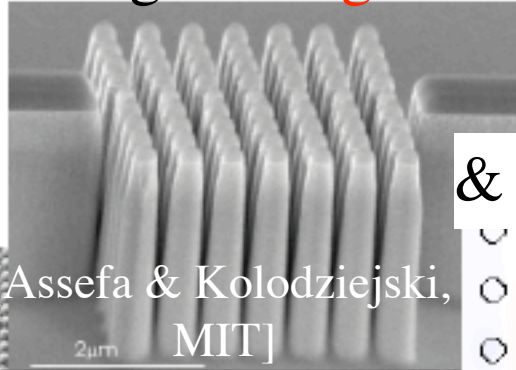


Computational Photonics:
Frequency and Time Domain Methods

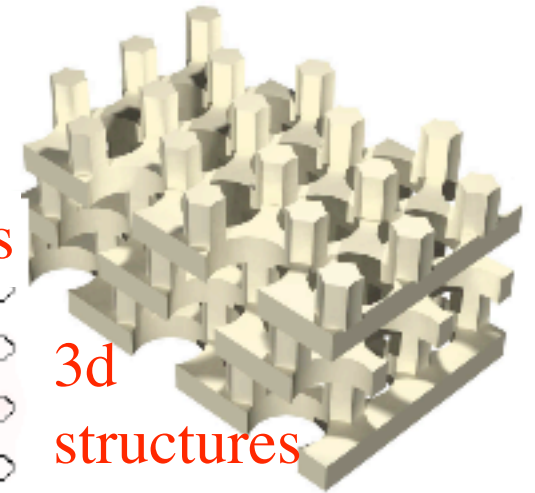
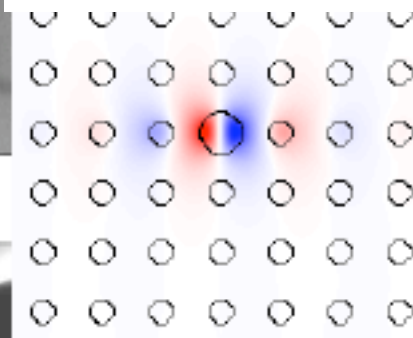
Steven G. Johnson
MIT Applied Mathematics

Nano-photonic media (\square -scale)

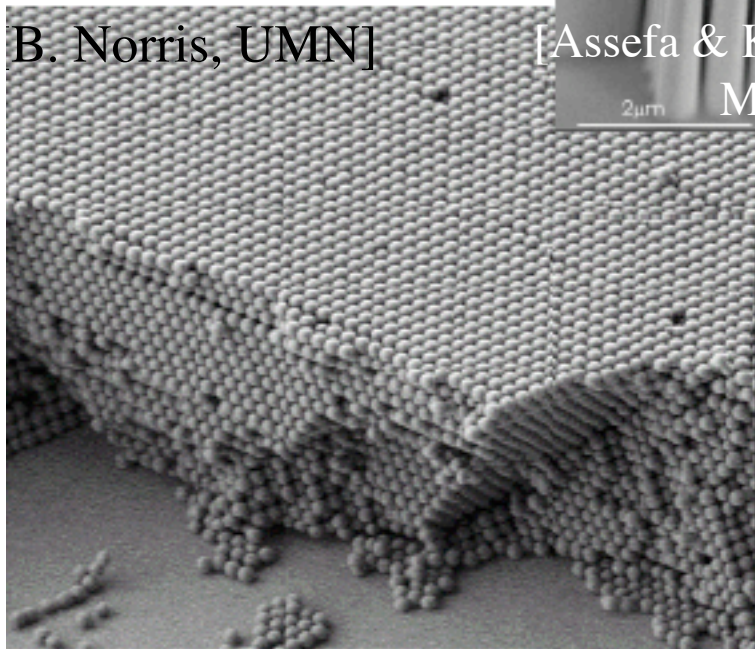
strange waveguides



& microcavities

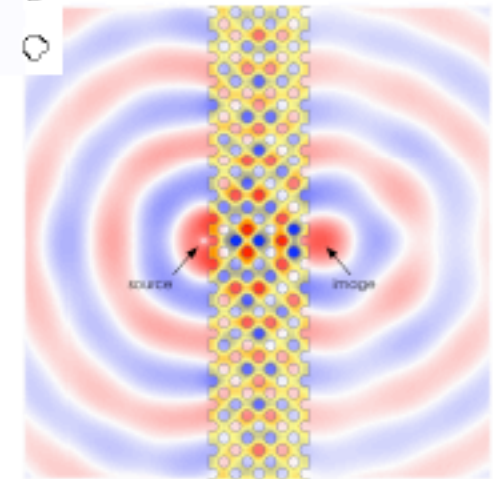
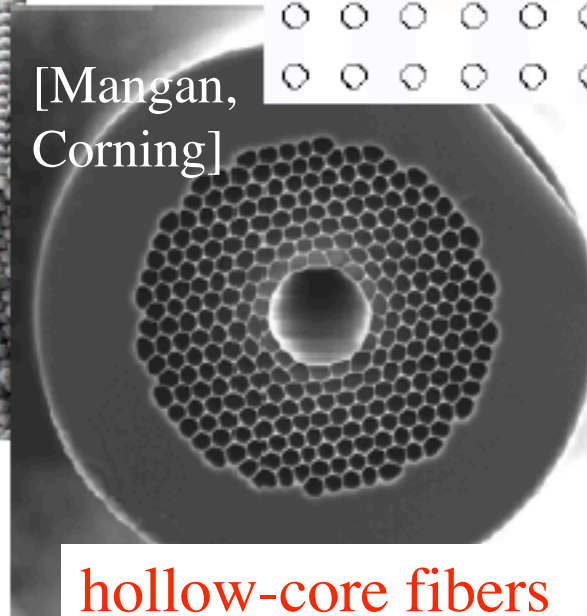


B. Norris, UMN]



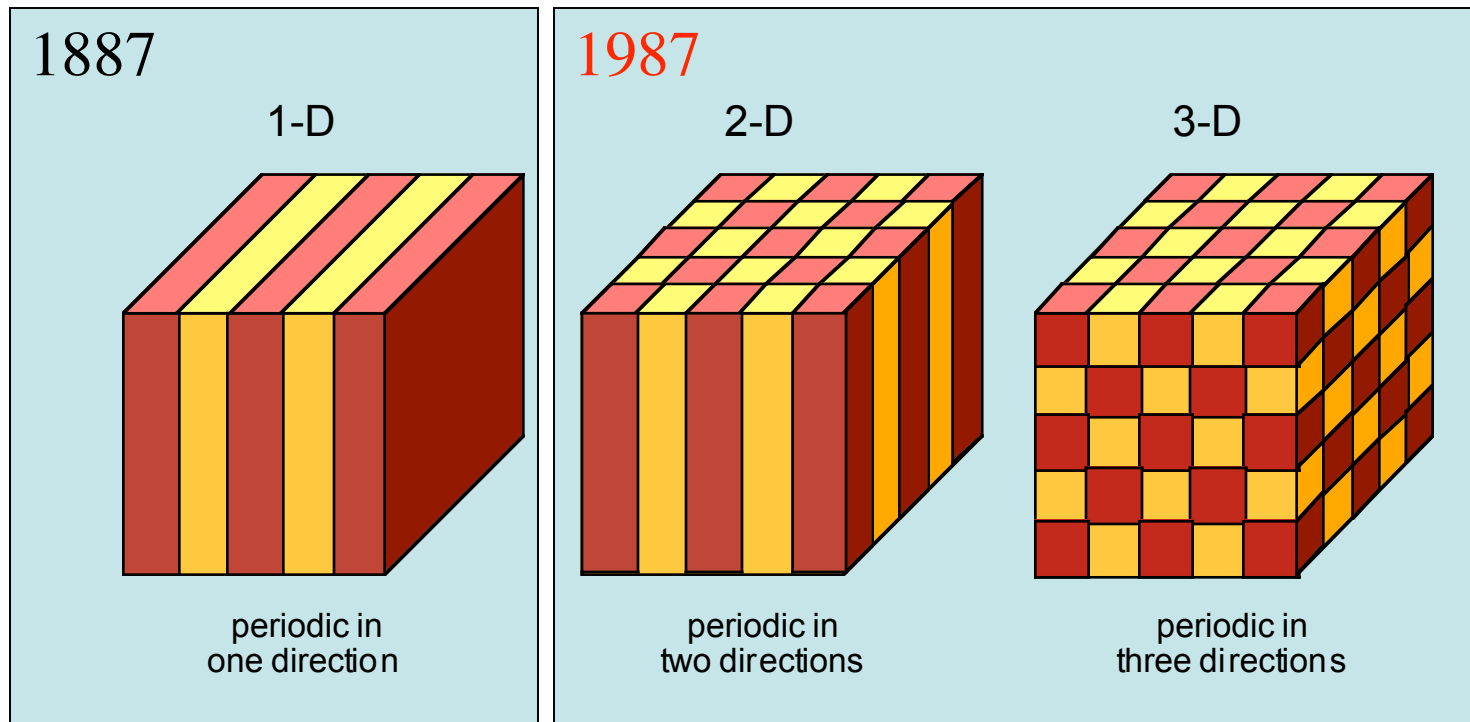
synthetic materials

[Mangan, Corning]



Photonic Crystals

periodic electromagnetic media

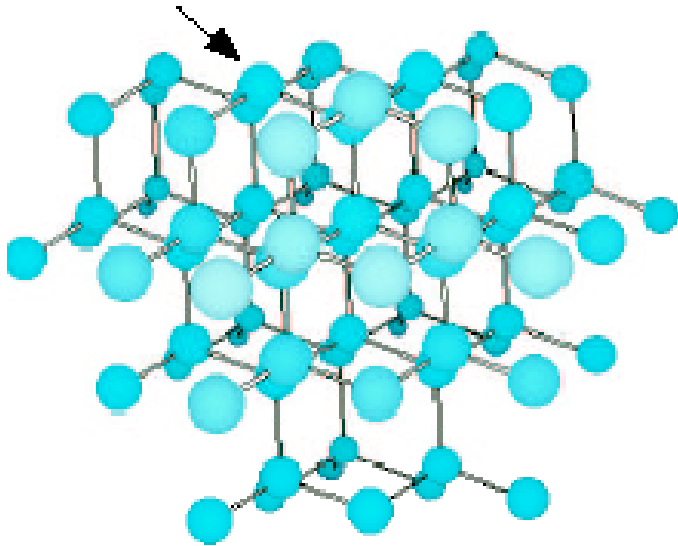


can have a band gap: optical “insulators”

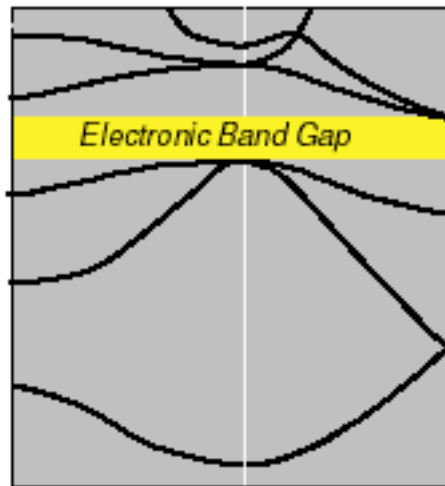
Electronic and Photonic Crystals

Periodic Medium
Bloch waves:
Band Diagram

atoms in diamond structure

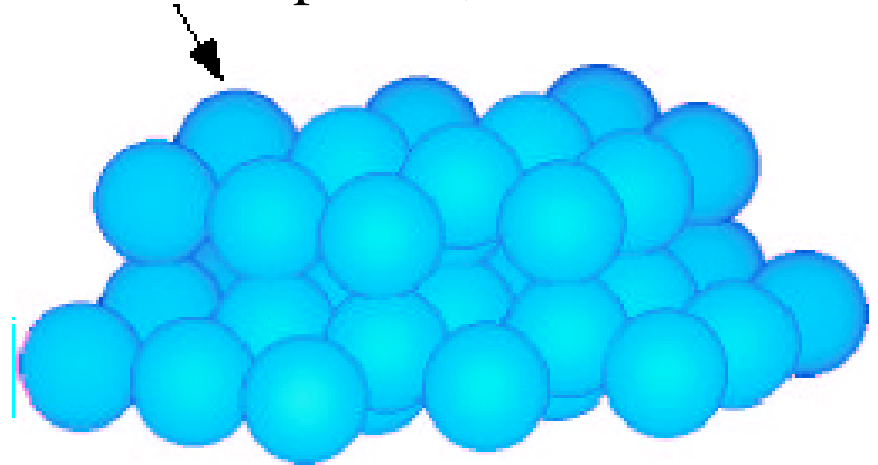


electron energy

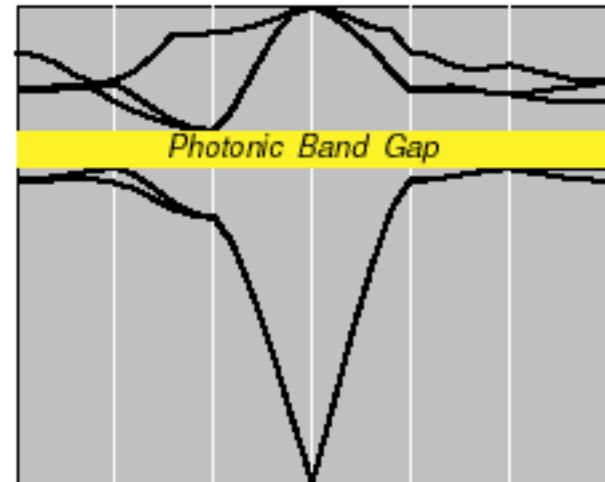


wavevector

dielectric spheres, diamond lattice



photon frequency



wavevector

Electronic & Photonic Modeling

Electronic

- **strongly interacting**
 - entanglement, Coulomb
 - tricky approximations
- **lengthscale** dependent
(from Planck's h)

Photonic

- **non-interacting** (or weakly),
 - simple approximations
(finite resolution)
 - **any desired accuracy**
- **scale-invariant**
 - *e.g.* size $\ll 10 \mu\text{m}$ $\ll 10 \mu\text{m}$
 - (except materials may change)

Computational Photonics Problems

- Time-domain simulation

- start with current $\mathbf{J}(\mathbf{x}, t)$
- run “numerical experiment” to simulate $\mathbf{E}(\mathbf{x}, t)$, $\mathbf{H}(\mathbf{x}, t)$

- Frequency-domain linear response

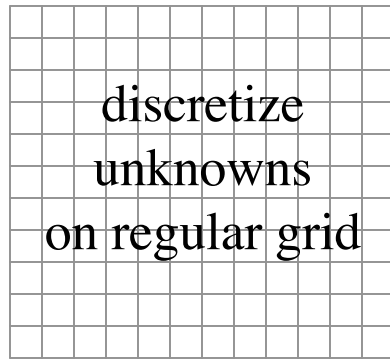
- start with harmonic current $\mathbf{J}(\mathbf{x}, t) = e^{-i\omega t} \mathbf{J}(\mathbf{x})$
- solve for steady-state harmonic fields $\mathbf{E}(\mathbf{x})$, $\mathbf{H}(\mathbf{x})$
- involves solving linear equation $\mathbf{Ax}=\mathbf{b}$

- Frequency-domain eigensolver

- solve for source-free harmonic eigenfields
 $\mathbf{E}(\mathbf{x}), \mathbf{H}(\mathbf{x}) \sim e^{-i\omega t}$
- involves solving eigenequation $\mathbf{Ax}=\omega^2\mathbf{x}$

