ON THE SOFTWARE PACKAGE AnT 4.669 FOR THE INVESTIGATION OF DYNAMICAL SYSTEMS

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Abstract
A software package for the simulation and investigation of the behavior of dynamical systems called AnT will be presented in this paper. Due to its flexible architecture, AnT is able to simulate various classes of dynamical systems, e.g. maps, ordinary and delay differential equations, etc., as well as many sub–classes derived from these. A main feature aimed at during the development of AnT is the support of the investigation of the dynamics of the simulated systems with several provided investigation methods, like e.g. period analysis, Lyapunov exponents calculation, generalized Poincaré section analysis, symbolic image analysis and much more. Another important feature of AnT are so–called scan runs, i.e. the ability to investigate a dynamical system by varying some relevant influence quantities, such as the control parameters, initial values, or even some parameters of the investigation methods.

Keywords
simulation, dynamical systems, non–linear dynamics, numerical investigation methods, distributed computing

1 Introduction

Efficient simulation of dynamical systems is an important field in research, industrial applications and education as well. The project presented here is focused on the development and implementation of a software package AnT for the simulation and investigation of a broad spectrum of dynamical systems. The AnT package comes along with a set of investigation methods, thus enabling the user to analyze various aspects of different classes of dynamical systems. Hereby, the user must only provide an equation of motion corresponding to one of the supported classes of dynamical systems and do the appropriate initialization of the simulator, e.g. by means of a configuration file or, more comfortably, by using a corresponding graphical user interface. The ability to turn several investigation methods either on or off leads to an increase in flexibility and also efficiency, since one only has to pay for resources that are really needed.
The AnT simulation package is a powerful tool which provides the user with data resulting from the performed computations. The user of the software may further process and interpret the produced data in order to get valuable insights concerning the dynamics of the investigated system. Compared to other known tools for the simulation and investigation of dynamical systems, like for instance AUTO, XPP, DsTool, Dynamics,

DDE-BIFTOOL, etc., `AnT` has some advantages. Firstly, the spectrum of dynamical system classes and investigation methods supported by `AnT` is broader than that of any other tool which we know of. Secondly, `AnT` allows the investigation of dynamical systems while varying some settings. Although other tools are also able to perform similar tasks, `AnT` is by now the only tool running in client-server mode. Hence, computation intensive tasks may be distributed among many clients automatically.

2 Classes of dynamical systems supported by `AnT`

According to the aims of the `AnT` project, the term of a dynamical system was kept very general. In this section we present a brief overview of several classes of dynamical systems which can be simulated and investigated using `AnT`. Currently, the simulator is able to deal with the following *basic classes* of dynamical systems:

- **standard discrete maps**: $\vec{x}_{n+1} = \vec{f}(\vec{x}_n, \{\sigma\})$
- **ordinary differential equations** (ODE): $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \{\sigma\})$
- **delay differential equations** (DDE): $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \vec{x}(t-\tau), \{\sigma\})$
- **functional differential equations** (FDE): $\dot{\vec{x}}(t) = \vec{\mathcal{F}}\left[\vec{x}_t, \{\sigma\}\right]$
  with $\vec{x}_t(\theta) = \vec{x}(t+\theta)$, $\theta \in [-\tau, 0]$
- **partial differential equations** (PDE) with one spatial component:
  $\frac{\partial}{\partial t}\vec{x}(q,t) = \vec{f}\left(\vec{x}(q,t), \frac{\partial}{\partial q}\vec{x}(q,t), \ldots, \vec{\sigma}\right)$ with a scalar spatial component q defined on the domain $[q_{\min}, q_{\max}]$.

Here $\vec{x}_n$ and $\vec{x}(t)$ denote the real–valued state vector of the system, σ a set of parameters, and τ the time delay. The vector $\vec{x}_t(\theta)$ is an element of the extended state space given by the space of vector–valued functions on the interval $[-\tau, 0]$ and $\vec{\mathcal{F}}$ is a non–linear functional defined on this space. Dealing with partial differential equations, one can use several types of von Neumann boundary conditions (fluxless, cyclic, interpolated, constant), as well as Dirichlet boundary conditions.
In addition to standard discrete maps it is also possible to use

