. In this case, we would write it as

$$\left(1-x^2\right) y'' - 2xy' + \lambda\left(\lambda+1\right) y = 0, \tag{C.136}$$

where $\lambda \in \mathbb{R}$ and the symbol ℓ are reserved for integers. Like any other second-order differential equation, this equation has two independent solutions. The first is denoted $P_\lambda(x)$ and is known as the Legendre function of the first kind. The second solution is denoted $Q_\lambda(x)$, i.e. the Legendre function of the second kind. In general, the functions $P_\lambda(x)$ are finite at $x = 1$, but diverge at $x = -1$ if $\lambda\ \not{\mathbb{Z}}$. The functions $Q_\lambda(x)$ are singular at $x = \pm 1$.

This generalized view of the Legendre equation shows that Eq. (C.81) admits solutions that are regular (do not diverge, i.e. do not contain one or more singularities) everywhere on the interval $\langle -1, 1\rangle$, namely Legendre polynomials. If we change the integer ℓ to a non-integer λ, the regularity of the solution does not hold.

C.3.7 Some other types of orthogonal polynomials

We will only present other orthogonal polynomials here in a brief overview.

- **Laguerre polynomials** $L_n^s(x)$, are used, for example, in quantum mechanics to describe the wave function corresponding to the states of the hydrogen atom. They are usually defined as a system of real polynomials, orthogonal in the case of the scalar product

$$\int_0^\infty P(x)P'(x)\, x^s \mathrm{e}^{-x}\,\mathrm{d}x, \tag{C.137}$$

where $s > -1$. Laguerre polynomials are the normalized solutions of *Laguerre equation*

$$xy'' + (\alpha - x)\, y' - \nu y = 0, \tag{C.138}$$

where $\alpha = s + 1$, $\nu = -n$ and where in general $\alpha, \nu \in \mathbb{C}$, $\alpha \neq 0$, $\alpha \neq \mathbb{Z}^-$ (i.e. $\alpha \neq 0, -1, -2, ...$), which is a homogeneous linear differential equation of the 2nd order. Equation (C.138) expresses the generalized (associated) form of Laguerre polynomials, when the so-called *classical Laguerre polynomials* $L_n(x)$ are the normalized solution of Eq. (C.138) for $s = 0$, i.e.

$$xy'' + (1 - x)\, y' + ny = 0. \tag{C.139}$$

The explicit expression of Laguerre polynomials, both general and classical, using Rodrigues' formula has the form

$$L_n^s(x) = \frac{1}{n!}\,\mathrm{e}^x x^{-s} \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\mathrm{e}^{-x} x^{s+n}\right), \qquad L_n(x) = \frac{\mathrm{e}^x}{n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\mathrm{e}^{-x} x^n\right). \tag{C.140}$$

The recursive relation for Laguerre polynomials has the form

$$xL_n^s(x) = -\left(n+1\right) L_{n+1}^s(x) + \left(s + 2n + 1\right) L_n^s(x) - \left(s + n\right) L_{n-1}^s(x), \tag{C.141}$$

while the norm of the Laguerre polynomials has the value

$$\|L_n^s\|^2 = \frac{\Gamma\left(s + n + 1\right)}{n!}. \tag{C.142}$$

Here are the first seven classical Laguerre polynomials:

$$L_0(x) = 1, \tag{C.143}$$
$$L_1(x) = -x + 1, \tag{C.144}$$
$$L_2(x) = \frac{1}{2}\left(x^2 - 4x + 2\right), \tag{C.145}$$
$$L_3(x) = \frac{1}{6}\left(-x^3 + 9x^2 - 18x + 6\right), \tag{C.146}$$
$$L_4(x) = \frac{1}{24}\left(x^4 - 16x^3 + 72x^2 - 96x + 24\right), \tag{C.147}$$
$$L_5(x) = \frac{1}{120}\left(-x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120\right), \tag{C.148}$$
$$L_6(x) = \frac{1}{720}\left(x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720\right). \tag{C.149}$$

- **Hermite polynomials**: There are several definitions of these polynomials, here we will only mention the so-called *physical Hermite polynomials* $H_n(x)$, which describe, for example, the quantum states of a harmonic oscillator, appear in numerical mathematics as the so-called Gauss quadrature rule, etc. They are the normalized solution of the equation

$$y'' - 2xy' + 2ny = 0. \tag{C.150}$$

The explicit expression of physical Hermite polynomials using Rodrigues' formula has the form

$$H_n(x) = (-1)^n \, \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(\mathrm{e}^{-x^2} \right). \tag{C.151}$$

The recursive relation for physical Hermite polynomials has the form

$$H_{n+1} - 2x \, H_n + 2n \, H_{n-1} = 0 \tag{C.152}$$

and the norm of physical Hermite polynomials has the value

$$\|H_n\|^2 = 2^n n! \sqrt{\pi}. \tag{C.153}$$

Here are the first seven physical Hermite polynomials:

$$H_0(x) = 1, \tag{C.154}$$
$$H_1(x) = 2x, \tag{C.155}$$
$$H_2(x) = 4x^2 - 2, \tag{C.156}$$
$$H_3(x) = 8x^3 - 12x, \tag{C.157}$$
$$H_4(x) = 16x^4 - 48x^2 + 12, \tag{C.158}$$
$$H_5(x) = 32x^5 - 160x^3 + 120x, \tag{C.159}$$
$$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120. \tag{C.160}$$

- **Chebyshev polynomials** (more precisely, the Chebyshev polynomials of the 1st type) $T_n(x)$ are the normalized solution of the generic equation

$$\left(1 - x^2\right) y'' - xy' + n^2 y = 0. \tag{C.161}$$

For interpolation by Chebyshev polynomials, any interval is linearly transformed (scaled) to the interval $\langle -1, 1 \rangle$. To each $t \in \langle a, b \rangle$ we assign the value $x \in \langle -1, 1 \rangle$ by the functional prescription

$$x = \frac{t - \frac{1}{2}\,(a+b)}{b-a}. \tag{C.162}$$

The explicit expression of Chebyshev polynomials using the Rodrigues formula has the form

$$T_n(x) = \cos\left(n \arccos x\right). \tag{C.163}$$

The recursive relation for Chebyshev polynomials has the form

$$T_{n+1} - 2x \, T_n + T_{n-1} = 0. \tag{C.164}$$

The norm of Chebyshev polynomials has the value

$$\|T_n\|^2 = \frac{\pi}{2} \text{ pro } n > 0, \quad \|T_n\|^2 = \pi \text{ pro } n = 0. \tag{C.165}$$

Here are the first five Chebyshev polynomials:

$$T_0(x) = 1, \tag{C.166}$$
$$T_1(x) = x, \tag{C.167}$$
$$T_2(x) = 2x^2 - 1, \tag{C.168}$$
$$T_3(x) = 4x^3 - 3x, \tag{C.169}$$
$$T_4(x) = 8x^4 - 8x^2 + 1. \tag{C.170}$$

Chebyshev polynomials are important, for example, in the theory of approximation of linear systems, etc.

There are a number of other orthogonal polynomial functions, for example Gegenbauer (ultraspherical) polynomials or other types of the already mentioned polynomials and the like, we will not discuss them here. I refer those interested to the relevant literature, for example Abramowitz & Stegun (1972).

C.4 Spherical harmonics

Spherical harmonics $Y_\ell^m(\theta, \phi)$ are functions of the polar angle $\theta \in (0, \pi)$ and the azimuthal angle $\phi \in (0, 2\pi)$ in spherical coordinates (r, θ, ϕ). The spherical functions are defined using the associated Legendre polynomials $P_\ell^m(\cos\theta)$, which depend only on the polar angle θ, multiplied by the complex function of the azimuthal angle ϕ, i.e. the exponential $\mathrm{e}^{\mathrm{i}m\phi} = \cos(m\phi) + \mathrm{i}\sin(m\phi)$. By introducing additional, yet "unjustified" numerical factors, we define the spherical function as

$$Y_\ell^m(\theta, \phi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi}, \tag{C.171}$$

where m is an integer in the interval $\langle -\ell, \ell \rangle$. The reason for introducing the square root will also be explained later. The factor $(-1)^m$ is given by convention and whether or not it is used depends on the author. The angles θ and ϕ determine the position of an arbitrary point on the surface of the sphere $r = \text{const.}$ and any functions θ and ϕ can therefore be considered as functions on the surface of the sphere. Spherical harmonics thus represent the set of functions on a spherical surface.

If $m = 0$, Eq. (C.171) becomes

$$Y_\ell^0 = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell^0(\cos\theta) \tag{C.172}$$

and we see that Y_ℓ^0 is a scaled version of the Legendre polynomials; these functions depend only on θ. We obtain spherical harmonics with negative m from those with positive ones by

$$Y_\ell^{-m} = (-1)^m (Y_\ell^m)^*, \tag{C.173}$$

with an asterisk denoting a complex conjugation. This property follows directly from Eq. (C.171) after we use the Eq. (C.91) and recall that $\mathrm{e}^{-\mathrm{i}m\phi} = (\mathrm{e}^{\mathrm{i}m\phi})^*$.

The first few spherical harmonics have the form

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \tag{C.174}$$

$$Y_1^0 = \frac{3}{\sqrt{4\pi}} \cos\theta, \tag{C.175}$$

$$Y_1^1 = -\frac{3}{\sqrt{8\pi}} \sin\theta\, \mathrm{e}^{\mathrm{i}\phi}, \tag{C.176}$$

$$Y_2^0 = \frac{5}{\sqrt{16\pi}}(3\cos^2\theta - 1), \tag{C.177}$$

$$Y_2^1 = -\frac{15}{\sqrt{8\pi}} \sin\theta\cos\theta\, \mathrm{e}^{\mathrm{i}\phi}, \tag{C.178}$$

$$Y_2^2 = \frac{15}{\sqrt{32\pi}} \sin^2\theta\, \mathrm{e}^{2\mathrm{i}\phi}, \tag{C.179}$$

$$Y_3^0 = \frac{7}{\sqrt{16\pi}}(5\cos^3\theta - 3\cos\theta), \tag{C.180}$$

$$Y_3^1 = -\frac{21}{\sqrt{64\pi}} \sin\theta \left(5\cos^2\theta - 1\right) \mathrm{e}^{\mathrm{i}\phi}, \tag{C.181}$$

$$Y_3^2 = \frac{105}{\sqrt{32\pi}} \sin^2\theta\cos\theta\, \mathrm{e}^{2\mathrm{i}\phi}, \tag{C.182}$$

$$Y_3^3 = -\frac{35}{\sqrt{64\pi}} \sin^3\theta\, \mathrm{e}^{3\mathrm{i}\phi}. \tag{C.183}$$

C.4.1 Orthonormality of spherical harmonics

In the paragraph C.3.4 we established that the functions P_ℓ^m and $P_{\ell'}^m$ are mutually orthogonal in the sense of Eq. (C.105),

$$\int_0^\pi P_\ell^m(\cos\theta) P_{\ell'}^m(\cos\theta)\sin\theta\,\mathrm{d}\theta = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\ell'}, \tag{C.184}$$

where we have simply replaced the variable x with the function $\cos\theta$ in the argument of the polynomial. As already mentioned, both functions must have the same value of m, for this statement to be valid. The functions $\mathrm{e}^{\mathrm{i}m\phi}$ and $\mathrm{e}^{\mathrm{i}m'\phi}$ are also orthogonal to each other in the sense of the scalar product, given by the equation

$$\int_0^{2\pi} (\mathrm{e}^{\mathrm{i}m\phi})^* \mathrm{e}^{\mathrm{i}m'\phi}\,\mathrm{d}\phi = 2\pi\delta_{mm'}. \tag{C.185}$$

Since the spherical harmonics are the result of the coupling of the associated Legendre polynomials with complex exponential functions of the azimuthal angle, we can consider the unification of both orthogonality statements. We can express this as

$$\int_0^{2\pi}\int_0^\pi \left[P_\ell^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}\right]^* \left[P_{\ell'}^{m'}(\cos\theta)\,\mathrm{e}^{\mathrm{i}m'\phi}\right]\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \frac{4\pi}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\ell'}\,\delta_{mm'}, \tag{C.186}$$

and we conclude that the double integral vanishes if $\ell' = \ell$ and $m' = m$. Both conditions must be satisfied; equality between m' and m is required by the integral ϕ and, if this first condition is satisfied, equality between ℓ' and ℓ is required by the integral θ. Note that it is not necessary to verify this condition for $m' \neq m$ in the integral θ, since the integral ϕ always vanishes under these circumstances.

The combined orthogonality statement (C.186) can be reexpressed in terms of spherical harmonics using the definition of Eq. (C.171). Since the double integral vanishes if $\ell' = \ell$ and $m' = m$, the numerical factor on the right-hand side of Eq. (C.186) can be written as

$$(-1)^m \sqrt{\frac{4\pi}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}} \cdot (-1)^{m'} \sqrt{\frac{4\pi}{2\ell'+1}\frac{(\ell'+m')!}{(\ell'-m')!}} \tag{C.187}$$

and transfer this expression to the left-hand side. The "alternating factor" $(-1)^{m+m'}$ is easy to deal with, because if $m' = m$, then we get $(-1)^{2m}$ and since $2m$ is always even, $(-1)^{2m} = 1$. The factor $(-1)^m$ and the first of the two square roots are then combined with $P_\ell^m(\cos\theta)\,\mathrm{e}^{im\phi}$ inside the integral on the left-hand side, giving the spherical harmonic $Y_\ell^m(\theta,\phi)$. Absorbing $(-1)^{m'}$ and the second of the two roots, we obtain $Y_{\ell'}^{m'}(\theta,\phi)$ in a similar way. We thus get

$$\int_0^{2\pi}\int_0^{\pi} \left[Y_\ell^m(\theta,\phi)\right]^* \left[Y_{\ell'}^{m'}(\theta,\phi)\right] \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi = \delta_{\ell\ell'}\delta_{mm'}, \tag{C.188}$$

which is an orthogonality statement for spherical functions. Since these functions depend on two variables, θ and ϕ, this is a two-dimensional form of orthogonality, defined in terms of the integral over the surface of the sphere. We emphasize that the integral approaches zero, except for $\ell' = \ell$ and $m' = m$. However, if both of these conditions are met, the integral is equal to

$$\int_0^{2\pi}\int_0^{\pi} \left|Y_\ell^m(\theta,\phi)\right|^2 \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi = 1, \tag{C.189}$$

in other words, the norm of spherical harmonics is equal to one. Alternatively, we can say that spherical harmonics are normalized functions of θ. and ϕ. This is why we inserted those "unjustified" factors into the definition of spherical harmonics in Eq. (C.171): we wanted to ensure that spherical harmonics were normalized.

C.4.2 Using spherical harmonics in solving differential equations

Since spherical harmonics are also functions of the azimuthal coordinate ϕ, Eq. (C.171) must satisfy the following identity for a fixed value of θ,

$$\frac{\partial^2 Y_\ell^m}{\partial\phi^2} = -m^2 Y_\ell^m. \tag{C.190}$$

If we insert the Eq. (C.190), or its equivalent representation using the associated Legendre polynomial, into Eq. (C.112), we can write m^2 as a partial derivative with respect to the azimuthal coordinate ϕ. We get

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial Y_\ell^m}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_\ell^m}{\partial\phi^2} + \ell\,(\ell+1)\,Y_\ell^m = 0. \tag{C.191}$$

This is a second-order partial differential equation for spherical harmonics.

The significance of this equation lies in the fact that it is closely related to the Laplacian in spherical coordinates, see Eq. (B.72) in the Appendix B.3. For a simpler explanation, we will present this spherical Laplacian $\nabla^2 f$ in its general form again,

$$\nabla^2 f = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial f}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}\right] \tag{C.192}$$

and we immediately see the agreement between the last two terms in Eq. (C.192) and the first two terms in Eq. (C.191). This agreement is not random and is in fact the main reason for the introduction and use of spherical harmonics.

Appendix D

Brief introduction to partial differential equations ★

Unlike ordinary differential equations (ODEs - see Chapter 3), partial differential equations (PDEs) contain partial derivatives according to several variables. These are, for example, first-order evolutionary (transport) equations (e.g., the so-called *Burgers'* equation) that are one-way in time and usually converge to a steady state. Second-order equations describe thermodynamic processes, i.e., the so-called *parabolic* partial differential equations, periodic processes (wave equation) - the so-called *hyperbolic* partial differential equations, or the so-called *elliptical* partial differential equations (Poisson equation, Laplace equation), etc. The classification of partial differential equations into individual types is important also from the practical point of view because each of them is usually solved differently.

D.1 First-order partial differential equations

D.1.1 Homogeneous first-order partial differential equations

The simplest partial differential equations are linear homogeneous first-order equations of two independent variables x, y; therefore, only the first-order (partial) derivatives occur in a linear expression

$$a(x,y)\frac{\partial u(x,y)}{\partial x} + b(x,y)\frac{\partial u(x,y)}{\partial y} = 0. \tag{D.1}$$

The solution to such an equation will be a function $u(x, y)$. The function of two variables, represented by a surface, can be characterized by contour lines $x = x(s)$, $y = y(s)$, where s is a parameter. The function $u\big[x(s), y(s)\big]$ is thus constant on contour lines, it can be considered as a function of a single variable (parameter s),

$$\frac{\mathrm{d}u\big[x(s), y(s)\big]}{\mathrm{d}s} = \frac{\partial u}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial u}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s} = 0, \tag{D.2}$$

where we search a solution of a system of ordinary differential equations (the so-called *characteristic system*)

$$\frac{\mathrm{d}x}{\mathrm{d}s} = a(x,y),\ \frac{\mathrm{d}y}{\mathrm{d}s} = b(x,y), \tag{D.3}$$

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

which we refer to as the *characteristics* (or also the 1st integral). A general equation of characteristics is then defined as $\varphi(x, y) = C$ and a general solution of an equation of two variables can be written as $u(x, y) = \Phi\big[\varphi(x, y)\big]$, where the function Φ can be considered as a function of a single variable φ. In the case of an equation of n independent variables, the general solution will take the form

$$u(x_1, \ldots, x_n) = \Phi\big[\varphi_1(x_1, \ldots, x_n), \ldots, \varphi_{n-1}(x_1, \ldots, x_n)\big]. \tag{D.4}$$

- **Solved examples of first-order linear homogeneous partial differential equations:**

1. Let us have a simple homogeneous equation of two independent variables,

$$x^2 \frac{\partial u}{\partial x} + y^2 \frac{\partial u}{\partial y} = 0. \tag{D.5}$$

The characteristic system thus will be $\mathrm{d}x/\mathrm{d}s = x^2$, $\mathrm{d}y/\mathrm{d}s = y^2$; its solution will be characteristics $-1/x = s + C_1$, $-1/y = s + C_2$, and excluding the parameter s, we get $1/y - 1/x = C = \varphi(x, y)$. The resulting general solution will therefore be

$$u(x, y) = \Phi\left(\frac{1}{y} - \frac{1}{x}\right). \tag{D.6}$$

2. Another simple example may be, for example, the homogeneous equations

$$\frac{\partial u}{\partial x} = 6x^2 \frac{\partial u}{\partial y} \tag{D.7}$$

whose characteristic system will be $\mathrm{d}x/\mathrm{d}s = 1$, $\mathrm{d}y/\mathrm{d}s = -6x^2$, where the solution of the first equation of the system will be the characteristic $x = s+C_1$. Since $\mathrm{d}y = -6\,(s+C_1)^2\mathrm{d}s$, the second characteristic will be $y = -2s^3 - 6s^2\,C_1 - 6s\,C_1^2 + C_2$. If we express from the first characteristic $s = x - C_1$ and substitute this expression into the second characteristic, we get the equation $y + 2x^3 = 2\,C_1^3 + C_2 = C = \varphi(x, y)$. Therefore, the resulting general solution will be

$$u(x, y) = \Phi\big(y + 2x^3\big). \tag{D.8}$$

However, this result can be reached much faster if one realizes that in case of a homogeneous equation, we obtain the ordinary first-order differential equation by dividing the equations of the characteristic system, i.e., $(\mathrm{d}y/\mathrm{d}s)/(\mathrm{d}x/\mathrm{d}s) = \mathrm{d}y/\mathrm{d}x = -6x^2$, and so $y = -2x^3 + C$.

3. Assume a homogeneous equation of three variables x, y, z,

$$(z - y)\frac{\partial u}{\partial x} + (x - z)\frac{\partial u}{\partial y} + (y - x)\frac{\partial u}{\partial z} = 0, \tag{D.9}$$

with the boundary condition $u(0, y, z) = yz$. The characteristic system will be $\mathrm{d}x/\mathrm{d}s = (z - y)$, $\mathrm{d}y/\mathrm{d}s = (x - z)$, $\mathrm{d}z/\mathrm{d}s = (y - x)$ in this case; after its summing, we get $\mathrm{d}x/\mathrm{d}s + \mathrm{d}y/\mathrm{d}s + \mathrm{d}z/\mathrm{d}s = 0$, and after integration with respect to s, we get $x + y + z = C_1$. Since the given equation contains three variables, we need one more general equation of characteristics, for example, by multiplying each characteristic by the corresponding variable, we get the expressions $x\,\mathrm{d}x/\mathrm{d}s = (z-y)x$, $y\,\mathrm{d}y/\mathrm{d}s = (x-z)y$, $z\,\mathrm{d}z/\mathrm{d}s = (y-x)z$.

After its summing (again with zero-sum), integration according to s, and multiplication by two (where $x' = \mathrm{d}x/\mathrm{d}s$, etc.), we get $2xx' + 2yy' + 2zz' = 0$, and so $x^2 + y^2 + z^2 = C_2$. Thus, the general solution will be

$$u(x, y, z) = \Phi\big(x + y + z, x^2 + y^2 + z^2\big). \tag{D.10}$$

After substituting the boundary condition, we get $\Phi\big(y + z, y^2 + z^2\big) = yz$, denoting $y + z = \xi$, $y^2 + z^2 = \eta$, we can write $\Phi\big(\xi, \eta\big) = (\xi^2 - \eta)/2$. The explicit solution of the boundary problem will be the function

$$u(x, y, z) = \frac{(x + y + z)^2 - (x^2 + y^2 + z^2)}{2} = xy + xz + yz. \tag{D.11}$$

• **Nonlinear homogeneous partial differential equation - non-viscous *Burgers'* equation:**

It is a nonlinear equation (also called *transport* equation) of a function $u(t, x)$ of two independent variables t, x (where, in the spatial term, this function is a multiple, i.e. of the second power), which describes the nonlinear progressive wave. In a one-dimensional case, it has the form

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0. \tag{D.12}$$

Characteristic equations, following from Equation (D.12), will be

$$\frac{\mathrm{d}t}{\mathrm{d}s} = 1,\ \frac{\mathrm{d}x}{\mathrm{d}s} = u,\ \text{and also}\ \frac{\mathrm{d}u}{\mathrm{d}t} = 0. \tag{D.13}$$

From the first equation we get $t = s$, so that we can choose t directly as a parameter. The third equation says that u is constant along the characteristics; from the second equation, it follows that the characteristics will be straight lines in the x, t plane. Solving the second and third characteristic equations is simple:

$$x = ut + C_1,\ u = C_2. \tag{D.14}$$

Considering that C_2 must be a function of C_1, that is, $C_2 = C_2(C_1)$, substituting $x - ut$ for C_1, we get a general solution of the partial differential equation:

$$u(x, t) = C_2(x - ut) = \Phi(x - ut). \tag{D.15}$$

To uniquely determine the general function Φ, we adopt an initial (boundary) condition $u(x, 0) = x$, for example. Then we can write $u(x, 0) = C_2\big[x - u(x, 0) \cdot 0\big] = x$ and thus $C_2(x) = x$. We get the equation $u = x - ut$, and the resulting unambiguous solution will be

$$u(x, t) = \frac{x}{1 + t} \tag{D.16}$$

in this case.

D.1.2 Inhomogeneous first-order partial differential equations

Inhomogeneous partial differential equations of the first-order of two independent variables can generally be written in the form

$$a(x, y)\frac{\partial u(x, y)}{\partial x} + b(x, y)\frac{\partial u(x, y)}{\partial y} = f(x, y). \tag{D.17}$$

Similar to the homogeneous equation, we can write

$$\frac{\mathrm{d}u\big[x(s),y(s)\big]}{\mathrm{d}s} = \frac{\partial u}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial u}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s} = f(x,y), \tag{D.18}$$

where we then search for a solution of the system of characteristic equations

$$\frac{\mathrm{d}x}{\mathrm{d}s} = a(x,y),\ \frac{\mathrm{d}y}{\mathrm{d}s} = b(x,y),\ \frac{\mathrm{d}u}{\mathrm{d}s} = f(x,y). \tag{D.19}$$

- **Solved examples of linear inhomogeneous partial differential equations:**

1. Consider a simple inhomogeneous partial differential equation of two independent variables

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = x \text{ with the boundary condition } u(x,a) = 1, \tag{D.20}$$

where a is a constant. From the system of Equations (D.19) follows the characteristic system $\mathrm{d}x/\mathrm{d}s = 1$, $\mathrm{d}y/\mathrm{d}s = 1$, $\mathrm{d}u/\mathrm{d}s = x$. By dividing the first two characteristic equations and, for example, the third and the first, we get the characteristics $C_1 = y - x$, $C_2 = u - x^2/2$. Thus we get a general solution of the partial differential equation in the form

$$\Phi(y-x, u-x^2/2) = 0, \tag{D.21}$$

where Φ is an arbitrary function of the characteristics. We will now rewrite the equation using the boundary condition as a function of the characteristics and constants, i.e., $\Phi(a-x, 1-x^2/2) = \Phi(C_1, C_2) = 0$. Then the first characteristic results in $x = a - C_1$, and from the second characteristic, we get $C_2 = 1 - (a-C_1)^2/2$. The last expression can be rewritten as $1 - (a-C_1)^2/2 - C_2 = \Phi(C_1, C_2) = 0$; after substituting this into the characteristics, we get the explicit expression $1 - \big[a^2 - 2a(y-x) + (y-x)^2\big]/2 - u + x^2/2 = 0$. The resulting solution of the boundary value problem for the given equation will then be

$$u(x,y) = xy + a(y-x) - \frac{y^2+a^2}{2} + 1. \tag{D.22}$$

2. Inhomogeneous partial differential equation of two independent variables has the form

$$y\frac{\partial u}{\partial x} - x\frac{\partial u}{\partial y} = y^2 - x^2, \text{ with the boundary condition } u(x,a) = x^2 - a^2, \tag{D.23}$$

where a is a constant. From the system of equations (D.19) follows the characteristic system $\mathrm{d}x/\mathrm{d}s = y$, $\mathrm{d}y/\mathrm{d}s = -x$, $\mathrm{d}u/\mathrm{d}s = y^2 - x^2$. Note that $y\,\mathrm{d}x/\mathrm{d}s + x\,\mathrm{d}y/\mathrm{d}s = \mathrm{d}u/\mathrm{d}s$ holds in this case. Equation $\mathrm{d}y/\mathrm{d}x = -x/y$, its integration gives first characteristic $x^2 + y^2 = C_1$. Equation $y\,\mathrm{d}x/\mathrm{d}s + x\,\mathrm{d}y/\mathrm{d}s = \mathrm{d}u/\mathrm{d}s$ can be written as $\mathrm{d}(xy)/\mathrm{d}s = \mathrm{d}u/\mathrm{d}s$. We get the second characteristic $u - xy = C_2$ after its integration. General solution of the partial differential equation will be:

$$\Phi(x^2+y^2, u-xy) = 0, \tag{D.24}$$

where Φ is an arbitrary function of the characteristics. We will now rewrite the equation again using the boundary condition as a function of the characteristics and constants, i.e., $\Phi(x^2+a^2, x^2-a^2-ax) = \Phi(C_1, C_2) = 0$. The first characteristic results in $x = \pm\sqrt{C_1 - a^2}$, the second characteristic results in the equation for both characteristics in the form $C_1 - 2a^2 \mp a\sqrt{C_1 - a^2} - C_2 = 0$. After substituting the original expressions into the characteristics, we get the explicit expression $x^2+y^2-2a^2 \mp a\big(\pm\sqrt{x^2+y^2-a^2}\big) - u + xy = 0$. Resulting solution of the boundary value problem for the given equation will be

$$u(x,y) = x^2 + y^2 + xy - a\sqrt{x^2+y^2-a^2} - 2a^2. \tag{D.25}$$

- **Solved examples of nonlinear inhomogeneous partial differential equations:**

1. An inhomogeneous nonlinear partial differential equation of two independent variables has the form

$$xu\frac{\partial u}{\partial x} + yu\frac{\partial u}{\partial y} = -xy, \text{ with the boundary value } u\left(x, \frac{a^2}{x}\right) = h, \tag{D.26}$$

where a, h are constants. From the system of equations (D.19) follows the characteristic system $\mathrm{d}x/\mathrm{d}s = xu$, $\mathrm{d}y/\mathrm{d}s = yu$, $\mathrm{d}u/\mathrm{d}s = -xy$. Integration of the equation $\mathrm{d}y/\mathrm{d}x = y/x$ gives the first characteristic, $y/x = C_1$. Note that $y\,\mathrm{d}x/\mathrm{d}s + x\,\mathrm{d}y/\mathrm{d}s = 2\,uxy$ holds in this case; thus, we can write this equation as $\mathrm{d}(xy)/\mathrm{d}s = -2u\,\mathrm{d}u/\mathrm{d}s = -\mathrm{d}u^2/\mathrm{d}s$, and after its integration, we get the second characteristic $u^2 + xy = C_2$. The general solution of the partial differential equation will be

$$\Phi\left(\frac{y}{x}, u^2 + xy\right) = 0, \tag{D.27}$$

where Φ is an arbitrary function of the characteristics. We will now rewrite the equation again using the boundary condition as a function of the characteristics and constants, i.e., $\Phi(a^2/x^2, h^2+a^2) = \Phi(C_1, C_2) = 0$. The first characteristic results in $x = \pm\sqrt{a^2/C_1}$, the second characteristic results in the equation for both characteristics, $h^2 + a^2 - C_2 = 0$. After substituting the original expressions into the characteristics, we get the explicit expression $h^2 + a^2 - u^2 - xy = 0$. The resulting solution of the boundary value problem for the given equation will be

$$u(x,y) = \sqrt{h^2 + a^2 - xy}. \tag{D.28}$$

2. An inhomogeneous nonlinear partial differential equation of two independent variables has the form

$$yu\frac{\partial u}{\partial x} - xu\frac{\partial u}{\partial y} = x - y, \text{ with the boundary value } u(x,x) = h, \tag{D.29}$$

where h is a constant. From the system of Equations (D.19) follows the characteristic system $\mathrm{d}x/\mathrm{d}s = yu$, $\mathrm{d}y/\mathrm{d}s = -xu$, $\mathrm{d}u/\mathrm{d}s = x - y$. Again, the integration of the equation $\mathrm{d}y/\mathrm{d}x = -x/y$ gives the first characteristic $x^2 + y^2 = C_1$. We can rewrite the equation $\mathrm{d}x/\mathrm{d}s + \mathrm{d}y/\mathrm{d}s = \mathrm{d}(x+y)/\mathrm{d}s$ as $\mathrm{d}(x+y)/\mathrm{d}s = u(y-x) = -u\,\mathrm{d}u/\mathrm{d}s$. After its integration, we get the second characteristic $u^2 + 2x + 2y = C_2$. The general solution of the partial differential equation will be:

$$\Phi(x^2 + y^2, u^2 + 2x + 2y) = 0, \tag{D.30}$$

where Φ is an arbitrary function of the characteristics. We will now rewrite the equation again using the boundary condition as a function of the characteristics and constants, i.e.,

$\Phi(2x^2, h^2 + 4x) = \Phi(C_1, C_2) = 0$. The first characteristic results in $x = \pm\sqrt{C_1/2}$, the second characteristic results in the equation for both characteristics, $h^2 \pm 4\sqrt{C_1/2} - C_2 = 0$. After substituting the original expressions into the characteristics, we get the explicit expression $h^2 + 2\sqrt{2}\sqrt{x^2 + y^2} - u^2 - 2x - 2y = 0$. The resulting solution of the boundary value problem for the given equation will be

$$u(x, y) = \sqrt{2\sqrt{2(x^2 + y^2)} - 2x - 2y + h^2}. \tag{D.31}$$

Analogously, it is possible to solve (almost) any first-order partial differential equation. It is always important to find a certain symmetry in the equation, which enables the construction of characteristic equations and finding the corresponding characteristics. For those interested in a deeper understanding of this problematics, I refer to the textbooks Arsenin (1977); Pospíšíl (2006); Franců (2011).