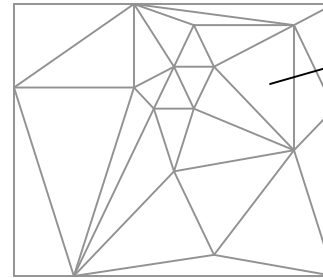
Numerical Methods: Basis Choices

finite difference



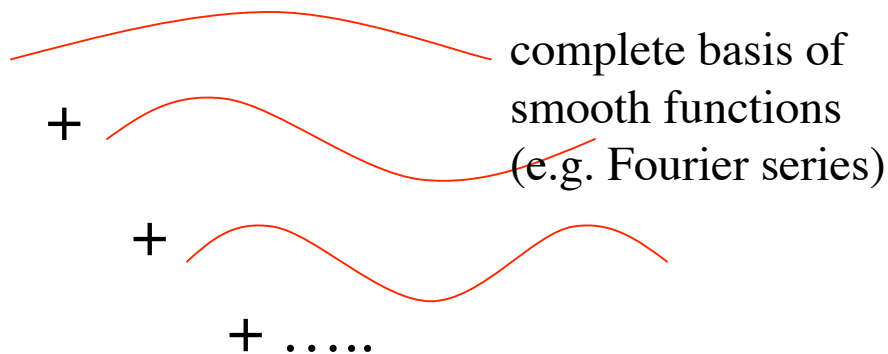
$$\frac{df}{dx} \approx \frac{f(x + \Delta x) - f(x - \Delta x)}{\Delta x} + O(\Delta x^2)$$

finite elements

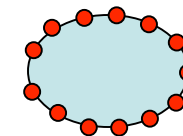
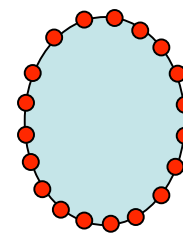


in irregular "elements,"
approximate unknowns
by low-degree polynomial

spectral methods



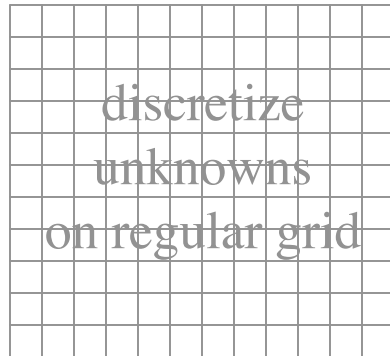
boundary-element methods



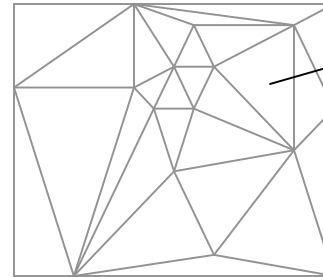
...solve
integral equation
via Green's functions

Numerical Methods: Basis Choices

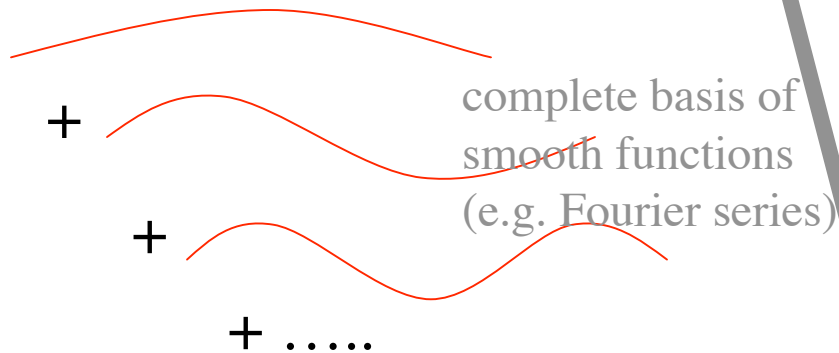
finite difference



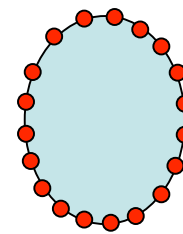
finite elements



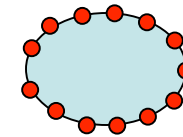
spectral methods



boundary-element methods



discretize only the
boundaries between
homogeneous media



...solve
integral equation
via Green's functions

Much easier to analyze, implement,
generalize, parallelize, optimize, ...

Potentially much more efficient,
especially for high resolution

Computational Photonics Problems

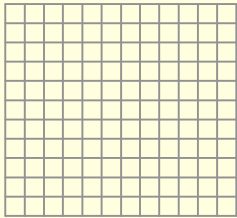
- **Time-domain simulation**
 - start with current $\mathbf{J}(\mathbf{x}, t)$
 - run “numerical experiment” to simulate $\mathbf{E}(\mathbf{x}, t)$, $\mathbf{H}(\mathbf{x}, t)$

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 - start with harmonic current $\mathbf{J}(\mathbf{x}, t) = e^{-i\omega t} \mathbf{J}(\mathbf{x})$
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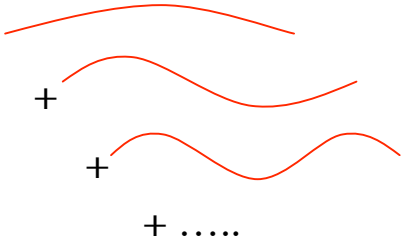
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Numerical Methods: Basis Choices

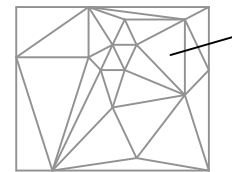
finite difference


$$\frac{df}{dx} \approx \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + O(\Delta x^2)$$

spectral methods

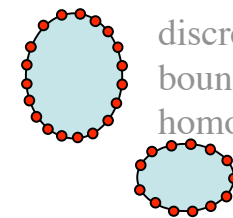


finite elements



in irregular “elements,” approximate unknowns by low-degree polynomial

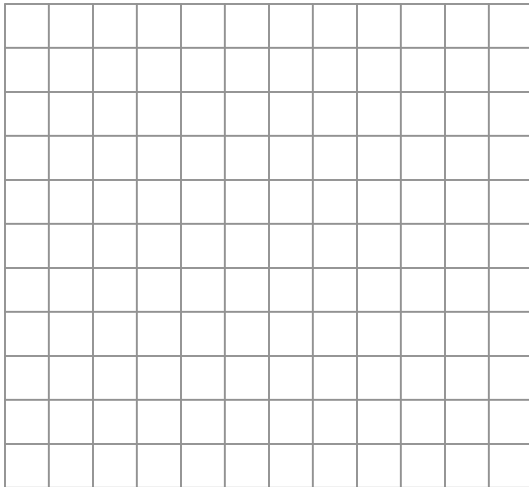
boundary-element methods



discretize only the boundaries between homogeneous media

FDTD

Finite-Difference Time-Domain methods



Divide *both* space and time into discrete grids

- spatial resolution Δx
- temporal resolution Δt

Very general: arbitrary geometries, materials, nonlinearities, dispersion, sources, ...

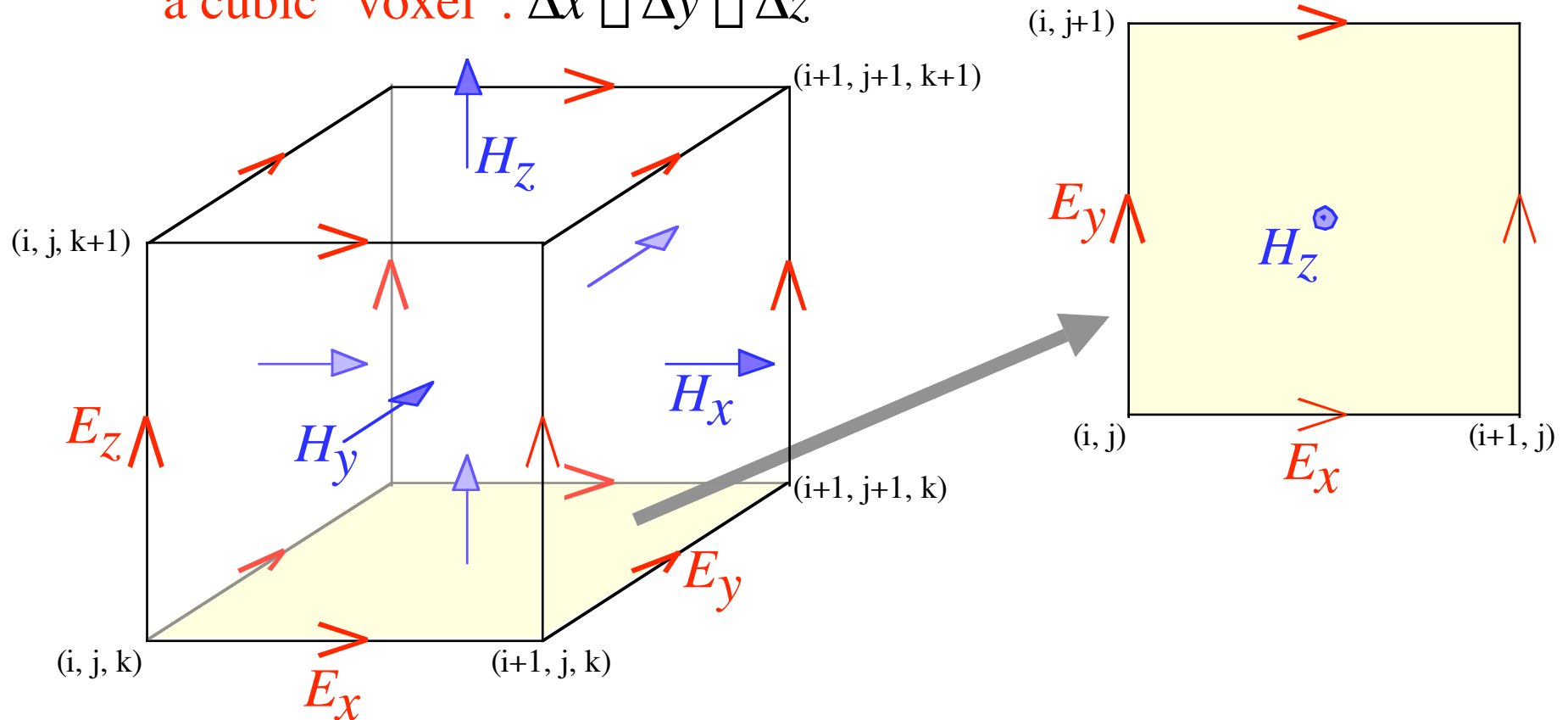
— *any photonics calculation, in principle*

$$\frac{\partial \mathbf{H}}{\partial t} = \nabla \times \vec{\mathbf{D}} \quad \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\epsilon} \nabla \times \mathbf{H} - \mathbf{J}$$

dielectric function $\epsilon(\mathbf{x}) = n^2(\mathbf{x})$

The Yee Discretization (1966)

a cubic “voxel”: $\Delta x \square \Delta y \square \Delta z$

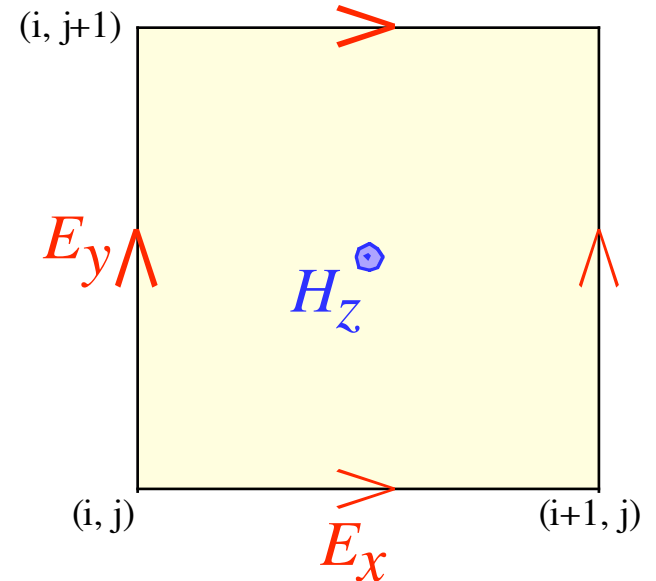


Staggered grid in space:

- every field component is stored on a different grid

The Yee Discretization (1966)

$$\frac{\partial \mathbf{H}}{\partial t} = \frac{1}{\Delta} \mathbf{E} \dots$$



$$\left. \frac{\partial H_z}{\partial t} \right|_{i+\frac{1}{2}, j+\frac{1}{2}} = \frac{1}{\Delta} \left[\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right]$$

$$\frac{1}{\Delta} \left[\frac{E_y(i+1, j+\frac{1}{2}) - E_y(i, j+\frac{1}{2})}{\Delta x} - \frac{E_x(i+\frac{1}{2}, j+1) - E_x(i+\frac{1}{2}, j)}{\Delta y} \right] + O(\Delta x^2) + O(\Delta y^2)$$

all derivatives become *center differences*...

The Yee Discretization (1966)

all derivatives become *center differences*...
including derivatives in *time*

$$\left. \frac{\partial \mathbf{H}}{\partial t} \right|_{t=n\Delta t} = \frac{1}{\Delta t} \left. \mathbf{E} \right|_{t=n\Delta t} = \frac{\mathbf{H}(n + \frac{1}{2}) - \mathbf{H}(n - \frac{1}{2})}{\Delta t} + O(\Delta t^2)$$

Explicit time-stepping:

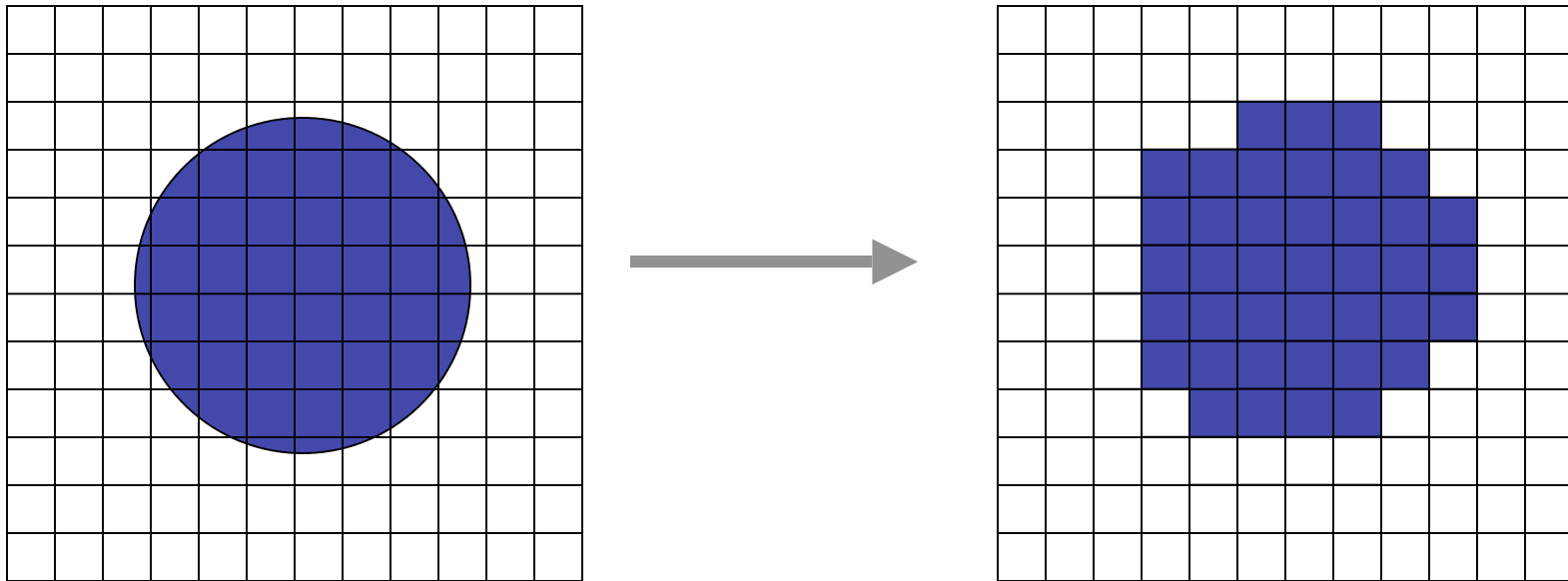
stability requires $\Delta t < \frac{\Delta x}{\sqrt{\# \text{ dimensions}}}$

(vs. *implicit* time steps: invert large matrix at each step)

FDTD Discretization Upshot

- For stability, space and time resolutions are proportional
 - doubling resolution in 3d requires at least $16 = 2^4$ times the work!
- But at least the error goes quadratically with resolution
 - ...right?
 - ...not necessarily!