- **recurrent maps** $\vec{x}_{n+1} = \vec{f}(\vec{x}_n, \vec{x}_{n-1}, ..., \vec{x}_{n-n_\tau}, \{\sigma\})$

with $n_\tau \in \mathbb{N}$, $n_\tau > 1$. Of course, the recurrent maps can be transformed into standard discrete maps by extending the state space accordingly. Hence, one is in principle always able to do the work with standard maps only, but using the more natural form of recurrent maps simplifies the modeling of time discrete systems with delay and is therefore supported by `AnT`. As a side note, we have to remark that this kind of elimination of the delay by state space extension is not possible for delay differential equations ([8], [6]).
Non–autonomous systems are not supported by `AnT` directly, but this is not a restriction, since they can be transformed into autonomous ones by a standard extension of the state space, i.e. by introducing a new state variable representing the time.
Additionally, `AnT` can be used with two more classes of dynamical systems, denoted as *composite* or *cellular* dynamical systems. These are known as coupled map lattices (CML) and coupled ordinary differential

equations lattices (CODEL) respectively. Given local couplings and closed ring topology, these systems can be defined by

- **CML:** $\vec{x}_{n+1}^{(i)} = \vec{f}\left(\vec{x}_n^{(i-l)\text{mod } N}, \ldots, \vec{x}_n^{(i)}, \vec{x}_n^{(i+r)\text{mod } N}, \{\sigma\}\right)$
- **CODEL:** $\dot{\vec{x}}^{(i)}(t) = \vec{f}\left(\vec{x}^{(i-l)\text{mod } N}(t), \ldots, \vec{x}^{(i)}(t), \ldots, \vec{x}^{(i+r)\text{mod } N}(t), \{\sigma\}\right)$

Hereby, N denotes the number of cells in the lattice, i is the cell index ($i = 1 \ldots N$) and l and r the ranges of the coupling interval. `AnT` provides also more general types of lattices with global coupling, where a cell is coupled arbitrarily with other existing cells. Hence, arbitrary lattice topology is also possible, as well as lattices with more than one space direction.
Furthermore, `AnT` has support for *hybrid dynamical systems*, which became more and more important during the past few years. A basic property of these systems is that their state space consists of two parts, a continuous–valued vector $\vec{x}_n \in \mathbb{R}^{n_c}$ and a vector $\vec{m} \in \mathbb{M}^{n_d}$ where $\mathbb{M}$ is a set of discrete values and $n_c, n_d \in \mathbb{N}^+$. `AnT` provides three types of hybrid systems, i.e.

- **hybrid maps**: $\vec{x}_{n+1} = \vec{f}(\vec{x}_n, \vec{m}_n, \{\sigma\}), \quad \vec{m}_{n+1} = \vec{\phi}(\vec{x}_n, \vec{m}_n, \{\sigma\})$
- **hybrid ODEs**: $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \vec{m}(t), \{\sigma\}), \quad \vec{m}(t^+) = \vec{\phi}(\vec{x}(t), \vec{m}(t), \{\sigma\})$
- **hybrid DDEs** $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \vec{x}(t-\tau), \vec{m}(t), \{\sigma\}), \quad \vec{m}(t^+) = \vec{\phi}(\vec{x}(t), \vec{m}(t), \{\sigma\})$

The notation $\vec{m}(t^+)$ means that the vector $\vec{m}$ is assumed to be left-side continuous with respect to time.
`AnT` is also able to deal with some classes of *stochastic systems* with additive noise η, although it should be remarked, that currently only a limited set of integration and investigation methods is available for these systems. The stochastic system classes supported by `AnT` are:

- **maps with additive noise**: $\vec{x}_{n+1} = \vec{f}(\vec{x}_n, \{\sigma\}) + \vec{\eta}_n$
- **ODEs with additive noise**: $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \{\sigma\}) + \vec{\eta}(t)$
- **DDEs with additive noise**: $\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), \vec{x}(t-\tau), \{\sigma\}) + \vec{\eta}(t)$