D.2 Second-order partial differential equations

D.2.1 Classification of second-order partial differential equations

A general partial differential equation of the second-order of the function $u(x, y)$ (for simplicity, we restrain ourselves to functions of only two variables) has the form:

$$\begin{aligned} a_{11}(x, y)\frac{\partial^2 u}{\partial x^2} + a_{12}(x, y)\frac{\partial^2 u}{\partial x \partial y} + a_{22}(x, y)\frac{\partial^2 u}{\partial y^2} + \\ + b_1(x, y)\frac{\partial u}{\partial x} + b_2(x, y)\frac{\partial u}{\partial y} + c(x, y)u + d(x, y) = 0, \end{aligned} \tag{D.32}$$

or, in a simplified notation used hereafter ($u_x = \partial u/\partial x$, $u_{xx} = \partial^2 u/\partial x^2$, etc.),

$$\begin{aligned} a_{11}(x, y)u_{xx} + a_{12}(x, y)u_{xy} + a_{22}(x, y)u_{yy} + \\ + b_1(x, y)u_x + b_2(x, y)u_y + c(x, y)u + d(x, y) = 0. \end{aligned} \tag{D.33}$$

The type of an equation (in case of a function of two variables) is determined by the following conditions:

$$a_{11}a_{22} - a_{12}^2 = 0 \qquad \text{parabolic equation,} \tag{D.34}$$

$$a_{11}a_{22} - a_{12}^2 < 0 \qquad \text{hyperbolic equation,} \tag{D.35}$$

$$a_{11}a_{22} - a_{12}^2 > 0 \qquad \text{elliptic equation.} \tag{D.36}$$

By adjusting the general form of an equation by transforming it into new variables through a quadratic form, the canonical form of equations can be obtained:

$$\begin{aligned} a_{11}(x, y)u_x \;\; - a_{22}(x, y)u_{yy} + \ldots = 0 \qquad & \text{parabolic equation,} \\ a_{11}(x, y)u_{xx} - a_{22}(x, y)u_{yy} + \ldots = 0 \qquad & \text{hyperbolic equation,} \\ a_{11}(x, y)u_{xx} + a_{22}(x, y)u_{yy} + \ldots = 0 \qquad & \text{elliptic equation.} \end{aligned} \tag{D.37}$$

In the case of an equation of several variables is the situation more complicated, the so-called *matrix of quadratic form* strictly determines the type of equation by its *definiteness*. An example of a transformation of a general second-degree polynomial to a quadratic form is

$$3x^2 + 2xy + 2y^2 = 3\left(x^2 + \frac{2}{3}xy + \frac{2}{3}y^2\right) = 3\left[\left(x + \frac{1}{3}y\right)^2 - \frac{1}{9}y^2 + \frac{2}{3}y^2\right] =$$

$$= 3\left[\left(x + \frac{1}{3}y\right)^2 + \frac{5}{9}y^2\right] = 3\left(x + \frac{1}{3}y\right)^2 + \frac{5}{3}y^2. \tag{D.38}$$

Substituting $\left\{\begin{matrix} x + \frac{1}{3}y = \xi_1 \\ y = \xi_2 \end{matrix}\right\}$, we get $3\,\xi_1^2 + \dfrac{5}{3}\,\xi_2^2$, which can be written as

$$\begin{pmatrix}\xi_1 & \xi_2\end{pmatrix} \begin{pmatrix} 3 & 0 \\ 0 & \frac{5}{3} \end{pmatrix} \begin{pmatrix}\xi_1 \\ \xi_2\end{pmatrix}. \tag{D.39}$$

Similarly, we can transform a general second-order partial differential equation. If the diagonal matrix of the quadratic form is positive or negative definite, i.e., its eigenvalues (see Equations (2.17)-(2.19)) are either all positive or all negative, then it is an elliptic equation. If the diagonal matrix of the quadratic form is indefinite (i.e., if some eigenvalues are positive, some are negative), then it is either a hyperbolic equation (the sign of only one eigenvalue is different) or ultrahyperbolic. If the diagonal matrix of the quadratic form is semidefinite (some eigenvalues are zero), then it is a parabolic equation (one eigenvalue is zero), or the so-called parabolic equation in the broader sense.

Canonical form of the particular types of equations, for example for a general function of the four variables $u = u(x_1, x_2, x_3, x_4)$, then schematically looks as follows:

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} \pm \frac{\partial u}{\partial x_4} + \ldots\ldots = 0 \qquad \text{parabolic,} \tag{D.40}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \pm \frac{\partial u}{\partial x_3} \pm \frac{\partial u}{\partial x_4} + \ldots\ldots = 0 \qquad \text{parabolic in the broader sense,} \tag{D.41}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} - \frac{\partial^2 u}{\partial x_4^2} + \ldots\ldots = 0 \qquad \text{hyperbolic,} \tag{D.42}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} - \frac{\partial^2 u}{\partial x_3^2} - \frac{\partial^2 u}{\partial x_4^2} + \ldots\ldots = 0 \qquad \text{ultrahyperbolic,} \tag{D.43}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} + \frac{\partial^2 u}{\partial x_4^2} + \ldots\ldots = 0 \qquad \text{elliptic.} \tag{D.44}$$

In the next explanation, we will show solutions to some selected types of parabolic, hyperbolic, and elliptic partial differential equations.

- **Physical applications of parabolic partial differential equations**

The most common form of a parabolic partial differential equation (e.g., the heat conduction equation) is

$$u_t = k(u_{xx} + u_{yy} + \ldots), \tag{D.45}$$

where a "constant" k (which need not have to be really a constant, the term k only does not contain the function of the declared variables $x, y, \ldots$) has the meaning $k = \lambda/(c_p\rho)$, where λ is the thermal conductivity coefficient, c_p is the heat capacity (at constant pressure), and ρ is the density.

D.2.2 Method of fundamental solution (Green's function method)

The solution of equations using the Fourier transform formalism and convolution of functions introduced in Section 10.2 will be shown in more detail in the following solved examples (in the following text we will always use the abbreviations LHS for the left-hand side of the equation and RHS for its right-hand side) of parabolic partial differential equations:

- **Homogeneous equations, non-homogeneous general initial condition:**

A homogeneous problem means an equation without a heat source, i.e., without RHS, while inhomogeneous (with RHS) means an additional heat source. In the case of homogeneous initial or boundary conditions, the corresponding function at time $t = 0$ or defined edges is zero. Consider an equation in the form

$$u_t = a^2 u_{xx}, \quad t > 0, \tag{D.46}$$

with the inhomogeneous initial condition $u(0,x) = \varphi(x)$. LHS and RHS of the equation are

$$\text{LHS:} \quad \widehat{u}_t(t,\xi) = \int_{-\infty}^{\infty} u_t(t,x)\, \mathrm{e}^{-\mathrm{i}x\xi}\, \mathrm{d}x = \widehat{u}_t(t,x), \tag{D.47}$$

$$\text{RHS:} \quad \widehat{u}_{xx}(t,\xi) = \int_{-\infty}^{\infty} u_{xx}(t,x)\, \mathrm{e}^{-\mathrm{i}x\xi}\, \mathrm{d}x = \underbrace{\Big[u_x\, \mathrm{e}^{-\mathrm{i}x\xi}\Big]_{-\infty}^{\infty}}_{0} + \mathrm{i}\xi \int_{-\infty}^{\infty} u_x(t,x)\, \mathrm{e}^{-\mathrm{i}x\xi}\, \mathrm{d}x = -\xi^2\, \widehat{u}(\xi). \tag{D.48}$$

So we get a simple first-order differential equation with directly separable variables, $\widehat{u}_t(\xi) = -a^2\xi^2\, \widehat{u}(\xi)$, whose solution is easy to identify as $\widehat{u}(\xi) = C\, \mathrm{e}^{-a^2\xi^2 t}$, or $\widehat{u}(t,\xi) = C(\xi)\, \mathrm{e}^{-a^2\xi^2 t}$. We determine the function $C(\xi)$ from the initial condition (D.46), $\widehat{u}(0,\xi) = \widehat{\varphi}(\xi) = C(\xi)$, $\widehat{u}(t,\xi) = C(\xi)\, \mathrm{e}^{-a^2\xi^2 t}$. We introduce a function $G(t,x)$ (Green's function) as the inverse Fourier image of the function $\widehat{G}(t,\xi) = \mathrm{e}^{-a^2\xi^2 t}$, so we get $\widehat{u}(t,\xi) = \widehat{\varphi}(\xi)\cdot\widehat{G}(t,\xi) = \widehat{(\varphi * G)}(t,\xi)$, and so $u(t,x) = (\varphi * G)(t,x)$:

$$G(t,x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{G}(t,\xi)\, \mathrm{e}^{\mathrm{i}\xi x}\, \mathrm{d}\xi = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-a^2\xi^2 t}\, \mathrm{e}^{\mathrm{i}\xi x}\, \mathrm{d}\xi = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-(a^2\xi^2 t - \mathrm{i}\xi x)}\, \mathrm{d}\xi =$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-(a\xi\sqrt{t} - \frac{\mathrm{i}x}{2a\sqrt{t}})^2}\, \mathrm{e}^{-\frac{x^2}{4a^2 t}}\, \mathrm{d}\xi = \left\{\begin{matrix} a\xi\sqrt{t} - \frac{\mathrm{i}x}{2a\sqrt{t}} = \eta \\ a\sqrt{t}\, \mathrm{d}\xi = \mathrm{d}\eta \end{matrix}\right\} = \frac{1}{2a\sqrt{\pi t}}\, \mathrm{e}^{-\frac{x^2}{4a^2 t}} = G(x,t). \tag{D.49}$$

The resulting solution of the given parabolic partial differential equation will thus be

$$u(t,x) = (\varphi * G)(t,x) = \int_{-\infty}^{\infty} \varphi(y)\, G(t, x-y)\, \mathrm{d}y = \frac{1}{2a\sqrt{\pi t}}\int_{-\infty}^{\infty} \varphi(y)\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2 t}}\, \mathrm{d}y. \tag{D.50}$$

In a general case, where $u(\tau,x) = \varphi(x)$, we get the resulting function in the form

$$u(t,x) = \frac{1}{2a\sqrt{\pi t}}\int_{-\infty}^{\infty} \varphi(y)\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2(t-\tau)}}\, \mathrm{d}y. \tag{D.51}$$

- **Next homogeneous equation, inhomogeneous general initial condition:**

Consider the 3D heat conduction equation (de facto diffusion equation)

$$\frac{\partial\phi}{\partial t} = D\nabla^2\phi, \tag{D.52}$$

where D is the (constant) diffusion coefficient, with homogeneous Dirichlet boundary conditions and the inhomogeneous initial condition

$$\lim_{|\boldsymbol{x}|\to\infty} \phi\,(t, \boldsymbol{x}) = 0\ \forall\ t, \qquad \phi\,(0, \boldsymbol{x}) \equiv \phi\,(\boldsymbol{x}) = \left(\frac{a}{\pi}\right)^{3/2} \phi_0\, \mathrm{e}^{-a|\boldsymbol{x}|^2}, \tag{D.53}$$

(where a is a positive constant) normalized so that $\int_{\mathbb{R}^3} \phi\,(\boldsymbol{x})\ \mathrm{d}^3x = \phi_0$. Let us find the fundamental solution of such an equation using Green's function.

Using the spatial Fourier transform of both sides, we get the ordinary differential equation

$$\widehat{\phi}_t\,(t, \boldsymbol{k}) = -D|\boldsymbol{k}|^2 \widehat{\phi}\,(t, \boldsymbol{k})\,, \qquad \text{so} \qquad \widehat{\phi}\,(t, \boldsymbol{k}) = \widehat{\phi}\,(\boldsymbol{k})\ \mathrm{e}^{-D|\boldsymbol{k}|^2 t}. \tag{D.54}$$

The general rule $\widehat{u} = \widehat{f}\,\widehat{G}$ implies $u = f * G$, where

$$G(t, \boldsymbol{x}) = \frac{1}{2\pi} \int_{\mathbb{R}^3} \mathrm{e}^{-D|\boldsymbol{k}|^2 t}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\, \mathrm{d}^3k = \frac{1}{(4\pi Dt)^{3/2}} \exp\left(-\frac{|\boldsymbol{x}|^2}{4Dt}\right). \tag{D.55}$$

The convolution $\phi(t, \boldsymbol{x}) = \phi(\boldsymbol{x}) * G(t, \boldsymbol{x})$ will have the explicit form

$$\phi(t, \boldsymbol{x}) = \phi_0 \left(\frac{a}{4\pi^2 Dt}\right)^{3/2} \int_{\mathbb{R}^3} \mathrm{e}^{-a|\boldsymbol{y}|^2} \exp\left(-\frac{|\boldsymbol{x}-\boldsymbol{y}|^2}{4Dt}\right)\, \mathrm{d}^3y, \tag{D.56}$$

where the function $G(t, \boldsymbol{x})$ acts as a convolution kernel. By successive modifications we obtain

$$\begin{aligned}
\phi(t, \boldsymbol{x}) &= \phi_0\, \alpha^{3/2} \int_{\mathbb{R}^3} \exp\left[-\left(a|\boldsymbol{y}|^2 + \frac{|\boldsymbol{x}-\boldsymbol{y}|^2}{4Dt}\right)\right]\, \mathrm{d}^3y = \\
&= \phi_0\, \alpha^{3/2} \int_{\mathbb{R}^3} \exp\left(-\frac{4aDt|\boldsymbol{y}|^2 + |\boldsymbol{x^2} - 2\boldsymbol{x}\boldsymbol{y} + \boldsymbol{y^2}|}{4Dt}\right)\, \mathrm{d}^3y = \\
&= \phi_0\, \alpha^{3/2} \exp\left(-\frac{|\boldsymbol{x}|^2}{4Dt}\right) \int_{\mathbb{R}^3} \exp\left[-\frac{(1+4aDt)\,|\boldsymbol{y}|^2 - 2|\boldsymbol{x}||\boldsymbol{y}|}{4Dt}\right]\, \mathrm{d}^3y = \\
&= \phi_0\, \alpha^{3/2} \exp\left(-\frac{|\boldsymbol{x}|^2}{4Dt}\right) \int_{\mathbb{R}^3} \exp\left[-\frac{\left(\sqrt{1+4aDt}\,|\boldsymbol{y}| - \frac{|\boldsymbol{x}|}{2\sqrt{1+4aDt}}\right)^2 - \frac{|\boldsymbol{x}|^2}{4(1+4aDt)}}{4Dt}\right]\, \mathrm{d}^3y = \\
&= \phi_0\, \alpha^{3/2} \exp\left(-\frac{a|\boldsymbol{x}|^2}{1+4aDt}\right) \int_{\mathbb{R}^3} \exp\left[-\frac{\left(\sqrt{1+4aDt}\,|\boldsymbol{y}| - \frac{|\boldsymbol{x}|}{2\sqrt{1+4aDt}}\right)^2}{4Dt}\right]\, \mathrm{d}^3y,
\end{aligned} \tag{D.57}$$

where $\alpha = a/(4\pi^2 Dt)$. Substitution

$$\frac{\sqrt{1+4aDt}\,|\boldsymbol{y}| - \frac{|\boldsymbol{x}|}{2\sqrt{1+4aDt}}}{2\sqrt{Dt}} = |\boldsymbol{z}|, \qquad \mathrm{d}^3y = \left(\frac{4Dt}{1+4aDt}\right)^{3/2} \mathrm{d}^3z, \tag{D.58}$$

gives

$$\phi_0 \left(\frac{a}{4\pi^2 Dt}\right)^{3/2} \left(\frac{4Dt}{1+4aDt}\right)^{3/2} \exp\left(-\frac{a|\boldsymbol{x}|^2}{1+4aDt}\right) \int_{\mathbb{R}^3} \mathrm{e}^{-|\boldsymbol{z}|^2}\, \mathrm{d}^3z, \tag{D.59}$$

where the value of the last integral is $\pi^{3/2}$. This gives us the resulting solution

$$\phi\,(t, \boldsymbol{x}) = \phi_0 \left(\frac{a/\pi}{1+4aDt}\right)^{3/2} \exp\left(-\frac{a|\boldsymbol{x}|^2}{1+4aDt}\right). \tag{D.60}$$

- **Inhomogeneous equation with homogeneous initial condition:**

Suppose an inhomogeneous equation in the form

$$u_t = a^2 u_{xx} + f, \quad t > 0, \tag{D.61}$$

with a homogeneous initial condition $u(0, x) = 0$. Its solution is assumed in the form

$$u(t, x) = \int_0^t w(t, x, \sigma)\, \mathrm{d}\sigma, \tag{D.62}$$

Its time derivative gives

$$\begin{gathered} u_t(t, x) = w(t, x, t) + \int_0^t w_t(t, x, \sigma)\, \mathrm{d}\sigma,\ u_{xx}(t, x) = \int_0^t w_{xx}(t, x, \sigma)\, \mathrm{d}\sigma, \\ w(t, x, t) + \int_0^t w_t(t, x, \sigma)\, \mathrm{d}\sigma = a^2 \int_0^t w_{xx}(t, x, \sigma)\, \mathrm{d}\sigma + f(t, x). \end{gathered} \tag{D.63}$$

Assuming

$$\int_0^t \left[w_t(t, x, \sigma) - a^2 w_{xx}(t, x, \sigma) \right] \mathrm{d}\sigma = f(t, x) - w(t, x, t) = 0, \tag{D.64}$$

its solution $w_t(t, x, \sigma) = a^2 w_{xx}(t, x, \sigma)$ with the initial condition $w(\sigma, x, \sigma) = f(\sigma, x)$ will have the form

$$w(t, x, \sigma) = \frac{1}{2a\sqrt{\pi(t-\sigma)}} \int_{-\infty}^{\infty} f(\sigma, y)\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2(t-\sigma)}}\, \mathrm{d}y. \tag{D.65}$$

The resulting solution will be

$$u(t, x) = \frac{1}{2a} \int_0^t \int_{-\infty}^{\infty} \frac{f(\sigma, y)}{\sqrt{t-\sigma}}\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2(t-\sigma)}}\, \mathrm{d}\sigma\, \mathrm{d}y. \tag{D.66}$$

- **Inhomogeneous equations with inhomogeneous initial condition:**

Suppose an inhomogeneous equation in the form

$$u_t = a^2 u_{xx} + f, \quad t > 0, \tag{D.67}$$

with the inhomogeneous initial condition $u(0, x) = \varphi(x)$. The linearity implies that the function u can be separated into two functions $u(t, x) = v(t, x) + w(t, x)$, where

$$\text{function I:} \qquad v_t(t, x) = a^2 v_{xx} + f, \qquad v(0, x) = 0, \tag{D.68}$$

$$\text{function II:} \qquad w_t(t, x) = a^2 w_{xx}, \qquad w(0, x) = \varphi(x). \tag{D.69}$$

From the initial condition $\varphi(x) = v(0, x) + w(0, x) = w(0, x)$, where $v(0, x) = 0$, we get

$$\begin{aligned} u(t, x) &= \int_{-\infty}^{\infty} \varphi(y)\, G(x, y, t)\, \mathrm{d}y + \int_0^t \int_{-\infty}^{\infty} f(\sigma, y)\, G(x, y, t-\sigma)\, \mathrm{d}\sigma\, \mathrm{d}y = \\ &= \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^{\infty} \varphi(y)\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2 t}}\, \mathrm{d}y + \frac{1}{2a} \int_0^t \int_{-\infty}^{\infty} \frac{f(\sigma, y)}{\sqrt{t-\sigma}}\, \mathrm{e}^{-\frac{(x-y)^2}{4a^2(t-\sigma)}}\, \mathrm{d}\sigma\, \mathrm{d}y. \end{aligned} \tag{D.70}$$

D.2.3 Solution of parabolic partial differential equations by the Fourier method (Method of separation of variables)

The method, which is very often used in solving second-order partial differential equations, will be again shown in more detail in the examples of parabolic partial differential equations.

- **Homogeneous one-dimensional problem, homogeneous boundary conditions, general initial condition:**

Assume an equation in the form

$$u_t = a^2 u_{xx}, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.71}$$

with the conditions $u(0,x) = \varphi(x)$, $u(t,0) = 0 = u(t,\ell)$. Suppose, further, that the function $u(t,x)$ can be expressed as the product of two functions of only one of the two variables, $u(t,x) = T(t)X(x)$. Equation (D.71) can thus be expressed as follows: $\dot{T}X = a^2 T X''$, the equation is then separated to the form

$$\frac{\dot{T}}{a^2 T} = \frac{X''}{X} = -\lambda. \tag{D.72}$$

Solution of the RHS thus will be $X'' + \lambda X = 0$, which implies $X(x) = v(x) = A \sin \sqrt{\lambda} x + B \cos \sqrt{\lambda} x$. Including the boundary condition, we get the corresponding coefficients of the RHS: $X(0) = B = 0$, $X(\ell) = A \sin \sqrt{\lambda} \ell = 0$, and so

$$\sqrt{\lambda} = \frac{k\pi}{\ell}, \tag{D.73}$$

where constant A can take any value (e.g., $A = 1$). RHS can thus be written as

$$X_k = v_k = \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.74}$$

We solve the LHS as an ordinary first-order differential equation, $\dot{T}/T = -a^2\lambda$, which implies

$$T = C_k \,\mathrm{e}^{-a^2 \lambda_k t} = C_k \,\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t}. \tag{D.75}$$

We then combine the two found separate functions into the product

$$u(t,x) = \sum_{k=1}^{\infty} C_k \,\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.76}$$

The so-called Fourier coefficient C_k is obtained from the initial condition,

$$\varphi(x) = \sum_{k=1}^{\infty} C_k \sin\left(\frac{k\pi}{\ell} x\right) = \sum_{k=1}^{\infty} C_k v_k, \quad \text{so} \quad C_k = \frac{1}{\|v_k\|^2} \int_0^{\ell} \varphi(\xi)\, v_k(\xi)\, \mathrm{d}\xi. \tag{D.77}$$

We solve the norm $\|v_k\|$ as a norm of a continuously defined vector (see Equation (2.1)), so

$$\|v_k\|^2 = \int_0^{\ell} v_k^2(\xi)\, \mathrm{d}\xi = \int_0^{\ell} \sin^2\left(\frac{k\pi}{\ell}\xi\right) \mathrm{d}\xi = \frac{\ell}{2}, \quad C_k = \frac{2}{\ell} \int_0^{\ell} \varphi(\xi) \sin\left(\frac{k\pi}{\ell}\xi\right) \mathrm{d}\xi. \tag{D.78}$$

The resulting function can then be written in the form

$$u(t,x) = \frac{2}{\ell} \sum_{k=1}^{\infty} \int_0^{\ell} \left[\varphi(\xi) \sin\left(\frac{k\pi}{\ell}\xi\right) \mathrm{d}\xi\right] \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.79}$$

• Homogeneous two-dimensional problem, homogeneous boundary conditions, general initial condition:

Heat conduction in orthogonal directions: suppose an equation in the form

$$u_t = a^2\left(u_{xx} + u_{yy}\right), \quad t > 0, \quad x \in \langle 0, \ell_1\rangle, \quad y \in \langle 0, \ell_2\rangle, \tag{D.80}$$

with conditions $u(0,x,y) = \varphi(x,y)$, $u(t,0,y) = 0 = u(t,\ell_1,y)$, $u(t,x,0) = 0 = u(t,x,\ell_2)$. We assume the product of three functions (compare with Equation (D.72)), where each is a function of only one of three variables: $u = T(t)X(x)Y(y)$. Both sides of Equation (D.80) can then be expressed as follows:

$$\dot{T}XY = a^2(TX''Y + TXY''), \quad \text{so} \quad \frac{\dot{T}}{a^2T} = \frac{X''}{X} + \frac{Y''}{Y} = -(\lambda_1 + \lambda_2). \tag{D.81}$$

We further assume $X''/X = -\lambda_1$, $Y''/Y = -\lambda_2$, which is justified with respect to the subsequent adjustment of the LHS of the equation. We get a solution of the RHS in the form

$$X_m = \sin\left(\frac{m\pi}{\ell_1}x\right), \quad Y_n = \sin\left(\frac{n\pi}{\ell_2}y\right). \tag{D.82}$$

We again solve the LHS as an ordinary first-order differential equation

$$T = C_{mn}\,\mathrm{e}^{-a^2\left[\left(\frac{m\pi}{\ell_1}\right)^2 + \left(\frac{n\pi}{\ell_2}\right)^2\right]t}. \tag{D.83}$$

Then we combine all three separate functions into the product

$$u(t,x,y) = \sum_{m,n=1}^{\infty} C_{mn}\,\mathrm{e}^{-a^2\left[\left(\frac{m\pi}{\ell_1}\right)^2 + \left(\frac{n\pi}{\ell_2}\right)^2\right]t} \times \sin\left(\frac{m\pi}{\ell_1}x\right)\sin\left(\frac{n\pi}{\ell_2}y\right). \tag{D.84}$$

We get the Fourier coefficient C_{mn} from the initial condition,

$$C_{mn} = \frac{1}{\|v_{mn}\|^2}\int_0^{\ell_1}\int_0^{\ell_2} \varphi(\xi,\eta)\sin\left(\frac{m\pi\xi}{\ell_1}\right)\sin\left(\frac{n\pi\eta}{\ell_2}\right)\mathrm{d}\xi\,\mathrm{d}\eta. \tag{D.85}$$

The norm $\|v_{mn}\|$ of the function $v_{mn} = X_mY_n$ is, analogously to Equation (D.78), given as

$$\|v_{mn}\|^2 = \int_0^{\ell_1}\int_0^{\ell_2} \sin^2\left(\frac{m\pi\xi}{\ell_1}\right)\sin^2\left(\frac{n\pi\eta}{\ell_2}\right)\mathrm{d}\xi\,\mathrm{d}\eta = \frac{1}{2}\Big[\xi\Big]_0^{\ell_1} \times \frac{1}{2}\Big[\eta\Big]_0^{\ell_2} = \frac{\ell_1\,\ell_2}{4}. \tag{D.86}$$

The resulting function can be written in the form

$$\begin{aligned} u(t,x,y) = \frac{4}{\ell_1\,\ell_2}\sum_{m,n=1}^{\infty}\int_0^{\ell_1}\int_0^{\ell_2}\left[\varphi(\xi,\eta)\sin\left(\frac{m\pi\xi}{\ell_1}\right)\sin\left(\frac{n\pi\eta}{\ell_2}\right)\mathrm{d}\xi\,\mathrm{d}\eta\right] \times \\ \times\,\mathrm{e}^{-a^2\left[\left(\frac{m\pi}{\ell_1}\right)^2 + \left(\frac{n\pi}{\ell_2}\right)^2\right]t} \times \sin\left(\frac{m\pi}{\ell_1}x\right)\sin\left(\frac{n\pi}{\ell_2}y\right). \end{aligned} \tag{D.87}$$

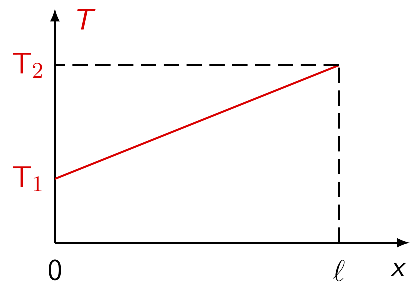

Figure D.1: Schematic representation of the profile of the function $w(x) = T_1 + \frac{T_2 - T_1}{\ell} x$.