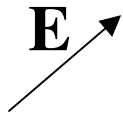
Difficulty with a grid: representing discontinuous materials?



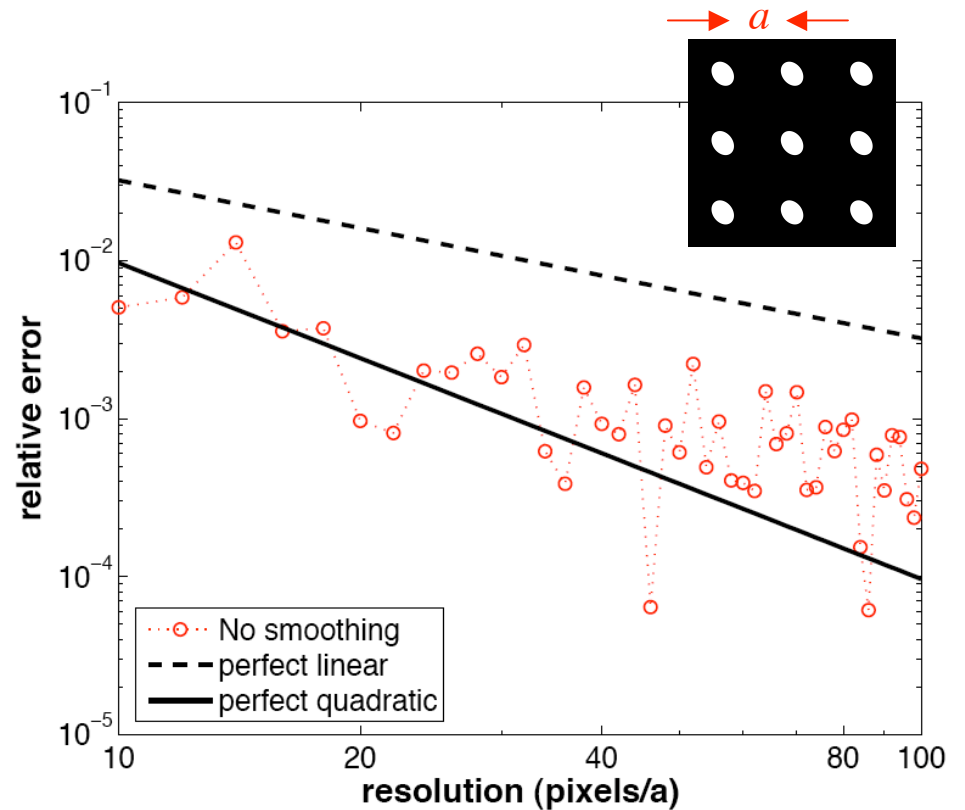
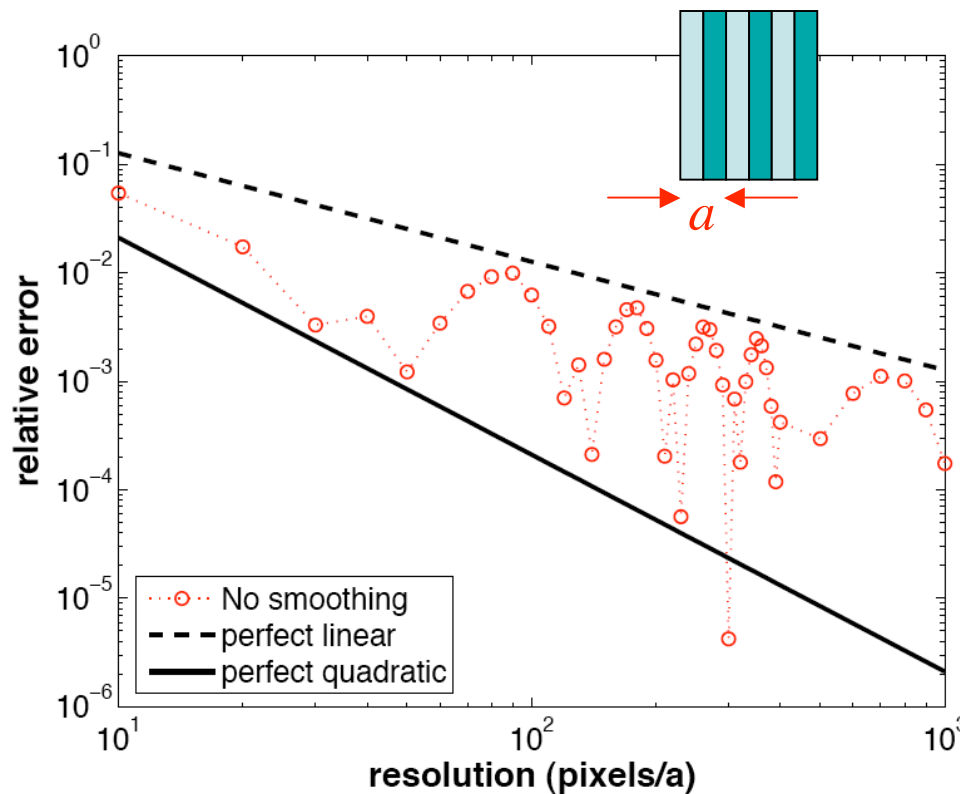
“staircasing”

... how does this affect accuracy?

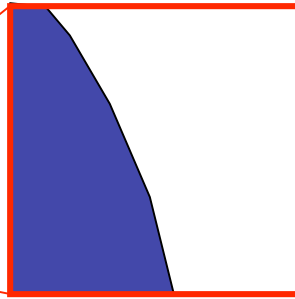
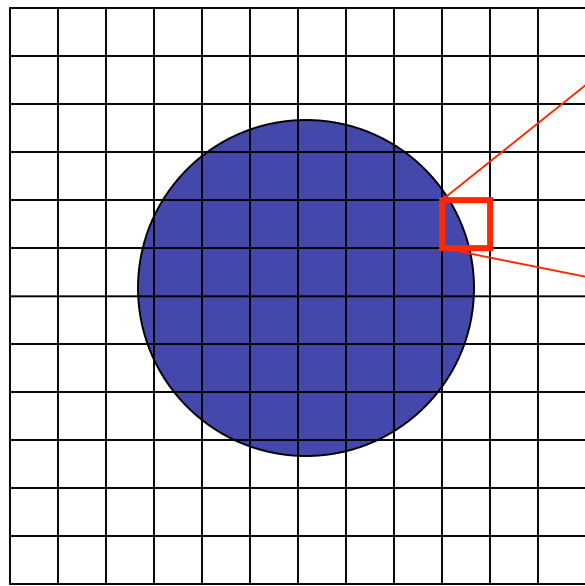
Field Discontinuity Degrades *Order of Accuracy*



TE polarization (\mathbf{E} in plane: discontinuous)

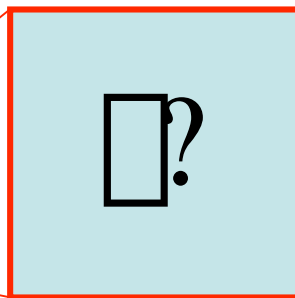
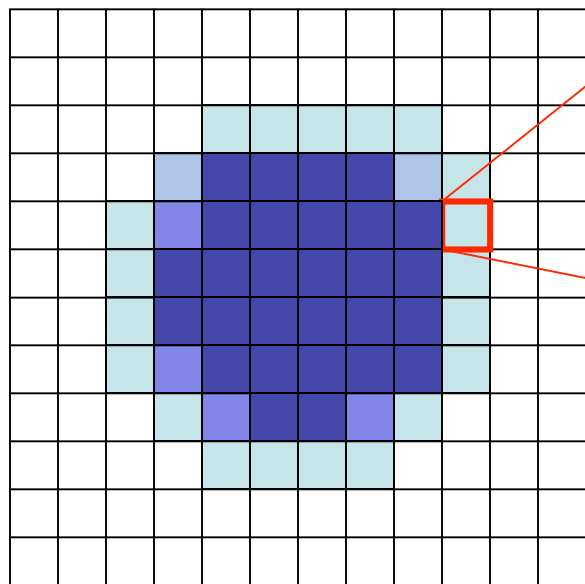


Sub-pixel smoothing



Can eliminate
discontinuity
by “grayscaleing”

— assign some *average*  to each pixel



= discretizing a *smoothed* structure

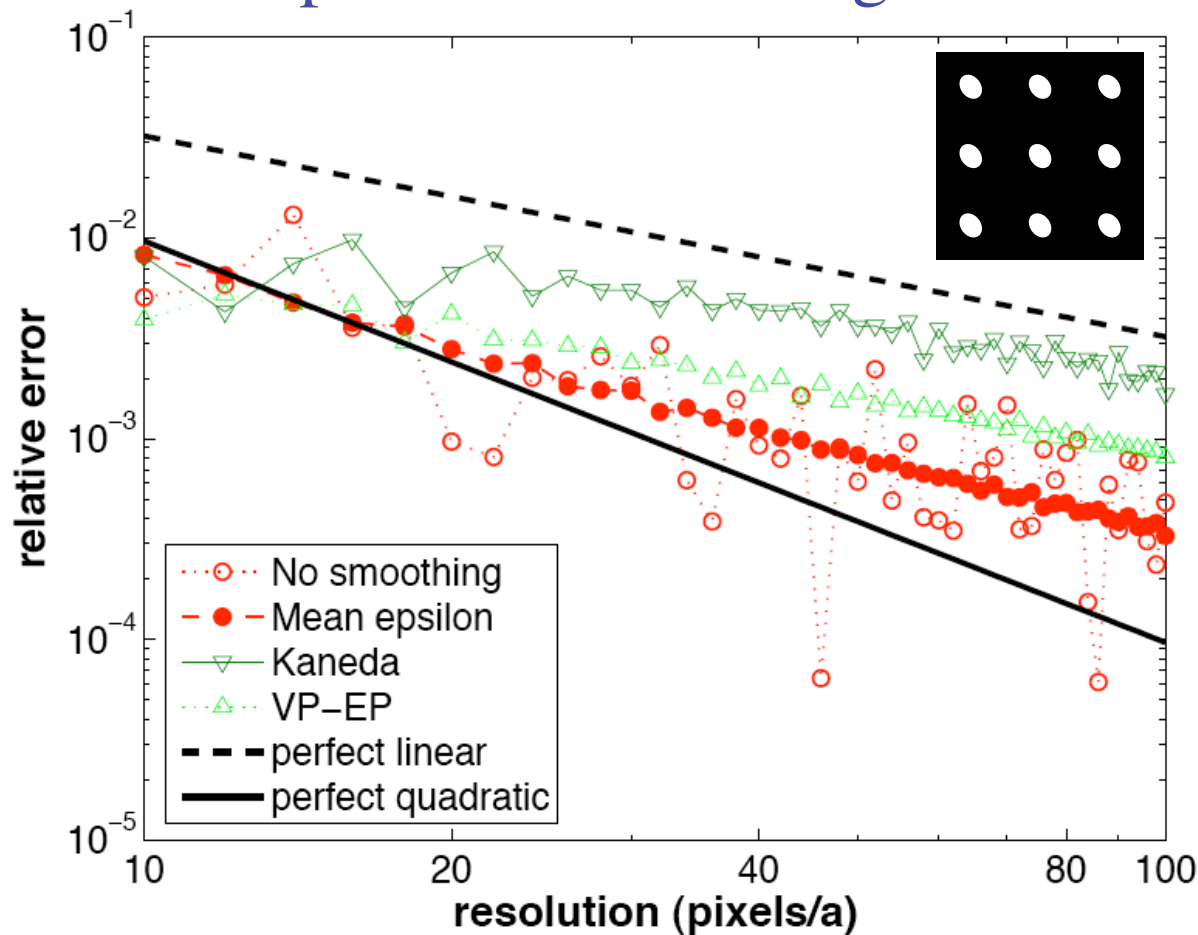
— that means we are *changing* geometry

— can actually *add* to error

Past sub-pixel smoothing methods can *make error worse!*

& convergence is
still only linear

Three previous smoothing methods



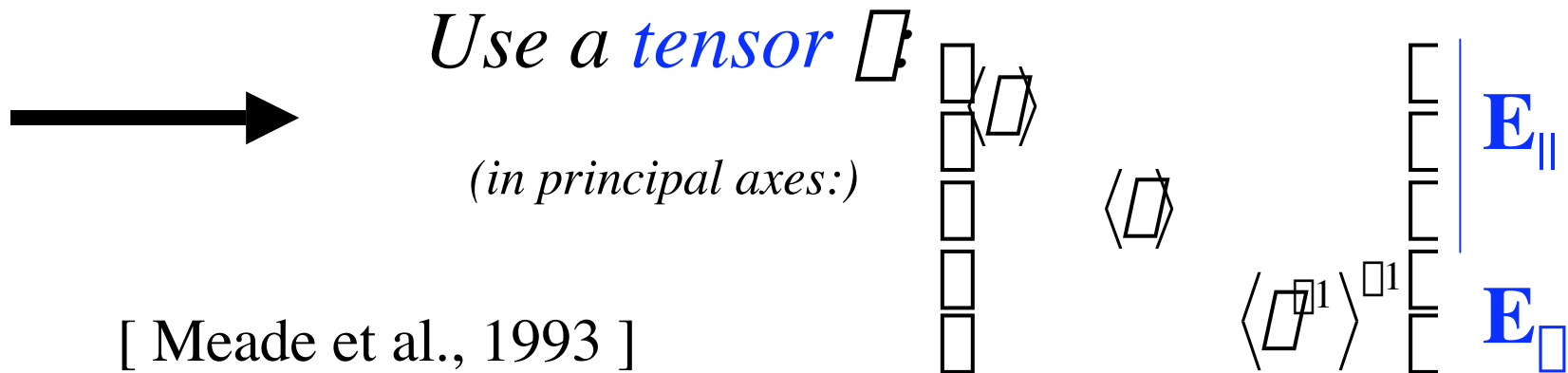
[Dey, 1999]
[Kaneda, 1997]
[Mohammadi, 2005]