Here $\vec{\eta}$ means the additive white noise vector, which can be distributed differently, e.g., uniform or Gaussian.
A remarkable feature of `AnT` is the very general implemented concept of **Poincaré sections**. According to this concept, the orbit of a discrete map is resulting from the orbit of some other dynamical system, whereby only those points are selected which satisfy a specific condition. In the case of classical Poincaré sections, this condition is given by the cross–section of the orbit with a plane. `AnT` supports two variants of classical Poincaré sections, which behave differently in the context of scan runs. On the one hand, the plane can be fixed, i.e. the plane remains the same even if the parameters of the investigated dynamical system are varied. For instance, the behavior of the Rössler system ([11]) can be investigated by varying the parameter a using Poincaré sections with the fixed plane $y = 0$ (see Fig. 1). On the other hand, in some cases it can be interesting to define the plane depending on the system parameters, and hence the coefficients of the plane have to be varied together with the system parameters. A typical example of such a case is the well–known Lorenz–63 system ([9]). For instance, it is known that this system possesses three fixed points, which can be determined analytically. ([12]). Two of these fixed points depend on the system parameters r and b. Hence, for Poincaré sections of the Lorenz–63 system it is suitable to use planes containing these two fixed points.

In addition to the classical Poincaré section approach, `AnT` can use any other condition in order to calculate generalized Poincaré sections. Especially, in the case of hybrid systems, there is a specific condition generating the Poincaré section, which is fulfilled whenever a change in the discrete state part occurs. Additionally, any user defined condition may be used as well. It has to be mentioned that, due to the architecture of `AnT`, Poincaré sections are represented as discrete maps with a special kind of system function, which iterates the given dynamical system until the Poincaré condition gets fulfilled. Hence, all investigation methods applicable for maps are also applicable for numerical calculated Poincaré maps.
At last, we ought to remark that `AnT` can also proceed **external input data**. Although this topic was not intended to be the main application area of the `AnT` package, we were able to achieve this functionality by implementing our system function as an external data reader. Hence, this dynamical system belongs to the class of standard discrete maps and may be described informally by

- $\vec{x}_{n+1}$ = next input vector

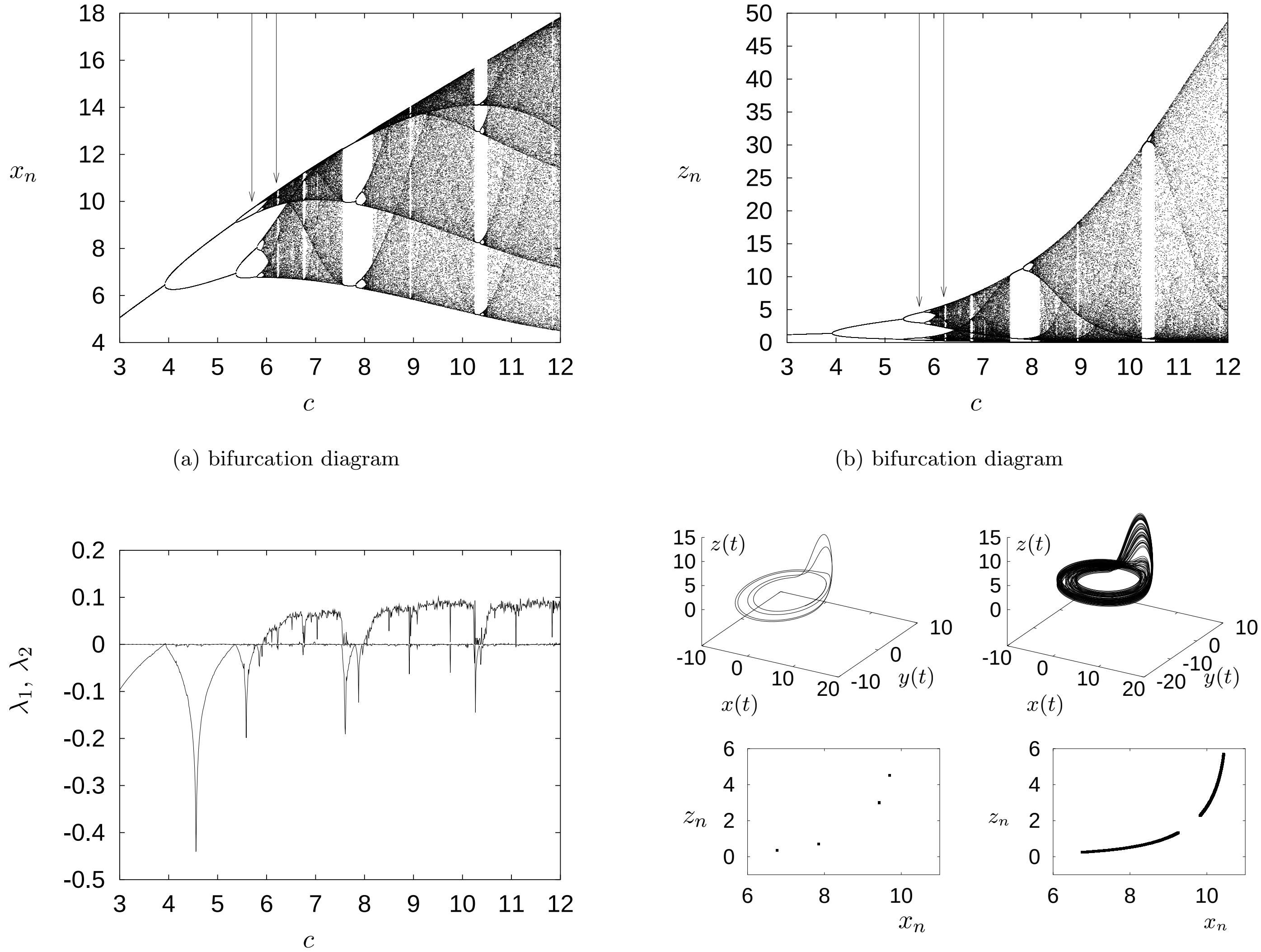
Summarizing, it has to be remarked that the support of such a broad spectrum of dynamical systems was not a primary aim in the early phases of the `AnT` project. However, it turned out that the software architecture concepts designed and used in the project allow this support generically. As a consequence hereof, we were able to implement many of our investigation methods at a high level of abstraction, thus reusing this functionality for many classes of dynamical systems and avoiding source code duplication.