- **Homogeneous one-dimensional problem, inhomogeneous boundary conditions, homogeneous initial condition:**

In the case of inhomogeneous boundary conditions, finding a particular solution will be more complicated. Consider an equation of cooling of a bar,

$$u_t = a^2 u_{xx}, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.88}$$

with the conditions $u(0,x) = 0$, $u(t,0) = T_1$, $u(t,\ell) = T_2$. We linearize the function $u(t,x) = v(t,x) + w(t,x)$, where the function $w(t,x)$ transforms to a stationary function $w(x)$ and meets the boundary conditions as follows, $w(t,0) = T_1$, $w(t,\ell) = T_2$, $v(t,0) = v(t,\ell) = 0$. For stationary functions further applies,

$$w(x) = T_1 + \frac{T_2 - T_1}{\ell} x, \quad v(0,x) = -T_1 + \frac{T_1 - T_2}{\ell} x, \quad v(0,x) + w(0,x) = 0. \tag{D.89}$$

We will rewrite the equation (D.88) for both functions of v and w, $v_t = a^2 v_{xx}$, $w_t = a^2 w_{xx}$. Spatial derivatives of a function w will be $w_x = (T_2 - T_1)/\ell$, $w_{xx} = 0$. Including further the conditions for a function v, $v_t = a^2 v_{xx}$, $v = XT$, $v(t,0) = 0 = v(t,\ell)$, we get

$$X(x) = A \sin \sqrt{\lambda} x + B \cos \sqrt{\lambda} x, \quad \text{so} \quad X_k = \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.90}$$

We can write the function v in the form

$$v(x,t) = \sum_{k=1}^{\infty} C_k \, \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.91}$$

From the initial condition (D.89), there also follows

$$v(0,x) = \sum_{k=1}^{\infty} C_k \sin\left(\frac{k\pi}{\ell} x\right) = -T_1 + \frac{T_1 - T_2}{\ell} x, \tag{D.92}$$

from which we calculate the Fourier coefficient,

$$\begin{aligned} C_k &= \frac{2}{\ell} \int_0^{\ell} \left(-T_1 + \frac{T_1 - T_2}{\ell} x\right) \sin\left(\frac{k\pi}{\ell} \xi\right) \mathrm{d}\xi = \\ &= \frac{2T_1}{k\pi}\left[(-1)^k - 1\right] - \frac{2(T_1 - T_2)}{k\pi}(-1)^k = (-1)^k \left(\frac{2T_2}{k\pi}\right) - \left(\frac{2T_1}{k\pi}\right). \end{aligned} \tag{D.93}$$

The resulting function will have the form

$$u(t,x) = T_1 + \frac{T_2 - T_1}{\ell} x + \sum_{k=1}^{\infty} \left[(-1)^k \left(\frac{2T_2}{k\pi}\right) - \left(\frac{2T_1}{k\pi}\right)\right] \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \sin\left(\frac{k\pi}{\ell} x\right). \tag{D.94}$$

- **Inhomogeneous one-dimensional problem with constant heat source T_0, with homogeneous conditions:**

Consider an equation of cooling of a bar with a constant heat source

$$u_t = a^2 u_{xx} + T_0, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.95}$$

with the conditions $u(0, x) = 0$, $u(t, 0) = 0 = u(t, \ell)$. We separate the function in a following way,

$$u(t, x) = TX, \quad X(x) = A \sin \sqrt{\lambda} x + B \cos \sqrt{\lambda} x, \quad X_k(x) = v_k(x) = \sin \left(\frac{k\pi}{\ell} x \right). \tag{D.96}$$

We assume a solution in the form

$$u(t, x) = \sum_{k=1}^{\infty} C_k(t) \sin \left(\frac{k\pi}{\ell} x \right). \tag{D.97}$$

By using another condition we obtain an inhomogeneous ordinary differential equation

$$\dot{C}_k(t) + a^2 \lambda_k C_k(t) = F_k(t), \tag{D.98}$$

where $F_k(t)$ is the so-called Fourier coefficient of inhomogeneity. We further solve this equation:

$$f(t, x) = \sum_{k=1}^{\infty} F_k(t) \sin \left(\frac{k\pi}{\ell} x \right), \tag{D.99}$$

$$F_k(t) = \frac{2}{\ell} \int_0^{\ell} f(t, \xi) \sin \left(\frac{k\pi}{\ell} \xi \right) \mathrm{d}\xi = \frac{2T_0}{\ell} \frac{\ell}{k\pi} \left[-\cos \frac{k\pi}{\ell} \xi \right]_0^{\ell} = \frac{2T_0}{k\pi} \left[1 - (-1)^k \right]. \tag{D.100}$$

We first solve a homogeneous equation

$$\dot{C}_k(t) = -a^2 \left(\frac{k\pi}{\ell} \right)^2 C_k(t) = -\left(\frac{ak\pi}{\ell} \right)^2 K(t)\, \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} + \dot{K}(t)\, \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t}. \tag{D.101}$$

Substituting this into the inhomogeneous equation, we get

$$\dot{C}_k(t) + \left(\frac{ak\pi}{\ell} \right)^2 K(t)\, \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} = \frac{2T_0}{k\pi} \left[1 - (-1)^k \right], \tag{D.102}$$

$$K(t) = \left(\frac{\ell}{ak\pi} \right)^2 \frac{2\,T_0}{k\pi} \left[1 - (-1)^k \right] \mathrm{e}^{\left(\frac{ak\pi}{\ell}\right)^2 t} + K_2. \tag{D.103}$$

The initial condition $C_k(0) = 0$ implies,

$$K_2 = \left(\frac{\ell}{ak\pi} \right)^2 \frac{2T_0}{k\pi} \left[(-1)^k - 1 \right], \tag{D.104}$$

$$C_k(t) = \left[1 - \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \right] \frac{2T_0}{k\pi} \left(\frac{\ell}{ak\pi} \right)^2 \left[1 - (-1)^k \right]. \tag{D.105}$$

The resulting function will have the form

$$u(t, x) = \sum_{k=1}^{\infty} \left[1 - \mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} \right] \frac{2T_0}{k\pi} \left(\frac{\ell}{ak\pi} \right)^2 \left[1 - (-1)^k \right] \sin \left(\frac{k\pi}{\ell} x \right). \tag{D.106}$$

- **Inhomogeneous one-dimensional problem with non-constant heat source, homogeneous conditions:**

Consider an equation of a cooling of a bar with a spatially and time-dependent heat source,

$$u_t = a^2 u_{xx} + tx, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.107}$$

with the conditions $u(0,x) = 0$, $u(t,0) = 0 = u(t,\ell)$. We first separate the function,

$$u(t,x) = TX, \quad X(x) = A \sin\sqrt{\lambda}x + B\cos\sqrt{\lambda}x, \quad X_k(x) = v_k(x) = \sin\left(\frac{k\pi}{\ell}x\right). \tag{D.108}$$

We again assume a solution in the form

$$u(t,x) = \sum_{k=1}^{\infty} C_k(t) \sin\left(\frac{k\pi}{\ell}x\right) \quad \text{where} \quad \dot{C}_k(t) + a^2\lambda_k C_k(t) = F_k(t). \tag{D.109}$$

We further solve this equation:

$$f(t,x) = \sum_{k=1}^{\infty} F_k(t) \sin\left(\frac{k\pi}{\ell}x\right), \quad F_k(t) = (-1)^{k+1}\frac{2\ell}{k\pi}\,t. \tag{D.110}$$

The solution of the homogeneous ordinary differential equations is

$$\dot{C}_k(t) = -\left(\frac{ak\pi}{\ell}\right)^2 K(t)\,\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} + \dot{K}(t)\,\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t}. \tag{D.111}$$

We substitute this again into the inhomogeneous equation, we get

$$\dot{C}_k(t) + \left(\frac{ak\pi}{\ell}\right)^2 K(t)\,\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} = (-1)^{k+1}\frac{2\ell}{k\pi}\,t, \tag{D.112}$$

$$K(t) = \frac{2\ell}{k\pi}(-1)^{k+1}\left[t\left(\frac{\ell}{ak\pi}\right)^2 \mathrm{e}^{\left(\frac{ak\pi}{\ell}\right)^2 t}\right] - \left(\frac{\ell}{ak\pi}\right)^4 \mathrm{e}^{\left(\frac{ak\pi}{\ell}\right)^2 t} + K_2. \tag{D.113}$$

The initial condition $C_k(0) = 0$ implies

$$K_2 = \frac{2\,\ell}{k\pi}(-1)^{k+1}\left(\frac{\ell}{ak\pi}\right)^4, \tag{D.114}$$

$$C_k(t) = \frac{2\ell}{k\pi}(-1)^{k+1}\left(\frac{\ell}{ak\pi}\right)^4\left[\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} + t\left(\frac{ak\pi}{\ell}\right)^2 - 1\right]. \tag{D.115}$$

The resulting function has the form

$$u(t,x) = \sum_{k=1}^{\infty}\frac{2\ell}{k\pi}(-1)^{k+1}\left(\frac{\ell}{ak\pi}\right)^4\left[\mathrm{e}^{-\left(\frac{ak\pi}{\ell}\right)^2 t} + t\left(\frac{ak\pi}{\ell}\right)^2 - 1\right]\sin\left(\frac{k\pi}{\ell}x\right). \tag{D.116}$$

- **Inhomogeneous one-dimensional problem with inhomogeneous conditions** ("outline" of a solution)**:**

Consider the equation

$$u_t = a^2 u_{xx} + tx, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.117}$$

with the conditions $u(0,x) = \varphi(x)$, $u(t,0) = u_1(t)$, $u(t,\ell) = u_2(t)$. We again separate the function $u(t,x)$ into the sum of $u(t,x) = v(t,x) + w(t,x)$, where w will satisfy the boundary conditions. If we write the equation (D.117) as $v_t + w_t = a^2 v_{xx} + a^2 w_{xx} + tx$, we get

$$v_t = a^2 v_{xx} + tx + a^2 w_{xx} - w_t, \tag{D.118}$$

where the last three terms represent the inhomogeneity. The initial condition for the function u gives $\varphi(x) = v(0,x) + w(0,x)$, that is, $v(0,x) = \varphi(x) - w(0,x)$. Using the functions v and w, we solve the problem principally in the same way as in the previous cases.

D.2.4 Simple examples of spatial problems

- **Temperature in an infinitely long rotational cylinder** (using the Bessel functions) **:**

Consider an equation (where c is radius of the cylinder)

$$u_t = a^2 \left(u_{\rho\rho} + \frac{1}{\rho} u_\rho \right), \quad t > 0, \quad \rho \in \langle 0, c \rangle, \tag{D.119}$$

representing the radial part of Laplacian in the cylindrical coordinates (B.46), with the conditions $u(0,\rho) = f(\rho)$, $u(t,0) = 0 = u(t,c)$. By separating the function $u = R(\rho)T(t)$, we can separate the equation

$$\frac{\dot{T}}{a^2 T} = \frac{R''}{R} + \frac{1}{\rho}\frac{R'}{R} = -\lambda^2. \tag{D.120}$$

After an adjustment, we obtain for the both sides

$$\text{LHS: } \dot{T} + a^2\lambda^2 T = 0, \quad \text{RHS: } \rho R'' + R' + \lambda^2 \rho R = 0. \tag{D.121}$$

By substituting $\lambda\rho = z$ and adjusting,

$$\frac{\mathrm{d}R}{\mathrm{d}\rho} = \lambda \frac{\mathrm{d}R}{\mathrm{d}z}, \quad \frac{\mathrm{d}^2 R}{\mathrm{d}\rho^2} = \lambda^2 \frac{\mathrm{d}^2 R}{\mathrm{d}z^2}, \tag{D.122}$$

we get the so-called *Bessel equation* with the index $\nu = 0$,

$$z\frac{\mathrm{d}^2 R}{\mathrm{d}z^2} + \frac{\mathrm{d}R}{\mathrm{d}z} + zR = 0, \tag{D.123}$$

where the general Bessel equation has the form $x^2 y'' + xy' + (x^2 - \nu^2)y = 0$. The solution of Equation (D.123) and the solution of the general Bessel equation are the functions

$$J_0(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(k!)^2} \left(\frac{x}{2}\right)^{2k}, \quad J_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{k=1}^{\infty} \frac{(-1)^k}{k!\,\Gamma(\nu + k + 1)} \left(\frac{x}{2}\right)^{2k}, \tag{D.124}$$

where the expression $\Gamma(\nu + k + 1)$ is the so-called Γ function, defined as $\Gamma(x) = \int_0^\infty \mathrm{e}^{-t} t^{x-1}\,\mathrm{d}t$. In our case, we get the solution of the RHS of Equation (D.121) in the form $R(z) = J_0(z)$, i.e., $R(\rho) = J_0(\lambda\rho)$, and so $J_0(\lambda_n \rho) = R_n(\rho)$, with the boundary condition $J_0(\lambda_n c) = 0$, where λ_n is the root of this equation for $n = 1, 2, 3, \ldots$. The solution of LHS of Equation (D.121) will be the function

$$T_n(t) = \mathrm{e}^{-a^2 \lambda_n^2 t}. \tag{D.125}$$

Using the so-called Fourier-Bessel expansion defined as $\sum_{k=1}^{\infty} C_n J_\nu(\lambda_n x) = f(x)$, we obtain at each point where the function $f(x)$ is continuous, the coefficient C_n (Fourier-Bessel coefficient), where for J_0 and general J_ν from Equation (D.124) applies

$$C_n = \frac{2}{c^2 J_1^2(\lambda_n c)} \int_0^c \xi\, J_0(\lambda_n \xi) f(\xi)\,\mathrm{d}\xi, \quad C_n = \frac{2}{c^2 J_{\nu+1}^2(\lambda_n c)} \int_0^c \xi\, J_\nu(\lambda_n \xi) f(\xi)\,\mathrm{d}\xi. \tag{D.126}$$

The resulting function will take the form

$$u(t,\rho) = \frac{2}{c^2} \sum_{n=1}^{\infty} \frac{J_0(\lambda_n \rho)}{J_1^2(\lambda_n c)} \int_0^c [\xi\, J_0(\lambda_n \xi) f(\xi)\,\mathrm{d}\xi]\,\mathrm{e}^{-a^2\lambda_n^2 t}. \tag{D.127}$$

- **Cooling of a sphere** (homogeneous equation) **:**

Consider a function with the Laplacian

$$u_t = a^2 \Delta u, \quad t > 0, \quad r \in \langle 0, R \rangle, \tag{D.128}$$

for the Cartesian coordinates $x^2 + y^2 + z^2 \leq R^2$, where R is the radius of the sphere, with the conditions $u(0,x,y,z) = f\left(\sqrt{x^2+y^2+z^2}\right) = f(r)$, and so $u(0,r) = f(r)$, $u(t,x,y,z) = u(t,r)$, $u(t,0) = T_1$, $u(t,R) = 0$. The successive partial derivatives will be

$$u_x = u_r r_x + \underbrace{u_\theta \theta_x + u_\phi \phi_x}_{0}, \quad \text{so} \quad u_x = u_r \frac{x}{r}, \tag{D.129}$$

$$u_{xx} = u_{rr}\frac{x^2}{r^2} + u_r \frac{r - x\frac{x}{r}}{r^2} = u_{rr}\frac{x^2}{r^2} + u_r \frac{r^2 - x^2}{r^3}, \tag{D.130}$$

$$\Delta u = u_{rr}\frac{x^2+y^2+z^2}{r^2} + u_r \frac{3r^2 - \left(x^2+y^2+z^2\right)}{r^3} = u_{rr} + \frac{2}{r}u_r, \quad \text{so} \tag{D.131}$$

$$u_t = a^2\left(u_{rr} + \frac{2}{r}u_r\right) \ \text{(spherical radial part of Laplacian - see Equation (B.72))}. \tag{D.132}$$

Using the substitution $v(r) = r u(r)$ so $u = v/r$, we get

$$u_t = \frac{1}{r}v_t,\ u_r = -\frac{1}{r^2}v + \frac{1}{r}v_r,\ u_{rr} = \frac{2}{r^3}v - \frac{1}{r^2}v_r - \frac{1}{r^2}v_r + \frac{1}{r}v_{rr} = \frac{2}{r^3}v - \frac{2}{r^2}v_r + \frac{1}{r}v_{rr}, \tag{D.133}$$

$$u_t = a^2\left(u_{rr} + \frac{2}{r}u_r\right), \quad \text{so} \frac{1}{r}v_t = a^2\left(\frac{2}{r^3}v - \frac{2}{r^2}v_r + \frac{1}{r}v_{rr} - \frac{2}{r^3}v + \frac{2}{r^2}v_r\right), \ \text{and so} \tag{D.134}$$

$$v_t = a^2 v_{rr}, \ \text{where } v(0,r) = r f(r)\ v(t,0) = rT_1,\ v(t,R) = 0. \tag{D.135}$$

With help of the linearization $u = z + w$, we obtain:

$$u(0,r) = f(r), \quad \text{so} \quad z(0,r) = u(0,r) - w(r), \tag{D.136}$$

$$w(r) = T_1 - \frac{T_1}{R}r,\ z(0,r) = f(r) - T_1 + \frac{T_1}{R}r,\ \tilde{z}(0,r) = r z(0,r). \tag{D.137}$$

$$v(0,r) = r f(r),\ \text{so}\ \tilde{z}(0,r) = r\left[f(r) - T_1 + \frac{T_1}{R}r\right] \quad \text{gives} \tag{D.138}$$

$$v = ru = r(z+w),\ z_t = a^2 z_{rr},\ z(t,0) = z(t,R) = 0,\ z = TX, \quad \text{so} \tag{D.139}$$

$$z(t,r) = \sum_{k=1}^{\infty} C_k\,\mathrm{e}^{-\left(\frac{ak\pi}{R}\right)^2 t} \sin\left(\frac{k\pi}{R}r\right). \tag{D.140}$$

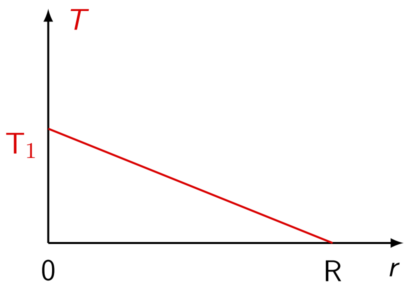

Figure D.2: Schematic representation of the profile of the function $w(r) = T_1 - \frac{T_1}{R} r$.

The Fourier coefficient will have the form

$$C_k = \frac{2}{R} \int_0^R r \left[f(r) - T_1 + \frac{T_1}{R} r \right] \sin\left(\frac{k\pi}{R} r\right) \mathrm{d}r. \tag{D.141}$$

The resulting function will be

$$u(t,r) = \underbrace{T_1 - \frac{T_1}{R} r}_{w} + \frac{2}{R} \int_0^R \left[f(r) - T_1 + \frac{T_1}{R} r \right] \times \sum_{k=1}^{\infty} \mathrm{e}^{-\left(\frac{ak\pi}{R}\right)^2 t} \sin\left(\frac{k\pi}{R} r\right) \mathrm{d}r. \tag{D.142}$$

D.2.5 Solution of hyperbolic partial differential equations by Fourier method

The following two simple solved examples illustrate the principle of using this method for hyperbolic PDEs:

- **Homogeneous wave equation:**

Consider the equation

$$u_{tt} = a^2 u_{xx}, \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.143}$$

with the Cauchy initial conditions (see Section 3.1.1)

$$u(0,x) = \varphi(x), \quad u_t(0,x) = \psi(x), \tag{D.144}$$

and with the mixed boundary conditions (see Section 3.2.1)

$$\alpha\, u(t,0) + \beta\, u_x(t,0) = 0, \quad \alpha\, u(t,\ell) + \beta\, u_x(t,\ell) = 0, \tag{D.145}$$

where α, $\beta \neq 0$. By separation of variables,

$$u(t,x) = T(t) X(x) \quad \text{and so} \quad \frac{\ddot{T}}{a^2 T} = \frac{X''}{X} = -\lambda^2, \tag{D.146}$$

we get after an adjustment,

$$\text{LHS: } \ddot{T} + a^2 \lambda^2 T = 0, \quad \text{RHS: } X'' + \lambda^2 X = 0. \tag{D.147}$$

From Equation (D.147), we get

$$T_k(t) = a_k \cos(\lambda_k a\, t) + b_k \sin(\lambda_k a\, t), \quad X_k(x) = c_k \cos(\lambda_k\, x) + d_k \sin(\lambda_k\, x), \tag{D.148}$$

Similarly to Equation (D.73), we get from the mixed boundary conditions (D.145)

$$\alpha + \beta\lambda = 0, \;\; \beta - \alpha\lambda = \beta^2 + \alpha^2 \neq 0, \quad \text{so} \quad \sin(\lambda_k\, x) = 0 \quad \text{and so} \quad \lambda_k = \frac{k\pi}{\ell}. \tag{D.149}$$

We thus get a solution for the spatial function (see Equation(D.74)),

$$X_k = c_k \cos\left(\frac{k\pi}{\ell}x\right) + d_k \sin\left(\frac{k\pi}{\ell}x\right). \tag{D.150}$$

Therefore, the general solution can be written in the form

$$u(t,x) = \sum_{k=1}^{\infty}\left[A_k \cos\left(\frac{ak\pi}{\ell}t\right) + B_k \sin\left(\frac{ak\pi}{\ell}t\right)\right]\left[\cos\left(\frac{k\pi}{\ell}x\right) + \sin\left(\frac{k\pi}{\ell}x\right)\right]. \tag{D.151}$$

From the Cauchy initial condition (D.144), we get

$$u(0,x) = \sum_{k=1}^{\infty} A_k \left[\cos\left(\frac{k\pi}{\ell}x\right) + \sin\left(\frac{k\pi}{\ell}x\right)\right] = \varphi(x), \tag{D.152}$$

and from the condition (D.144) we get

$$u_t(0,x) = \sum_{k=1}^{\infty} \frac{ak\pi}{\ell} B_k \left[\cos\left(\frac{k\pi}{\ell}x\right) + \sin\left(\frac{k\pi}{\ell}x\right)\right] = \psi(x) = \sum_{k=1}^{\infty} \frac{ak\pi}{\ell} B_k\, v_k. \tag{D.153}$$

The Fourier coefficients A_k, B_k can be found from Equations (D.152) and (D.153) (see also Equation (D.77)),

$$A_k = \frac{1}{\|v_k\|^2}\int_0^{\ell} \varphi(\xi)\, v_k(\xi)\, \mathrm{d}\xi, \quad B_k = \frac{\ell}{ak\pi\|v_k\|^2}\int_0^{\ell} \psi(\xi)\, v_k(\xi)\, \mathrm{d}\xi. \tag{D.154}$$

We solve the norm $\|v_k\|$ of the function v_k as a norm of a continuously defined vector (see Equation (2.1)), i.e.,

$$\|v_k\|^2 = \int_0^{\ell} v_k^2(\xi)\, \mathrm{d}\xi = \int_0^{\ell} \left[\cos\left(\frac{k\pi}{\ell}\xi\right) + \sin\left(\frac{k\pi}{\ell}\xi\right)\right]^2 \mathrm{d}\xi = \int_0^{\ell} \mathrm{d}\xi = \ell. \tag{D.155}$$

After substitution, we get the equation identical to Equation (D.151) in the form

$$\begin{aligned} u(t,x) = \sum_{k=1}^{\infty} &\left[\cos\left(\frac{k\pi}{\ell}x\right) + \sin\left(\frac{k\pi}{\ell}x\right)\right] \times \\ &\times \left[\frac{1}{\ell}\int_0^{\ell} \varphi(\xi)\, v_k(\xi)\cos\left(\frac{ak\pi}{\ell}t\right) \mathrm{d}\xi + \frac{1}{ak\pi}\int_0^{\ell} \psi(\xi)\, v_k(\xi)\, \sin\left(\frac{ak\pi}{\ell}t\right) \mathrm{d}\xi\right]. \end{aligned} \tag{D.156}$$

- **Inhomogeneous wave equation with homogeneous initial conditions:**

Consider the equation

$$u_{tt} = a^2 u_{xx} + f \quad (\text{where } f \text{ is the source of a wave energy}), \quad t > 0, \quad x \in \langle 0, \ell \rangle, \tag{D.157}$$

with the homogeneous Cauchy initial conditions (see Section 3.1.1)

$$u(0,x)=0, \quad u_t(0,x)=0, \tag{D.158}$$

and with the mixed boundary conditions (see Section 3.2.1)

$$\alpha\, u(t,0)+\beta\, u_x(t,0)=0, \quad \alpha\, u(t,\ell)+\beta\, u_x(t,\ell)=0, \tag{D.159}$$

where α, $\beta \neq 0$. As in the previous example,

$$u(t,x)=TX, \quad X(x)=A\sin(\lambda x)+B\cos(\lambda x)\,, \quad X_k(x)=v_k(x)=\sin\left(\frac{k\pi}{\ell}x\right). \tag{D.160}$$

We choose the equation in the form

$$u(t,x)=\sum_{k=1}^{\infty}C_k(t)\,v_k(x)=\sum_{k=1}^{\infty}C_k(t)\sin\left(\frac{k\pi}{\ell}x\right). \tag{D.161}$$

Using another condition, we get the inhomogeneous ordinary differential equation

$$\ddot{C}_k(t)+a^2\lambda_k^2C_k(t)=F_k(t), \quad \text{where} \quad F_k(t) \text{ is the so-called } \textit{Fourier coefficient of inhomogeneity}, \tag{D.162}$$

$$f(t,x)=\sum_{k=1}^{\infty}F_k(t)\sin\left(\frac{k\pi}{\ell}x\right), \quad \text{and so} \quad F_k(t)=\frac{2}{\ell}\int_0^{\ell}f(t,\xi)\sin\left(\frac{k\pi}{\ell}\xi\right)\mathrm{d}\xi. \tag{D.163}$$

Furthermore, we would have to solve the non-homogeneous differential equation of the second order (D.162) (for example by the method of variation of parameters - see Section 3.2.1) for a particular function $F_k(t)$. By including the initial conditions (D.158), we obtain the solution of Equation (D.162) at least in a general integrable form

$$C_k(t)=\frac{\ell}{ak\pi}\int_0^t F_k(\sigma)\sin\left[\frac{ak\pi}{\ell}(t-\sigma)\right]\mathrm{d}\sigma. \tag{D.164}$$

By substituting this into the equation of the general solution (D.161), we get (see the solution of the similar type equation in the case of a parabolic partial differential equations in Section D.2.3)

$$u(t,x)=\sum_{k=1}^{\infty}\frac{\ell}{ak\pi}\sin\left(\frac{k\pi}{\ell}x\right)\int_0^t F_k(\sigma)\sin\left[\frac{ak\pi}{\ell}(t-\sigma)\right]\mathrm{d}\sigma. \tag{D.165}$$

D.2.6 Demonstration of possible ways of solving simple elliptic partial differential equations

The following solved examples demonstrate some basic ways of calculating elliptical PDEs:

- **Laplace equation:**

The Laplace equation in Cartesian coordinates is in the simplest form defined as

$$u_{xx}(x,y) + u_{yy}(x,y) = 0. \tag{D.166}$$

In this example, we will solve the Laplace equation on the rectangular domain with dimensions a, b, with mixed Dirichlet and Neumann conditions (see Section 3.2.1), in the form

$$u(x,0) = 0,\ u(0,y) = 0,\ u_x(a,y) = 0\ (y \neq 0),\ u_y(x,b) = u_0 \sin\left(\frac{\pi}{2a}x\right)\ (x \neq 0). \tag{D.167}$$

By separating the variables $u(x,y) = X(x)Y(y)$ we get the equation

$$X''Y + XY'' = 0 \text{ and so } \frac{X''}{X} = -\frac{Y''}{Y} = \lambda, \tag{D.168}$$

where the constant λ can take the values $\lambda = 0,\ \lambda > 0,\ \lambda < 0$.

1. $\lambda = 0$: We will assume separate functions $X(x)$ and $Y(y)$ in the form of polynomials. According to the boundary conditions, the appropriate degree of the polynomials will be the first, so $X(x) = Ax + B$, $Y(y) = Cy + D$. From the boundary condition $u(0,y) = 0$ follows $B = 0 \vee C = D = 0$ but if $C = D = 0$, then $Y(y) = 0$ and so $u(x,y) = 0$ everywhere. If we continue with $B = 0$, we get $Ax(Cy + D) = 0$, and including another boundary condition $u(x,0) = 0$, then $AxD = 0$ must apply. Case $A = 0$ gives $X(x) = 0$, so $u(x,y) = 0$ everywhere. Considering also $D = 0$, then $u(x,y) = AxCy = 0$, and the next boundary condition $u_x(a,y) = 0$ implies $ACy = 0$, i.e., $A = 0 \vee C = 0$. However, in both cases $u(x,y) = 0$. Thus, the case $\lambda = 0$ gives only a trivial solution.

2. $\lambda > 0$: From Equation (D.168), we get a general solution in the form

$$u(x,y) = \left[A\cosh(\sqrt{\lambda}x) + B\sinh(\sqrt{\lambda}x)\right]\left[C\cos(\sqrt{\lambda}y) + D\sin(\sqrt{\lambda}y)\right]. \tag{D.169}$$

   The boundary condition $u(0,y) = 0$ implies $A[C\cos(\sqrt{\lambda}y) + D\sin(\sqrt{\lambda}y)] = 0$, hence $C = D = 0$. Then of course $Y(y) = 0$ and hence $u(x,y) = 0$ everywhere. If we continue with $A = 0$, we get $u(x,y) = B\sinh(\sqrt{\lambda}x)[C\cos(\sqrt{\lambda}y) + D\sin(\sqrt{\lambda}y)]$. Including another boundary condition $u(x,0) = 0$, then $BC\sinh(\sqrt{\lambda}x) = 0$ must apply. Case $B = 0$ gives $X(x) = 0$, i.e., $u(x,y) = 0$ everywhere. If we continue with $C = 0$, then $u(x,y) = BD\sinh(\sqrt{\lambda}x)\sin(\sqrt{\lambda}y)$, and another boundary condition $u_x(a,y) = 0$ implies $\sqrt{\lambda}BD\cosh(\sqrt{\lambda}a)\sin(\sqrt{\lambda}y) = 0$, that is, $B = 0 \vee D = 0$, and in both cases $u(x,y) = 0$. Thus, the case $\lambda > 0$ also gives only a trivial solution.

3. $\lambda < 0$: From Equation (D.168), we get a general solution in the form

$$u(x,y) = \left[A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)\right]\left[C\cosh(\sqrt{\lambda}y) + D\sinh(\sqrt{\lambda}y)\right]. \tag{D.170}$$

   The boundary condition $u(0,y) = 0$ implies $A[C\cosh(\sqrt{\lambda}y) + D\sinh(\sqrt{\lambda}y)] = 0$ hence $C = D = 0$, then $Y(y) = 0$ and hence $u(x,y) = 0$ everywhere. We continue with $A = 0$, we get $u(x,y) = B\sin(\sqrt{\lambda}x)[C\cosh(\sqrt{\lambda}y) + D\sinh(\sqrt{\lambda}y)]$. Including another boundary condition $u(x,0) = 0$, then $BC\sin(\sqrt{\lambda}x) = 0$ must hold. Case $B = 0$ gives $X(x) = 0$, i.e., $u(x,y) = 0$ everywhere. If we continue with $C = 0$, then $u(x,y) = BD\sin(\sqrt{\lambda}x)\sinh(\sqrt{\lambda}y)$, and another boundary condition $u_x(a,y) = 0$ obviously implies

$\sqrt{\lambda}BD\cos(\sqrt{\lambda}a)\sinh(\sqrt{\lambda}y) = 0$, that is, $B = 0 \vee D = 0$ (but in both cases $u(x,y) = 0$) $\vee \cos(\sqrt{\lambda}a) = 0$. The last case gives a solution

$$\cos(\sqrt{\lambda}a) = 0, \text{ so } \sqrt{\lambda} = \frac{(2k-1)\pi}{2a} \text{ and so}$$

$$u(x,y) = \sum_{k=1}^{\infty} K_k \sin\left[\frac{(2k-1)\pi}{2a}\,x\right] \sinh\left[\frac{(2k-1)\pi}{2a}\,y\right], \text{ where } K_k = BD. \tag{D.171}$$

If we also apply the fourth boundary condition, we get

$$u_0 \sin\frac{\pi}{2a}x = \sum_{k=1}^{\infty} K_k \sin\left[\frac{(2k-1)\pi}{2a}\,x\right] \sinh\left[\frac{(2k-1)\pi}{2a}\,b\right]. \tag{D.172}$$

The arguments of the sine function result in a solution only for $k = 1$, i.e., $K_1 = u_0 \,/\, \sinh[\pi b/(2a)]$. The resulting solution including all the boundary conditions will be

$$u(x,y) = u_0 \left[\sinh\left(\frac{\pi b}{2a}\right)\right]^{-1} \sin\left(\frac{\pi x}{2a}\right) \sinh\left(\frac{\pi y}{2a}\right). \tag{D.173}$$

Another typical elliptic partial differential equation can be the so-called *Poisson equation* of the type $\Delta u(x,y) = f(x,y)$, i.e., an inhomogeneous elliptical equation, most frequently used in the form of the gravitational Poisson equation, $\Delta\Phi = 4\pi G\rho$, where Φ is the gravitational potential, ρ is the density of matter and G is the gravitational constant, or the Poisson electrostatic potential equation, $\Delta\Phi = -\rho/\epsilon$, where ρ is the electric charge density, and ϵ is the permittivity. The solution of the multidimensional Poisson equation is analogous to the solution of the Laplace equation, and, for example, also to inhomogeneous hyperbolic partial differential equation.