A Criterion for Accurate Smoothing

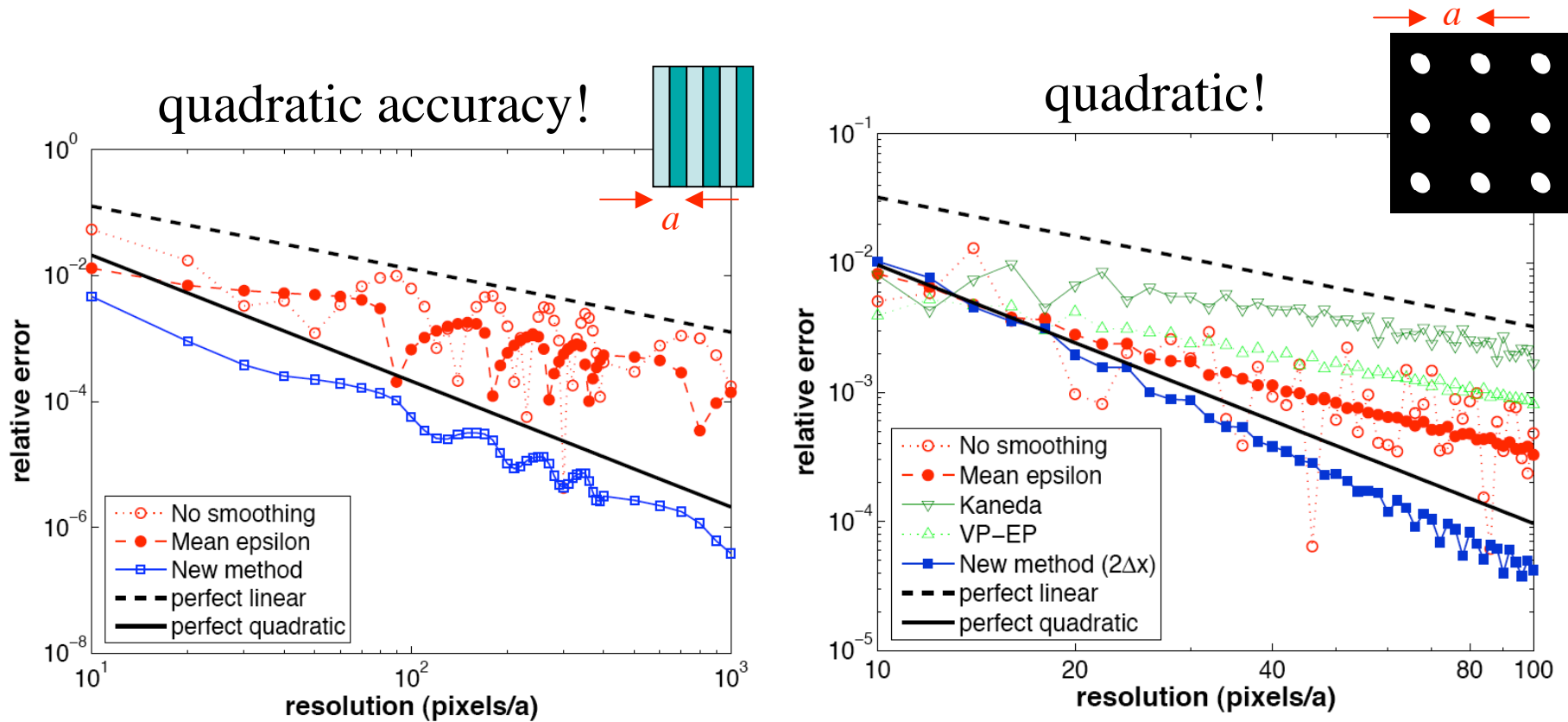
1st-order errors
from
smoothing $\square\square$

$$\sim \langle \square \square \square \rangle \|\mathbf{E}_{\parallel}\|^2 \square\square \left(\frac{1}{\square}\right) |D_{\square}|^2 \begin{bmatrix} \square \\ \square \\ \square \\ \square \\ \square \end{bmatrix}$$

We want the smoothing errors to be *zero* to 1st order
— minimizes error *and* 2nd-order convergent!

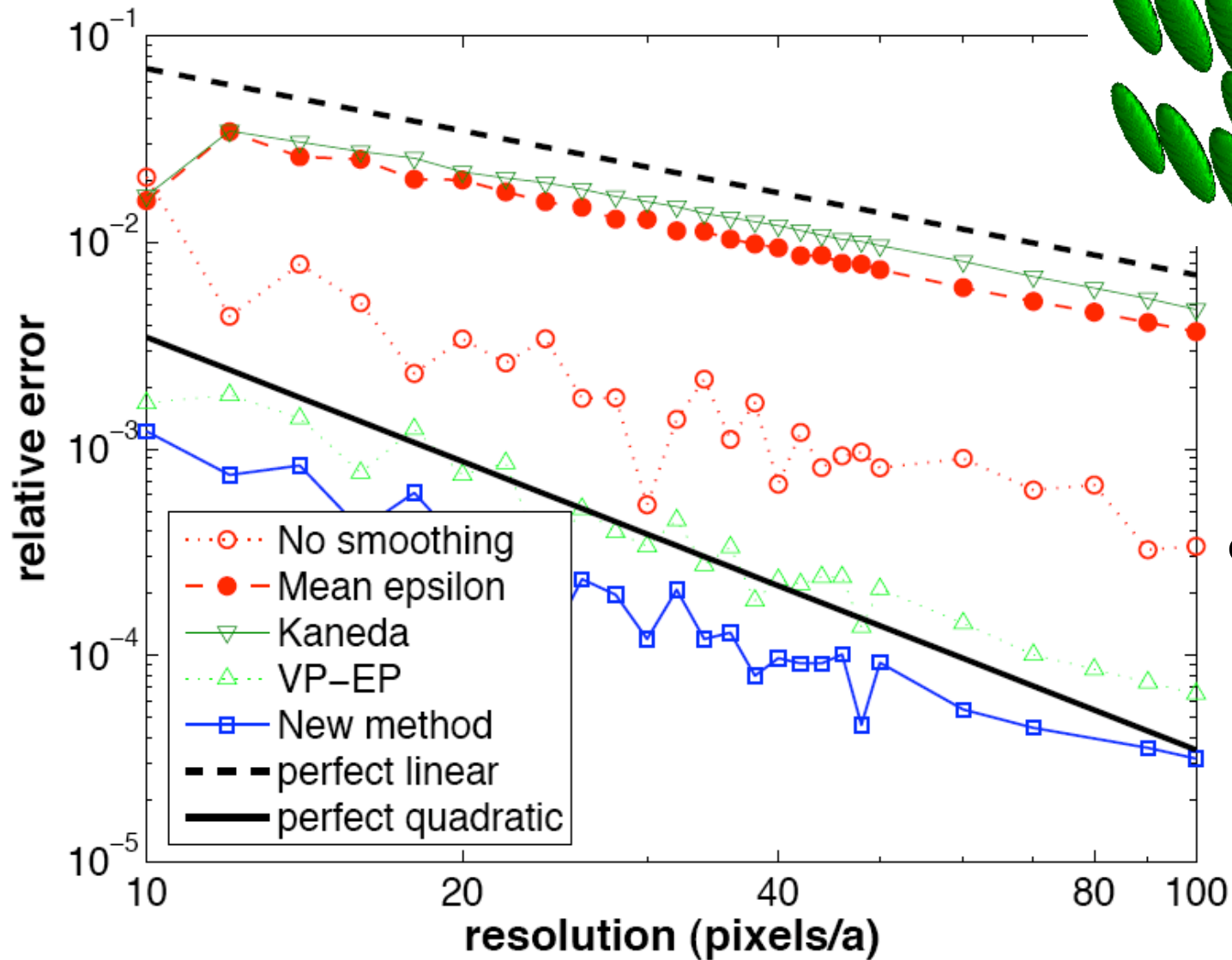
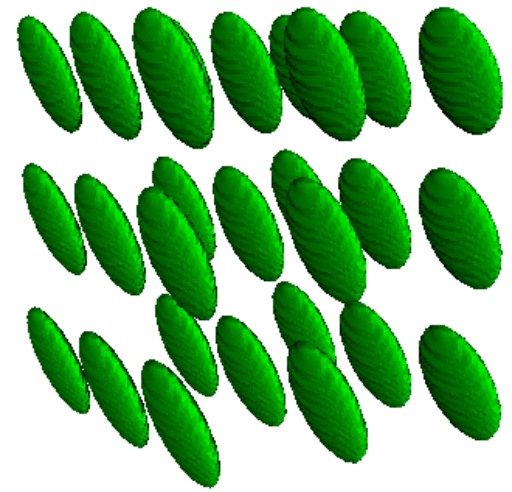


Consistently the Lowest Error



[Farjadpour *et al.*, *Opt. Lett.* 2006]

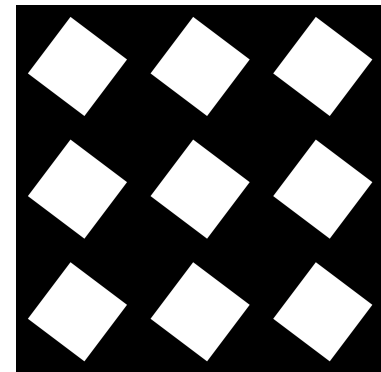
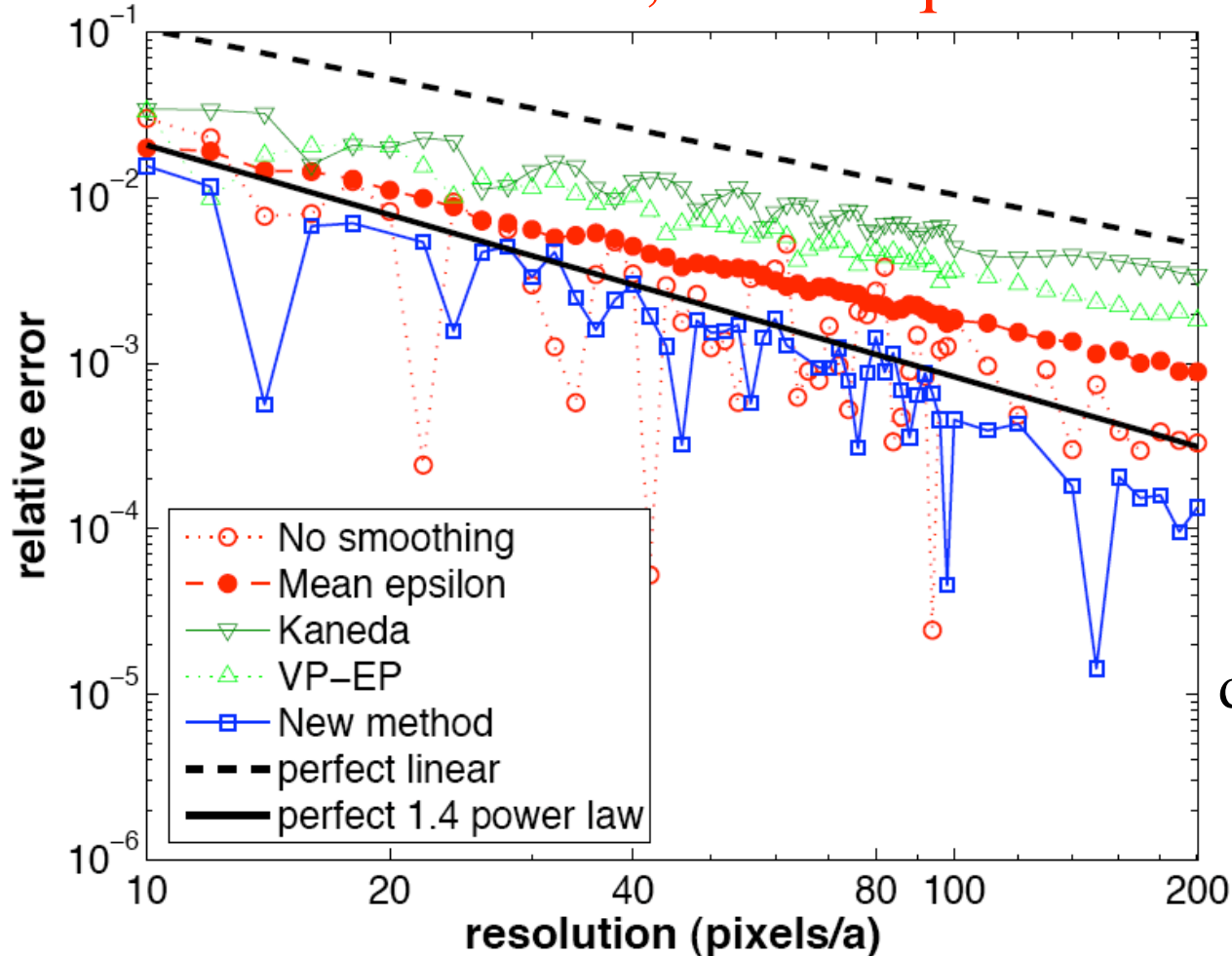
... & in 3d too



(notice that ranking of other methods has shuffled!)

A qualitatively different case: **corners**

still \sim lowest error, but *not* quadratic



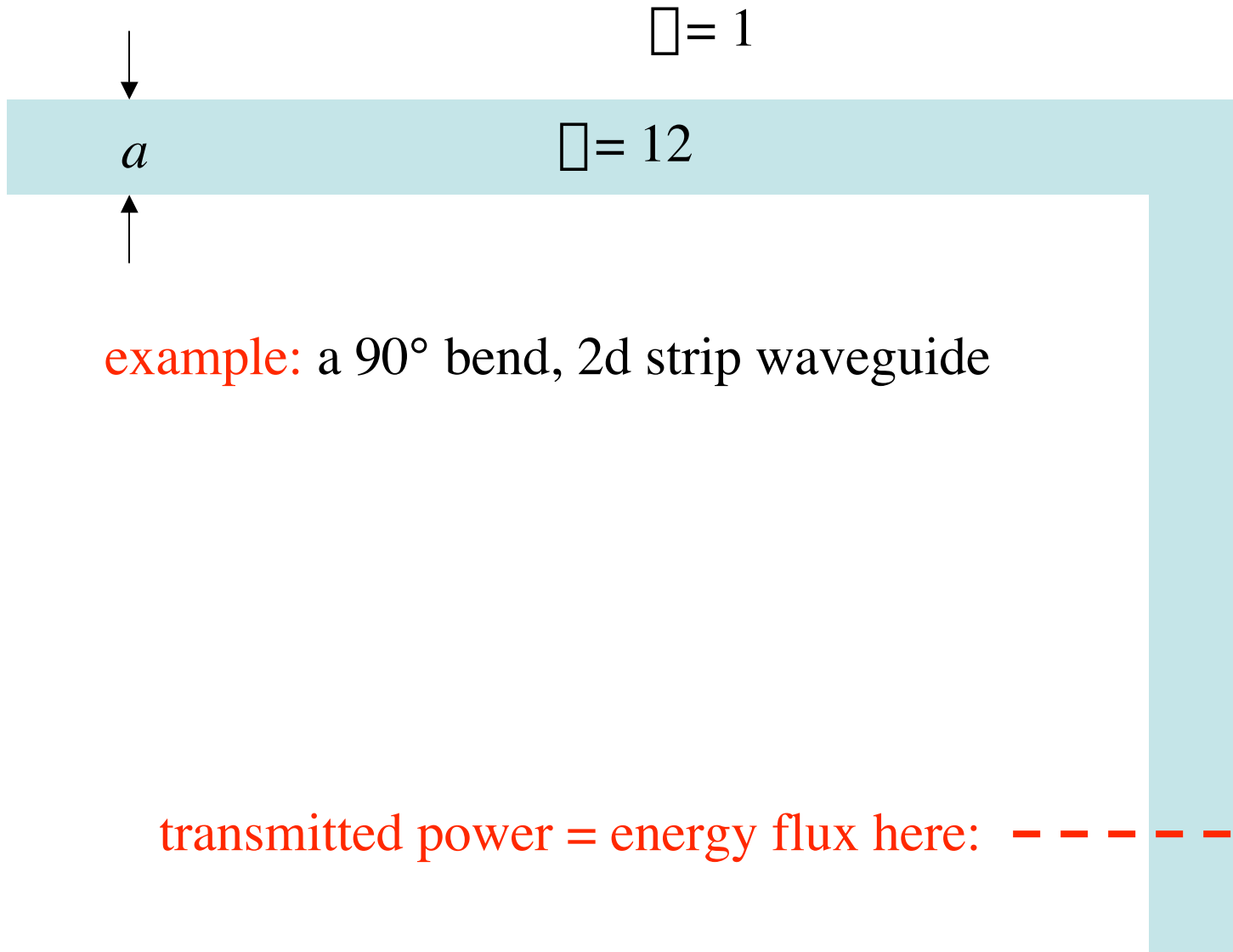
zero-perturbation
criterion
not satisfied
due to **E divergence**
at corner
— analytically,
error $\sim \Delta x^{1.404}$

Yes, but what can you *do* with FDTD?