3 Integration methods

In order to investigate dynamical systems continuous in time, i.e. ODEs, DDEs, etc., `AnT` integrates them numerically. Hereby, the continuous trajectory has to be approximated by a sequence of discrete states resulting from the applied integration method. To cope with typical problems arising by the numerical integration, like for instance by the integration of the so–called stiff differential equations or the integration of stochastic systems, `AnT` provides several classes of integration methods. Currently implemented methods with fixed step size include the well–known one–step methods of Runge–Kutta type defined by their corresponding pre–implemented Butcher arrays. Additionally, the Butcher arrays can be supplied by the user. Hence, `AnT` supports user defined integration methods of this type. Furthermore a large collection of different integration methods is implemented, containing among others some implicit methods like Heun–backward, some multi–step methods with memory like the backward differentiation approach (Gear method) and some predictor–corrector methods like the Adams–Moulton approach. Additionally, `AnT` supports several methods with adjustable step size.

4 Scans

An important issue within the theory of non-linear dynamical systems is the investigation of the system dynamics depending on various settings. `AnT` can handle this kind of investigation by allowing so–called scan–runs, which incorporate the analysis of the system dynamics for varying settings. During such a scan–run, not only one or more parameters of the investigated dynamical system can be varied, but also the initial values as well as specific parameters of the applied investigation methods. One possible application



(a) bifurcation diagram

(b) bifurcation diagram

(c) Lyapunov exponents

(d) attractors and Poincaré sections

Figure 1: *Investigation of the Rössler system.*

The Rössler system, given by $\dot{x}(t) = -(x(t) + z(t))$, $\dot{y}(t) = x(t) + ay(t)$, $\dot{z}(t) = b + z(t)(x(t) - c)$, is here investigated using the parameter settings $a = 0.15$, $b = 0.2$ and varying c.

(a),(b) *Bifurcation diagrams for the Poincaré map, defined by the cross–sections of the trajectory with the half–plane $\left\{(x, y, z)^T \,|\, y = 0,\, x > 0\right\}$.*

(c) *The figure shows the largest two Lyapunov exponents of this three–dimensional system continuous in time.*

(d) *A periodic and a chaotic (two–band) attractor and the corresponding Poincaré sections. The parameter values used here ($c = 5.7$ and $c = 6.2$) are marked with arrows in the bifurcation diagrams shown in (a) and (b).*

of the scan–run is the investigation of bifurcation scenarios showing the dependency of the system dynamics on some control parameters. `AnT` supports one–dimensional scan–runs, where only one control parameter is varied (see Fig. 1, and Fig. 3), as well as higher–dimensional scans (see Fig. 4). Another domain of application for scan–runs is the investigation of basins of attraction in the case of coexisting attractors. Furthermore, one can empirically determine the parameter settings of certain investigation methods for which these methods operate optimally. A sample application of this case is presented below, but we have to remark that such scans are rather unusual, since scan–runs normally concern the parameters or initial values of the system.