- **Poisson equation with constant right-hand side:**

Let's solve a simple equation defined on the domain $x > y^2$, i.e., in the region bounded by the parabola $x = y^2$ with vertex at the point $[0,0]$ whose axis coincides with the positive part of the x-axis,

$$u_{xx}(x,y) + u_{yy}(x,y) = 2, \tag{D.174}$$

with the Dirichlet condition at the boundary, $u(y^2, y) = 0$. Let us assume a solution in the form containing all terms of a second-degree polynomial with undetermined coefficients,

$$u(x,y) = A + Bx + Cy + Dx^2 + Exy + Fy^2, \tag{D.175}$$

where, after the partial differentiation in the sense of Equation (D.174), we can easily find $F = 1 - D$. After substituting the boundary condition, i.e., from the equation

$$A + Cy + (B - D + 1)\,y^2 + Ey^3 + Dy^4 = 0, \tag{D.176}$$

we obtain nonzero coefficients only for $B = -1$, $F = 1$. So the sought solution will be

$$u(x,y) = y^2 - x. \tag{D.177}$$

- **Poisson equation with constant right-hand side on circular region, with inhomogeneous boundary condition:**

Within a circular area with a radius R, the following equation apply,

$$u_{xx}(x,y) + u_{yy}(x,y) = 4, \tag{D.178}$$

where the Dirichlet condition $u(x, y_1) = 1$ applies at the boundary of the region, resulting in $y_1 = \pm\sqrt{R^2 - x^2}$. Analogously to parabolic equations with inhomogeneous boundary conditions, we separate the searched function $u(x,y)$ into the sum of two functions, for example, $U(x,y)$ and $v(x,y)$, for which the following relations

$$u(x,y) = U(x,y) + v(x,y),\ U_{xx} + U_{yy} = 4,\ U(x,y_1) = 0,\ v_{xx} + v_{yy} = 0,\ v(x,y_1) = 1 \tag{D.179}$$

hold. As in the previous case, we assume for each function a complete polynomial of the second degree with undetermined coefficients,

$$U(x,y) = A + Bx + Cy + Dx^2 + Exy + Fy^2, \tag{D.180}$$

$$v(x,y) = a + bx + cy + dx^2 + exy + fy^2, \tag{D.181}$$

which gives $F = 2 - D$, $f = -d$. After substituting the boundary condition, Equations (D.180) and (D.181) can be rewritten in the form

$$A + Bx \pm (C + Ex)\sqrt{R^2 - x^2} + 2(D-1)x^2 + (2-D)R^2 = 0, \tag{D.182}$$

$$a + bx \pm (c + ex)\sqrt{R^2 - x^2} + 2dx^2 - dR^2 = 1. \tag{D.183}$$

The particular non-zero coefficients will be $A = -R^2$, $D = 1$, $F = 1$, $a = 1$. Summing Equations (D.182) and (D.183) gives the desired resulting function

$$u(x,y) = 1 - R^2 + x^2 + y^2. \tag{D.184}$$

- **Poisson equation with general right-hand side, mixed boundary conditions:**

Let's solve in a similar way the Poisson equation given as

$$u_{xx}(x,y) + 4u_{yy}(x,y) = xy, \tag{D.185}$$

with the boundary conditions $u(0,y) = y^2$, $u_x(0,y) = 0$. In order to get the terms of the required degree after differentiation, we must now assume a solution in the form of a complete polynomial of the fourth degree with undetermined coefficients,

$$\begin{aligned} u(x,y) = A + Bx + Cy + Dx^2 + Exy + Fy^2 + Gx^3 + Hx^2y + Ixy^2 + Jy^3 + \\ + Kx^4 + Lx^3y + Mx^2y^2 + Nxy^3 + Qy^4. \end{aligned} \tag{D.186}$$

Thus, the corresponding second derivatives in this case will be

$$u_{xx} = 2D + 6Gx + 2Hy + 12Kx^2 + 6Lxy + 2My^2, \tag{D.187}$$

$$u_{yy} = 2F + 2Ix + 6Jy + 2Mx^2 + 6Nxy + 12Qy^2. \tag{D.188}$$

For the particular coefficients, we get

$$D = -4F,\ G = -\frac{4}{3}I,\ H = -12J,\ K = -\frac{2}{3}M,\ L = \frac{1-24N}{6},\ M = -24Q. \tag{D.189}$$

Substituting the Dirichlet boundary condition, we get $A = 0$, $C = 0$, $F = 1$, $J = 0$, $Q = 0$, and the relations (D.189) immediately result in $D = -4$, $H = 0$, $K = 0$, $M = 0$. By substituting the Neumann boundary condition we get $B = 0$, $E = 0$, $I = 0$, $N = 0$, then the relations (D.189) result in $G = 0$, $L = 1/6$. Substituting nonzero coefficients into equation (D.186) gives the desired resulting function,

$$u(x, y) = -4x^2 + y^2 + \frac{1}{6}x^3y. \tag{D.190}$$

This problematic is described in detail in the textbook Franců (2011).

Appendix E

Practical basics of numerical calculations ★

The aim of this chapter is not to give a systematic description of basic methods of numerical mathematics but only briefly and illustratively clarify some principles and possible procedures in practical numerical modeling of the most frequent (above described) analytical topics. In this respect, I refer those interested, for example, to lecture notes Humlíček (2009) or the corresponding textbooks (for example Přikryl, 1985; Vitásek, 1987; Čermák & Hlavička, 2006, etc.). Selected problems of simple modeling are also accompanied by examples of very elementally written programming scripts for a given problem (with explanatory notes in blue letters), occasionally even by pictures and graphs of the resulting models. Programming scripts are demonstrated here in the most elementary form, without any subroutines, modules, and other "program improvements", in which, however, the nature of the algorithm, especially for beginners, may be lost.

The extensive use of numerical mathematics in most science and technology disciplines has also resulted in the development of many completed libraries written in major programming languages; their well-arranged repositories can be found on the pages GAMS (Guide to Available Mathematical Software) `http://gams.nist.gov/`. Some of them are commercial (and quite complex), such as NAG (Numerical Algorithmus Group) `https://www.nag.com/content/nag-library` or IMSL (International Mathematics and Statistics Library) `http://www.roguewave.com/products-services/imsl-numerical-libraries`, others are freely available and are usually focused on a specific area, such as FFTPACK `http://www.netlib.org/fftpack/` - (fast) Fourier transform, LAPACK (see Section E.1) - linear algebra, MINPACK `http://www.netlib.org/minpack/` - nonlinear equations, etc. Their full or partial implementation can significantly speed up and facilitate the creation and quality of the eventual user's own algorithms.

E.1 Numerical methods of linear algebra

In this section, we will not discuss individual methods of numerical solutions of linear algebra, there is an extensive literature (e.g., Humlíček (2009)), describing both the numerical equations and their stability and the *condition number* (i.e., the determination of the precision of numerical matrix algorithms), error estimates, etc. Currently, there are many ready-made packages

★ are marked paragraphs, and examples, intended primarily for students of higher semesters and years of bachelor study.

(procedures), consisting of particular subroutines (libraries), designed to solve specific or even combined algebraic problems (for example, solving systems of linear equations, solving the so-called *tridiagonal* matrices (i.e., matrices with nonzero elements only on the main and both adjacent diagonals), finding determinants, inverse matrices, eigenvalues and eigenvectors, etc. One of the most powerful such packages that we will present in more detail here is the software package LAPACK (Linear Algebra PACKage, Anderson et al. (1999)), which evolved from older packages EISPACK and LINPACK and is designed for Fortran 77, Fortran 90; there are also C++ versions. There are extended versions of this package or other libraries based on it, with built-in subroutines for parallelization on powerful computer clusters (see Section E.6) such as ScaLAPACK, MAGMA, MORSE, CHAMELEON, etc.

The LAPACK software package is a freely available software library and can be installed either from the software distribution center of the used system distribution or from the web address `http://www.netlib.org/lapack`. When compiling the program file we use, we have to enter a reference to LAPACK, for example: `gfortran filename.f95 -llapack`. Descriptions of individual subroutines and their use (e.g., the DGBSV library for solving systems of real linear equations of any number of variables, or DGTSV that is appropriate for solving tridiagonal matrices, etc.) are available in user guides such as Anderson et al. (1999).

- Sample scheme of DGBSV subroutine, designed for solving a system of linear equations:

N	(entry, INTEGER) = number of equations = order of square matrix A, N $\geq$ 0.
KL	(entry, INTEGER) = number of subdiagonals within the band of A, KL $\geq$ 0.
KU	(entry, INTEGER) = number of superdiagonals within the band of A, KU $\geq$ 0.
NRHS	(entry, INTEGER) = number of right-hand sides, i.e., the number of columns of the matrix B, NRHS $\geq$ 0.
AB	(entry/exit, DOUBLE PRECISION) = array, dimension (LDAB,N). On entry: the matrix A in band storage, in rows KL+1 to 2*KL+KU+1; rows 1 to KL of the array need not be set. The j-th column of A is stored in the j-th column of the array AB as follows: AB(KL+KU+1+i-j, j) = A(i,j) for max(1, j-KU) $\leq$ i $\leq$ min(N, j+KL). On exit, details of the factorization: the matrix U is stored as an upper triangular band matrix with KL+KU superdiagonals in rows 1 to KL+KU+1, and the multipliers used during the factorization are stored in rows KL+KU+2 to 2*KL+KU+1 (see the scheme below).
LDAB	(entry, INTEGER) = leading dimension of the array AB. LDAB $\geq$ 2*KL+KU+1.
IPIV	(exit, INTEGER) = array, dimension N, pivot indices that define the permutation matrix; row i of the matrix was interchanged with row IPIV(i).
B	(entry/exit, DOUBLE PRECISION) = array, dimension (LDB,NRHS), on entry, the N-by-NRHS right-hand side matrix B, on exit, if INFO = 0, the N-by-NRHS solution matrix X.
LDB	(entry, INTEGER) = leading dimension of the array B, LDB $\geq$ max(1,N).
INFO	(exit, INTEGER) = 0: successful exit, < 0: if INFO = -i, the i-th argument had an illegal value, > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and the solution has not been computed.

FURTHER DETAILS:

The band storage scheme is illustrated by the following example, where M = N = 6, KL = 2, KU = 1:

On entry:

*	*	*	+	+	+
*	*	+	+	+	+
*	a12	a23	a34	a45	a56
a11	a22	a33	a44	a55	a66
a21	a32	a43	a54	a65	*
a31	a42	a53	a64	*	*

On exit:

*	*	*	u14	u25	u36
*	*	u13	u24	u35	u46
*	u12	u23	u34	u45	u56
u11	u22	u33	u44	u55	u66
m21	m32	m43	m54	m65	*
m31	m42	m53	m64	*	*

Array elements marked * are not used by the routine; elements marked + need not be set on entry, but are required by the routine to store elements of U because of fill-in resulting from the row interchanges.

- Sample scheme of DGTSV subroutine, designed for solving a tridiagonal matrices:

  N (entry, INTEGER) = number of equations = order of the squared tridiagonal matrix A, N $\geq$ 0.

  NRHS (entry, INTEGER) = number of right-hand sides, i.e., the number of columns of the matrix B, NRHS $\geq$ 0.

  DL (entry/exit, DOUBLE PRECISION) = array, dimension N-1, on entry, DL must contain the N-1 sub-diagonal elements of A, on exit, DL is overwritten by the N-2 elements of the second super-diagonal of the upper triangular matrix U from the LU factorization.

  D (entry/exit, DOUBLE PRECISION) = array, dimension N, on entry, D must contain the diagonal elements of A, on exit, D is overwritten by the N diagonal elements of U.

  DU (vstup/výstup, DOUBLE PRECISION) = array, dimension N-1, on entry, DU must contain the N-1 super-diagonal elements of A, on exit, DU is overwritten by the N-1 elements of the first super-diagonal of U.

  B (entry/exit, DOUBLE PRECISION) = array, dimension (LDB,NRHS), on entry, the N by NRHS matrix of right-hand side matrix B, on exit, if INFO = 0, the N by NRHS solution matrix X.

  LDB (vstup, INTEGER) = leading dimension of the array B, LDB $\geq$ max(1,N).

  INFO (výstup, INTEGER) = 0: successful exit, < 0: if INFO = -i, the i-th argument had an illegal value, > 0: if INFO = i, U(i,i) is exactly zero, and the solution has not been computed.

Other libraries are constructed in a similar way. Examples of solutions and program scripts with reference to LAPACK are given in the following Sections E.2.1, E.3.1, E.3.2, E.3.3, E.5.1, E.5.7, etc.

E.2 Interpolation

By interpolation we mean substitution of more complex functional dependence by a simpler, i.e., an approximation of a given function by another appropriate function. By interpolation approximation we mean an interpolation of a discrete function, i.e., of a function given by a finite set of points of its domain and their assigned functional values (usually represented by a table), using the function (or its derivatives), which at these points have the same values as the original function. The most suitable interpolation functions are polynomials of various (selected) degree, e.g., the so-called *Lagrange* and *Newton* interpolation polynomial (Humlíček, 2009; Vitásek, 1987) or the so-called *splines*. The following Section E.2.1 briefly shows frequently used the so-called *cubic interpolation spline* for one-dimensional interpolations. Two-dimensional *bilinear* and *bicubic* interpolations using two-dimensional polynomials of the 1st and 3rd degree, respectively, are documented in Sections E.2.2 and E.2.3.

In practical calculations, it is always necessary to consider or test which type of interpolation best fits to the given task. For example, if there are large disproportions between the spacing of the specified points (i.e. the "grid" of points being dense or very sparse in different regions), it is better to use simpler "piecewise" linear interpolation, because interpolation by a continuous function (for example by the cubic interpolation spline, see Section E.2.1) may strongly "oscillate" in the sparse areas. Alternatively, it is possible to use different types of approximations for different regions of the interpolated dependence (and to connect them appropriately in the "meeting" points).

E.2.1 Cubic interpolation spline

is one of the most frequently used interpolation functions. This is the so-called *piecewise* interpolation polynomial of the third degree s_i in the form

$$S(x) = s_1(x) \text{ for } x_1 \le x < x_2,\ s_2(x) \text{ for } x_2 \le x < x_3, \ldots, s_{n-1}(x) \text{ for } x_{n-1} \le x < x_n, \tag{E.1}$$

defined as

$$s_i(x) = a_i(x-x_i)^3 + b_i(x-x_i)^2 + c_i(x-x_i) + d_i, \tag{E.2}$$

whose second derivatives we denote as M_i. It is thus a set of cubic functions (pieces) that are joined to each other at the specified points (knots) $[x_i, y_i]$ by the functional value and the first and second derivatives. There are different types of these splines according to boundary conditions, for example, the so called *natural spline* is determined by the boundary conditions $M_1 = M_n = 0$, the *parabolically terminated spline* is determined by the boundary conditions $M_1 = M_2$, $M_n = M_{n-1}$ (the extrapolation of zeroth-order), the *cubic terminated spline* is determined by the boundary conditions $M_1 = 2M_2 - M_3$, $M_n = 2M_{n-1} - M_{n-2}$ (the extrapolation of first-order or also linear extrapolation), etc.

From the conditions of the continuity of the functional values and the first and second derivatives at the points x_i, for $i = 0, \ldots, n-1$ the following implies:

$$s_i(x_i) = y_i, \qquad s_i(x_{i+1}) = y_{i+1}, \tag{E.3}$$

$$s'_{i-1}(x_i) = s'_i(x_i) = c_i, \qquad s''_{i-1}(x_i) = s''_i(x_i) = M_i = 2b_i. \tag{E.4}$$

These internal conditions are further supplemented by the two boundary conditions given by the spline type. By comparing all of these conditions at all knots $[x_i, y_i]$, we get a set of linear equations for unknown second derivatives M_i at the inner knots:

$$(x_{i+1}-x_i)\,M_{i+1} + 2\,(x_{i+1}-x_{i-1})\,M_i + (x_i - x_{i-1})\,M_{i-1} = 6\left(\frac{y_{i+1}-y_i}{x_{i+1}-x_i} - \frac{y_i - y_{i-1}}{x_i - x_{i-1}}\right). \tag{E.5}$$

This system of equations can be written using the so-called *tridiagonal matrix* in the form (where we introduce $\Delta x_i = x_{i+1} - x_i$, $\Delta^+ x_i = x_{i+1} - x_{i-1}$, $\Delta y_i = y_{i+1} - y_i$, $\Delta_j = \Delta y_j / \Delta x_j$, $\Delta_j^i = \Delta y_i / \Delta x_i - \Delta y_j / \Delta x_j$):

$$\begin{pmatrix} 2\Delta x_{n-1} & \Delta x_{n-1} & & & & \\ \Delta x_{n-1} & 2\Delta^+ x_{n-1} & \Delta x_{n-2} & & & \\ & \Delta x_{n-2} & 2\Delta^+ x_{n-2} & \Delta x_{n-3} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \Delta x_2 & 2\Delta^+ x_2 & \Delta x_1 \\ & & & & \Delta x_1 & 2\Delta x_1 \end{pmatrix} \begin{pmatrix} M_n \\ M_{n-1} \\ M_{n-2} \\ \vdots \\ M_2 \\ M_1 \end{pmatrix} = 6 \begin{pmatrix} -\Delta_{n-1} \\ \Delta_{n-2}^{n-1} \\ \Delta_{n-3}^{n-2} \\ \vdots \\ \Delta_1^2 \\ \Delta_1 \end{pmatrix}, \quad \text{(E.6)}$$

which we solve, for example, using an appropriate package library LAPACK (see Section E.1). The particular coefficients of Equation (E.2) can then be easily calculated:

$$d_i = y_i, \quad c_i = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} - (M_{i+1} + 2M_i) \frac{x_{i+1} - x_i}{6}, \quad b_i = \frac{M_i}{2}, \quad a_i = \frac{M_{i+1} - M_i}{6\,(x_{i+1} - x_i)}. \quad \text{(E.7)}$$

In the case of a constant step of an independent variable $x_{i+1} - x_i = h = \text{const.}$, Equation (E.5) simplifies to the form

$$M_{i+1} + 4M_i + M_{i-1} = \frac{6}{h^2} (y_{i+1} - 2y_i + y_{i-1}), \quad \text{(E.8)}$$

the matrix (E.6) will thus take the form

$$\begin{pmatrix} 2 & 1 & & & & \\ 1 & 4 & 1 & & & \\ & 1 & 4 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 2 \end{pmatrix} \begin{pmatrix} M_n \\ M_{n-1} \\ M_{n-2} \\ \vdots \\ M_2 \\ M_1 \end{pmatrix} = \frac{6}{h^2} \begin{pmatrix} -\Delta y_{n-1} \\ \Delta y_{n-1} - \Delta y_{n-2} \\ \Delta y_{n-2} - \Delta y_{n-3} \\ \vdots \\ \Delta y_2 - \Delta y_1 \\ \Delta y_1 \end{pmatrix}. \quad \text{(E.9)}$$

- Example of a program script for natural cubic interpolation spline (Fortran 95):

program nat3_splajn	program name declaration
implicit none	command that prevents automatic assignment of letters i, j, k, l, m, n for integer variables and other letters for real variables (i.e., expressed by numbers with decimal expansion)

table of the values $[x_i, y_i]$:
[1,1], [2,3], [3,4], [4,1.5], [5,1.5], [6,5], [7,7], [8,5], [9,2], [10,0]

integer :: i, j, np	declaration of integer variables: i = sequence number of independent variable, j = sequence number of linear equation, np = total number of discrete values
parameter (np=10)	enter fixed value of np that cannot be changed in the program

```
integer :: INFO,KL,KU,LDAB,LDB,N,RHS
```
declaration of integer variables of the LAPACK procedure - see Section E.1

```
parameter(KL=np-3,KU=np-3,N=np-2,KUKL=KL+KU+1,LDAB=2*KL+KU+1,&
LDB=N,RHS=1)
```
enter fixed values of integer parameters

```
integer :: IPIV(N)
```
enter a parameter as an array of N elements

```
double precision, dimension(np) :: x, y
```
declaration of real quantities x, y as a field (vector) of np elements with the so-called double precision, allowing to calculate a number to 16 decimal places and to a power of about 10^{300} (depending on computer parameters)

```
double precision, dimension(np) :: M(N,N),AB(LDAB,N),B(LDB,RHS)
```
enter parameters as two-dimensional arrays

```
double precision :: f(np), res(np), a(np), b(np), c(np), d(np)
```
another way of declaring real quantities as an array (vector) with np elements with double precision

```
double precision :: h
```
declaration of real scalar quantities

```
parameter (h=1.d0)
```
enter a fixed interval value of an independent variable that cannot be changed in the program

```
x=(/(1.d0*i, i=1,np)/)
```
vector of values of independent variable

```
y=(/1.d0, 3.d0, 4.d0, 1.5d0, 1.5d0, 5.d0, 7.d0, 5.d0, 2.d0, 0.d0/)
```
y (measured) values, np = number of measured values

```
do i=1,N
   do j=1,N
      if(j.eq.i)then
         M(i,j)=4.d0
      elseif(j.eq.i-1)then
         M(i,j)=1.d0
      elseif(j.eq.i+1)then
         M(i,j)=1.d0
      else
         M(i,j)=0.d0
      endif
   end do
end do
```
cycle of calculation of second derivatives M, enter of tridiagonal matrix

```
do i=1,N
   do j=1,N
      AB(KUKL+i-j, j)=M(i,j)
   end do
end do
```
LAPACK calculation cycle

```
do i=1,N
   B(i,1)=6.d0/h**2.d0*(y(i)-2.d0*y(i+1)+y(i+2))
end do
```
right-hand side calculation

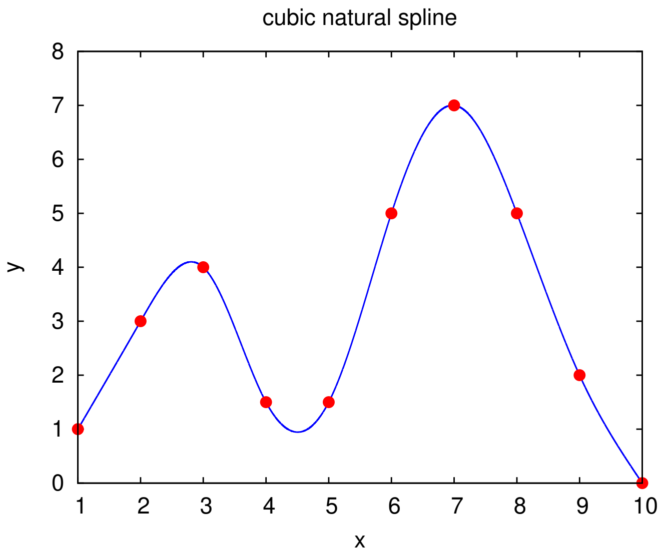

Figure E.1: Graph of the cubic natural interpolation spline described in Section E.2.1.

```
call the DGBSV subroutine (see Section E.1):
call DGBSV(N,KL,KU,1,AB,LDAB,IPIV,B,N,INFO)
if(INFO.ne.0) write(*,*) "INFO=",INFO,"!!!"
a(1)=B(1,1)/6.d0/h                        calculation of coefficients a, b, c, d in the
                                          first spline piece
b(1)=0.d0
c(1)=(y(2)-y(1))/h-B(1,1)/6.d0*h
d(1)=y(1)
do i=2,np-2                               cycle of calculation of coefficients a, b, c, d
                                          in internal spline pieces
   a(i)=(B(i,1)-B(i-1,1))/6.d0/h
   b(i)=B(i-1,1)/2.d0
   c(i)=(y(i+1)-y(i))/h-(B(i,1)+2.d0*B(i-1,1))/6.d0*h
   d(i)=y(i)
end do
a(np-1)=-B(N,1)/6.d0/h                    calculation of coefficients in the last piece
b(np-1)=B(N,1)/2.d0
c(np-1)=(y(np)-y(np-1))/h-2.d0*B(N,1)/6.d0*h
d(np-1)=y(np-1)
do i=1,np-1                               writing coefficients to file fort.1
   write(1,*) a(i), b(i), c(i), d(i)
end do
end program nat3_splajn                   exit the program
```

E.2.2 Bilinear interpolation

In practice, interpolations of functions of two or more variables are often very important. For example, we want to interpolate a table of measured values of a certain quantity at different times and at different distances from the selected reference point, both for intermediate times

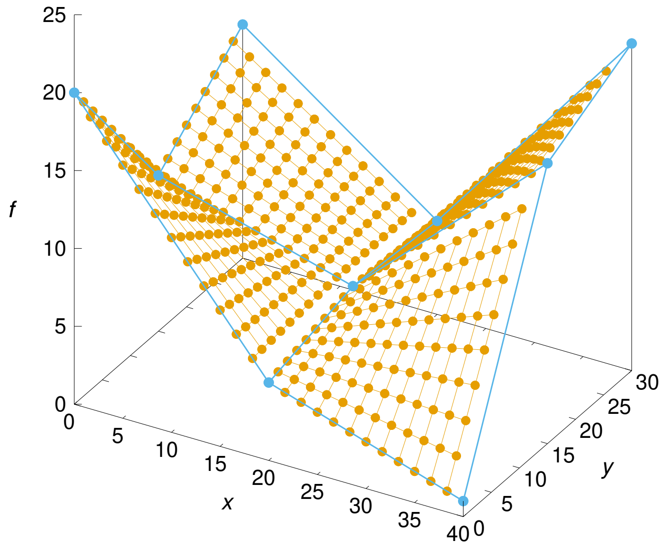

Figure E.2: Schematic representation of bilinear interpolation. The points of the function $f(x_\alpha, y_\beta)$ are located in the knots of the blue grid (highlighted by blue rings), the yellow grid represents its interpolation, where each cell of the blue grid is in the x-direction divided into 12 sub-intervals, and in the y-direction into nine sub-intervals. Due to the chosen computational algorithm, the interpolation at the "outer" edges of the blue cells is incomplete; in case of other adjacent blue cells, they would be counted at their "inner" edges.

and intermediate positions. These interpolations are also very often used in digital image processing, where the color and intensity values of individual scanned pixels are recalculated for intermediate points to achieve an (apparently) higher resolution.

The simplest two-dimensional interpolation is the so-called *bilinear interpolation* of a two-variable function, which is an extension of the linear interpolation to two dimensions. We assign the values 0 and 1 to the indexes i, j for the "inner" and "outer" of the piecewise interpolated area (grid cell) in both directions in each intermediate step. For both the entered and interpolated function values (we note that $\lim_{x\to 0} x^0 = 1$) holds

$$f(x,y) = \sum_{i=0}^{1}\sum_{j=0}^{1} a_{ij} x^i y^j = a_{00} + a_{01}y + a_{10}x + a_{11}xy, \tag{E.10}$$

with unknown elements of a *constant* 1×4 matrix $\boldsymbol{a} = a_{ij}$ (where the superscripts i, j in Equation (E.10) mean powers). Let's denote x, y the *relative* (with respect to the cell origin) coordinates of the interpolated value (of the "interpolant"), and x_α, y_β $(\alpha, \beta = 0, 1)$ coordinates of cell edges with the specified values $\boldsymbol{f}_0 = [f(x_0, y_0), f(x_0, y_1), f(x_1, y_0), f(x_1, y_1)]$, $\boldsymbol{k} = x^i y^j$ and $\boldsymbol{A} = x_\alpha^i y_\beta^j$ (matrix 4×4). From Equation (E.10) one gets $\boldsymbol{f}_0 = \boldsymbol{a}\boldsymbol{A}$ and so $\boldsymbol{a} = \boldsymbol{A}^{-1}\boldsymbol{f}_0$. At the same time $f(x,y) = \boldsymbol{a} \cdot \boldsymbol{k} = \boldsymbol{k} \cdot \boldsymbol{a}$ must hold, so

$$f(x,y) = \boldsymbol{k}\boldsymbol{A}^{-1}\boldsymbol{f}_0. \tag{E.11}$$

We will illustrate this principle using an example of one "cell" with the coordinates of the edges $x_0 = 0$, $x_1 = 20$, $y_0 = 0$, $y_1 = 15$ and with the entered values $f(x_0, y_0) = 20$, $f(x_0, y_1) = 10$, $f(x_1, y_0) = 5$, $f(x_1, y_1) = 6.5$ ("left bottom" blue cell in Figure E.2). Within this cell we want to find the bilinear interpolant $f(x, y)$, for example, at the point $x = 10$, $y = 5$. The explicit notation of Equation (E.11) in this case will be

$$f(10,5) = (1,5,10,50)\begin{pmatrix}1 & 0 & 0 & 0\\ 1 & 15 & 0 & 0\\ 1 & 0 & 20 & 0\\ 1 & 15 & 20 & 300\end{pmatrix}^{-1}\begin{pmatrix}20\\ 10\\ 5\\ 6.5\end{pmatrix} = \frac{133}{12}. \tag{E.12}$$

In the same way, interpolations in other entered cells will be calculated.

The following numerical algorithm illustrates how to calculate the bilinear interpolation of a two-dimensional mesh consisting of four cells with specified values at the corners, where each grid cell is divided into 12 sub-intervals in the x-direction and into nine sub-intervals in the y-direction. The result of the interpolation is shown in Figure E.2.

- Example of a script for bilinear interpolation on four spatial cells of a two-dimensional discrete function (Fortran 95):

```
program bilinear                              program name declaration
implicit none
integer :: i, j, ii, jj                       declaration of integer variables: i, j = se-
                                              rial numbers of "blue" points (nodes) of the
                                              grid, ii, jj = serial numbers of bilinear in-
                                              terpolation knots (yellow grid)
parameter (ni=3, nj=3, nii=13, njj=10)        enter a range of declared variables
double precision :: x(ni), y(nj), f(ni,nj)    entering real variables with double precision
double precision :: p(ni,nii), q(nj,njj), ff(ni,nj, nii,njj)
double precision, parameter :: dx=40.d0, dy=30.d0
                                              enter the size of the entire domain
calculation of coordinates of grid nodes with specified values of function f:
do i=1,ni
   x(i)=dx/dfloat(ni-1)*dfloat(i-1)
end do
do j=1,nj
   y(j)=dy/dfloat(nj-1)*dfloat(j-1)
end do
tabular enumeration of the values of the function f at the nodes (the 1st sequence number
corresponds to the x direction, the 2nd to the direction y):
f(1,1)=20.d0
f(2,1)=5.d0
f(3,1)=1.d0
f(1,2)=10.d0
f(2,2)=6.5d0
f(3,2)=18.d0
f(1,3)=15.d0
f(2,3)=6.d0
f(3,3)=21.d0
print a (node) grid with the specified values of the function f into the file fort.10:
do i=1,ni
```

```
    do j=1,nj
        write(10,*) x(i), y(j), f(i,j)
    end do
    write(10,*)
end do

calling the subroutine to calculate interpolations in particular cells of a nodal grid:
call interpol(ni,nj,nii,njj,x,y,p,q,dx,dy,f,ff)

stop
end program bilinear                              end of main program

- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

subroutine for interpolation calculation:
subroutine interpol(ni,nj,nii,njj,x,y,p,q,dx,dy,f,ff)
implicit none

integer :: i, j, k, ii, jj
integer, intent(in) :: ni, nj, nii, njj
double precision, intent(in) :: x(ni), y(nj), dx, dy, f(ni,nj)
double precision :: xx(nii), yy(njj)
double precision, intent(out) :: p(ni,nii), q(nj,njj), ff(ni,nj,nii,njj)

double precision :: B1(ni-1,nj-1), B2(ni-1,nj-1), B3(ni-1,nj-1), B4(ni-1,nj-1)

integer :: INFO
integer, parameter :: N=4
double precision, dimension(N,N) :: A
integer,dimension(size(A,1)) :: IPIV
double precision, dimension(size(A,1),size(A,2)) :: AINV
double precision, dimension(size(A,1)) :: WORK

matrix A:
do i=1,N                                          zero matrix initialization
    do j=1,N
        A(i,j)=0.d0
    end do
end do

A(1,1)=1.d0                                       nonzero elements of the matrix A
A(2,1)=1.d0
A(2,3)=dy/dfloat(nj-1)
A(3,1)=1.d0
A(3,2)=dx/dfloat(ni-1)
A(4,1)=1.d0
A(4,2)=dx/dfloat(ni-1)
A(4,3)=dy/dfloat(nj-1)
A(4,4)=dx/dfloat(ni-1)*dy/dfloat(nj-1)


We save A as AINV to avoid overwriting it
AINV=A

- - - - - LAPACK procedure to calculate the inverse matrix - - - - -
```

```
the DGETRF procedure calculates the LU factorization of a general matrix A.
call DGETRF(N,N,AINV,N,IPIV,INFO)
if(INFO.ne.0) write(*,*) "Matrix is numerically singular!"
   stop
endif
the DGETRI procedure calculates the inverse matrix
call DGETRI(N,AINV,N,IPIV,WORK,N,INFO)
if(INFO.ne.0) write(*,*) "Matrix inversion failed!"
   stop
endif
- - - - - End of the LAPACK procedure - - - - -
do ii=1,nii
   xx(ii)=dx/dfloat(ni-1)/dfloat(nii-1)*dfloat(ii-1)
end do
do jj=1,njj
   yy(jj)=dy/dfloat(nj-1)/dfloat(njj-1)*dfloat(jj-1)
end do
do i=1,ni-1
   do j=1,nj-1
      B1(i,j)=AINV(1,1)*f(i,j)+AINV(1,2)*f(i,j+1)+AINV(1,3)*f(i+1,j) &
             +AINV(1,4)*f(i+1,j+1)
      B2(i,j)=AINV(2,1)*f(i,j)+AINV(2,2)*f(i,j+1)+AINV(2,3)*f(i+1,j) &
             +AINV(2,4)*f(i+1,j+1)
      B3(i,j)=AINV(3,1)*f(i,j)+AINV(3,2)*f(i,j+1)+AINV(3,3)*f(i+1,j) &
             +AINV(3,4)*f(i+1,j+1)
      B4(i,j)=AINV(4,1)*f(i,j)+AINV(4,2)*f(i,j+1)+AINV(4,3)*f(i+1,j) &
             +AINV(4,4)*f(i+1,j+1)
   end do
end do
absolute coordinates p,q:
do i=1,ni-1
   do ii=1,nii-1
      p(i,ii)=xx(ii)+x(i)
   end do
end do
do j=1,nj-1
   do jj=1,njj-1
      q(j,jj)=yy(jj)+y(j)
   end do
end do
interpolant calculation:
do i=1,ni-1
   do j=1,nj-1
      do ii=1,nii-1
         do jj=1,njj-1
            ff(i,j,ii,jj)=B1(i,j)+yy(jj)*B2(i,j)+xx(ii)*B3(i,j)+xx(ii)*yy(jj)*B4(i,j)
         end do
```

```
            end do
        end do
    end do

    writing interpolants of function f into the file fort.11:
    do i=1,ni-1
        do j=1,nj-1
            do ii=1,nii-1
                do jj=1,njj-1
                    write(11,*) p(i,ii), q(j,jj), ff(i,j,ii,jj)
                end do
                write(11,*)
            end do
            write(11,*)
        end do
        write(11,*)
    end do

    return
    end subroutine interpol
```

E.2.3 Bicubic interpolation

Bilinear interpolation is often inappropriate, since the interpolated surfaces of individual cells of a given function form a discontinuous surface as a whole. Therefore, it is preferable to use the so-called *bicubic interpolation*, which is a two-dimensional analogue of continuous interpolation of a one-dimensional function by the third-degree polynomial, for example, by a cubic interpolation spline (see Section E.2.1).