Some common tasks:

- **Frequency-domain response:**
 - put in harmonic source and wait for steady-state
- **Transmission/reflection spectra:**
 - get **entire spectrum from a single simulation**
(Fourier transform of impulse response)
- **Eigenmodes and resonant modes:**
 - get all modes from a single simulation
(some tricky signal processing)

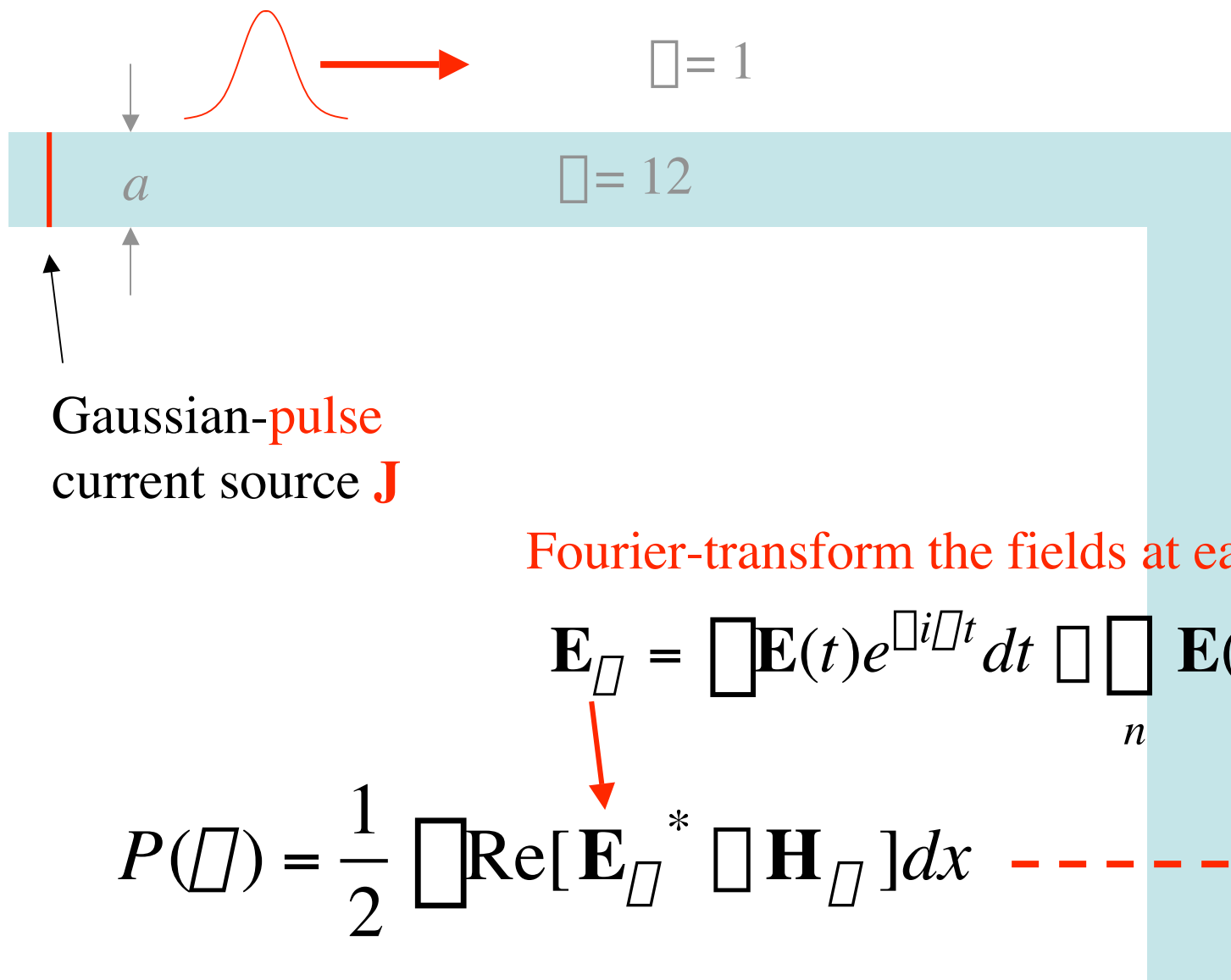
Transmission Spectra in FDTD



example: a 90° bend, 2d strip waveguide

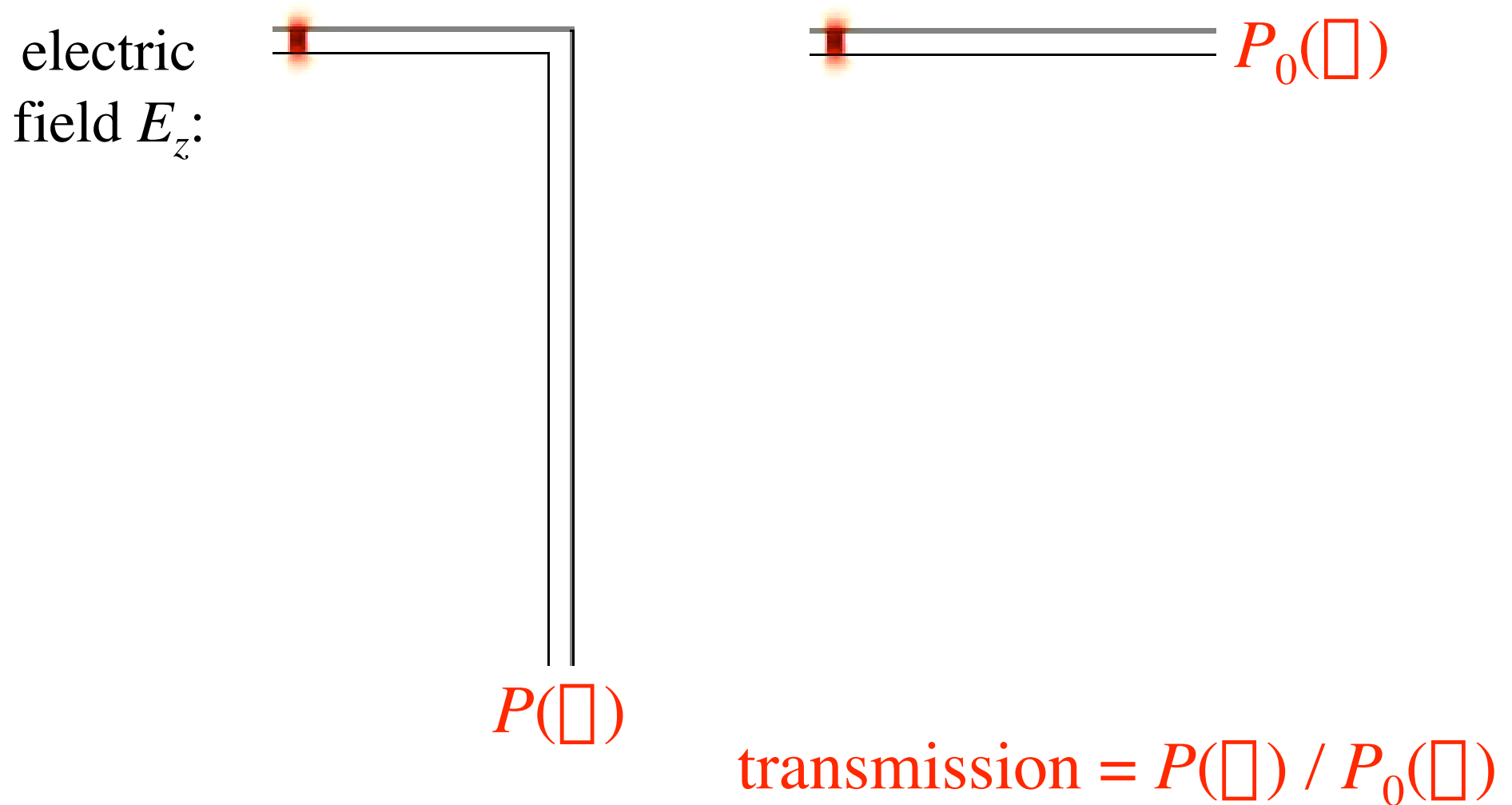
transmitted power = energy flux here: - - - - -

Transmission Spectra in FDTD

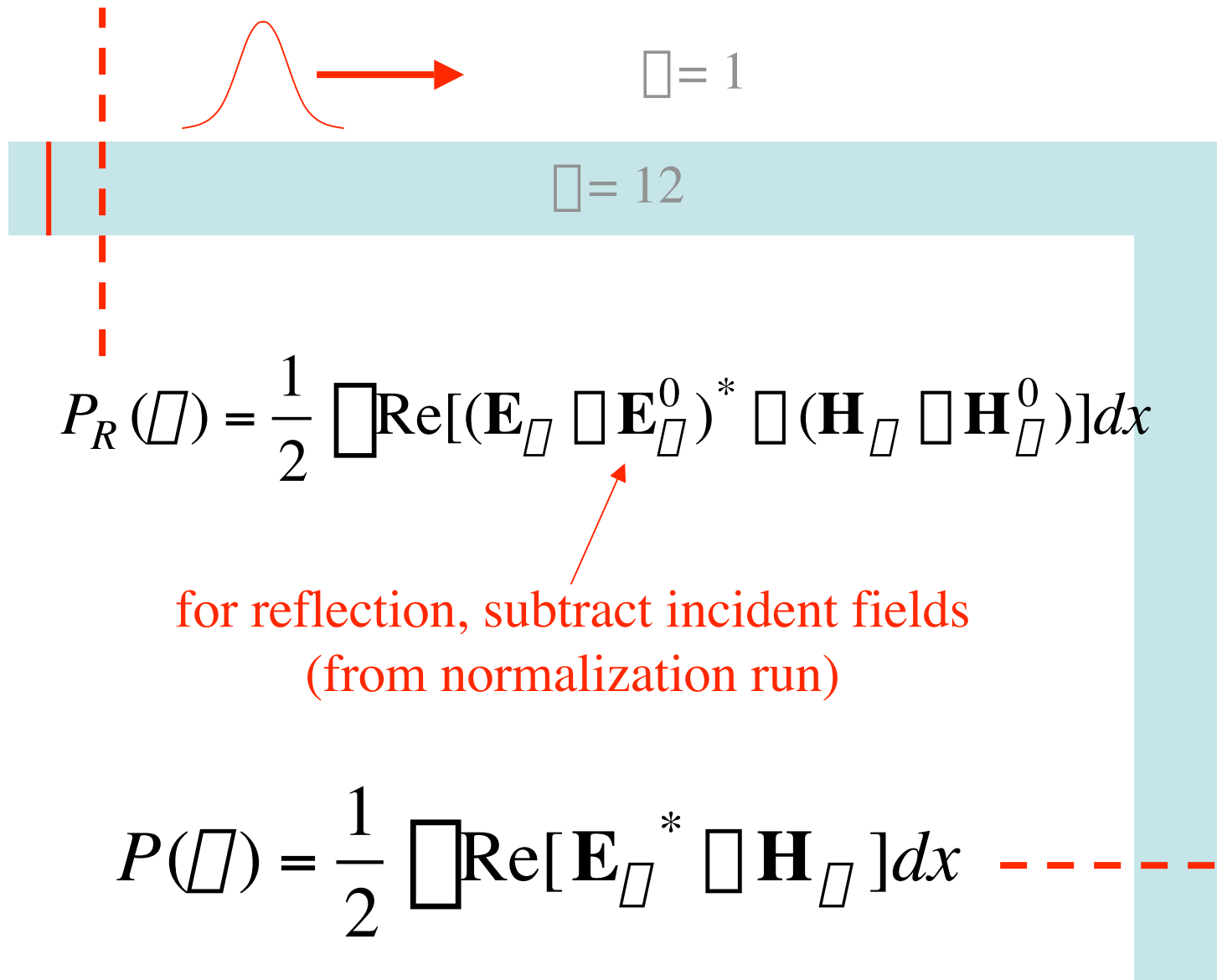


Transmission Spectra in FDTD

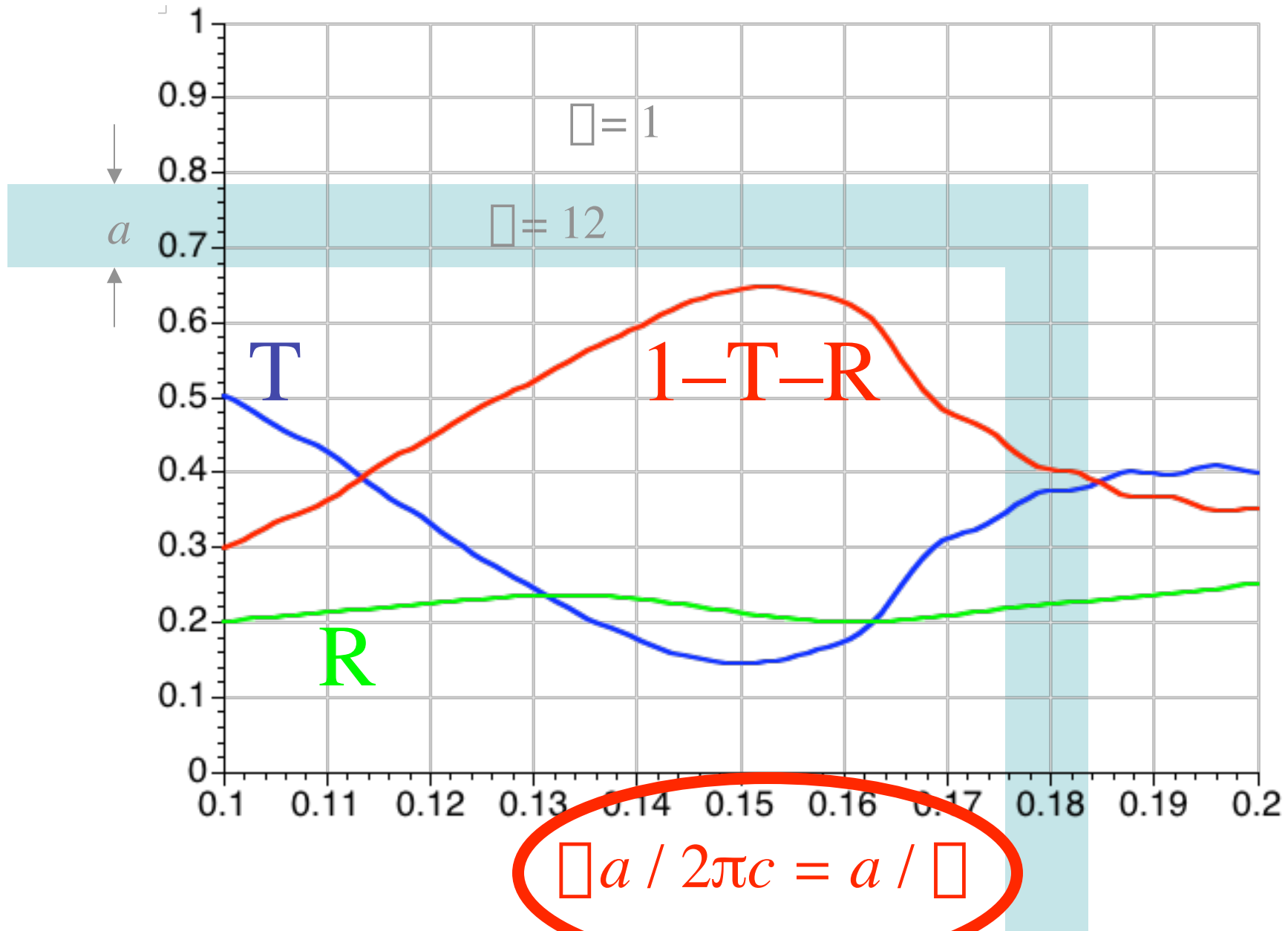
must always do *two* simulations: one for normalization