One of the approaches for the calculation of the Lyapunov exponents, implemented by `AnT` (some modification of the approach of Wolf *et al.* [13]), possesses as parameters the length of a small deviation vector $|\vec{\varepsilon}|$ and the number N_{GSO} of iteration steps between two subsequent applications of the Gram–Schmidt ortho–normalization procedure. These parameters must be provided by the user. In order to determine the suitable settings for the parameters, one can investigate their influence on the calculated values of Lyapunov exponents by using them as scan parameters in a scan–run. In the example presented in Fig. 2, the correct value of the Lyapunov exponent can be determined analytically, which yields $\lambda^* = \ln(2)$. In Fig 2.a, the accuracy of the numerical calculation is shown depending on the length of the deviation vectors $|\vec{\varepsilon}|$. The Gram–Schmidt ortho–normalization procedure is applied in each step. As one can see, the appropriate setting for $|\vec{\varepsilon}|$ lies between $\varepsilon_{\min} \propto 10^{-9}$ and $\varepsilon_{\max} \propto 10^{-7}$. If one sets $|\vec{\varepsilon}| \gg \varepsilon_{\max}$, the results are not precise enough due to approach specific requirements, by $|\vec{\varepsilon}| \ll \varepsilon_{\min}$ the accumulated numerical errors made by the computer become perceptible. By increasing the number of iterations, one achieves more precise results, but the suitable ranges for ε will be smaller. In Fig. 2.b, the accuracy of the numerical calculation is shown depending on the number of iteration steps between two subsequent applications of the Gram–Schmidt ortho–normalization procedure. As one can see, the best results are achieved if the procedure is applied in each step. We remark that for other dynamical systems, especially continuous in time, the optimal setting for the parameter N_{GSO} may be larger, depending on the used step size.

Another important feature of `AnT` concerning scan-runs is the possibility of distributing them automatically among several nodes (processors, machines), thus executing the simulations in parallel.

5 Investigation methods

As already mentioned, `AnT` provides a lot of investigation methods, considering various aspects of the behavior of a dynamical system. In order to acquire a rough idea of the investigated dynamical system, one can use the basic trajectory evaluations. For instance, one can calculate one or more trajectories of the system, the orbital and average velocities as well as other values like e.g. the wave numbers ([3], Fig. 3.d). The period analysis makes it possible to calculate bifurcation and period diagrams. This is particularly useful in combination with one– or higher–dimensional scan runs (compare Fig. 3.a, Fig. 3.b and Fig. 4). The stability properties of a dynamical system can be investigated by calculating the Lyapunov exponents of its attractors (Fig. 2, Fig. 3.c). This investigation method is implemented not only for maps and ordinary differential equations, but also for dynamical systems with memory, such as delay differential equations. Due to its generality, this method can also be applied to the more general class of functional differential equations.