Not only the functional values of interpolation cubic curves, but also their first derivative and the mixed second derivative must coincide at the interface of particular interpolated cells. By analogy to Equation (E.10) (including the notation method introduced in Section E.2.2), we get

$$f(x,y) = \sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij}x^i y^j, \tag{E.13}$$

$$f_x(x,y) = \sum_{i=1}^{3}\sum_{j=0}^{3} i a_{ij}x^{i-1} y^j, \tag{E.14}$$

$$f_y(x,y) = \sum_{i=0}^{3}\sum_{j=1}^{3} j a_{ij}x^i y^{j-1}, \tag{E.15}$$

$$f_{xy}(x,y) = \sum_{i=1}^{3}\sum_{j=1}^{3} ij a_{ij}x^{i-1} y^{j-1}, \tag{E.16}$$

where the superscripts $i, j, i-1, j-1$ mean powers.

For the same given function $\boldsymbol{f}_0(x_\alpha, y_\beta)$ as in Section E.2.2, Equations (E.13) - (E.16) for the

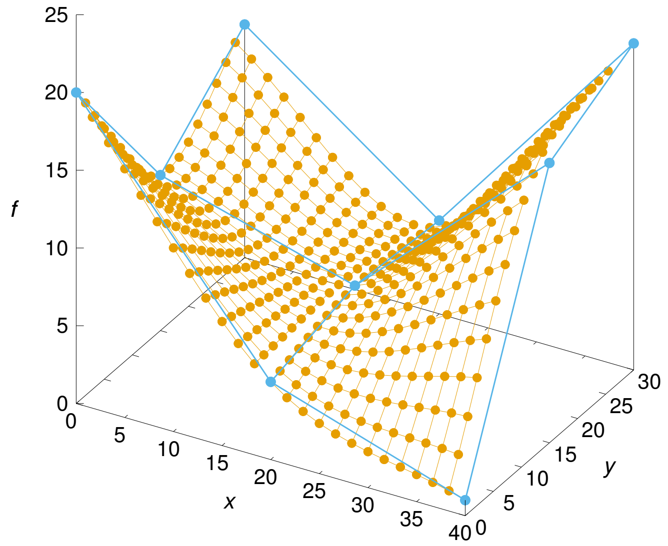

Figure E.3: Schematic representation of bicubic interpolation of the same (blue) grid as in Figure E.2.

"bottom left" cell will be explicitly written as:

$$f_0(0,0) = a_{00}, \tag{E.17}$$
$$f_0(0,15) = a_{00} + 15a_{01} + 225a_{02} + 3375a_{03}, \tag{E.18}$$
$$f_0(20,0) = a_{00} + 20a_{10} + 400a_{20} + 8000a_{30}, \tag{E.19}$$
$$\begin{aligned} f_0(20,15) &= a_{00} + 15a_{01} + 225a_{02} + 3375a_{03} + 20a_{10} + 300a_{11} + 4500a_{12} + 67\,500\,a_{13}+ \\ &+ 400a_{20} + 6000a_{21} + 90\,000\,a_{22} + 1\,350\,000\,a_{23} + 8000a_{30} + 120\,000\,a_{31} + 1\,800\,000\,a_{32}+ \\ &+ 27\,000\,000\,a_{33}. \end{aligned} \tag{E.20}$$

$$f_{0x}(0,0) = a_{10}, \tag{E.21}$$
$$f_{0x}(0,15) = a_{10} + 15a_{11} + 225a_{12} + 3375a_{13}, \tag{E.22}$$
$$f_{0x}(20,0) = a_{10} + 40a_{20} + 1200a_{30}, \tag{E.23}$$
$$\begin{aligned} f_{0x}(20,15) &= a_{10} + 15a_{11} + 225a_{12} + 3375a_{13} + 40a_{20} + 600a_{21} + 9000a_{22} + 135\,000\,a_{23}+ \\ &+ 1200a_{30} + 18\,000\,a_{31} + 270\,000\,a_{32} + 4\,050\,000\,a_{33}. \end{aligned} \tag{E.24}$$

$$f_{0y}(0,0) = a_{01}, \tag{E.25}$$
$$f_{0y}(0,15) = a_{01} + 30a_{02} + 675a_{03}, \tag{E.26}$$
$$f_{0y}(20,0) = a_{01} + 20a_{11} + 400a_{21} + 8000a_{31}, \tag{E.27}$$
$$\begin{aligned} f_{0y}(20,15) &= a_{01} + 30a_{02} + 675a_{03} + 20a_{11} + 600a_{12} + 13\,500\,a_{13} + 400a_{21} + 12\,000\,a_{22}+ \\ &+ 270\,000\,a_{23} + 8000a_{31} + 240\,000\,a_{32} + 5\,400\,000\,a_{33}. \end{aligned} \tag{E.28}$$

$$f_{0xy}(0,0) = a_{11}, \tag{E.29}$$
$$f_{0xy}(0,15) = a_{11} + 30a_{12} + 675a_{13}, \tag{E.30}$$
$$f_{0xy}(20,0) = a_{11} + 40a_{21} + 1200a_{31}, \tag{E.31}$$
$$\begin{aligned} f_{0xy}(20,15) &= a_{11} + 30a_{12} + 675a_{13} + 40a_{21} + 1200a_{22} + 27\,000\,a_{23} + 1200a_{31} + 36\,000\,a_{32}+ \\ &+ 810\,000\,a_{33}. \end{aligned} \tag{E.32}$$

We again denote (see Section E.2.2) x, y the *relative* coordinates of the interpolant and x_α, y_β the coordinates of the cell edges with the specified values $\boldsymbol{f}_0 = [f(x_0, y_0), f(x_0, y_1), f(x_1, y_0), f(x_1, y_1)]$. Unlike the bilinear interpolation, the matrix $\boldsymbol{a} = a_{ij}$ will be of the dimension 1×16. We introduce a vector with 16 components,

$$
\begin{aligned}
\boldsymbol{F}_0 =& [f(x_0, y_0), f(x_0, y_1), f(x_1, y_0), f(x_1, y_1), f_x(x_0, y_0), f_x(x_0, y_1), \\
& f_x(x_1, y_0), f_x(x_1, y_1), f_y(x_0, y_0), f_y(x_0, y_1), f_y(x_1, y_0), f_y(x_1, y_1), \\
& f_{xy}(x_0, y_0), f_{xy}(x_0, y_1), f_{xy}(x_1, y_0), f_{xy}(x_1, y_1)],
\end{aligned}
\tag{E.33}
$$

the vector

$$
\boldsymbol{K} = x^i y^j = 1, y, y^2, y^3, x, xy, xy^2, \dots, x^3 y^3, \tag{E.34}
$$

where $i, j = 0, 1, 2, 3$ will also have 16 components, and the matrix $\boldsymbol{A}$ given in this case by the coefficients of Equations (E.17) - (E.32),

$$
\boldsymbol{A} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
1 & y_1 & y_1^2 & y_1^3 & 0 & 0 & \cdots & 0 \\
1 & x_1 & x_1^2 & x_1^3 & 0 & 0 & \cdots & 0 \\
1 & y_1 & y_1^2 & y_1^3 & x_1 & x_1 y_1 & \cdots & x_1^3 y_1^3 \\
0 & 0 & 0 & 0 & 1 & y_1 & \cdots & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & 1 & \cdots & 9x_1^2 y_1^2
\end{pmatrix}, \tag{E.35}
$$

will be of the dimension 16×16. The derivatives at the knots of the grid will take the following form: at the internal points they will be defined as

$$
f_x(x_\alpha, y_\beta) = \frac{f(x_{\alpha+1}, y_\beta) - f(x_{\alpha-1}, y_\beta)}{x_{\alpha+1} - x_{\alpha-1}}, \tag{E.36}
$$

$$
f_y(x_\alpha, y_\beta) = \frac{f(x_\alpha, y_{\beta+1}) - f(x_\alpha, y_{\beta-1})}{y_{\beta+1} - y_{\beta-1}}, \tag{E.37}
$$

$$
f_{xy}(x_\alpha, y_\beta) = \frac{f(x_{\alpha+1}, y_{\beta+1}) - f(x_{\alpha-1}, y_{\beta+1}) - f(x_{\alpha+1}, y_{\beta-1}) + f(x_{\alpha-1}, y_{\beta-1})}{(x_{\alpha+1} - x_{\alpha-1})(y_{\beta+1} - y_{\beta-1})}, \tag{E.38}
$$

at the "upper" endpoints they will be

$$
f_x(x_\alpha, y_\beta) = \frac{f(x_\alpha, y_\beta) - f(x_{\alpha-1}, y_\beta)}{x_\alpha - x_{\alpha-1}}, \tag{E.39}
$$

$$
f_y(x_\alpha, y_\beta) = \frac{f(x_\alpha, y_\beta) - f(x_\alpha, y_{\beta-1})}{y_\beta - y_{\beta-1}}, \tag{E.40}
$$

$$
f_{xy}(x_\alpha, y_\beta) = \frac{f(x_\alpha, y_\beta) - f(x_{\alpha-1}, y_\beta) - f(x_\alpha, y_{\beta-1}) + f(x_{\alpha-1}, y_{\beta-1})}{(x_\alpha - x_{\alpha-1})(y_\beta - y_{\beta-1})} \tag{E.41}
$$

and at the "bottom" endpoints they will be

$$
f_x(x_\alpha, y_\beta) = \frac{f(x_{\alpha+1}, y_\beta) - f(x_\alpha, y_\beta)}{x_{\alpha+1} - x_\alpha}, \tag{E.42}
$$

$$
f_y(x_\alpha, y_\beta) = \frac{f(x_\alpha, y_{\beta+1}) - f(x_\alpha, y_\beta)}{y_{\beta+1} - y_\beta}, \tag{E.43}
$$

$$
f_{xy}(x_\alpha, y_\beta) = \frac{f(x_{\alpha+1}, y_{\beta+1} - f(x_\alpha, y_{\beta+1}) - f(x_{\alpha+1}, y_\beta) + f(x_\alpha, y_\beta)}{(x_{\alpha+1} - x_\alpha)(y_{\beta+1} - y_\beta)}. \tag{E.44}
$$

The derivatives at interpolated points (knots) will be defined similarly. Analogously to Equation (E.11), the resulting equation for calculation of interpolants will have the form:

$$f(x, y) = \boldsymbol{K}\boldsymbol{A}^{-1}\boldsymbol{F}_0. \tag{E.45}$$

The numerical algorithm will be in this case considerably more extensive than in Section E.2.2; however, it can be constructed in a similar way as in the case of the bilinear interpolation. For this reason, we present here only the form of the matrix $\boldsymbol{A}$, the term B1 (while the other terms of B will be completely similar, always with the first summation index) and the calculation of the resulting interpolants, the other operations (except for the dimension) will be the same as in Section E.2.2:

```
matrix A (N=16):
do i=1,N                                            initialization of the zero matrix
   do j=1,N
      A(i,j)=0.d0
   end do
end do
A(1,1)=1.d0                                         nonzero elements of the matrix A
A(2,1)=1.d0
A(2,2)=dy/dfloat(nj-1)
A(2,3)=(dy/dfloat(nj-1))**2.d0
A(2,4)=(dy/dfloat(nj-1))**3.d0
A(3,1)=1.d0
A(3,5)=dx/dfloat(ni-1)
A(3,9)=(dx/dfloat(ni-1))**2.d0
A(3,13)=(dx/dfloat(ni-1))**3.d0
A(4,1)=1.d0
A(4,2)=dy/dfloat(nj-1)
A(4,3)=(dy/dfloat(nj-1))**2.d0
A(4,4)=(dy/dfloat(nj-1))**3.d0
A(4,5)=dx/dfloat(ni-1)
A(4,6)=dx/dfloat(ni-1)*dy/dfloat(nj-1)
A(4,7)=dx/dfloat(ni-1)*(dy/dfloat(nj-1))**2.d0
A(4,8)=dx/dfloat(ni-1)*(dy/dfloat(nj-1))**3.d0
A(4,9)=(dx/dfloat(ni-1))**2.d0
A(4,10)=(dx/dfloat(ni-1))**2.d0*dy/dfloat(nj-1)
A(4,11)=(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))**2.d0
A(4,12)=(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))**3.d0
A(4,13)=(dx/dfloat(ni-1))**3.d0
A(4,14)=(dx/dfloat(ni-1))**3.d0*dy/dfloat(nj-1)
A(4,15)=(dx/dfloat(ni-1))**3.d0*(dy/dfloat(nj-1))**2.d0
A(4,16)=(dx/dfloat(ni-1))**3.d0*(dy/dfloat(nj-1))**3.d0
A(5,5)=1.d0
A(6,5)=1.d0
A(6,6)=dy/dfloat(nj-1)
A(6,7)=(dy/dfloat(nj-1))**2.d0
A(6,8)=(dy/dfloat(nj-1))**3.d0
A(7,5)=1.d0
```

```
A(7,9)=2.d0*dx/dfloat(ni-1)
A(7,13)=3.d0*(dx/dfloat(ni-1))**2.d0
A(8,5)=1.d0
A(8,6)=dy/dfloat(nj-1)
A(8,7)=(dy/dfloat(nj-1))**2.d0
A(8,8)=(dy/dfloat(nj-1))**3.d0
A(8,9)=2.d0*dx/dfloat(ni-1)
A(8,10)=2.d0*dx/dfloat(ni-1)*dy/dfloat(nj-1)
A(8,11)=2.d0*dx/dfloat(ni-1)*(dy/dfloat(nj-1))**2.d0
A(8,12)=2.d0*dx/dfloat(ni-1)*(dy/dfloat(nj-1))**3.d0
A(8,13)=3.d0*(dx/dfloat(ni-1))**2.d0
A(8,14)=3.d0*(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))
A(8,15)=3.d0*(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))**2.d0
A(8,16)=3.d0*(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))**3.d0
A(9,2)=1.d0
A(10,2)=1.d0
A(10,3)=2.d0*dy/dfloat(nj-1)
A(10,4)=3.d0*(dy/dfloat(nj-1))**2.d0
A(11,2)=1.d0
A(11,6)=dx/dfloat(ni-1)
A(11,10)=(dx/dfloat(ni-1))**2.d0
A(11,14)=(dx/dfloat(ni-1))**3.d0
A(12,2)=1.d0
A(12,3)=2.d0*dy/dfloat(nj-1)
A(12,4)=3.d0*(dy/dfloat(nj-1))**2.d0
A(12,6)=dx/dfloat(ni-1)
A(12,7)=dx/dfloat(ni-1)*2.d0*dy/dfloat(nj-1)
A(12,8)=dx/dfloat(ni-1)*3.d0*(dy/dfloat(nj-1))**2.d0
A(12,10)=(dx/dfloat(ni-1))**2.d0
A(12,11)=(dx/dfloat(ni-1))**2.d0*2.d0*dy/dfloat(nj-1)
A(12,12)=(dx/dfloat(ni-1))**2.d0*3.d0*(dy/dfloat(nj-1))**2.d0
A(12,14)=(dx/dfloat(ni-1))**3.d0
A(12,15)=(dx/dfloat(ni-1))**3.d0*2.d0*dy/dfloat(nj-1)
A(12,16)=(dx/dfloat(ni-1))**3.d0*3.d0*(dy/dfloat(nj-1))**2.d0
A(13,6)=1.d0
A(14,6)=1.d0
A(14,7)=2.d0*dy/dfloat(nj-1)
A(15,10)=2.d0*dx/dfloat(ni-1)
A(15,14)=3.d0*(dx/dfloat(ni-1))**2.d0
A(16,6)=1.d0
A(16,7)=2.d0*dy/dfloat(nj-1)
A(16,8)=3.d0*(dy/dfloat(nj-1))**2.d0
A(16,10)=2.d0*dx/dfloat(ni-1)
A(16,11)=4.d0*dx/dfloat(ni-1)*dy/dfloat(nj-1)
A(16,12)=6.d0*dx/dfloat(ni-1)*(dy/dfloat(nj-1))**2.d0
A(16,15)=6.d0*(dx/dfloat(ni-1))**2.d0*dy/dfloat(nj-1)
A(16,16)=9.d0*(dx/dfloat(ni-1))**2.d0*(dy/dfloat(nj-1))**2.d0
do j=1,nj-1                     terms of B: fx, fy, fxy are the corresponding partial
                                derivatives
```

```
    do j=1,nj-1
        B1(i,j)= &
        AINV(1,1)*f(i,j)+AINV(1,2)*f(i,j+1)+AINV(1,3)*f(i+1,j)+AINV(1,4)*f(i+1,j+1)+ &
        AINV(1,5)*fx(i,j)+AINV(1,6)*fx(i,j+1)+AINV(1,7)*fx(i+1,j)+AINV(1,8)*fx(i+1,j+1)+ &
        AINV(1,9)*fy(i,j)+AINV(1,10)*fy(i,j+1)+AINV(1,11)*fy(i+1,j)+AINV(1,12)*fy(i+1,j+1)+ &
        AINV(1,13)*fxy(i,j)+AINV(1,14)*fxy(i,j+1)+AINV(1,15)*fxy(i+1,j)+AINV(1,16)*fxy(i+1,j+1)
        other terms of B2 - B16 will be similar to B1, the 1st matrix index is always summation
    end do
end do

     calculation of interpolants:
do i=1,ni-1
    do j=1,nj-1
        do ii=1,nii-1
            do jj=1,njj-1
                ff(i,j,ii,jj)=
                B1(i,j)+yy(jj)*B2(i,j)+yy(jj)**2.d0*B3(i,j)+yy(jj)**3.d0*B4(i,j)+ &
                xx(ii)*B5(i,j)+xx(ii)*yy(jj)*B6(i,j)+ &
                xx(ii)*yy(jj)**2.d0*B7(i,j)+xx(ii)*yy(jj)**3.d0*B8(i,j)+ &
                xx(ii)**2.d0*B9(i,j)+xx(ii)**2.d0*yy(jj)*B10(i,j)+ &
                xx(ii)**2.d0*yy(jj)**2.d0*B11(i,j)+xx(ii)**2.d0*yy(jj)**3.d0*B12(i,j)+ &
                xx(ii)**3.d0*B13(i,j)+xx(ii)**3.d0*yy(jj)*B14(i,j)+ &
                xx(ii)**3.d0*yy(jj)**2.d0*B15(i,j)+xx(ii)**3.d0*yy(jj)**3.d0*B16(i,j)
            end do
        end do
    end do
end do
```

The resulting form of bicubic interpolation of the same grid as in Section E.2.2, described by Equations (E.17) - (E.32), is plotted in Figure E.3.

E.3 Regression

Regression (*regression analysis*) is called the searching for such a function (the so-called *regression function*), which best describes the relationship between two groups of variables, e.g., the dependence of random variables (measured values) on time, etc. It is predetermined which variable is independent (explanatory or also regressor) and which variable is dependent (explained or also response). Single regression describes the dependence of the response variable on a single regressor, while multiple regression describes a situation where the response variable depends on multiple regressors. Depending on the nature and a profile of the dependency examined, we choose the type of the *regression model*, for example, the *linear regression* (fitting the values of the dependent variables with a straight line), regression by a polynomial of nth degree, etc., as well as the most appropriate statistical method such as *least squares* or *robust regression*, which eliminates extremely deviated or biased values, etc. (see also concepts and statistical methods in the web address `http://physics.muni.cz/~mikulas/zvc.html`.

E.3.1 Least squares linear regression

Using the set of n discrete response values (explained variables) y_i, $i = 1, \dots, n$, which is determined by the enumeration of ordered pairs $[x_i, y_i]$, we fit a straight line (polynomial of the 1st degree) $f^{\mathrm{I}}(x) = kx + q$, so that the sum S of squares of the so-called *residues*, i.e. the distance of points y_i from functional values $f(x_i)$ at the points x_i is minimal (the squares are used here because of the independence of the sign of deviation). So we get the equation

$$S = \sum_i \left[y_i - f^{\mathrm{I}}(x_i)\right]^2 = \sum_i \left[y_i - (kx_i + q)\right]^2 = \min, \tag{E.46}$$

for two unknown values of k and q. To minimize this function, we set $\partial S/\partial k = 0$ and $\partial S/\partial q = 0$ at the same time. We can write the result using matrix formalism as

$$\begin{pmatrix} \sum_i x_i^2 & \sum_i x_i \\ \sum_i x_i & n \end{pmatrix} \begin{pmatrix} k \\ q \end{pmatrix} = \begin{pmatrix} \sum_i x_i y_i \\ \sum_i y_i \end{pmatrix}. \tag{E.47}$$

This makes it easy to find expressions for both the searched parameters depending on the ordered n-tuple $[x_i, y_i]$ (e.g., on the measured values depending on time or position),

$$k = \frac{n\sum_i x_i y_i - \sum_i x_i \sum_i y_i}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2}, \qquad q = \frac{\sum_i x_i^2 \sum_i y_i - \sum_i x_i \sum_i x_i y_i}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2}. \tag{E.48}$$

The method was suggested and first used by Karl Friedrich Gauss for the calculation of geodetic errors.

- Example of a linear least squares regression script, program Fortran 95:

```
program linear_regression                          declaration of the program name
implicit none
table of the values [x_i, y_i]:
[1,2], [2,1], [3,4], [4,12], [5,7], [6,8], [7,10], [8,14], [9,19], [10,17]
integer :: i, np                                   declaration of integer variables: i = se-
                                                   quence number of a pair of variables, np
                                                   = total number of discrete values
parameter (np=10)                                  enter a fixed value np
double precision, dimension(np) :: x, y            declaration of real quantities x, y as an ar-
                                                   ray (vector) of np elements
double precision :: f(np), res(np)                 another way of declaring real quantities f,
                                                   res as an array (vector) of np elements
double precision :: k, q, sumres                   declaration of real scalar quantities
x=(/(1.d0*i, i=1,np)/)                             vector of regressor values
y=(/2.d0, 1.d0, 4.d0, 12.d0, 7.d0, 8.d0, 10.d0, 14.d0, 19.d0, 17.d0/)
                                                   vector of response values
```

Option I - direct application of the formula (E.48)**:**

```
searched coefficients of the linear function:
k=(np*SUM(x*y)-SUM(x)*SUM(y))/(np*SUM(x**2.d0)-(SUM(x))**2.d0)
q=(SUM(x**2.d0)*SUM(y)-SUM(x)*SUM(x*y))/(np*SUM(x**2.d0)-(SUM(x))**2.d0)
```

Option II - using the set of equations (E.47) and the LAPACK procedure - see Section E.1:

```
in the program header you must also declare these variables:
integer :: j, INFO, KL, KU, LDAB, LDB, N, RHS
parameter(KL=1,KU=1,N=2,KUKL=KL+KU+1,LDAB=2*KL+KU+1,LDB=N,RHS=1)
integer :: IPIV(N)
double precision :: M(N,N),AB(LDAB,N),B(LDB,RHS)
double precision :: max
M(1,1)=SUM(x**2.d0)                 matrix of the left-hand side, M(N,N)
M(1,2)=SUM(x)
M(2,1)=SUM(x)
M(2,2)=np
do i=1,N                            LAPACK calculation cycle
   do j=1,N
      AB(KUKL+i-j, j)=M(i, j)
   end do
end do
B(1,1)=SUM(x*y)                     calculation of right-hand side by the LAPACK
                                    procedure
B(2,1)=SUM(y)
call of the DGBSV process:
call DGBSV(N,KL,KU,1,AB,LDAB,IPIV,B,N,INFO)
if(INFO.ne.0) write(*,*) "INFO=",INFO,"!!!"
k=B(1,1)
q=B(2,1)

joint continuation:
write(1,*) k, q                     print the calculated values to file "fort.1"
write(1,*)                          separating line
do i=1,np                           calculation cycle
   f(i)=k*x(i)+q                    calculation of the linear function values
   res(i)=(f(i)-y(i))**2.d0         calculation of residues
   sumres=SUM(res)                  calculation of the sum of residues
end do
do i=1,np                           writing cycle to the file
   write(1,*) x(i), y(i), f(i), res(i)
end do
write(1,*)
write(1,*) sumres                   writing the sum of residues to the file
end program linear_regression       exit the program
```

E.3.2 Least squares polynomial regression

The procedure described in the previous Section E.3.1 can be generalized for a polynomial of any (mth) degree, where the analogy of Equation (E.46) can be rewritten into the form

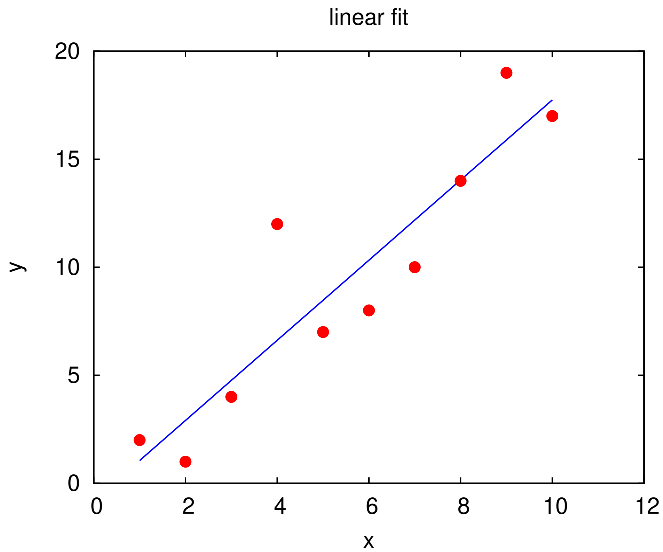

Figure E.4: Plot of the example of the linear regression, i.e., the fit of the 10 points with a straight line with parameters calculated by the least squares method.

(superscripts always mean powers)

$$S = \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{m} p_j x_i^j \right)^2 = \min, \tag{E.49}$$

where the coefficients p_j are coefficients of the jth-degree polynomial, thus for linear regression $p_0 = q$, $p_1 = k$ holds (see Equation (E.47)). At the same time, it is clear that the number N of Equations in the LAPACK procedure corresponds to $m+1$. We find the minimum of Equation (E.49) by setting $\partial S/\partial p_j = 0$, we thus get the system of $m+1 = N$ linear equations, which can be expressed by the matrix notation in the form

$$\begin{pmatrix} \sum_i x_i^{2m} & \cdots & \sum_i x_i^{m+1} & \sum_i x_i^m \\ \vdots & \ddots & \vdots & \vdots \\ \sum_i x_i^{m+1} & \cdots & \sum_i x_i^2 & \sum_i x_i \\ \sum_i x_i^m & \cdots & \sum_i x_i & n \end{pmatrix} \begin{pmatrix} p_m \\ \vdots \\ p_1 \\ p_0 \end{pmatrix} = \begin{pmatrix} \sum_i x_i^m y_i \\ \vdots \\ \sum_i x_i y_i \\ \sum_i y_i \end{pmatrix}. \tag{E.50}$$

The computational cycle of the LAPACK procedure (see the program script in Section E.3.1) can be generalized as follows (Fortran 95):

```
do i=1,N-1                          matrix of the left-hand side, M(N,N)
   do j=1,N
      M(i,j)=SUM(x**(2*N-i-j))
   end do
end do
i=N
do j=1,N-1
   M(N,j)=SUM(x**(N-j))
```

```
end do
M(N,N)=np
do i=1,N                          LAPACK calculation cycle
  do j=1,N
    AB(KUKL+i-j, j)=M(i, j)
  end do
end do
do i=1,N                          calculation of the right side by the LAPACK
                                  procedure
  B(i,1)=SUM(x**(N-i)*y)
end do
```

Otherwise, the program procedure described in Section E.3.1 remains practically unchanged.

E.3.3 Robust regression

If we want to eliminate the effect of very biased (deviated or "blown") values, we choose the so called *weighted* or *robust* regression. There are a number of robust regression models (see, for example, Huber & Ronchetti (2009)), for all of these, we will mention the simple so-called *Tukey method of M-estimate* (Tukey's bisquare method), based on residual weighting using a double square. First, we calculate the unweighted residues $\text{res\_}i = y_i - f(x_i)$ (as in Sections, e.g., E.3.1, E.3.2), and then use the following weighting function:

$$w_i(\text{res\_}i) = \left[1 - \left(\frac{\text{res\_}i}{6\,\text{med}}\right)^2\right]^2 \tag{E.51}$$

where med is the median of absolute deviation of the residues that we can regard as the residue itself, or the deviation of each residue from its own median. The weight $w_i = 0$ if the absolute value of the residue $|\text{res\_}i| > 6\,\text{med}$. The extremely deviated values are thus completely excluded, less deviated values are retained but with a reduced weight.