Reflection Spectra in FDTD



Transmission/Reflection Spectra



Dimensionless Units

Maxwell's equations are *scale invariant*

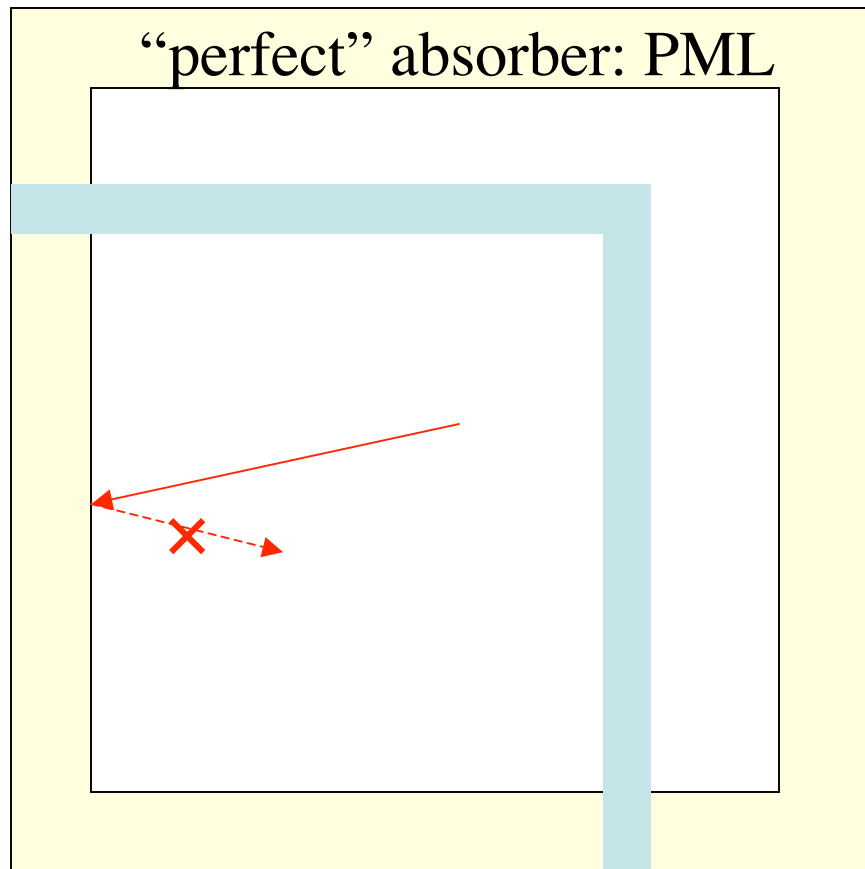
- most useful quantities are dimensionless ratios like a / λ , for a characteristic lengthscale a
- same ratio, same λ , $\lambda = a / \text{ratio}$ = same solution regardless of whether $a = 1\mu\text{m}$ or 1km

Our (typical) approach:

pick characteristic lengthscale a

- measure distance in units of a
- measure time in units of a/c
- measure λ in units of $2\pi c/a = a / \lambda$
-

Absorbing Boundaries: Perfectly Matched Layers



Artificial absorbing material
overlapping the computation

Theoretically reflectionless

... but PML is no longer perfect
with **finite resolution**,
so “gradually turn on” absorption
over finite-thickness PML

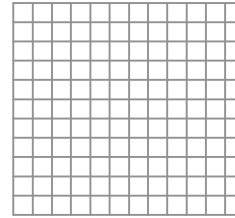
Computational Photonics Problems

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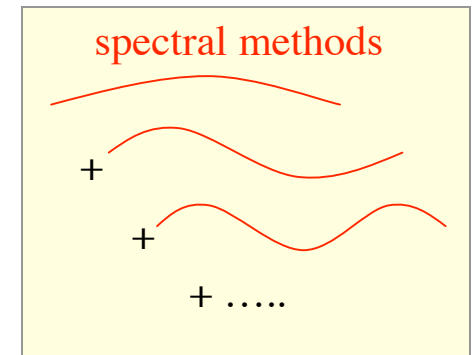
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finite difference

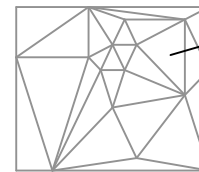


$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x^2)$$

spectral methods

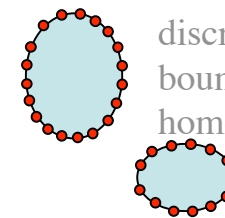


finite elements



in irregular “elements,”
approximate unknowns
by low-degree polynomial

boundary-element methods



discretize only the
boundaries between
homogeneous media

A Maxwell Eigenproblem

$$\vec{\nabla} \times \vec{E} = \frac{1}{c} \frac{\partial \vec{H}}{\partial t} = i \frac{\epsilon}{c} \vec{H}$$

First task:
get rid of this mess

$$\vec{\nabla} \times \vec{H} = \frac{1}{c} \frac{\partial \vec{E}}{\partial t} + \vec{J} = i \frac{\epsilon}{c} \vec{E}$$

dielectric function $\epsilon(\mathbf{x}) = n^2(\mathbf{x})$

$$\underbrace{\vec{\nabla} \times \frac{1}{\epsilon} \vec{\nabla} \times}_{\text{eigen-operator}} \vec{H} = \underbrace{\frac{\epsilon}{c^2}}_{\text{eigen-value}} \vec{H} \quad \underbrace{\vec{H}}_{\text{eigen-state}} \quad + \text{constraint} \quad \vec{\nabla} \cdot \vec{H} = 0$$

Electronic & Photonic Eigenproblems

Electronic

$$\nabla^2 \psi + V(\psi) \psi = E \psi$$

nonlinear eigenproblem
(V depends on e density $|\psi|^2$)

Photonic

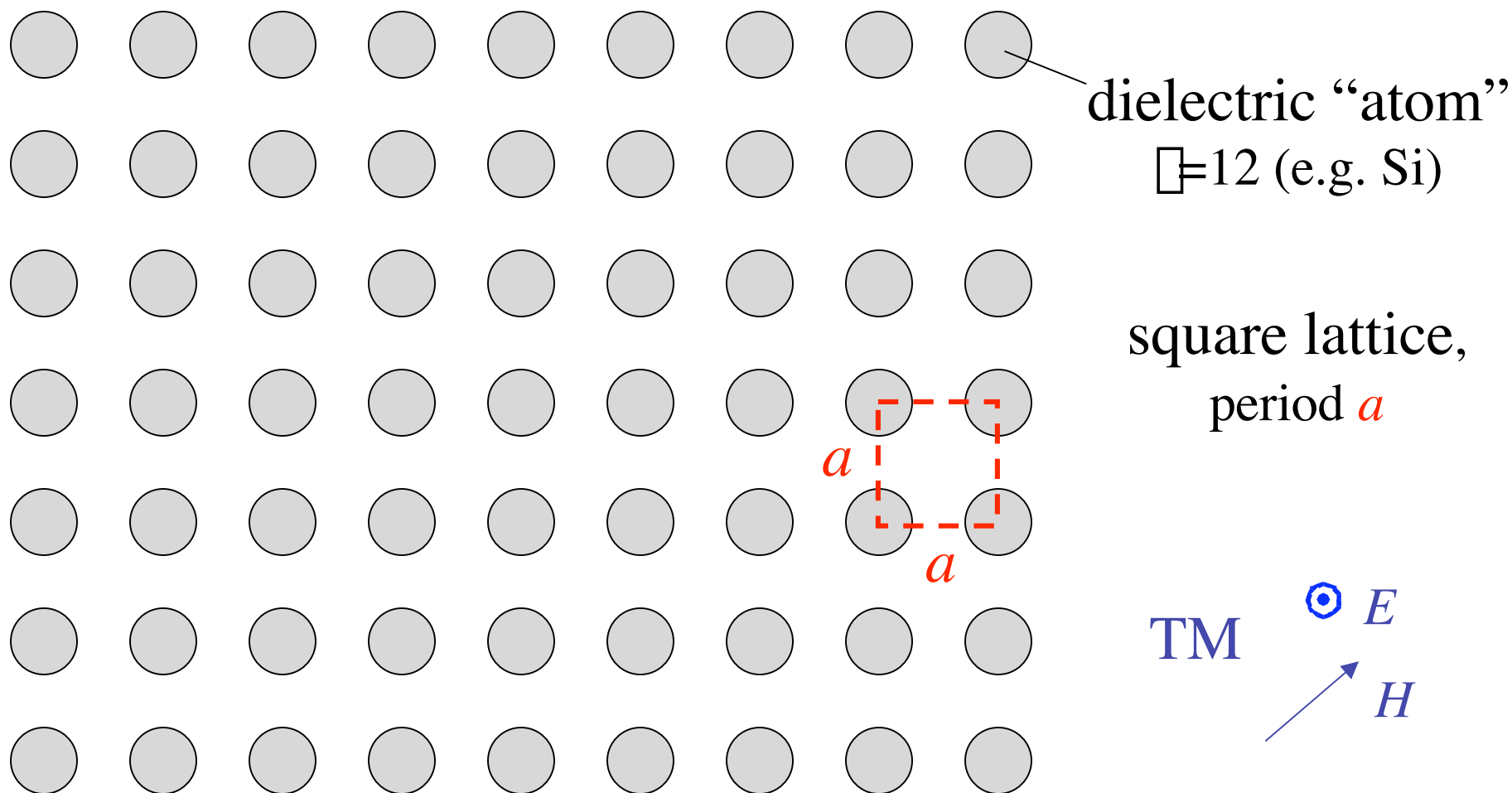
$$\nabla \cdot \left(\frac{1}{c^2} \nabla \vec{H} \right) = \vec{H}$$

simple **linear eigenproblem**
(for linear materials)

— many **well-known**
computational **techniques**

Hermitian = real E & ψ , ... Periodicity = Bloch's theorem...

A 2d Model System



Periodic Eigenproblems

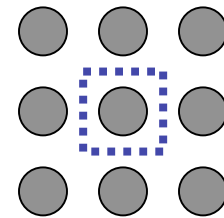
if eigen-operator is periodic, then Bloch-Floquet theorem applies:

can choose:
$$\vec{H}(\vec{x}, t) = e^{i(\vec{k} \cdot \vec{x} - \omega t)} \vec{H}_{\vec{k}}(\vec{x})$$

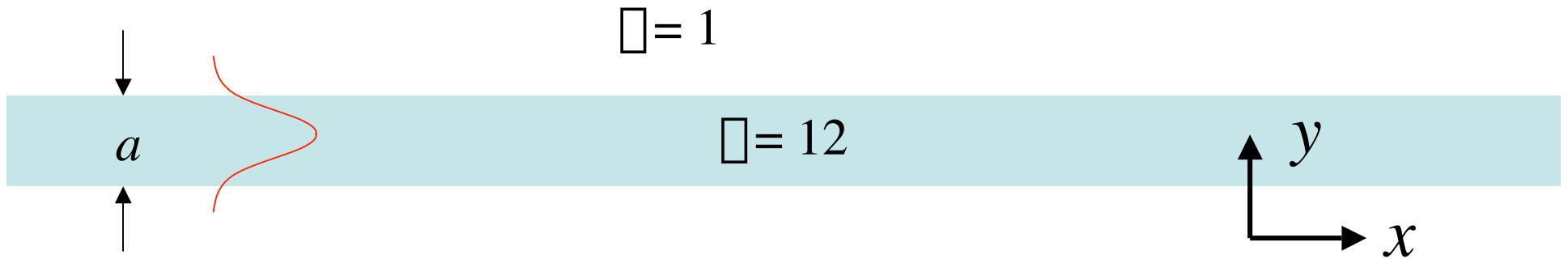
planewave
periodic “envelope”

Corollary 1: \mathbf{k} is conserved, *i.e.* no scattering of Bloch wave

Corollary 2: $\vec{H}_{\vec{k}}$ given by finite unit cell,
so ω are discrete $\omega_n(\mathbf{k})$



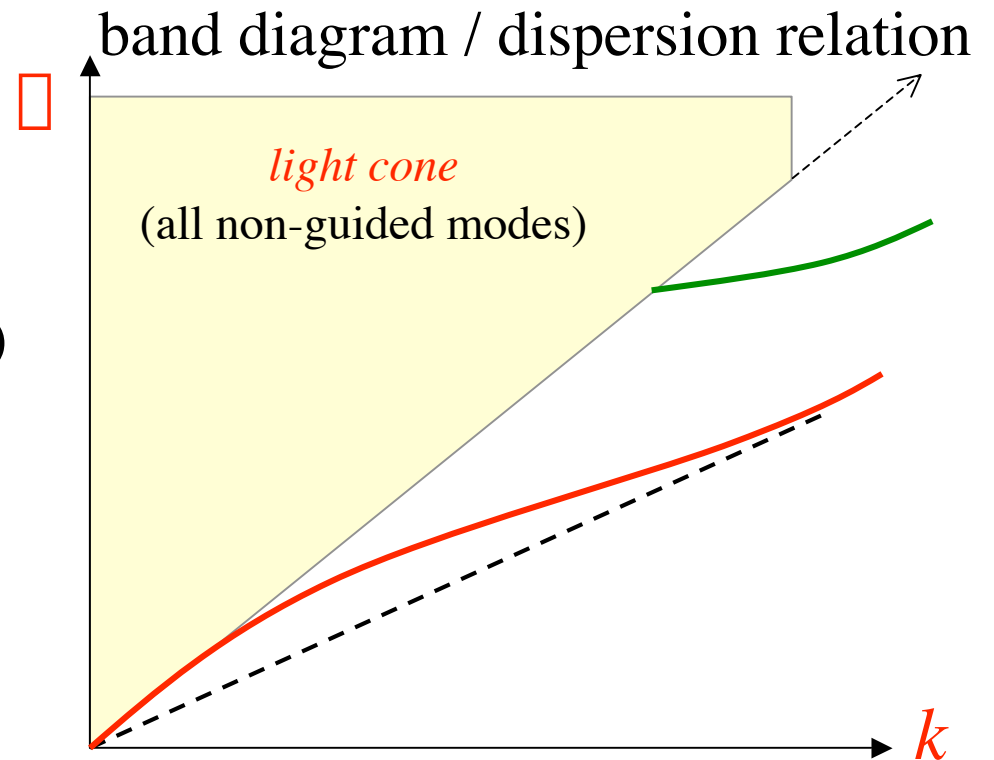
A More Familiar Eigenproblem



find the **normal modes**
of the waveguide:

$$\mathbf{H}(y, t) = \mathbf{H}_k(y) e^{i(kx - \omega t)}$$

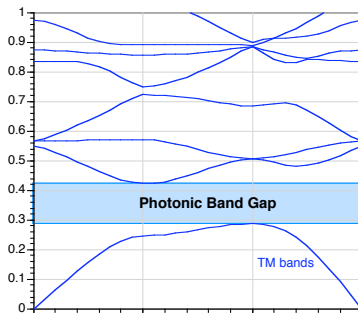
(propagation constant k
a.k.a. β)



Solving the Maxwell Eigenproblem

Finite cell → discrete eigenvalues ω_n

Want to solve for $\omega_n(\mathbf{k})$,
& plot vs. “all” \mathbf{k} for “all” n ,



$$(\omega + i\mathbf{k}) \frac{1}{\omega} (\omega + i\mathbf{k}) \mathbf{H}_n = \frac{\omega_n^2}{c^2} \mathbf{H}_n$$

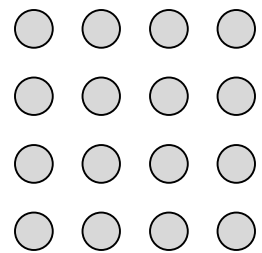
$$\text{constraint: } (\omega + i\mathbf{k}) \cdot \mathbf{H} = 0$$

$$\text{where: } \mathbf{H}(x,y) \propto e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$$

- 1 Limit range of \mathbf{k} : irreducible Brillouin zone
- 2 Limit degrees of freedom: expand \mathbf{H} in finite basis
- 3 Efficiently solve eigenproblem: iterative methods