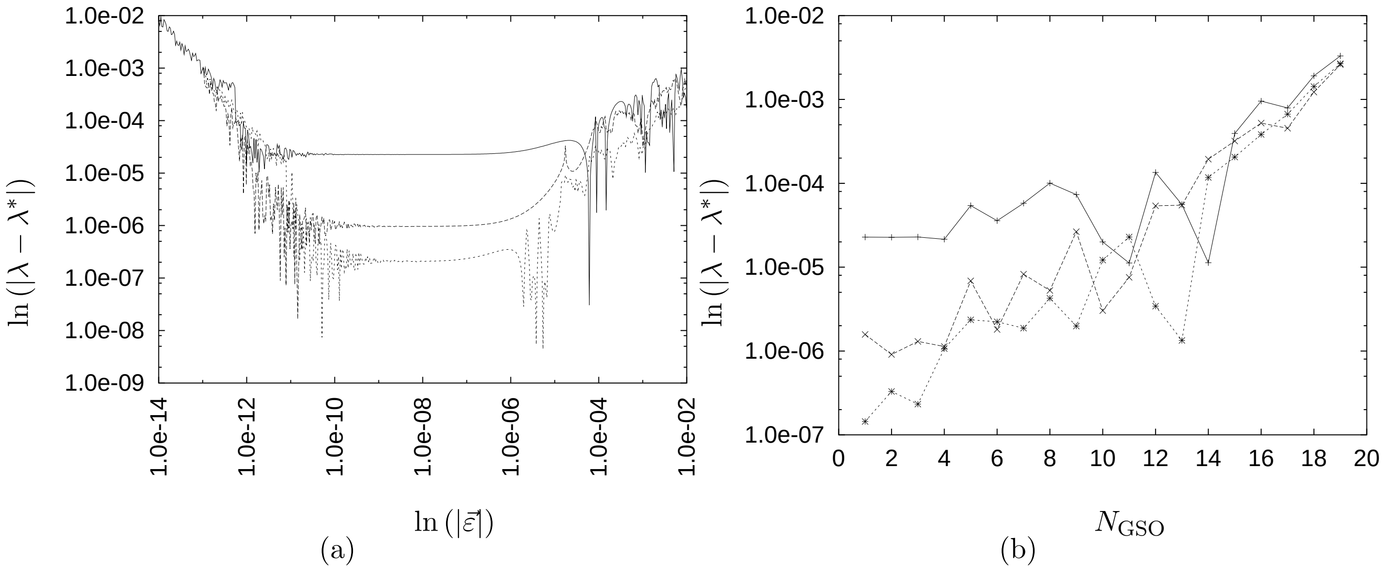
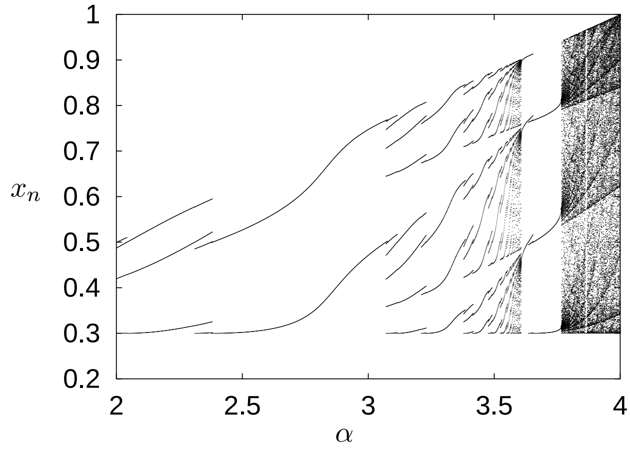


Figure 2: *Accuracy of the numerical calculation of the Lyapunov exponents for the logistic map* $x_{n+1} = \alpha x_n(1 - x_n)$ *for* $\alpha = 4.0$. *The number of iterations is* $25\,000$ *steps (solid line),* $250\,000$ *steps (dashed line) and* $2\,500\,000$ *steps (dotted line). The transient part is* 1000 *steps in all three cases. The initial value is* $x_0 = 0.1$.

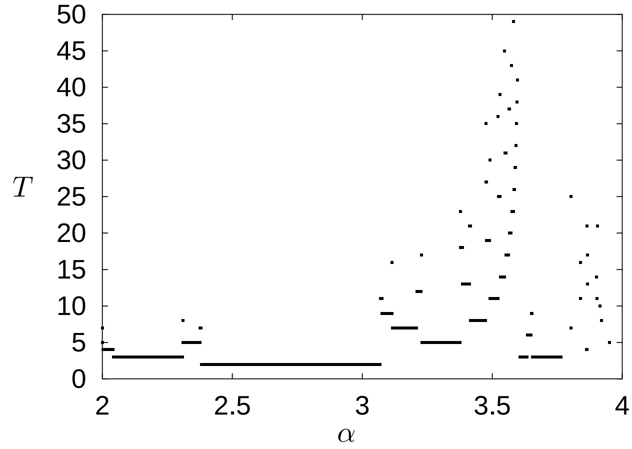
We have included some standard techniques from the field of frequency analysis, like e.g. the calculation of power spectra. Singular value decomposition is another useful method provided by `AnT`.
Methods based on symbolic dynamics provide a collection of generic techniques for the generation of symbolic sequences corresponding to the underlying trajectory. `AnT` supports n–dimensional extensions of the techniques, which are known for 1–dimensional systems, like for instance (LR)– and $(+-)$– symbolic dynamics. From the symbolic sequence, `AnT` is able to calculate some quantitative measures like e.g. its entropy ([7]).
A powerful part of `AnT` is the module for determination and evaluation of symbolic images ([4, 5, 10]). Using this analysis method one is able to find invariant sets of a vector field, especially including unstable orbits. Note, that the method is applicable for both dynamical systems discrete and continuous in time. Furthermore, it is possible to determine the basins of attraction at least for simple attractors, that is, for fixed points and for limit cycles.
The results of each investigation method are written to corresponding data files. After a simulation run, these results can be visualized and evaluated by the user. Additionally, 2D and 3D online-visualization modules are implemented, which can be used during single-run simulations.