Programming this robust (weighted) regression model is easy, we only enter the calculated weights into the right-hand side of Equation (E.50):

$$\begin{pmatrix} \sum_i x_i^{2m} & \cdots & \sum_i x_i^{m+1} & \sum_i x_i^m \\ \vdots & \ddots & \vdots & \vdots \\ \sum_i x_i^{m+1} & \cdots & \sum_i x_i^2 & \sum_i x_i \\ \sum_i x_i^m & \cdots & \sum_i x_i & n \end{pmatrix} \begin{pmatrix} p_m \\ \vdots \\ p_1 \\ p_0 \end{pmatrix} = \begin{pmatrix} \sum_i x_i^m w_i y_i \\ \vdots \\ \sum_i x_i w_i y_i \\ \sum_i w_i y_i \end{pmatrix}. \tag{E.52}$$

There are standard modules in each programming language to calculate the median. We can use, for example, the following subroutine; the result is included in Equation(E.51) (Fortran 95):

```
subroutine median(i, j, k, np, res, med)
implicit none
integer :: i, j, k, np
double precision :: res(np)
double precision, intent(out) :: med
double precision :: temp
```

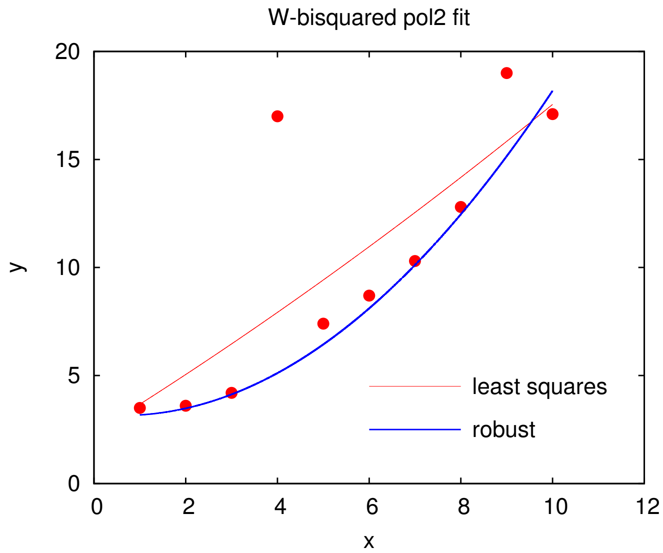

Figure E.5: Comparison of the quadratic regression, i.e., fitting by a polynomial of the 2nd degree with parameters calculated by the method of least squares according to Section E.3.2 (red line) and the robust Tukey method according to Section E.3.3 (blue line). The set of 10 points with the coordinates [1,3.5], [2,3.6], [3,4.2], [4,17], [5,7.4], [6,8.7], [7,10.3], [8,12.8], [9,19], [10,17.1] contains the strongly deviated values (gross errors) to which the robust curve responds poorly or not at all.

```
Sorting the numbers in ascending order:
do j=1,np-1
   do k=j+1,np
      if(res(j)>res(k))then
         temp=res(k)
         res(k)=res(j)
         res(j)=temp
      endif
   end do
end do
Calculating the median for an even or odd number:
if(mod(np,2)==0)then
   med=(res(np/2)+res(np/2+1))/2.d0
else
   med=res(np/2+1)
endif
end subroutine median
Calculation of weights follows: w(y(i))=(1.d0-(y(i)/6.d0*med)**2.d0)**2.d0, atd.
```

E.3.4 Cubic smoothing spline

The so-called *smoothing* can be useful in the case that a densely measured or calculated dependence shows a considerable local variance, yet its global trend (see Figure E.6), which is however sufficiently irregular or complicated and does not resemble any simple function (polynomial, exponential, etc.), is obvious. Fitting of such point dependence $[x_i, y_i]$ by the *cubic smoothing spline* represented by the function $S(x)$, whose simplest form we find using the minimization

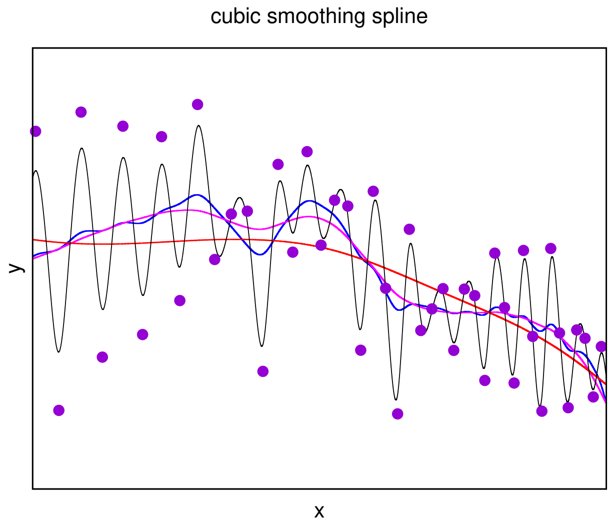

Figure E.6: Fitting a set of points (measured or calculated values) with a series of cubic smoothing splines with different values of the parameter λ; the black line with the lowest λ is closest to the fitted points, the red line with the highest λ smoothes the global dependency the most. For $\lambda = 0$, we get the cubic interpolation spline (see Section E.2.1) directly passing through the given points, while in the case of $\lambda \to \infty$, we get a linear regression of the set of points (see Section E.3.1).

(cf. Equation (E.46)),

$$S = \sum_{i=1}^{n} [y_i - S(x_i)]^2 + \lambda \int S''(x)^2 \, \mathrm{d}x = \min, \tag{E.53}$$

is done in fact in two steps. In the first step, we find new points $[x_i, \tilde{Y}_i]$ with less variance (where $S(x_i) = \tilde{Y}_i$), in the second step, we fit these new points $[x_i, \tilde{Y}_i]$ by the cubic interpolation spline according to Section E.2.1. The positive number λ in Equation (E.53) is the so-called *smoothing parameter*, which controls "roughness" or "subtlety" of the smoothing, where the higher λ means more robust smoothing (see comparison of curves with different parameters λ in Figure E.6).

Since it is a cubic spline, the particular segments (pieces) of the function $S''(x)$ (2nd derivative of the function $S(x)$) will be the linear abscissas, which must at the points x_i and x_{i+1} take the values $S''(x_i) = M_i$, $S''(x_{i+1}) = M_{i+1}$ (see Equation (E.3)). Thus, in a general point within the particular segments must apply

$$S''(x) = M_i + \frac{M_{i+1} - M_i}{x_{i+1} - x_i}(x - x_i). \tag{E.54}$$

The integral in Equation (E.53) will thus have the solution for each particular segment in the form

$$\int_{x_i}^{x_{i+1}} \left[M_i + \frac{M_{i+1} - M_i}{x_{i+1} - x_i}(x - x_i) \right]^2 \mathrm{d}x = \frac{x_{i+1} - x_i}{3} \left(M_{i+1}^2 + M_{i+1} M_i + M_i^2 \right). \tag{E.55}$$

By detailed analysis of Equation (E.6), however, now with searched values of $\tilde{Y}_i$ in the right-hand side, shortly written in the matrix notation as

$$\boldsymbol{W M} = \boldsymbol{R S}, \tag{E.56}$$

we find that Equation (E.55) is identically solvable using the matrix multiplication in the following order,

$$\int S''(x)^2 \,\mathrm{d}x = \boldsymbol{S}^{\boldsymbol{T}} \tilde{\boldsymbol{R}}^{\boldsymbol{T}} \tilde{\boldsymbol{W}}^{-1} \tilde{\boldsymbol{R}} \boldsymbol{S}, \tag{E.57}$$

where $\boldsymbol{S}$ is the (column) n-dimensional vector of the searched values $\tilde{Y}_i$, $\tilde{\boldsymbol{W}}$ is the tridiagonal symmetrical matrix of the dimension $(n-2) \times (n-2)$ with the elements

$$W_{i-1,i} = W_{i,i-1} = \frac{x_{i+1} - x_i}{6}, \quad W_{ii} = \frac{x_{i+2} - x_i}{3}, \tag{E.58}$$

and $\tilde{\boldsymbol{R}}$ is the matrix of the dimension $(n-2) \times n$ with the elements

$$\tilde{R}_{ii} = \frac{1}{x_{i+1} - x_i}, \quad \tilde{R}_{i,i+1} = -\left(\frac{1}{x_{i+1} - x_i} + \frac{1}{x_{i+2} - x_{i+1}}\right), \quad \tilde{R}_{i,i+2} = \frac{1}{x_{i+2} - x_{i+1}}. \tag{E.59}$$

Rewriting the minimalization Equation (E.53) in such a way, we get its left-hand side in the form

$$(\boldsymbol{Y} - \boldsymbol{S})^{\boldsymbol{T}} (\boldsymbol{Y} - \boldsymbol{S}) + \lambda\, \boldsymbol{S}^{\boldsymbol{T}} \tilde{\boldsymbol{R}}^{\boldsymbol{T}} \tilde{\boldsymbol{W}}^{-1} \tilde{\boldsymbol{R}} \boldsymbol{S}. \tag{E.60}$$

If we set its derivative with respect to $\boldsymbol{S}$ equal to zero, we get the resulting expression for the searched values within the above described first step,

$$\boldsymbol{S} = \left(\boldsymbol{E} + \lambda\, \tilde{\boldsymbol{R}}^{\boldsymbol{T}} \tilde{\boldsymbol{W}}^{-1} \tilde{\boldsymbol{R}}\right)^{-1} \boldsymbol{Y}, \tag{E.61}$$

where $\boldsymbol{E}$ is the unit matrix.

Calculation of the second step, that is, fitting of the found points $\tilde{Y}_i$ by the cubic interpolation spline, will now be done according to Section E.2.1. For numerical calculations of matrix multiplication, inverse matrices, tridiagonal matrices, etc., we may again use the procedures, for example, from the programming package LAPACK, according to the previously shown program scripts.

E.4 Numerical methods of calculation of functions of a single variable

E.4.1 Searching the root of a function of a single variable - Newton's method

The roots of a generally non-linear function (equation) $f(x) = 0$ is often impossible to express in the form of an explicit analytical formula. To find the solution of such an equation, we must use some of the numerical (iterative) methods, where, using a certain number of initial approximations of the searched root x_0, we generate the serie x_1, x_2, x_3, ... , which converges to the root x_0. In some cases, it is necessary to enter an interval a, b, which, according to a preliminary estimate, contains the searched root; the closer the initial evaluation is, the faster the applied method converges. We assume in the following examples the continuous real function $f(x)$ with the corresponding number of continuous derivatives in the input interval in which we expect the searched root $f(x_0) = 0$.

We make the initial estimate of an interval (intervals) where the root (roots) may be found, for example, by the graphical method: using the appropriate computing program or by listing the values of the given function into a table, we plot the function $f(x)$ and find its approximate intersections with the axis x. For example, in case of the function given by the formula

$$f(x) = x^3 - 3x^2 + 2x - 3, \tag{E.62}$$

we can wery easy recognize that there exists one real root, which must certainly lie within the interval $x_0 \in (2, 3)$.

There exist a lot of possible numerical procedures (for example the method of secants, etc.), probably the most frequently used is the so-called *Newton's method* or the method of tangents. We start with the initial approximation of x_0 and calculate x_1, x_2, x_3, $\ldots$, respectively. If we know the approximation x_k and want to determine a better approximation x_{k+1}, we pass a tangent to the curve $y = f(x)$ through the point $[x_k, f(x_k)]$. We regard the intersection of this tangent with the axis x as the value x_{k+1}. We get the equation of the tangent in the form

$$f'(x_k) = \{3x_k^2 - 6x_k + 2\} = \frac{f(x_k)}{x_k - x_{k+1}}, \tag{E.63}$$

from which we derive the relation for calculation of an each following step (iteration),

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}. \tag{E.64}$$

The calculation terminates, regarding the value x_{k+1} found in the last step as the searched root x_0 with required accuracy, (according to the selected magnitude of the tiny number ϵ which determines the required accuracy level) for example in these cases:

$$|x_{k+1} - x_k| \le \epsilon \qquad \text{or} \qquad |f(x_{k+1})| \le \epsilon. \tag{E.65}$$

- Example of possible way of programming Equation (E.62) - Fortran 95:

program newton	declaration of the name of the program
implicit none	
integer :: i	decleration of integer variables in the header of the program: i = sequence number of a spatial step
double precision :: x, dx, f, df	declaration of the real variables, where x = x_k, dx = $x_k - x_{k+1}$, f = $f(x_k)$, df = $f'(x_k)$, with double precision
x=3.d0	estimate of the enter value x_k
do	computing cycle
i = i+1	
f = x**3 - 3.d0*x**2 + 2.d0*x - 3.d0	Equation (E.62)
df = 3.d0*x**2 - 6.d0*x + 2.d0	derivative of the function (E.62)
dx = f/df	Equation (E.64)
x = x-dx	new value x_k
if (dabs(dx)**.lt.**1.d-12) **exit**	stop criterion: $\lvert x_k - x_{k+1}\rvert < 10^{-12}$
end do	
write (100,*) x	writing the root of the function f into the file fort.100
stop	stop of the whole process
end program newton	end of the program

- Table of the results of the program of computation of the root of the function $f(x_k)$ for the particular steps k:

k	x_k	$f(x_k)$	$x_k - x_{k+1}$
0	3.0000000000000000	3.0000000000000000	0.27272727272727271
1	2.7272727272727275	0.42599549211119836	5.3581553581554045E-002
2	2.6736911736911733	1.4723079585858834E-002	1.9886039436713345E-003
3	2.6717025697475019	1.9848200396133109E-005	2.6880854327577796E-006
4	2.6716998816620690	3.6242120415863610E-011	4.9083680000275664E-012
5	2.6716998816571604	1.7763568394002505E-015	2.4057679206275180E-016

E.4.2 Numerical differentiation

The simplest numerical approximation of the 1st derivative has the form of the so-called *forward difference*,

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \tag{E.66}$$

where $h = \Delta x > 0$, with an error of the approximation, $\delta f'(x)$, expressed using the Taylor expansion of x, i.e., $\delta f'(x) = -(h/2)f''(\xi)$, where $\xi \in (x, x+h)$. About the same simple is the so-called *backward difference*,

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}, \tag{E.67}$$

with the same order error. Approximation with higher accuracy is the so-called *central difference*,

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}, \tag{E.68}$$

with the error of approximation $\delta f'(x) = -(h^2/6)f'''(\xi)$, where $\xi \in (x-h, x+h)$, however, it takes up two spatial steps (cells) of the computational grid. In an analogous way, we can derive also the 2nd derivative in the form

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}, \tag{E.69}$$

with the error of approximation $\delta f''(x) = -(h^2/12)f^{(4)}(\xi)$, where $\xi \in (x-h, x+h)$.

There are also more accurate and sophisticated difference schemes (see, for example, van Leer, 1977, 1982; Vitásek, 1987; LeVeque, 2002), for example, a single-sided approximation of the 1st derivative, which is the second-order of accuracy,

$$f'(x) \approx \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}, \tag{E.70}$$

with the approximation error $\delta f'(x) = (h^2/3)f'''(\xi)$, where $\xi \in (x, x+2h)$, or an approximation of the 1st derivative, which is of the fourth-order of accuracy, in the form

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}, \tag{E.71}$$

i.e., with an error that is of the order of h^4, etc. However, their natural disadvantage is that they occupy several spatial steps (cells) of the computational grid, and also with extended and complicated calculations there increase the demands on the computational time. Therefore, it is always necessary to consider the calculation scheme adequate to the solved problem and its required accuracy, corresponding to the real capabilities of the computing device used.

E.4.3 Numerical integration

It is always based on substitution of a complexly bounded geometric formation (the area under the curve of a given function in case of a single variable) by a simpler formation or the sum of such formations. The name *numerical quadrature* is also used, in the sense of the construction of the areal (i.e., two-dimensional, quadrature) formations. We will show examples of the most common (in most cases quite sufficient) methods of numerical integration of functions of a single variable using the so-called *Newton-Cotes formulas.* There are, of course, a number of other methods of numerical integration, such as *Gaussian quadrature formulas*, *Romberg quadrature*, etc. We will not mention here the accuracy and methods of an error determination, etc., everything is standardly available in the literature.

- **Newton-Cotes (quadrature) formulas**

Rectangular method: This method is not formally regarded as the Newton-Cotes formula, although it is the simplest but at the same time the least accurate numerical integration method, where a definite integral of the given function (i.e., the area of the surface under the curve of the functional values of the function $f(x)$ within the interval $\langle a,b\rangle$) approximates by a rectangle. This approximation can be refined if, for example, we divide the interval $\langle a,b\rangle$ into a selected number of n equal sub-intervals, calculate the rectangular approximation for each sub-interval separately and sum the results, i.e.,

$$I=\int_a^b f(x)\,\mathrm{d}x\approx\frac{b-a}{n}\sum_{k=0}^{n-1} f\left(a+k\,\frac{b-a}{n}\right). \tag{E.72}$$

Trapezoidal method: represents more precise numerical integration method, where a definite integral of a given function is approximated by trapezoids (the points of the function are connected by straight lines). If we divide the interval $\langle a,b\rangle$ into a selected number of n equal sub-intervals, we calculate the trapezoidal approximation again for each sub-interval and sum the results, i.e.,

$$I=\int_a^b f(x)\,\mathrm{d}x\approx\frac{b-a}{2n}\sum_{k=0}^{n-1}\left[f(x_{k+1})+f(x_k)\right], \tag{E.73}$$

where $x_k=a+k(b-a)/n$.

Simpson's rule: based on quadratic (parabolic) interpolation of sub-intervals of the integrated function. In case of integration of polynomials, this method gives very accurate results. The composed approximation by the Simpson rule, where the interval $\langle a,b\rangle$ is divided into an even number of n sub-intervals, it has the form (where $x_k=a+k(b-a)/n$)

$$I=\int_a^b f(x)\,\mathrm{d}x\approx\frac{b-a}{3n}\sum_{k=1}^{n/2}\left[f(x_{2k-2})+4f(x_{2k-1})+f(x_{2k})\right]. \tag{E.74}$$

Simpson's 3/8 *rule* (or the second Simpson's rule): based on cubic interpolation of sub-intervals of the integrated function. Composed approximation by the Simpson's 3/8 rule, where the interval $\langle a,b\rangle$ is divided into n sub-intervals, where n is divisible by three, has the form (where again $x_k=a+k(b-a)/n$)

$$I=\int_a^b f(x)\,\mathrm{d}x\approx\frac{3(b-a)}{8n}\sum_{k=1}^{n/3}\left[f(x_{3k-3})+3f(x_{3k-2})+3f(x_{3k-1})+f(x_{3k})\right]. \tag{E.75}$$

Newton-Cotes formulas of arbitrarily higher orders can be constructed in a similar way, but the orders of magnitude higher than 4 (*Boolean rule*) are rarely used, their disadvantage is the very fast (even exponentially) increasing integration error.

- **Numerical integration in higher dimensions**

These methods can be applied in various ways also for multiple integration, their choice depends, for example, on the shape of the integration area and on the specific functions contained in the integrand. Here we show only two basic methods:

Trapezoidal method in 2D: Consider the double integral (see Equation (7.3))

$$I = \iint_{\mathcal{S}} f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_a^b \left[\int_{\phi_1(x)}^{\phi_2(x)} f(x,y)\,\mathrm{d}y \right] \mathrm{d}x. \tag{E.76}$$

The inner integral is approximated by a one-dimensional numerical quadrature, where x is a constant. The obtained values are then used to calculate the outer integral, also using a one-dimensional rule. Let us denote the two divided simple integrals as follows,

$$F(x) = \int_{\phi_1(x)}^{\phi_2(x)} f(x,y)\,\mathrm{d}y, \quad I = \int_a^b F(x)\,\mathrm{d}x. \tag{E.77}$$

For example, we calculate the inner quadrature $F(x)$ at a point x_j as (see Equation (E.73))

$$F(x) = h_j \left[\frac{1}{2} f(x_j, y_{j,0}) + f(x_j, y_{j,1}) + \ldots + f(x_j, y_{j,n_j-1}) + \frac{1}{2} f(x_j, y_{j,n_j}) \right], \tag{E.78}$$

where

$$h_j = \frac{\phi_2(x_j) - \phi_1(x_j)}{n_j}, \qquad y_{j,k} = \phi_1(x_j) + k h_j. \tag{E.79}$$

The number and the interval size of the steps n_j result from the fact that, in general, the number of calculation points in the y-direction may be different for different x_j (see Figure E.7), depending on the shape of the integration area. Then we approximate the integral I by the outer (composed) one-dimensional quadrature,

$$I = h \left[\frac{1}{2} F(x_0) + F(x_1) + \ldots + F(x_{m-1}) + \frac{1}{2} F(x_m) \right], \tag{E.80}$$

where, assuming a uniform step m in the x-direction, $h = (b-a)/m$, and $x_j = a + jh$. If the integrand $f(x,y)$ is a smooth and slowly increasing or decreasing function, we select the number of n_j points usually, so that $h_j \approx h$ for all j. This minimizes the computational cost within the required accuracy.

The total quadrature can therefore be written as

$$I \approx \sum_{j=0}^{m} \sum_{k=0}^{n_j} w_{j,k} f(x_j, y_{j,k}) h h_j, \tag{E.81}$$

where $w_{j,k} = 1$ at the points within the integration area ($j \neq 0 \wedge j \neq m \wedge k \neq 0 \wedge k \neq n_j$), $w_{j,k} = 1/2$ at the boundary of the integration area except the corners ($j = 0 \vee j = m \wedge k \neq 0 \wedge k \neq n_j$ or $j \neq 0 \wedge j \neq m \wedge k = 0 \vee k = n_j$), and $w_{j,k} = 1/4$ in the corners of the integration area ($j = 0 \vee j = m \wedge k = 0 \vee k = n_j$). The accuracy of the given method is of the second-order, its error $\delta I = \mathcal{O}(h^2 + \max h_j^2)$.

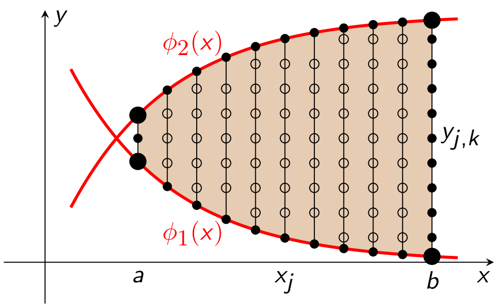

Figure E.7: Schematic representation of the grid density for numerical integration of double integral with the optimal distribution of the grid nodes according to Equation (E.81). To each node x_j in the horizontal direction x there is assigned a different number of nodes $y_{j,k}$ in the vertical direction y. The empty circles correspond to the internal nodes of the grid, where $w_{j,k} = 1$, the smaller solid circles correspond to the nodes at the boundary of the integration area (indicated by the brown area), where $w_{j,k} = 1/2$. The large solid circles correspond to the nodes at the corners of the integration area, where $w_{j,k} = 1/4$.

Trapezoidal method in 3D: In the case of the triple integral (see Equation (7.6))

$$I = \int_a^b \left[\int_{\phi_1(x)}^{\phi_2(x)} \left(\int_{\psi_1(x,y)}^{\psi_2(x,y)} f(x,y,z)\,\mathrm{d}z \right) \mathrm{d}y \right] \mathrm{d}x, \tag{E.82}$$

we will use a similar strategy as in 2D; the resulting formula (analogy to (E.81)) will be

$$I \approx \sum_{j=0}^{m} \sum_{k=0}^{n_j} \sum_{l=0}^{n_{j,k}} w_{j,k,l} f(x_j, y_{j,k}, z_{j,k,l}) h h_j h_{j,k}, \tag{E.83}$$

where, assuming again a uniform step m in the x-direction, $h = (b-a)/m$, $x_j = a + jh$, Further also

$$h_j = \frac{\phi_2(x_j) - \phi_1(x_j)}{n_j}, \qquad y_{j,k} = \phi_1(x_j) + kh_j, \tag{E.84}$$

$$h_{j,k} = \frac{\psi_2(x_j, y_k) - \psi_1(x_j, y_k)}{n_{j,k}}, \qquad z_{j,k,l} = \psi_1(x_j, y_k) + lh_{j,k}, \tag{E.85}$$

where $w_{j,k,l} = 1$ at the points within the integration area ($j \neq 0 \wedge j \neq m \wedge k \neq 0 \wedge k \neq n_j \wedge l \neq 0 \wedge l \neq n_{j,k}$), $w_{j,k} = 1/2$ within the surfaces at the boundary of the integration area, except at the edges where two of these surfaces meet, and except at the corners where all three meet, ($j = 0 \vee j = m \wedge k \neq 0 \wedge k \neq n_j \wedge l \neq 0 \wedge l \neq n_{j,k}$ or $j \neq 0 \wedge j \neq m \wedge k = 0 \vee k = n_j \wedge l \neq 0 \wedge l \neq n_{j,k}$ or $j \neq 0 \wedge j \neq m \wedge k \neq 0 \wedge k \neq n_j \wedge l = 0 \vee l = n_{j,k}$), $w_{j,k} = 1/4$ on the edges of the integration area, except at the corners ($j = 0 \vee j = m \wedge k = 0 \vee k = n_j \wedge l \neq 0 \wedge l \neq n_{j,k}$ or $j = 0 \vee j = m \wedge k \neq 0 \wedge k \neq n_j \wedge l = 0 \vee l = n_{j,k}$ or $j \neq 0 \wedge j \neq m \wedge k = 0 \vee k = n_j \wedge l = 0 \vee l = n_{j,k}$) and $w_{j,k} = 1/8$ at the corners of the integration area ($j = 0 \vee j = m \wedge k = 0 \vee k = n_j \wedge l = 0 \vee l = n_{j,k}$). The accuracy of the introduced method is again second-order, its error $\delta I = \mathcal{O}(h^2 + \max h_j^2 + \max h_{j,k}^2)$.

Simpson's rule in 2D: Using this rule (see the principles and notation, given in Equation (E.74)), Equations (E.78) and (E.80) will take the form

$$F(x) = \frac{h_j}{3n_j} \left[f(x_j, y_{j,0}) + 2 \sum_{k=1}^{\frac{n_j}{2}-1} f(x_j, y_{j,2k}) + 4 \sum_{k=1}^{\frac{n_j}{2}} f(x_j, y_{j,2k-1}) + f(x_j, y_{j,n_j}) \right], \tag{E.86}$$

$$I = \frac{h}{3m}\left[F(x_0) + 2\sum_{k=1}^{\frac{m}{2}-1} F(x_{2k}) + 4\sum_{k=1}^{\frac{m}{2}} F(x_{2k-1}) + F(x_m)\right], \tag{E.87}$$

respectively. By sequentially chaining the same principle, we would also easily construct Simpson's rule in 3D.

Similarly, multidimensional numerical quadratures based on higher order methods can be constructed. Given these analogies to a one-dimensional quadrature, we do not explicitly mention them here.

E.4.4 Simple numerical methods for solving ordinary differential equations

There are numerous variants of solutions of ordinary differential equations, for example, using the *Euler method* or the so-called *Runge-Kutta method* (methods), etc. (for further details - see, e.g., (Humlíček, 2009)).

- **Euler method**

is the simplest and also the least accurate method appropriate for numerical solution of ordinary first-order differential equations or their systems. The method is based on the definition of the first-order equation, $y' = f(x, y)$, where x is an independent variable and y is a dependent variable. Its transcription to a numerical scheme with $n + 1$ points of spatial grid and with the constant step $h = (y_n - y_0)/n$ (for example using forward difference) will take the following form:

$$\frac{y_{i+1} - y_i}{h} = f(x, y) \quad \text{and so} \quad y_{i+1} = y_i + hf, \tag{E.88}$$

where $i = 0, \ldots, n$. By analogy, we can extend this principle to a system of several first-order equations.

We will show the application of the method on a system of two (nonlinear, analytically very difficult to solve) first-order equations, formed by the decomposition of the second-order equation in the form $y'' - 5(y' - 1)^2 + 6y^2 = 0$, with the boundary conditions $y(0) = 1$, $y'(0) = 2$, in the interval $x \in \langle 0, 10\rangle$, i.e.,

$$\begin{aligned} y' &= z + 1, \\ z' &= 5z^2 - 6y^2. \end{aligned} \tag{E.89}$$

The numerical algorithm of the system of Equations (E.89) can be written as follows (Fortran 95):

• **program** Euler **implicit none**	declaration of the program name
double precision :: x, y, z, h, f, g	declaration of real quantities and functions
x=0.d0, y=1.d0, z=1.d0, h=1.d-3	declaration of parameters and boundary conditions
do	calculation cycle

```
   f=z+1.d0
   g=5.d0*z**2.–6.d0*y**2.
```

```
    y=y+h*f
    z=z+h*g
    write(1,*) x,y,z                    write to file fort.1
    x=x+h
    if(x>10.d0)exit                     stop criterion
  end do                                end of cycle
  end program Euler
```

By this calculation we actually obtain a discrete profile of the functions y and $z = y' - 1$ in the given interval $\langle 0, 10 \rangle$, with the step 10^{-3}. The values of both functions at the endpoint of the interval are now $y(10) = 0.91287365321267411$ and $z(10) = -1.0000034112031584$.

- **Runge-Kutta (RK) methods**

In general, these methods may be of different orders, the *Euler method* is actually the Runge-Kutta method of the first order. The most frequently used is the so-called "RK4" (fourth-order method), the "*classical Runge-Kutta method*" or often simply called the "*Runge-Kutta method*". This is defined (we use the notation introduced in the previous paragraph of the Euler method) as

$$x_{i+1} = x_i + h, \quad y_{i+1} = y_i + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right), \tag{E.90}$$

where the coefficients k_α are generally determined such that the method of an order p corresponds to the Taylor polynomial of the function $y(x)$ of the same order. So in the case of "RK4", they will be

$$k_1 = f(x_i, y_i), \tag{E.91}$$

$$k_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_1\right), \tag{E.92}$$

$$k_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_2\right), \tag{E.93}$$

$$k_4 = f\left(x_i + h, y_i + hk_3\right). \tag{E.94}$$

As an example, we show here the numerical algorithm of the same set of Equations (E.89) as in the previous Euler method (Fortran 95):

```
• program RK                                   program name declaration
  implicit none
  double precision :: x, y, z, h, f, g         declaration of real quantities and functions
  double precision :: k1y, k2y, k3y, k4y       declaration of coefficients for the variable y
  double precision :: k1z, k2z, k3z, k4z       declaration of coefficients for variable z
  x=0.d0, y=1.d0, z=1.d0, h=1.d-3              declaration of parameters and boundary condi-
                                               tions
  do                                           calculation cycle
    f=z+1.d0
    g=5.d0*z**2.–6.d0*y**2.
```

```
      k1y=f
      k1z=g
      k2y=(z+k1z*h/2.d0+1.d0)
      k2z=(5.d0*(z+k1z*h/2.d0)**2.-6.d0*(y+k1y*h/2.d0)**2.)
      k3y=(z+k2z*h/2.d0+1.d0)
      k3z=(5.d0*(z+k2z*h/2.d0)**2.-6.d0*(y+k2y*h/2.d0)**2.)
      k4y=(z+h*k3z)
      k4z=(5.d0*(z+h*k3z)**2.-6.d0*(y+h*k3y)**2.)

      y=y+h*(k1y+2.d0*k2y+2.d0*k3y+k4y)/6.d0
      z= z+h*(k1z+2.d0*k2z+2.d0*k3z+k4z)/6.d0

      write(1,*) x,y,z                    write to file fort.1

      x=x+h

      if(x>10.d0)exit                     stop criterion
   end do                                 end of cycle

   end program RK
```

We get a similar profile of the functions y and $z = y' - 1$ in a given interval $\langle 0, 10\rangle$, with the step 10^{-3}, as using the Euler method. The values of both functions at the endpoint of the interval are $y(10) = 0.91287365717860480$ and $z(10) = -1.0000034161695313$, respectively; therefore, the numerical values for both methods first differ in the order of 10^{-9}.

- **Half-step error estimate**

A popular simple method of error estimate is the so-called *half step method*, which in many practical applications gives reliable results (detailed description and theoretical analysis exist in virtually every numerical mathematics textbook). Its principle is that we perform the calculation again with the same boundary conditions but with a half step $h/2$, so that to determine the error (deviation from the exact solution) δy of the function y, this process is repeated twice within one step h. The resulting deviation estimate is then determined as

$$\delta y = \frac{y\left(x, \frac{h}{2}\right) - y(x, h)}{2^p - 1}, \tag{E.95}$$

where p is the order of the numerical method (for example, in the case of the Euler method, the denominator of Equation (E.95) is equal to 1, in the case of "RK4' will be equal to 15). For comparison, the error estimate of the calculations of the first-order differential equations systems from this Section (where $h = 10^{-3}$) will be $\delta y(10) \approx 3.973 \times 10^{-9}$ and $\delta z(10) \approx -4.976 \times 10^{-9}$ for the Euler method and $\delta y(10) \approx 4.441 \times 10^{-17}$ and $\delta z(10) \approx -1.480 \times 10^{-17}$ for the method "RK4".

- **Dormand-Prince method (DOPRI)**

This method is de facto the member (extension) of the Runge-Kutta family solutions, it corresponds, however, to Taylor polynomial of 6th or 7th order. Using this method, we obtain the 4th and 5th order of accuracy of the RK solutions (Dormand & Prince, 1980). The difference in accuracy between the 4th and 5th order in the RK solution, we then take as the error in the accuracy of the 4th order RK solution. Based on this error, we then implement an algorithm of the *adaptive iterative step* h for keeping the desired accuracy (see below).