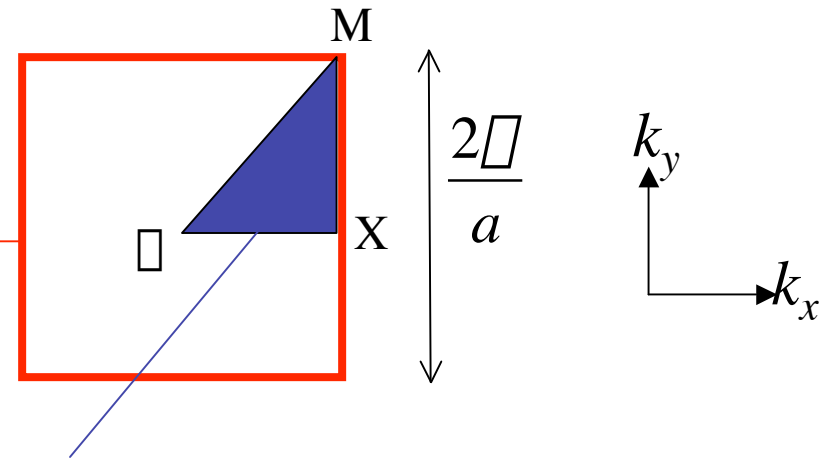
Solving the Maxwell Eigenproblem: 1

① Limit range of \mathbf{k} : irreducible Brillouin zone



— Bloch's theorem: solutions are **periodic in \mathbf{k}**

first Brillouin zone
= minimum $|\mathbf{k}|$ “primitive cell”



irreducible Brillouin zone: reduced by symmetry

② Limit degrees of freedom: expand \mathbf{H} in finite basis

③ Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2a

- 1 Limit range of \mathbf{k} : irreducible Brillouin zone
- 2 Limit degrees of freedom: expand \mathbf{H} in finite basis (N)

$$|\mathbf{H}\rangle = \mathbf{H}(\mathbf{x}_t) = \sum_{m=1}^N h_m \mathbf{b}_m(\mathbf{x}_t) \quad \text{solve: } \hat{A}|\mathbf{H}\rangle = \omega^2 |\mathbf{H}\rangle$$

finite matrix problem: $Ah = \omega^2 Bh$

$$\langle \mathbf{f} | \mathbf{g} \rangle = \mathbf{f}^* \cdot \mathbf{g} \quad A_{ml} = \langle \mathbf{b}_m | \hat{A} | \mathbf{b}_l \rangle \quad B_{ml} = \langle \mathbf{b}_m | \mathbf{b}_l \rangle$$

- 3 Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2b

- ① Limit range of \mathbf{k} : irreducible Brillouin zone
- ② Limit degrees of freedom: expand \mathbf{H} in finite basis
 - must satisfy constraint: $(\square + i\mathbf{k}) \cdot \mathbf{H} = 0$

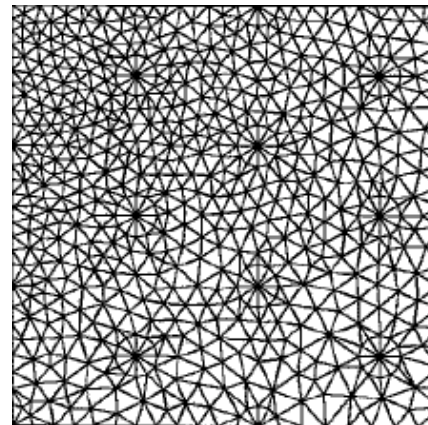
Planewave (FFT) basis

$$\mathbf{H}(\mathbf{x}_t) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{x}_t}$$

constraint: $\mathbf{H}_{\mathbf{G}} \cdot (\mathbf{G} + \mathbf{k}) = 0$

uniform “grid,” periodic boundaries,
simple code, $O(N \log N)$

Finite-element basis



[figure: Peyrilloux et al.,
J. Lightwave Tech.
21, 536 (2003)]

constraint, boundary conditions:

Nédélec elements

[Nédélec, *Numerische Math.*
35, 315 (1980)]

nonuniform mesh,
more arbitrary boundaries,
complex code & mesh, $O(N)$

- ③ Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 3a

- ① Limit range of \mathbf{k} : irreducible Brillouin zone
- ② Limit degrees of freedom: expand \mathbf{H} in finite basis
- ③ Efficiently solve eigenproblem: **iterative methods**

$$Ah = \nabla^2 Bh$$

Slow way: compute A & B , ask LAPACK for eigenvalues
— requires $O(N^2)$ storage, **$O(N^3)$ time**

Faster way:

- start with *initial guess* eigenvector h_0
- *iteratively* improve
- $O(Np)$ storage, $\sim O(Np^2)$ time for p eigenvectors
(p **smallest** eigenvalues)

Solving the Maxwell Eigenproblem: 3b

- ① Limit range of \mathbf{k} : irreducible Brillouin zone
- ② Limit degrees of freedom: expand \mathbf{H} in finite basis
- ③ Efficiently solve eigenproblem: iterative methods

$$Ah = \nabla^2 Bh$$

Many iterative methods:

- Arnoldi, Lanczos, Davidson, Jacobi-Davidson, ...,
Rayleigh-quotient minimization

Solving the Maxwell Eigenproblem: 3c

- 1 Limit range of \mathbf{k} : irreducible Brillouin zone
- 2 Limit degrees of freedom: expand \mathbf{H} in finite basis
- 3 Efficiently solve eigenproblem: iterative methods

$$Ah = \omega^2 Bh$$

Many iterative methods:

- Arnoldi, Lanczos, Davidson, Jacobi-Davidson, ...,
Rayleigh-quotient minimization

for Hermitian matrices, smallest eigenvalue ω_0 minimizes:

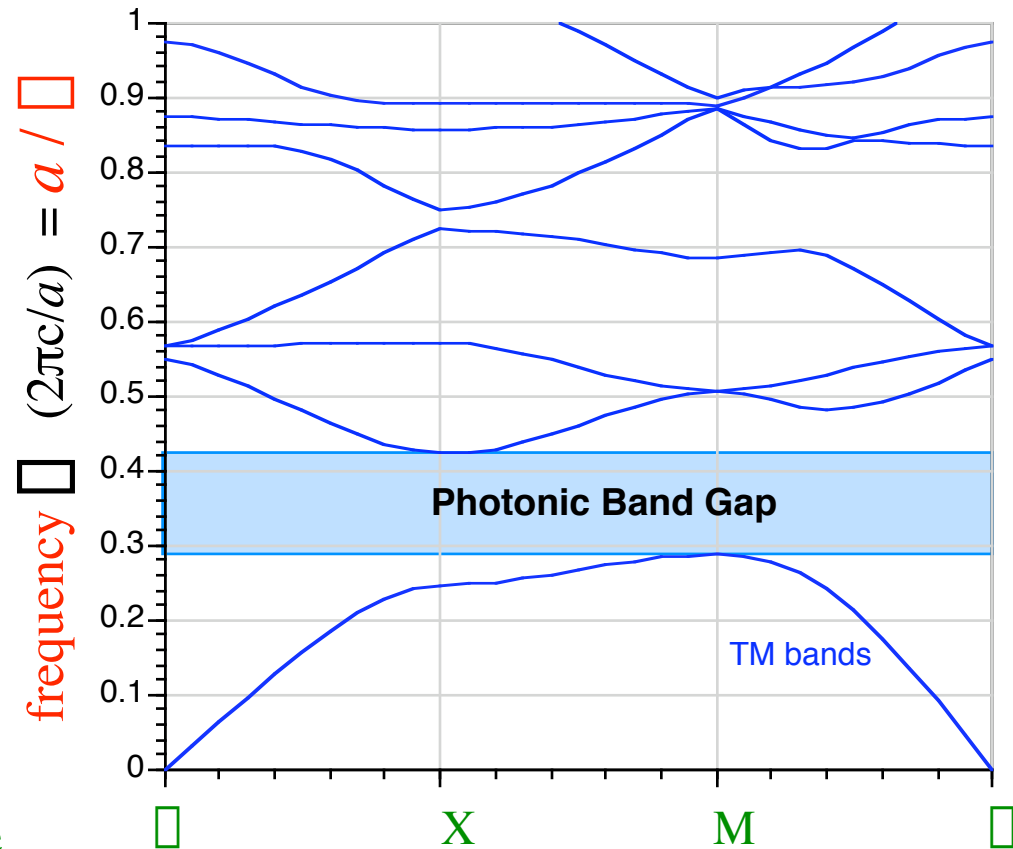
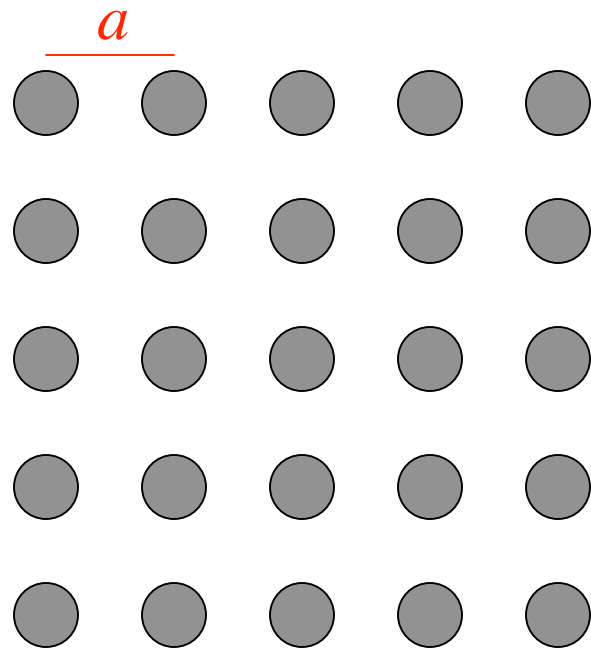
“variational theorem”

$$\omega_0^2 = \min_h \frac{h' Ah}{h' Bh}$$

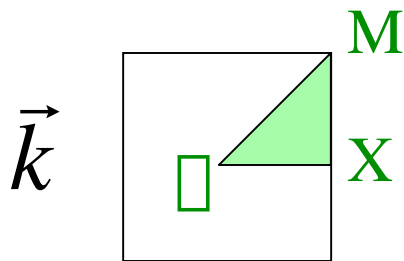
minimize by preconditioned conjugate-gradient (or...)

Band Diagram of 2d Model System

(radius $0.2a$ rods, $\epsilon_r=12$)



irreducible Brillouin zone



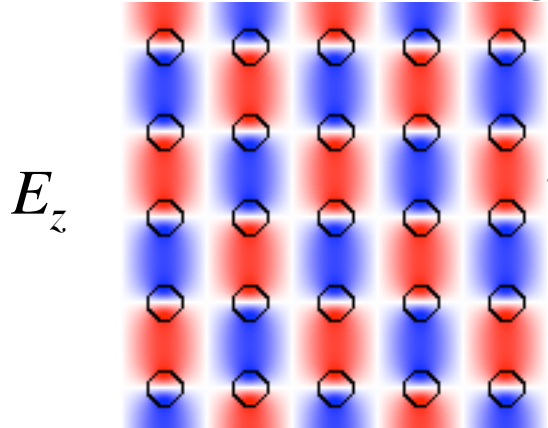
TM



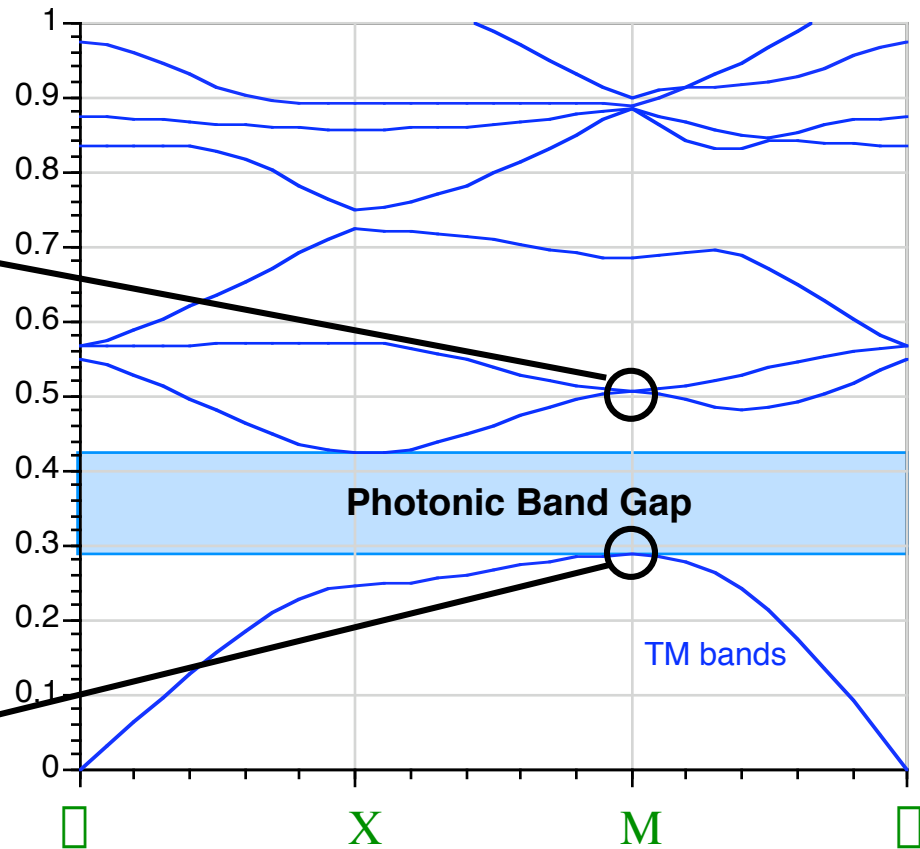
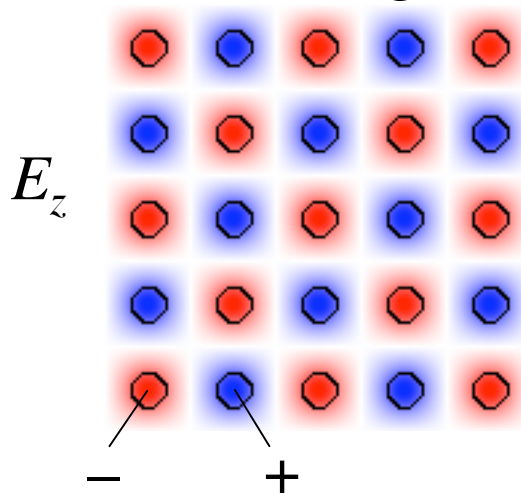
gap for
 $n > \sim 1.75:1$

Origin of Gap in 2d Model System

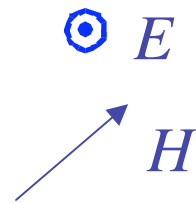
orthogonal: node in high \square



lives in high \square



TM



gap for
 $n > \sim 1.75:1$

The Iteration Scheme is *Important*

(minimizing function of 10^4 – 10^8 + variables!)