6 Conclusion

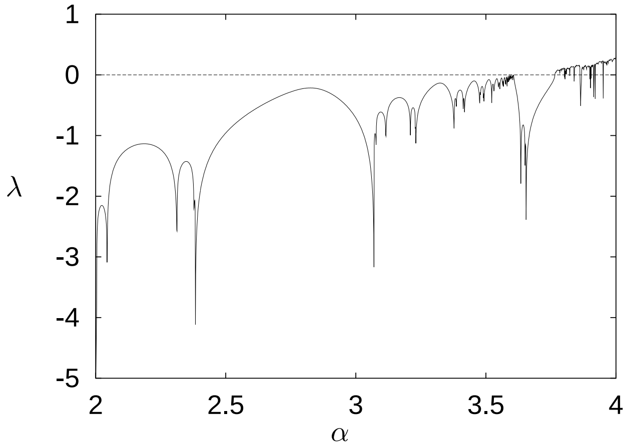
The `AnT` package is free software and is distributed under the GNU public license. It is available at the URL `http://www.AnT4669.de`. There, one can also find a more detailed description of the package.



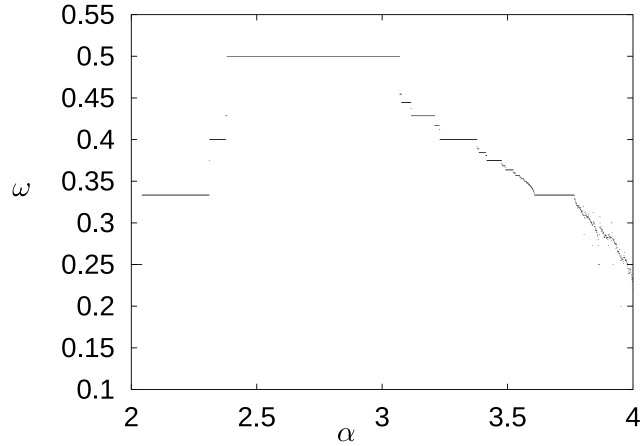
(a) bifurcation diagram



(b) period diagram



(c) Lyapunov exponent λ



(d) wave number ω

Figure 3: *Some investigation results.*

Presented are some aspects of the dynamical behavior of the following one–dimensional dynamical system discrete in time, with the piecewise defined system function

$$x_{n+1} = \begin{cases} \alpha x_n(1 - x_n) & \textit{if} \quad x_n \leq \frac{1}{2} \\ \beta x_n(x_n - 1) + 1 & \textit{if} \quad x_n > \frac{1}{2} \end{cases} \tag{1}$$

at $\beta = 2.8$ and various values of α.

(a) *Bifurcation diagram. Shown are the periodic and aperiodic dynamics of the system.*

(b) *From the period diagram one can see that the bifurcation scenario presented in Fig.* (a) *resembles a period adding scenario [1].*

(c) *As one can see from the diagram of the Lyapunov exponent, the bifurcations presented in Fig.* (a) *take mostly place on super–stable parameter values.*

(d) *In the wave number diagram one can recognize the typical "devil's staircase" structure [2].*