This method is especially useful in the case of ODEs with strong damping or "tough" (the so-called *stiff equations*), where simpler methods become quickly unstable and produce inaccurate results. An example of such a stiff equation may be $y' = 3\frac{y}{x} + x^3 + x$, $y(1) = 3$ which is also analytically solvable ($y = 3x^3 + x^4 - x^2$) so that we can compare the results given by different methods.

The 4th order solution in the point x_{i+1}, we obtain as

$$y_{i+1} = y_i + h\left(\frac{35}{384}k_1 + \frac{500}{1113}k_3 + \frac{125}{192}k_4 - \frac{2187}{6784}k_5 + \frac{11}{84}k_6\right). \tag{E.96}$$

The 5th order solution in the point x_{i+1} will be

$$Y_{i+1} = y_i + h\left(\frac{5179}{57600}k_1 + \frac{7571}{16695}k_3 + \frac{393}{640}k_4 - \frac{92097}{339200}k_5 + \frac{187}{2100}k_6 + \frac{1}{40}k_7\right). \tag{E.97}$$

where the coefficients k_α are (see the so-called *Butcher tableau*, Butcher (2008))

$$\begin{aligned}
k_1 &= f(x_i, y_i)\\
k_2 &= f\left(x_i + \frac{1}{5}h, y_i + \frac{1}{5}k_1\right)\\
k_3 &= f\left(x_i + \frac{3}{10}h, y_i + \frac{3}{40}k_1 + \frac{9}{40}k_2\right)\\
k_4 &= f\left(x_i + \frac{4}{5}h, y_i + \frac{44}{45}k_1 - \frac{56}{15}k_2 + \frac{32}{9}k_3\right)\\
k_5 &= f\left(x_i + \frac{8}{9}h, y_i + \frac{19372}{6561}k_1 - \frac{25360}{2187}k_2 + \frac{64448}{6561}k_3 - \frac{212}{729}k_4\right)\\
k_6 &= f\left(x_i + h, y_i + \frac{9017}{3168}k_1 - \frac{355}{33}k_2 - \frac{46732}{5247}k_3 + \frac{49}{176}k_4 - \frac{5103}{18656}k_5\right)\\
k_7 &= f\left(x_i + h, y_i + \frac{35}{384}k_1 + \frac{500}{1113}k_3 + \frac{125}{192}k_4 - \frac{2187}{6784}k_5 + \frac{11}{84}k_6\right).
\end{aligned} \tag{E.98}$$

The difference between 4th and 5th order solutions defines the error of the 4th order solution,

$$\delta y_{i+1} = |Y_{i+1} - y_{i+1}|. \tag{E.99}$$

If the error exceeds the selected upper limit in accuracy $\delta_{\max}$, the algorithm shrinks the magnitude of the iteration step h (typically to one half) and repeats the computation. The iteration step h shrinks for so long until the required accuracy is reached. On the other hand, if the error drops below the selected lower limit in accuracy $\delta_{\min}$, the magnitude of the iteration step h extends (typically doubles), and the calculation repeats until the required accuracy is reached. The substantial advantage is that the calculation in regions where the solution is already stable does not repeat, so the computational time is spared.

Here we show an example of solving ordinary second-order differential equations by the simple, often used, the so-called *shooting method*, and also using a tridiagonal matrix (see Section E.2.1):

- **Shooting method**

is a simple method of solving ordinary second-order differential equations where we need two boundary conditions, the position at "shot" and at "impact" (Dirichlet conditions), or the direction of "shot" and "impact" (Neumann conditions), or the mixed conditions (for example, the position and direction of the "shot"), based on the "firing" the function according to the given boundary conditions. We then search coefficients of the function that ensure that the "shot" function "falls" in the desired way to the desired point. We will show the method on the example of the solution of the so-called *Lane-Emden* equation, which is an ordinary second-order differential equation usually written in the implicit form

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}y}{\mathrm{d}x}\right)+y^n=0 \qquad \text{and so} \qquad y''+\frac{2}{x}y'+y^n=0, \tag{E.100}$$

where x is an independent variable, y is a dependent variable, and n is a constant. This equation is analytically solvable only for $n = 0$, 1, 5, for all the other n must be solved numerically. For $n = 0$, we get the solution by direct integration with an inclusion of the boundary conditions, for $n = 1$, we solve the spherical Bessel differential equation (see Equation (D.124)). For $n = 5$, we get a solution through the so-called Emden transformation, where $y = Ar^{\omega}s$, r, s are new variables, and $\omega = 2/(n-1)$.

We will calculate Equation (E.100) for $n = 1.5$ and with the mixed boundary conditions $y(0) = 1$, $y'(0) = 0$. The algorithm is "fired" horizontally from the point [0,1], the new value y is calculated in each spatial step as $y = y + (\Delta y/\Delta x)\Delta x$. The second derivative y'' is written as $(y')'$, that is, $\Delta(\Delta y/\Delta x)/\Delta x$, and every new value y'' is calculated as $(\Delta y/\Delta x)/\Delta x = (\Delta y/\Delta x)/\Delta x-[(2/x)(\Delta y/\Delta x)+y^n]$ in each spatial step. This can be rewritten after multiplying the whole equation by Δx as $(\Delta y/\Delta x) = (\Delta y/\Delta x) - [(2/x)(\Delta y/\Delta x) + y^n]\Delta x$. The numerical algorithm of Equation (E.100) can be written as follows (Fortran 95):

• **program** Emden **implicit none**	program name declaration
double precision :: x, y, dydx, n, dx	declaration of real quantities x, y, dydx, n, dx with double precision, where dydx $= y' = \Delta y/\Delta x$ and dx $= \Delta x$
x=0.d0	declaration of parameters and boundary conditions
y=1.d0 dydx=0.d0 dx=1.d-3 n=1.5d0	
do	calculation cycle
x=x+dx y=y+dydx*dx dydx=dydx-(2.d0*dydx/x+y**n)*dx	
if(x>15.d0)**exit**	stop criterion given by preliminary estimation
write(1,*) x,y,dydx	write to file fort.1
end do	end of cycle
end program Emden	

• Example of solving ordinary second-order differential equations using the tridiagonal matrix

The solution of the boundary value problem of the ordinary second-order equation $p(x)y''(x) + q(x)y'(x)+r(x)y(x) = f(x)$ on an interval a, b with the Dirichlet boundary conditions $y(a) = A$,

$y(b) = B$, can be easily solved using a tridiagonal matrix (see Section E.2.1). As an example of solution, we will use a simple equation with constant coefficients $y'' + 3y' + 2y = (20x + 29)\,\mathrm{e}^{3x}$ (easy to solve even analytically) on the interval $\langle 0, 1\rangle$ with the Dirichlet boundary conditions $y(0) = 0$, $y(1) = 1$.

After rewriting the given equation into the difference scheme with $n+2$ points of the spatial grid, where we derive the particular derivatives of the left-hand side according to Equations (E.68) and (E.69), we get the equation in the form

$$\left(p - \frac{h}{2}q\right) y_{i-1} + \left(h^2 r - 2p\right) y_i + \left(p + \frac{h}{2}q\right) y_{i+1} = h^2 f_i, \tag{E.101}$$

where $i = 0, 1, \dots, n, n+1$, with the coefficients $p = 1$, $q = 3$, $r = 2$, and with the constant spatial step $h = (x_{n+1} - x_0)/(n+1) = [x(1) - x(0)]/(n+1)$, at $n = 99$ it will be $h = 0.01$. If we denote the brackets on the left-hand side of Equation (E.101) successively P, Q, R, we get the equation with the tridiagonal matrix on the left-hand side in the form

$$\begin{pmatrix} Q & R & & & & \\ P & Q & R & & & \\ & & \ddots & \ddots & \ddots & \\ & & & P & Q & R \\ & & & & P & Q \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix} = \begin{pmatrix} h^2 f_1 - P y_0 \\ h^2 f_2 \\ \vdots \\ h^2 f_{n-1} \\ h^2 f_n - R y_{n+1} \end{pmatrix}. \tag{E.102}$$

The numerical algorithm is written as follows (Fortran 95):

• **program** tridiag **implicit none**	declaration of the program name
integer :: i, ni, N, LDB, NRHS, INFO	declaration of integer variables: i = sequence number of independent variable, ni = total number of discrete values, the others are the parameters of the LAPACK package subprogram DGTSV - see Section E.1
parameter(ni=99,N=ni,LDB=N,NRHS=1)	values of integer variables
double precision :: x(ni) ,y(ni), h(ni), p(ni), q(ni), r(ni), f(ni), B(LDB,NRHS), DL(N-1), DU(N-1), D(N)	declaration of real variables as a double precision array
double precision, parameter :: x0=0.d0, xn=1.d0, y0=0.d0, yn=1.d0	declaration of real constants with double precision
do i=1,N	spatial step calculation cycle
x(i)=x0+(xn-x0)*i/dfloat(ni+1)	The dfloat command changes the integer variable to real
end do	
do i=1,N	main calculation cycle
h(i)=x(i)-x(i-1)	the constant step h is written here in general
p(i)=1.d0	constant coefficients are written in general

```
    q(i)=3.d0
    r(i)=2.d0
    f(i)=(20.d0*x(i)+29.d0)*dexp(3.d0*x(i))
    if(i.eq.1) then                          lower boundary condition
       B(i,1)=h(i)**2.d0*f(i)-(p(i)-q(i)*h(i)/2.d0)*y0
    elseif((i.gt.1).and.(i.lt.N)) then       main array
       B(i,1)=h(i)**2.d0*f(i)
    else                                     upper boundary condition
       B(i,1)=h(i)**2.d0*f(i)-(p(i)+q(i)*h(i)/2.d0)*yn
    endif
 end do
 do i=1,N-1                                  enter the lower diagonal
    DL(i)=p(i)-q(i)*h(i)/2.d0
 end do
 do i=1,N                                    enter the main diagonal
    D(i)=r(i)*h(i)**2.d0-2.d0*p(i)
 end do
 do i=2,N                                    enter the upper diagonal
    DU(i)=p(i)+q(i)*h(i)/2.d0
 end do
 call the LAPACK DGTSV subroutine (see SectionE.1):
 call DGTSV(N, NRHS, DL, D, DU, B, LDB, INFO)
 if(INFO.ne.0) write(*,*) "INFO=",INFO,"!!!"
 write(1,*) x0, y0
 do i=1,N
    y(i)=B(i,1)
    write(1,*) x(i), y(i)                    write to file fort.1
 end do
 write(1,*) xn, yn
 end program tridiag
```

E.5 Numerical methods of calculating functions of several variables - solution of partial differential equations

E.5.1 Finding the roots of a system of functions of several variables - Newton-Raphson method

The Newton (Newton-Raphson) method is also a very effective tool for solving the general system of (non-linear) equations. A system P containing n equations can generally be written as

$$P_i\left(\vec{x}\right) = 0, \tag{E.103}$$

where $i = 1, \ldots, n$ and $\vec{x}$ is a vector of variables x_j. Using the Taylor expansion of Equation (E.103) to the first-order, we get a general expression for kth iteration (kth iterative step) of solving the system of equations P_i, which can be written in the compact form as

$$J^{\,k}\Delta\vec{x}^{\,k} = -\vec{P}^{\,k-1}\big(\vec{x}^{\,k-1}\big), \tag{E.104}$$

where the vector $\Delta\vec{x}$ represents the correction of the solution for each variable x_j with respect to the previous iterative step. The explicit notation of the vector $\Delta\vec{x}^{\,k}$ will have the form

$$\Delta\vec{x}^{\,k} = (x_1^k - x_1^{k-1}, \dots, x_n^k - x_n^{k-1})^T. \tag{E.105}$$

The expression $\vec{P}^{\,k}$ in Equation (E.104) represents the vector of kth iteration of all the system of equations $P_i^{\,k}$, while the expression $J^{\,k}$ denotes the corresponding Jacobi matrix whose each element $J_{ij}^{\,k}$ can be easily expressed analytically from the system of equations $P_i^{\,k}$, setting

$$J_{ij}^{\,k} = \frac{\partial P_i^{\,k}}{\partial x_j^k}. \tag{E.106}$$

For example, if we solve (as a simple model example) the set of equations:

$$\begin{array}{rrrcr} x^4 & +6y^2 & -12z & = & 16, \\ 5x^3 & -3y & +z^2 & = & 9, \\ x^3 & +7y^2 & -z & = & 0, \end{array} \tag{E.107}$$

we can write the explicit form of Equation (E.104) as

$$\begin{pmatrix} 4\,x_0^3 & 12\,y_0 & -12 \\ 15\,x_0^2 & -3 & 2\,z_0 \\ 3\,x_0^2 & 14\,y_0 & -1 \end{pmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \\ z - z_0 \end{pmatrix} = - \begin{pmatrix} x_0^4 + 6\,y_0^2 - 12\,z_0 - 16 \\ 5\,x_0^3 - 3\,y_0 + z_0^2 - 9 \\ x_0^3 + 7\,y_0^2 - z_0 \end{pmatrix}, \tag{E.108}$$

which we further solve iteratively by using, for example, the LAPACK package (see Section E.1) as a system of three linear equations for three unknown variables $\Delta x = x - x_0$, $\Delta y = y - y_0$, and $\Delta z = z - z_0$, from which at each step we get new values of x, y, and z as $x = \Delta x + x_0$, $y = \Delta y + y_0$, and $z = \Delta z + z_0$.

- An example of a possible way to program a system of equations (E.107) - Fortran 95:

```
program eqsystem                    declaration of the program name
implicit none

declaration of real variables in the program header, see Section E.1:
integer :: i,j,K,INFO,KL,KU,LDAB,LDB,N,NRHS
parameter(N=3,KL=2,KU=2,K=KU+KL+1,LDAB=2*KL+KU+1,LDB=N,NRHS=1)
integer :: IPIV(N)

declaration of real variables with double precision:
double precision :: AB(LDAB,N),B(LDB,NRHS),DER(N,N),C(N),x0,y0,z0
redirection of the final solution output to file "solve.dat":
open(10,file="solve.dat",status="unknown")

x0=-4.0d0                           estimate of entry value x_k
y0=-3.0d0                           estimate of entry value y_k
z0=14.0d0                           estimate of entry value z_k
do                                  calculation cycle
   matrix of derivatives of left-hand sides:
   DER(1,1)=4.d0*x0**3.d0
   DER(1,2)=12.d0*y0
```

```
    DER(1,3)=-12.d0
    DER(2,1)=15.d0*x0**2.d0
    DER(2,2)=-3.0
    DER(2,3)=2.d0*z0
    DER(3,1)=3.d0*x0**2.d0
    DER(3,2)=14.d0*y0
    DER(3,3)=-1.d0
```

transformed band matrix AB according to LAPACK scheme, see Section E.1:

```
    do j=1,N
       do i=max(1,j-KU),min(N,j+KL)
          AB(K+i-j,j)=DER(i,j)
       end do
    end do
```

matrix of right-hand sides:

```
    B(1,1)=-(x0**4.d0+6.d0*y0**2.d0-12.d0*z0-16.d0)
    B(2,1)=-(5.d0*x0**3.d0-3.d0*y0+z0**2.d0-9.d0)
    B(3,1)=-(x0**3.d0+7.d0*y0**2.d0-z0)
```

calculation cycle of the subprogram DGBSV, see Equation E.1:

```
    call DGBSV(N,KL,KU,1,AB,LDAB,IPIV,B,N,INFO)
    if (INFO.ne.0) write(*,*) "INFO=",INFO,"!!!"
    C=(/(dabs(B(i,1)),i=1,N)/)

    if (maxval(C).lt.1.d-15) exit
```

stop criterion: $\max|\Delta x, \Delta y, \Delta z| < 10^{-15}$

```
    x0=B(1,1)+x0
    y0=B(2,1)+y0
    z0=B(3,1)+z0
```

write resulting values $x, y, z, \Delta x, \Delta y, \Delta z$ from particular time steps to file:

```
   write(10,*)x0,y0,z0,(B(i,1),i=1,N)
 end do

 stop
 end program eqsystem
```

stops the process

end of program

- Table of the calculated values $x_k, y_k, z_k, \Delta x_k, \Delta y_k, \Delta z_k$ from all the time steps performed:

k	x_k	y_k	z_k
1	-3.5568659855769229	-2.8660523504273505	14.644631410256411
2	-3.4484177335542667	-2.8088357894123277	14.321062859837509
3	-3.4422190042021756	-2.8052747443938260	14.300861993036721
4	-3.4421993029036972	-2.8052630869488695	14.300795971729505
5	-3.4421993027044500	-2.8052630868291244	14.300795971052235
6	-3.4421993027044500	-2.8052630868291244	14.300795971052233

k	Δx_k	Δy_k	Δz_k
1	0.44313401442307693	0.13394764957264957	0.64463141025641035
2	0.10844825202265625	5.7216561015022732E-002	-0.32356855041890148
3	6.1987293520911584E-003	3.5610450185016187E-003	-2.0200866800787826E-002
4	1.9701298478486783E-005	1.1657444956463351E-005	-6.6021307216049201E-005
5	1.9924720437988766E-010	1.1974503494876664E-010	-6.7726957780015056E-010
6	6.2835370146182566E-017	1.8208999862070576E-016	-1.3650720993330078E-015

The initial estimate (if we do not know, unlike in the case of standard physical processes, some “predicted” values) can be rather difficult. Using this example, you can check that if you, for example, choose all the initial values equal to 1, the calculation converges as well, however, after 24 325 time steps (instead of 6 time steps in case of the above written close estimates of the initial integers).

E.5.2 Principles of finite differences

Simple example - one-dimensional equation with two variables: t-time, x-length - the Burgers' (transport) partial differential equation

$$\frac{\partial f(t,x)}{\partial t} + u\frac{\partial f(t,x)}{\partial x} = 0, \tag{E.109}$$

where u is the constant (velocity). Numerical form of the function $f(t,x)$ is represented on one-dimensional grid of M spatial points,

$$x_0,\, x_1,\, \dots,\, x_M \qquad (x_0 < x_1 < x_2 < \dots < x_M). \tag{E.110}$$

The calculation is repeated over N time steps,

$$t_1 = t_0 + \Delta t,\; t_2 = t_1 + \Delta t = t_0 + 2\Delta t,\; \dots,\; t_N = t_0 + N\Delta t. \tag{E.111}$$

The numerical solution of the function $f(t,x)$ in a general jth spatial and nth time step ($x = x_j$, $t = t_n$) is denoted as f_j^n. The Taylor expansion of the function $f(t,x)$ has the form

$$f(x+h,t) = f(x,t) + h\frac{\partial f(x,t)}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 f(x,t)}{\partial x^2} + \mathcal{O}(h^3) + \dots \tag{E.112}$$

$$f(x-h,t) = f(x,t) - h\frac{\partial f(x,t)}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 f(x,t)}{\partial x^2} - \mathcal{O}(h^3) + \dots, \tag{E.113}$$

where $h = \Delta x$ is the increment of the spatial variable x (see Equation (1.1)) and the symbol $\mathcal{O}$ denotes a negligible, not counted contribution of higher order terms. In the numerical mathematics, the derivatives are replaced by the so called *differences* (see Section E.4.2):

$$\frac{\partial f(x,t)}{\partial x} \approx \frac{f(x+h,t) - f(x,t)}{h} = \frac{f_{j+1}^n - f_j^n}{\Delta x}, \quad \text{etc.} \tag{E.114}$$

The types of the differences for approximations of the first-order derivatives:

$$\begin{aligned}
\left.\frac{\partial f}{\partial x}\right|_j^n &\approx \left(f_{j+1}^n - f_j^n\right)/\Delta x && \text{forward difference,}\\
\left.\frac{\partial f}{\partial x}\right|_j^n &\approx \left(f_j^n - f_{j-1}^n\right)/\Delta x && \text{backward difference,}\\
\left.\frac{\partial f}{\partial x}\right|_j^n &\approx \left(f_{j+1}^n - f_{j-1}^n\right)/(2\Delta x) && \text{central difference.}
\end{aligned} \tag{E.115}$$

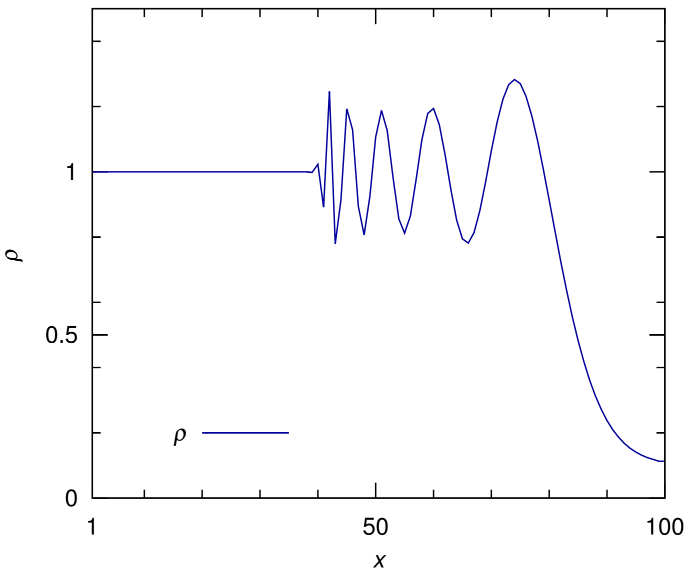

Figure E.8: Graph (time snapshot) of successive density waves, described by the Burgers' equation (E.109), modeled by the explicit Euler scheme based on finite difference principle (Equation (E.118), see also the program script presented in this Section). The graph obviously shows an unstable wave perturbation whose extent and amplitude permanently increases (see Section E.5.3).

Example of the numerical difference scheme for approximations of second-order derivatives:

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_j^n \approx \left(f_{j+1}^n - 2f_j^n + f_{j-1}^n\right)/(\Delta x)^2. \tag{E.116}$$

The numerical difference scheme of the transport (advection) equation (E.109) has the form

$$\frac{\left(f_j^{n+1} - f_j^n\right)}{\Delta t} = -u\frac{\left(f_{j+1}^n - f_{j-1}^n\right)}{2\Delta x}, \tag{E.117}$$

where the time step is calculated as the forward difference and the space step is calculated as the central difference. After a simple modification, we get the difference equation (E.117) in the programmable form:

$$f_j^{n+1} = f_j^n - \frac{u\Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right). \tag{E.118}$$

- An example of a possible way to program Equation (E.118) - Fortran 95:

program explicit **implicit none**	declaration of the program name
integer :: j, n, t	declaration of integer variables in the header of the program: j = sequence number of a spatial step, n = sequence number of a time step
integer :: nj, nn	declaration of integer variables in the header of the program: nj = total number of spatial steps j, n = total number of time steps n
parameter (nj=100, nn=200)	enter numeric values for nj, nn

```
double precision :: x(nj), f(nj), u(nj)   declaration of real quantities x, f, and u as an
                                          array (vector) of nj elements with double precision
double precision :: dt                    declaration of real quantity dt (time step)
parameter (dt = 1.d0, u = 1.2d0)          declaration of fixed values of constant real values
do j=1,nj                                 initial condition cycle (initial function)
   x(j) = dfloat(j)                       dfloat command converts integer variable to real
   if (j.le.nj/2) then                    the so called logic condition (where .le. means ≤)
      f(j) = 1.d0
   else
      f(j) = 0.1d0                        specified initial function: for x ≤ 0.5nj → f = 1.0,
                                          for x > 0.5nj → f = 0.1
   endif
end do                                    end of cycle
t=0.d0                                    change of the type of variable t to real with double
                                          precision
do                                        outer (time) cycle
   t = t+dt
   do j=2,nj-1                            inner (spatial) cycle
     f(j) = f(j)-u(j)*dt*(f(j+1)-f(j-1))/(x(j+1)-x(j-1))        Equation (E.118)
   end do                                 end of the inner cycle
   f(1) = f(1)                            inner the so-called fixed (inflow) boundary condition
   f(nj) = f(nj-1)                        outer the so-called free (outflow) boundary condition
   do j=1,nj                              write cycle to a file named fort.100
      write (100,*) x(j), f(j)            write the calculated values
   end do
   write (100,*)
   write (100,*)                          two-row space required for animation of time cycles
   if (t.gt.200.d0) exit                  exit from the time step cycle if t > 200
end do                                    end of the time step cycle
stop                                      stopping the whole process at t > 200
end program explicit                      end of program
```

This so-called explicit Euler numerical scheme is simple, clear, and illustrative but it is *always* numerically unstable (see Figure E.8 and Section E.5.3):

E.5.3 von Neumann stability analysis

A simple analytical method based on the assumption of a periodic numerical perturbation, i.e., the *Fourier decomposition* of a numerical error. The method was published in the year 1947 by the mathematicians John Crank and Phyllis Nicolson, co-authored by the prominent mathematician, physicist, and pioneer of digital computers, John von Neumann.

Suppose general disturbances of stability (periodic perturbations, vibrations) of the wave nature in the form

$$\xi^n e^{ikj\Delta x}, \tag{E.119}$$

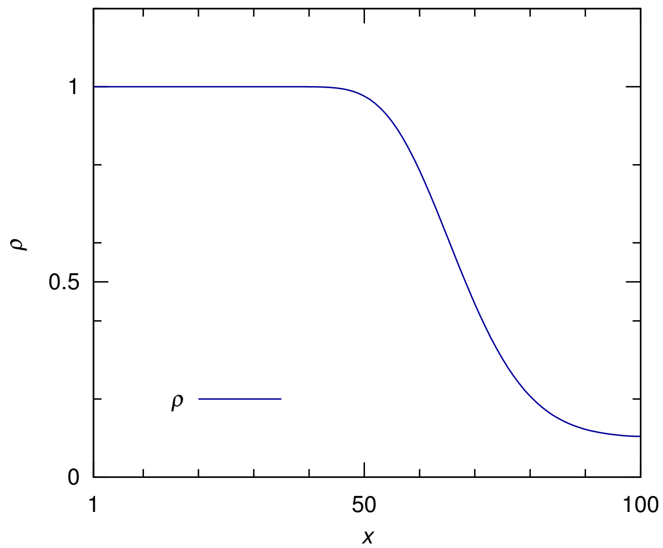

Figure E.9: Time snapshot of a progressive density wave, described by the Burgers' equation (E.109), modeled by the Lax method (Equation (E.125)). The density curve is stable in contrast to the explicit scheme, but there is too much of the so-called *numerical diffusivity*, manifested by the significant blur (defocusing) of the original sharp steep-wave shape (cf. the graph in Section E.5.8), caused by adding an expression corresponding to the second derivative of the advection term, i.e., where the expression $(f_{j+1} + f_{j-1})/2$ in Equation (E.125) can be regarded as $f_j + (f_{j+1} - 2f_j + f_{j-1})/2$.

where $\xi(k)$ is the amplitude of the wave, k is the wavenumber of an arbitrary value. If $|\xi| > 1$, for $n \to \infty$ there will be

$$|\xi|^n \to \infty, \tag{E.120}$$

the perturbation permanently grows, and the numerical scheme is unstable. If

$$|\xi| < 1, \tag{E.121}$$

the numerical scheme is stable. After substituting the perturbation of the wave function into the explicit solution (E.118), we get

$$\left(\xi^{n+1} - \xi^n\right) e^{ikj\Delta x} = -\frac{u\Delta t}{2\Delta x}\xi^n \left[e^{ik(j+1)\Delta x} - e^{ik(j-1)\Delta x}\right], \tag{E.122}$$

and after dividing the whole Equation (E.122) by the expression $\xi^n e^{ikj\Delta x}$, we get

$$\xi = 1 - \frac{u\Delta t}{2\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right) = 1 - i\frac{u\Delta t}{\Delta x}\sin(k\Delta x). \tag{E.123}$$

Since $|a + ib| = \sqrt{a^2 + b^2}$, the square of Equation (E.123) is equal to

$$|\xi|^2 = 1 + \left(\frac{u\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x), \tag{E.124}$$

where the right-hand side almost always will be greater than 1 (exceptionally equal to 1). Obviously, in the case of the explicit numeric scheme, the inequality $|\xi| \geq 1$ must always apply; this scheme is therefore always unstable.

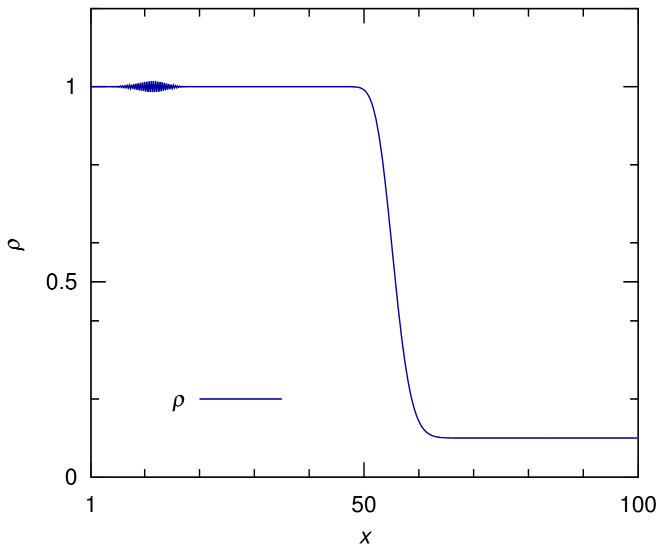

Figure E.10: Time snapshot of a progressive density wave (E.109), modeled by the implicit scheme method (Equation (E.134)). The density curve is stable and, unlike the Lax scheme, it is far not so blurred. The amplitude of the progressive "wave packet" of the perturbation in the left part of the graph decreases with time; however, its extent does not change.

E.5.4 Lax method

The numerical variant of the explicit scheme, which it substantially stabilizes, is named after the mathematician Peter David Lax. It is based on a simple modification of the time step term. The term f_j^n in the explicit solution is replaced here by the arithmetic mean of the neighboring values,

$$f_j^{n+1} = \frac{1}{2}\left(f_{j+1}^n + f_{j-1}^n\right) - \frac{u\Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right). \tag{E.125}$$

The von Neumann stability analysis in this case gives

$$\xi = \cos(k\Delta x) - i\frac{u\Delta t}{\Delta x}\sin(k\Delta x), \quad \text{and so} \quad |\xi|^2 = \cos^2(k\Delta x) + \left(\frac{u\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x). \tag{E.126}$$

The scheme is obviously stable if for the so-called *Courant-Friedrichs-Lewyho* number $u\Delta t/\Delta x$ (shortly the Courant number, usually abbreviated as cfl) holds

$$\frac{u\Delta t}{\Delta x} \leq 1 \qquad \text{Courant stability theorem.} \tag{E.127}$$

The same equation (E.109) modeled by the Lax method (E.125) is shown in the graph E.9.

E.5.5 Upwind method

The upwind method uses a backward difference in the spatial (advection) term,

$$f_j^{n+1} = f_j^n - \frac{u\Delta t}{\Delta x}(f_j^n - f_{j-1}^n), \tag{E.128}$$

the von Neumann stability analysis in this case gives (cfl $= \alpha$):

$$\xi = 1 - \alpha + \alpha\cos(k\Delta x) - i\alpha\sin(k\Delta x), \quad \text{and so,}$$
$$|\xi|^2 = [1 - \alpha + \alpha\cos(k\Delta x)]^2 + \alpha^2\sin^2(k\Delta x). \tag{E.129}$$

The condition $|\xi|^2 < 1$ implies the inequality

$$2\alpha(1-\alpha)[1-\cos(k\Delta x)] > 0. \tag{E.130}$$

Because, if $\alpha > 0$ then $\cos(k\Delta x) < 1$, the scheme will be stable if, as in the Section E.5.4, the Courant number $\alpha < 1$.

E.5.6 Lax-Wendroff method

The two-step method named after the already mentioned Peter Lax (see Section (E.5.4)) and another matematician Burt Wendroff, combines the advantages of the Lax and the explicit scheme in the following way:

1st step (Lax) and 2nd step (explicit):

$$f_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(f_{j+1}^n + f_j^n\right) - \frac{1}{2}\frac{u\Delta t}{\Delta x}\left(f_{j+1}^n - f_j^n\right), \qquad f_j^{n+1} = f_j^n - \frac{u\Delta t}{\Delta x}\left(f_{j+\frac{1}{2}}^{n+\frac{1}{2}} - f_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right). \tag{E.131}$$

The von Neumann stability analysis in this case gives (cfl $= \alpha$):

$$\xi = 1 - 2\alpha\sin\left(\frac{k\Delta x}{2}\right)\left[\alpha\sin\left(\frac{k\Delta x}{2}\right) + i\cos\left(\frac{k\Delta x}{2}\right)\right], \quad \text{and so,} \tag{E.132}$$
$$|\xi|^2 = 1 - 4\alpha^2\sin^2\left(\frac{k\Delta x}{2}\right)\left[1 - \alpha^2\sin^2\left(\frac{k\Delta x}{2}\right) - \cos^2\left(\frac{k\Delta x}{2}\right)\right]. \tag{E.133}$$

The requirement $|\xi|^2 < 1$ again implies the stability condition $\alpha < 1$.

E.5.7 Implicit scheme

The principle of the so-called implicit scheme is based on the fact that the values of a quantity f in the spatial (advection) term on the right-hand side of Equation (E.118) are given at the time t^{n+1}, that is, de facto in the future. After the following instant calculation,

$$f_j^{n+1} = f_j^n - \frac{u\Delta t}{2\Delta x}\left(f_{j+1}^{n+1} - f_{j-1}^{n+1}\right), \tag{E.134}$$

and the von Neumann stability analysis in this case gives (cfl $= \alpha$):

$$\xi = \frac{1}{1 + i\alpha\sin(k\Delta x)} = \frac{1 - i\alpha\sin(k\Delta x)}{1 + \alpha^2\sin^2(k\Delta x)}, \quad \text{and so} \quad |\xi|^2 = \frac{1}{1 + \alpha^2\sin^2(k\Delta x)}. \tag{E.135}$$

From Equation (E.135), it is therefore clear that the implicit scheme must satisfy the stability condition $|\xi| \leq 1$, so it is *always* numerically stable. The disadvantage of this method is the complicated calculation of f_j^{n+1} at every time step, where we calculate this unknown value using the so called *tridiagonal* matrix (see Sections E.1, E.2.1),

$$\frac{\alpha}{2}f_{j-1}^{n+1} - f_j^{n+1} - \frac{\alpha}{2}f_{j+1}^{n+1} = -f_j^n, \tag{E.136}$$

by any of the numerical linear algebra methods or libraries (see Section E.1). The same equation (E.109), modeled by the implicit method (E.134)-(E.136), is shown in the graph E.10.

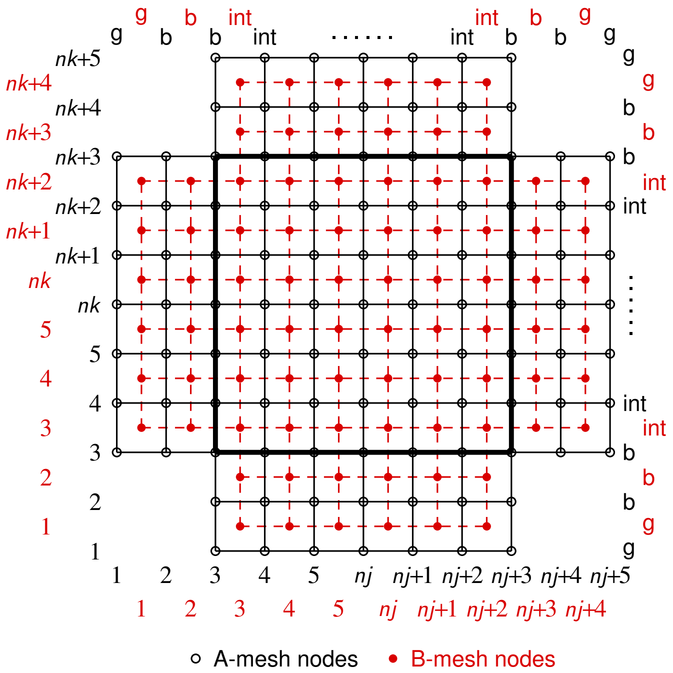

Figure E.11: *Staggered mesh* scheme. The A-mesh for computing vectors is shown in black, and the B-mesh for computing scalar quantities is shown in red. The internal computational domain ('int') is bounded by the thick line, the symbol 'b' indicates the boundary conditions counting zone, and the symbol 'g' indicates the so-called *ghost zone*, which is the another added boundary condition zone that is necessary for calculating differential equations of the second order, or for the case of symmetrical conditions that may be, for example, relative to the grid axis (periodic boundary conditions), or to the grid center, etc. The exact arrangement of the boundary conditions zones may vary in detail according to the type of boundary conditions (fixed, reflective, periodic, etc.

E.5.8 Example of the more advanced numerical scheme

- At present, there are a number of more modern, accurate and stable numeric methods (see, e.g., Thompson, 2006):

- The use of the so-called *staggered mesh*, allowing to separate fluxes of different types of quantities (flux splitting), for example, vector and scalar fields, etc.

- Gradual addition of individual members of the right-hand sides of the physical equations representing different force fields (operator splitting):

$$\begin{aligned}
(f^1 - f^0)/\Delta t &= L_1(f^0) \\
(f^2 - f^1)/\Delta t &= L_2(f^1) \\
\vdots \qquad & \qquad \vdots \\
(f^m - f^{m-1})/\Delta t &= L_m(f^{m-1}),
\end{aligned} \tag{E.137}$$

  where L_j represents the individual approximations of the right-hand side of equations by using the finite difference principle, m is the total number of terms on the right-hand side of the equation, and the superscripts indicate the sequence number of the time sub-step.

- The principle of the *staggered mesh*: on the A-mesh "live" the vector variables, on the

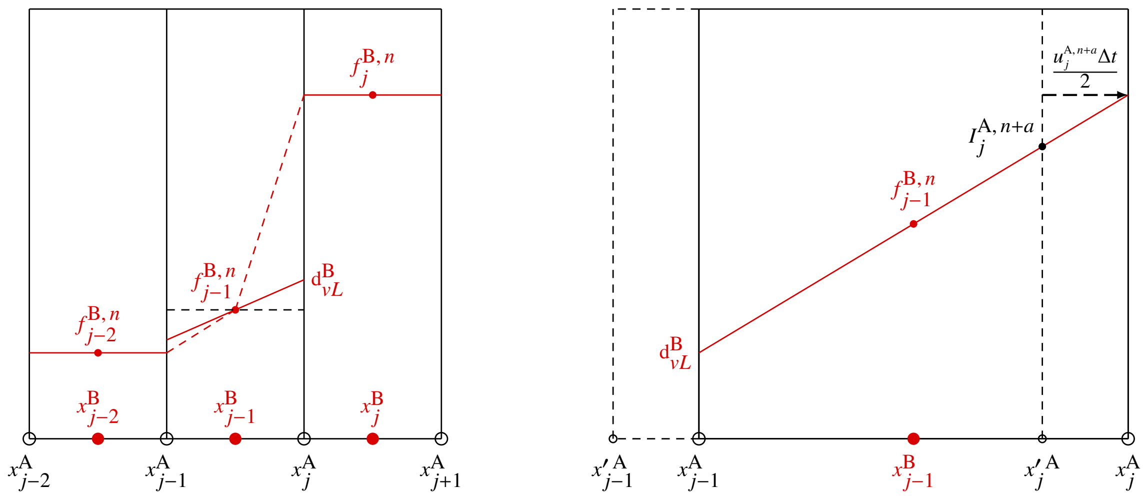

Figure E.12a Figure E.12b

Figure E.12: Schematic representation of the condition of the monotonicity of the van Leer derivative (Equation (E.139)) is shown in Figure E.12a: the slope of linear distribution of the quantity f in the central computational cell (dashed line) is reduced due to the van Leer derivative (solid line denoted as d^{B}_{vL}), so the values of linearly interpolated, advected scalar variable f at the cell interface must "fit" along the whole edge of this cell, between the values of this variable, *averaged* over the volumes of adjacent computational cells. Figure E.12b shows the predictor step of the advection of scalar variable f (Equation (E.140)). The quantity is linearly interpolated (the solid red line denoted by d^{B}_{vL} indicates the slope of the van Leer derivative). It is advected to the cell interface in the half-time step $t + \Delta t/2$. The cell boundaries, depicted by the solid line, symbolize the volume of matter advected in time while the "dashed" cell is fixed in space. The position of the linear interpolant I is denoted as $I^{A,n+a}_{j}$. The following corrector step (Equation (E.141)) advects the variable to the center of the B-mesh at the time $t + \Delta t$.

B-mesh "live" the scalar quantities (see Figure (E.11).

- An example of a two-step method (i.e., the calculation of the next time step is divided into the two intermediate sub-steps: an explicitly calculated *predictor* step followed by implicit the so-called *corrector* step) for calculation of the transport equation (E.109) of a scalar quantity f:

$$\Delta^{A}_{-} = \frac{f^{B}_{j} - f^{B}_{j-1}}{x^{B}_{j} - x^{B}_{j-1}}, \quad \Delta^{A}_{+} = \frac{f^{B}_{j+1} - f^{B}_{j}}{x^{B}_{j+1} - x^{B}_{j}}, \tag{E.138}$$

where Δ_{-}, Δ_{+} are the symbols for the backward and forward difference. To calculate the predictor step, we use the so-called *van Leer* derivative (van Leer, 1982), definned as:

$$d^{B}_{vL} = \begin{cases} \langle \Delta_{-}\Delta_{+} \rangle = \dfrac{2\Delta_{-}\Delta_{+}}{\Delta_{-} + \Delta_{+}}, & \text{if} \quad \Delta_{-}\Delta_{+} > 0 \\ 0, & \text{if} \quad \Delta_{-}\Delta_{+} < 0\,. \end{cases} \tag{E.139}$$

Therefore, the van Leer derivative is nonzero if the function f is monotonous and is zero in those fields of the spatial grid where the function f goes through extremes. An important feature of the van Leer derivative is that it conserves the monotonicity of the derivatives and prevents the formation of local extremes: it follows from Equation

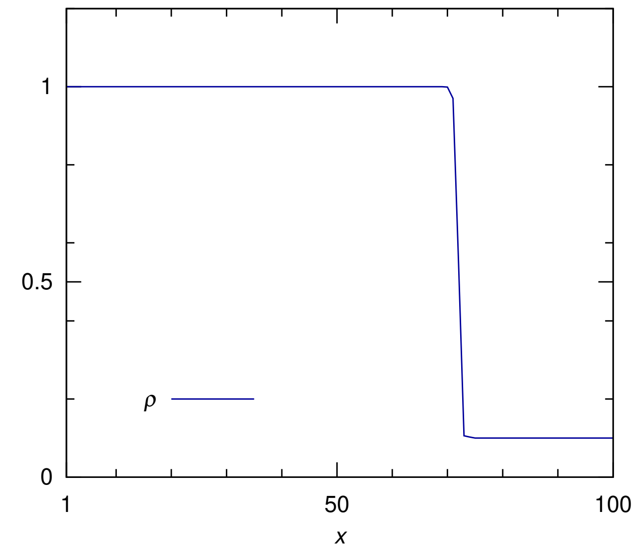

Figure E.13: Time snapshot of the progressive density wave, described by the Burgers' equation (E.109), modeled by the predictor-corrector method (using Equations (E.140) and (E.141)). The density curve is stable and sharp in contrast to the previous schemes, the mild slope of the wavefront is given by the density of the computational grid (the distance of neighboring spatial points). The waveform can be corrected by adding the so-called shear *Navier-Stokes viscosity* or by the volumetric the so-called *numerical (artificial) viscosity* often used in practical calculations (see, e.g., LeVeque, 2002, and others).

(E.139) that if $\Delta_- \approx \Delta_+ \approx \Delta$, then $\langle \Delta_- \Delta_+ \rangle \approx \Delta$, and if $\Delta_- \ll \Delta_+$, or $\Delta_- \gg \Delta_+$, then $\langle \Delta_- \Delta_+ \rangle \approx \min(\Delta_-, \Delta_+)$. This guarantees that the values of the derived function f at the boundaries of the computational cell will not locally "overshoot" the mean values of the function f in the neighboring cells (see Figure E.12).

- The result of the predictor step is the variable I (we call it, for example, the *interpolant*), which is during the predictor step advected at the interface of the other mesh, i.e., from the original B-mesh to the A-mesh and vice versa. In this case, the predictor step will have the form

$$I_j^{\mathrm{A},\,n+a} = f_{j-1}^{\mathrm{B},\,n} + \mathrm{d}_{vL}^{\mathrm{B}} \left(x_j^{\mathrm{A}} - x_{j-1}^{\mathrm{B}} - \frac{u_j^{\mathrm{A},\,n+a} \Delta t}{2} \right), \tag{E.140}$$

where u is the advection rate (cf. Equation (E.118)), and the superscript $n+a$ denotes an intercellular shift of the variable within the time step n.

- The following corrector step will be performed by the equation in the form

$$f_j^{\mathrm{B},\,n+1} = f_j^{\mathrm{B},\,n} - \frac{\Delta t}{x_{j+1}^{\mathrm{A}} - x_j^{\mathrm{A}}} \left(I_{j+1}^{\mathrm{A},\,n+a} u_{j+1}^{\mathrm{A},\,n+a} - I_j^{\mathrm{A},\,n+a} u_j^{\mathrm{A},\,n+a} \right). \tag{E.141}$$

Thus, after the corrector step, the scalar variable f returns to the B-mesh, i.e., in the middle between the positions $\mathrm{A}(j+1)$, $\mathrm{A}(j)$. Equation (E.141) is also a numerical form of one-dimensional divergence. A similar two- and three-dimensional scheme is called the *finite volume method* - see, e.g., LeVeque (2002)). The multidimensional form of Equation (E.141) (calculated in the coordinate direction j, where the k index symbolizes all the other coordinate directions, depending on the dimension of the computational grid) will be:

$$f_{j,k}^{\mathrm{B},\,n+1} = f_{j,k}^{\mathrm{B},\,n} - \frac{\Delta t}{V_{j,k}^{\mathrm{B}}}\left(I_{j+1,k}^{\mathrm{A},\,n+a}u_{j+1,k}^{\mathrm{A},\,n+a}S_{j+1,k}^{\mathrm{A}} - I_{j,k}^{\mathrm{A},\,n+a}u_{j,k}^{\mathrm{A},\,n+a}S_{j,k}^{\mathrm{A}}\right), \tag{E.142}$$

where the quantity $V_{j,k}^{\mathrm{B}}$ means the volume of one grid cell centered on the mesh B, the quantity $S_{j,k}^{\mathrm{A}}$ is then the edge of this cell (located on the mesh A), through which flows the quantity f in the direction j (see Sections B.1.2, B.2.2, B.3.2, and B.7.4, describing relations between these variables in different coordinate systems - see also Figure E.12). If we model the transport equation (E.109) for a vector quantity, the procedure will be quite similar but instead of the mesh B, we will start from the mesh A; the predictor step transports this quantity to the mesh B and then the corrector step moves it back again to the mesh A.

- The same Equation (E.118), modeled by the predictor-corrector method, is shown in Figure E.13. The Courant number cfl $= 0.5$.

- Special attention should be paid to the selection and writing of the *boundary conditions* (see the corresponding zones of the computational grid in Figure E.11). Their basic types include:

  – *fixed* (inflow) boundary conditions, where the values in b and g zones are entered in initial conditions (initial function) and do not change further.

  – *free* (outflow) boundary conditions, when the values in b and g zones in each time step are equal to the value in the first (nearest) computational zone (here it is appropriate to somehow fix that the scalar variables are always non-negative or non-zero).

  – *periodic* boundary conditions, when the values in the zone 1 are equal to the values in zone $nj+1$ in each time step, the values in the zone 2 to the values in the zone $nj+2$, values in the zone 3 (on the red mesh) to the values in the zone $nj+3$, and vice versa, the values in the zone $nj+4$ to the values in the zone 4, and the values in the zone $nj+5$ to values in zone 5. The values in the zones 3 and $nj+3$ on the black mesh are calculated separately from hydrodynamic equations (the same applies to other directions).

  – *reflective* (solid wall) boundary conditions, where the scalar variables q and components of the vector variables that are parallel to the given edge are calculated as $q(1) = q(4)$, $q(2) = q(3)$, $q(nj+3) = q(nj+2)$, and $q(nj+4) = q(nj+1)$. Components of the vector quantities that are perpendicular to the given edge are calculated as $q(1) = -q(5)$, $q(2) = -q(4)$, $q(3) = 0$, $q(nj+3) = 0$, $q(nj+4) = -q(nj+2)$, $q(nj+5) = -q(nj+1)$. The same applies for other directions.

- The numerical scheme given in this Section is far from being the only possible, it is just an example of the so-called *piecewise linear method*, where the numerical differences are simplified by straight pieces (lines). It is also possible to use more accurate the so-called *piecewise parabolic method* - PPM, see, e.g., Colella & Woodward (1984)). Its natural disadvantage, however, is the inherently higher computational cost, i.e., the demands on the computer power, etc. In addition, there are a number of other methods based on different principles of numerical differentiation, other types of spatial grids (such as the so-called *adaptive meshes* that change over time and adapt themselves to the physical distributions of a given problem), or do not use the spatial grids for calculations at all - for example the so-called *SPH method* (Smooth Particle Hydrodynamics), etc.

E.5.9 Examples of modeling of real physical processes

Riemann-Sod shock tube:

The basic test problem for most numerical codes with easily verifiable results. It is a closed tube, or box, divided into two compartments by a fixed partition, also called the *diaphragm*, where both the compartments are filled with a gas of different densities and pressures. Suddenly, the partition disappears, causing the gas starting to move, which is preceded by a shock wave propagating perpendicular to the plane of the original partition, in the direction of the thinner gas. Figure E.14 shows the snapshot of the density profile where the initial state of the gas (where the index L denotes the left side of the tube with higher initial density and pressure, the index R denotes the right side of the tube with lower initial density and pressure) is chosen in the following way: $\rho_L = 1.0$, $\rho_R = 0.125$, $P_L = 1.0$, $P_R = 0.1$, $\gamma = 5/3$, where ρ is the density, P is the pressure, and γ is the adiabatic constant. Figure E.15 shows a similar test problem with varying initial variables in the both directions x, y, with the following parameters: $\rho_L = \mathrm{e}^{-y^2}$, $\rho_R = 0.125\,\mathrm{e}^{-y^2}$, $P_L = \mathrm{e}^{-y^2}$, $P_R = 0.1\,\mathrm{e}^{-y^2}$, $\gamma = 5/3$. So the density and pressure profiles in the transverse direction y are "Gaussian". In this model, a "perturbation" is added, caused by the small initial velocity component $V_y = 0.05$.

Kelvin-Helmholtz instability

Another frequent test problem is the modeling of the Kelvin-Helmholtz instability (see, e.g., Chandrasekhar, 1961, see also Figure E.16). The rectangular area (box) is filled with a gas with two oppositely directed flows separated by a linear imaginary discontinuity. The boundary conditions are periodic at the front edges of the streams, i.e., on the sides with the coordinates $x = 0$ and $x = 1$ in Figure E.16. On the remaining two sides, they are again entered as the "solid walls". The initial conditions for the problem are taken from the parameters given by the instructions for the code ATHENA (Stone et al., 2008; Springel, 2013): for $y > 0.5$, the longitudinal flow rate $V_{x,1} = 0.3$ and the gas density $\rho_1 = 1$, for $y \le 0.5$ is the longitudinal flow rate $V_{x,2} = -0.3$ and the gas density $\rho_2 = 2$. The initial pressure $P = 1.0$ in the whole computational domain and the adiabatic exponent $\gamma = 5/3$. To avoid a too sharp interface between the two streams, we define a transition region between the two streams described by the equations (Springel, 2013):

$$\rho(x, y) = \rho_1 + (\rho_2 - \rho_1)\left(1 + \mathrm{e}^{\frac{y-0.5}{\sigma}}\right)^{-1}, \tag{E.143}$$

which characterizes the initial density perturbation in the y-direction, similarly

$$V_x(x, y) = V_{x,1} + (V_{x,2} - V_{x,1})\left(1 + \mathrm{e}^{\frac{y-0.5}{\sigma}}\right)^{-1}, \tag{E.144}$$

which characterizes the initial failure of the x-component of the velocity field in the y-direction, where the standard deviation of the velocity $\sigma = 0.01$. Into these initial conditions, we insert a periodic perturbation of the y-velocity component in the form

$$V_y(x, y) = A\cos(kx)\,\mathrm{e}^{-k\,|y-0.5|}, \tag{E.145}$$

with the wavenumber $k = 2 \times (2\pi/L)$ and the amplitude of the perturbation $A = 0.05$. The importance of this test also lies in the easy verification of the linearity of the perturbation growth

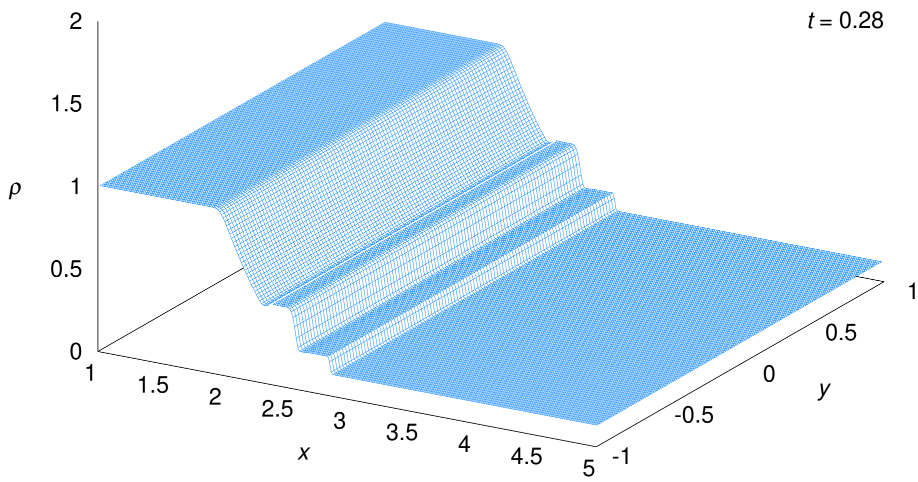

Figure E.14: Result of the density ρ simulation in the Riemann-Sod shock tube in the case of non-viscous flow at the time $t = 0.28$ (in units corresponding to the description in Section E.5.9). The initial state of the gas is static and is fixed by a solid partition (also called the *diaphragm*), located at $1/3$ of the length of the tube. The values of density ρ and pressure P on the left side of the partition are $\rho_L = 1.0$, $P_L = 1.0$, the values on the right side of the partition are $\rho_R = 0.125$, $P_R = 0.1$. The total length $\times$ the total width of the tube (box) is 4.0×2.0 in arbitrary units and the computational grid of 300×100 zones is used, the boundary conditions are "solid walls". The three characteristic "steps" in density are (from right to left) an intrinsic shock wave (whose propagation speed can exceed four times the actual speed of the moving gas), further, the so-called contact discontinuity, which is the location of the original barrier, spreading with the flow velocity of the moving gas, and finally the so-called rarefaction wave propagating in the opposite direction (see graphs of the same test problem, for example, in Stone & Norman, 1992).

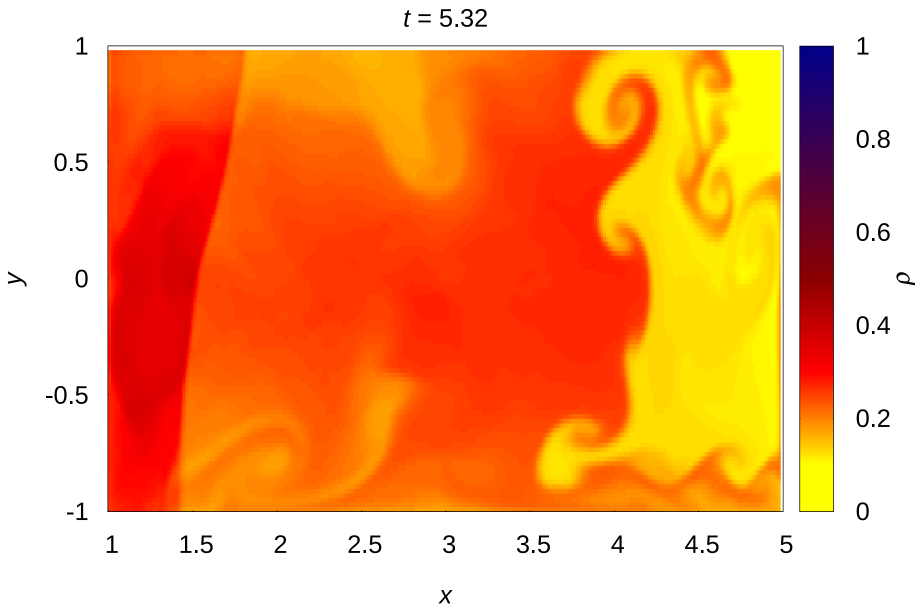

Figure E.15: Color graph of the density in the same Riemann-Sod shock tube at the time $t = 5.32$, with a small added initial y component of velocity, $V_y = 0.05$. This "perturbation" will cause some lateral flow distortions where the Kelvin-Helmholtz and Rayleigh-Taylor instabilities are also visible.

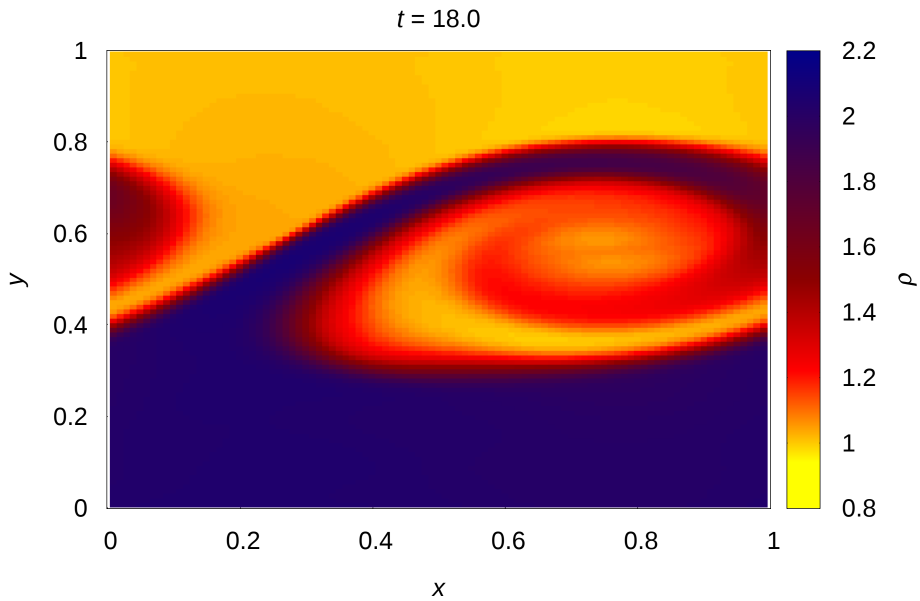

Figure E.16: Color graph of density in the Kelvin-Helmholtz instability (see Section E.5.9). The snapshot shows the flow in the advanced time, when the instability is already completely non-linear, i.e., with fully developed turbulences.

in the early phase of the computation, while later is the progress of the perturbation evolution clearly non-linear, which excludes the performance of quantitative analytical calculations. In addition, the "sharpness" of the interface between the two oppositely streaming flows can serve as an indicator of the so-called *numerical diffusivity* (i.e., the stabilization of the advection scheme algorithm using the 2nd derivatives of the flow) of the computational scheme (Stone et al., 2008).

E.6 Parallelization of computational algorithms

To speed up and often even allow the calculation of very large (one-dimensional or multidimensional) algorithms (codes), it is necessary to parallelize these algorithms, i.e., to divide them into multiple partitions (processes) that can be simultaneously (parallelly) computable on the corresponding number of computer processors. Therefore, the principle of the parallelization is to divide the total spatial computational domain (see, for example, Figure E.11) into a number of separate computational sub-domains (*ranks*). Depending on the nature of the problem, these ranks can be calculated either separately or if there is a need for mutual "communication", that is, a contact between these ranks (for example, in hydrodynamic calculations where traceability to boundary conditions at the boundaries of the entire computational area is necessary; the information about the values in the adjacent rank is transmitted at the ranks borders). This "inter-rank communication" should not cause any significant slowdown of the calculation.

There are a number of specialized libraries for creating parallel algorithms, probably the most widespread of them is the Message-Passing Interface (MPI) library, including several subtypes, created by a group of research and development staff from the academic and industrial field for wide use on parallel computers. The official source of the library, including the user's and programming manuals, is on the webpage `http://www.mpi-forum.org/`, I recommend the Lísal (2007) scripts (in the Czech language) for an introduction to the library and the parallel programming techniques, and the Pacheco (1998) manual for more detailed study. The library is programmed to transfer data from one process to another, using cooperative operations within each process (the so-called *point - to - point* communication between two processes). The main purpose of using parallel programming methods is to speed up the calculations significantly, both in the case of fully-independent ranks and in cases where the mutual "send and receive" communication is required. Often, the calculation on a single processor is even impossible; if the binary file indicates an excessively large computation process, the source file cannot be compiled at all. The MPI library is developed for various programming languages such as Fortran, C, C ++, Python and Java but there may be some minor differences in the organization of computation (for example, the different order of inclusion of spatial cells in a two-dimensional parallel computation for Fortran where the computation "runs" within each ranks first in the "vertical" direction, while in the case of the C language, the calculation "runs" always first "horizontally"). Since it is already a very large and specialized discipline, we will not describe here further details and techniques of the parallel programming.

In the framework of computer clusters working in the Czech Republic, it is possible to achieve the simultaneous involvement of several hundred processes. For example, the available and powerful computer clusters currently are:

- METACENTRUM, a virtual organization that manages and distributes the computing infrastructure of collaborating academic and university centers. Computing and storage devices are managed by the "Czech National Grid Infrastructure" project, which is a part of the "Project of Large Infrastructure for Research, Development, and Innovations" (LM2010005). The computer cluster METACENTRUM includes: Computer Center of Masaryk University in Brno (CERIT-SC center, Loschmidt Laboratories - Institute of Experimental Biology of the Faculty of Science MU and NCBR - National Center for Biomolecular Research of the Faculty of Science MU), Computer Center of the University of West Bohemia in Pilsen (KIV - Department of Informatics and Computer Science in the University of West Bohemia, KMA and KKY - Department of Mathematics and Department of Cybernetics in the University of West Bohemia), Computer Center of the University of South Bohemia in České Budějovice (Faculty of Science, University of South Bohemia), computer center of the Academy of Sciences of the Czech Republic, computer center of the Department of Telecommunications, Faculty of Electrical Engineering, Czech Technical University in Prague, etc., the umbrella organization is the e-infrastructure for science, research and education CESNET. The global parameters and cluster performance exceed 10 000 CPU cores (tens of TB of RAM), and with a storage capacity of about 1 PB (1 063 TB) for operating data and about 19 PB (19 000 TB) of storage space. The official website is `http://metavo.metacentrum.cz/`.

- Computer cluster ANSELM (National Supercomputing Center, VSB - Technical University of Ostrava), which consists of 3 344 computer cores CPU (15 TB of RAM) in total. The official website is `http://www.it4i.cz/`

- The new computer cluster SALOMON (National Supercomputing Center, VSB - Technical University of Ostrava) is now available to users, which according to the TOP 500 ranking is officially the 40th most powerful supercomputer in the world! Current parameters: 24 192 Intel Xeon CPU cores (Haswell-EP), 129 TB RAM, 52 704 Intel Xeon Phi accelerator coprocessors cores with 13.8 TB RAM, 2 PFLOP/s maximum computing power, 2 PB disk capacity, and 3 PB backup tape capacity. The official website is `http://www.it4i.cz/`.

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