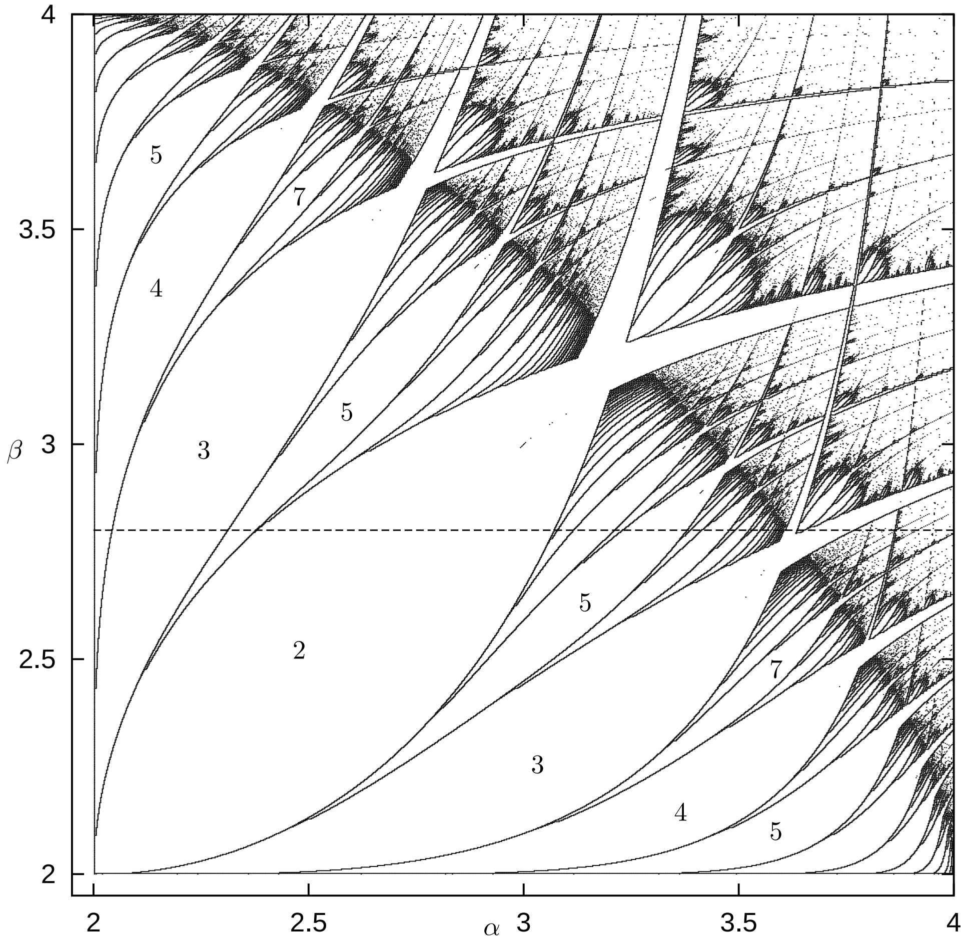


Figure 4: *Bifurcation structures of the system (1) in the 2-dimensional parameter space* $[\alpha \times \beta]$.

The white spaces denote regions with the same periodical behavior, calculated by the method denoted as region analysis. Some of the periods are written within the corresponding regions. The dashed line shows the section corresponding to a 1-dimensional parameter scan for α *with* $\beta = 2.8$*, as presented in Fig. 3.*

The software is yet available for UNIX-based operating systems like Linux, Solaris or FreeBSD and uses free libraries only. For instance, in some numerical investigation methods the libraries fftwlib (`http://www.fftw.org`) and CLAPACK (`http://www.netlib.org/clapack`) are used. If these libraries are not installed on the current system, then the corresponding numerical methods (Fourier analysis, principal values decomposition) can not be loaded. However, the simulator works even without them, since the other investigation methods are not affected anyway.

For future releases, it is planned to extend the `AnT` package with new system classes. Especially, partial differential equations (PDE) with more then one spatial direction and coupled delay and functional differential equations (CDDEL and CFDEL) will be considered. Another important goal is the extension of the list of supported investigation methods. Currently, we are working on more precise methods for the numerical calculation of entropies and several fractal dimensions, on including some new ideas from the field of symbolic dynamics, etc.

7 Acknowledgments

The authors wish to thank all peoples who were and are still involved in the development process of `AnT`. Many thanks to Prof. Levi (University of Stuttgart, Germany) for supporting our work.

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