$$\square_0^2 = \min_h \frac{h' Ah}{h' Bh} = f(h)$$

Steepest-descent: minimize $(h + \square \square f)$ over \square ... repeat

Conjugate-gradient: minimize $(h + \square d)$

— d is $\square f + (\text{stuff})$: *conjugate* to previous search dirs

Preconditioned steepest descent: minimize $(h + \square d)$

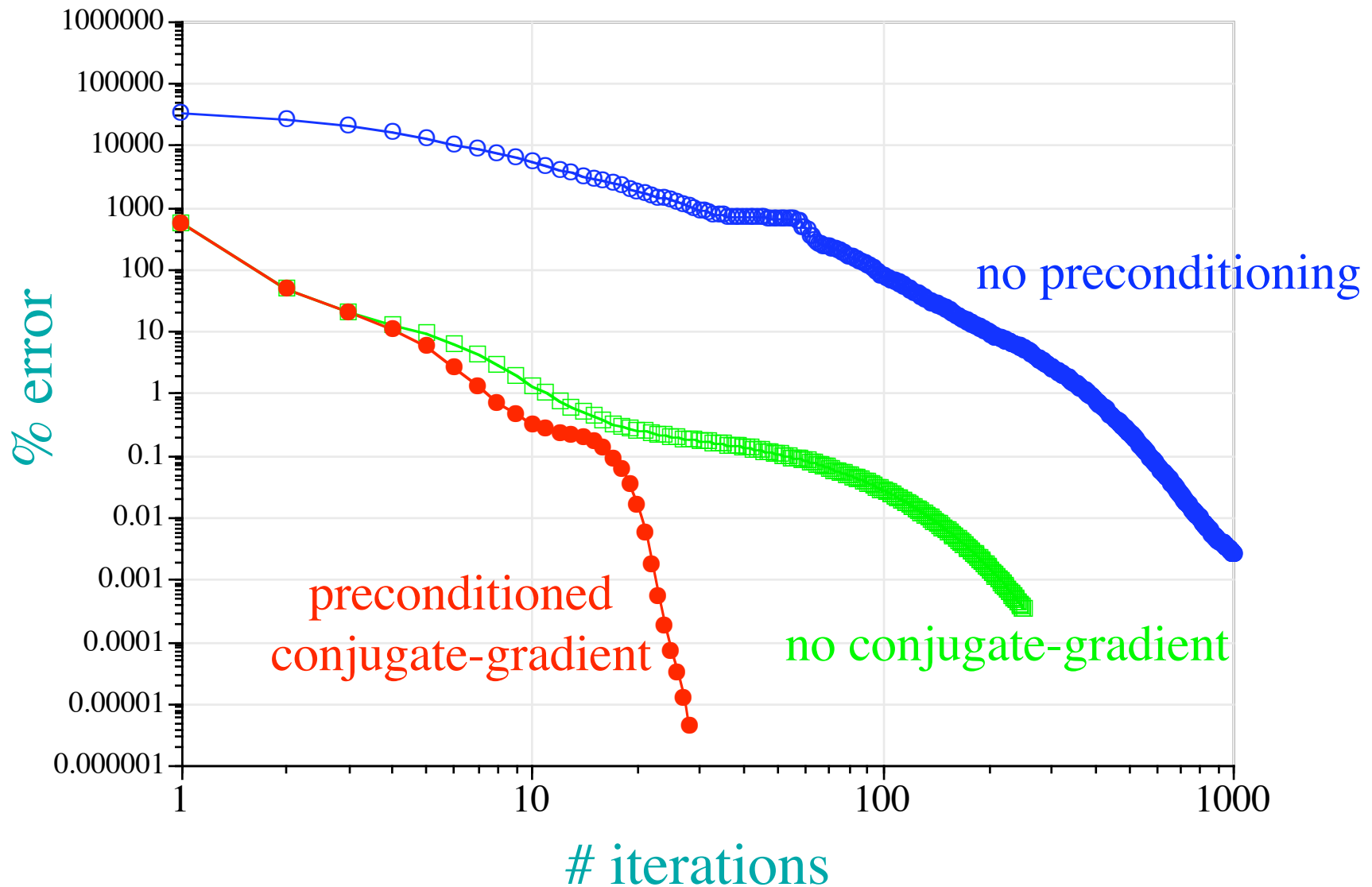
— $d = (\text{approximate } A^{-1}) \square f \sim$ Newton's method

Preconditioned conjugate-gradient: minimize $(h + \square d)$

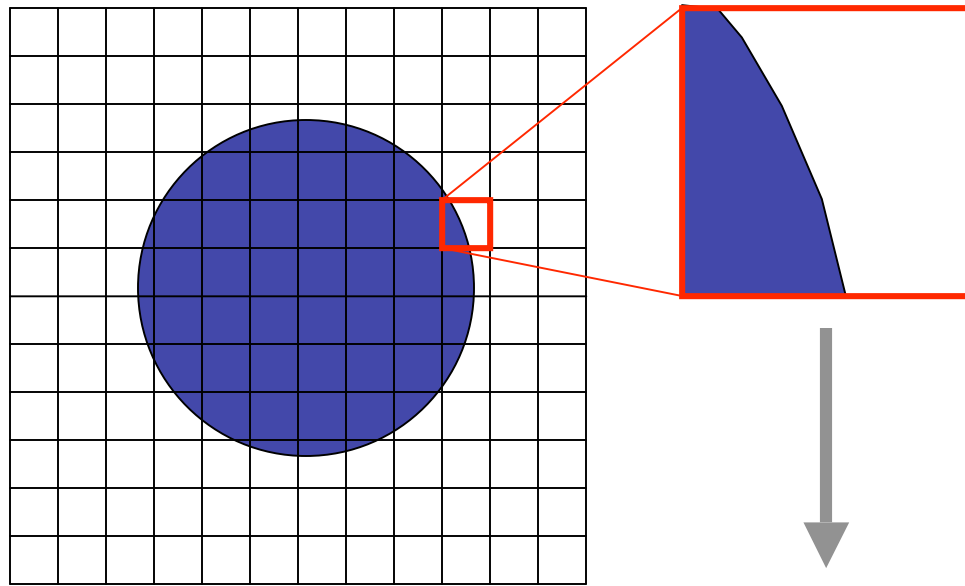
— d is $(\text{approximate } A^{-1}) [\square f + (\text{stuff})]$

The Iteration Scheme is *Important*

(minimizing function of $\sim 40,000$ variables)

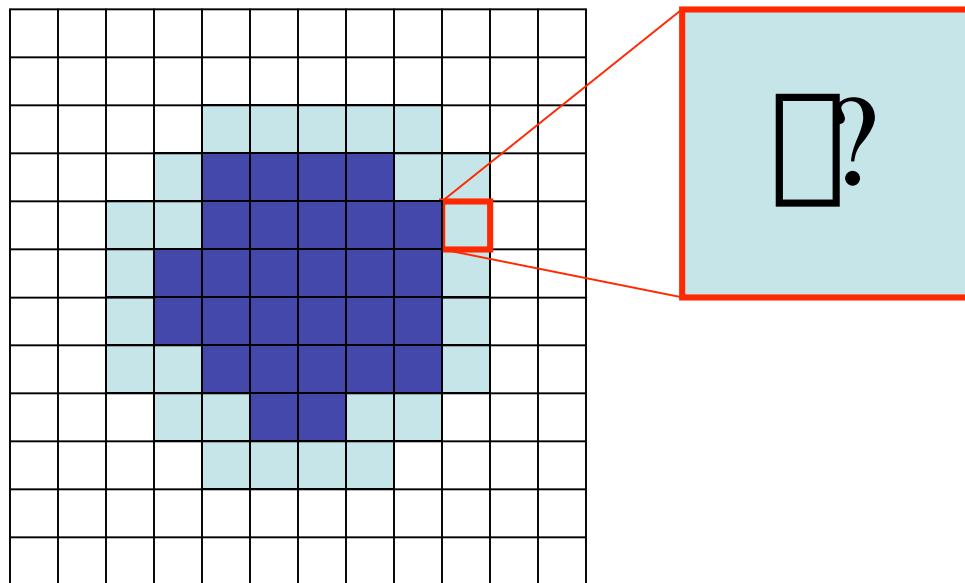


The Boundary Conditions are Tricky



\mathbf{E}_{\parallel} is continuous

\mathbf{E}_{\perp} is discontinuous
 ($\mathbf{D}_{\perp} = \epsilon \mathbf{E}_{\perp}$ is continuous)

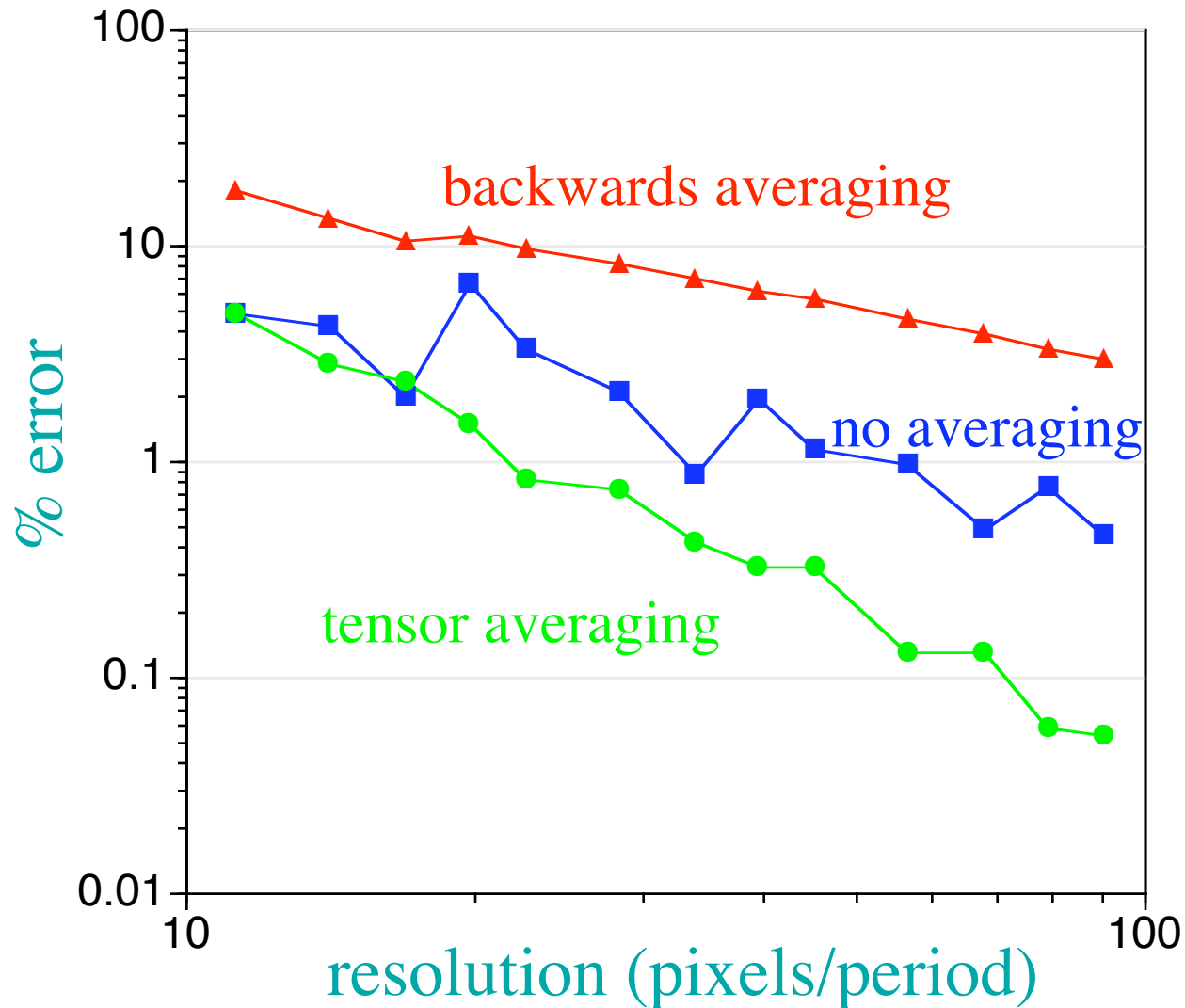


Any single scalar ϵ fails:
 (mean \mathbf{D}) \neq (any ϵ) (mean \mathbf{E})

Use a tensor ϵ

$$\begin{array}{c} \epsilon \end{array} \cdot \begin{array}{c} \mathbf{E}_{\parallel} \\ \mathbf{E}_{\perp} \end{array}$$

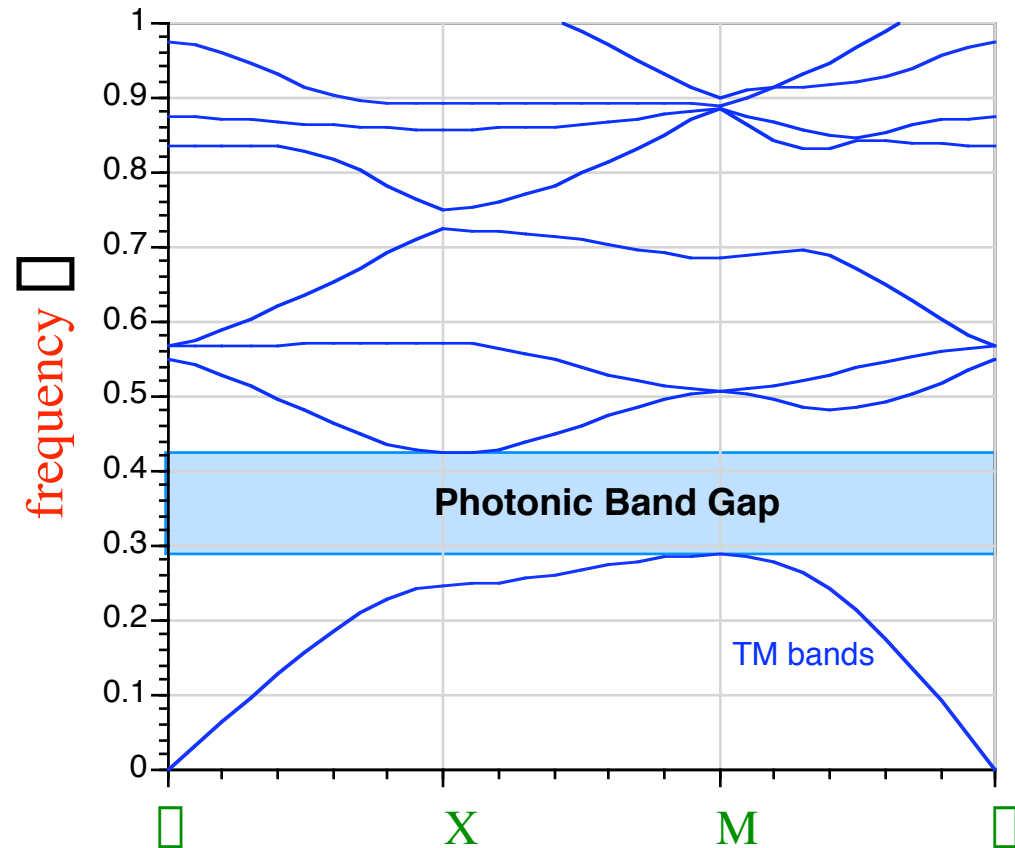
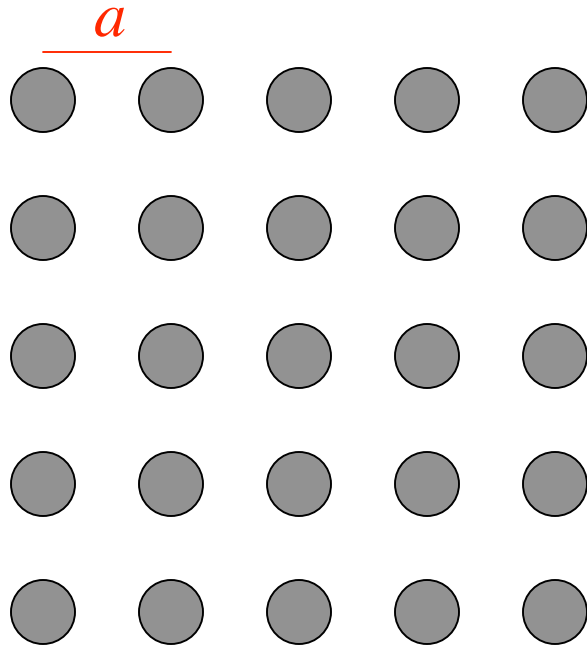
The \square -averaging is *Important*



correct averaging
changes *order*
of convergence
from Δx to Δx^2

(similar effects
in other E&M
numerics & analyses)

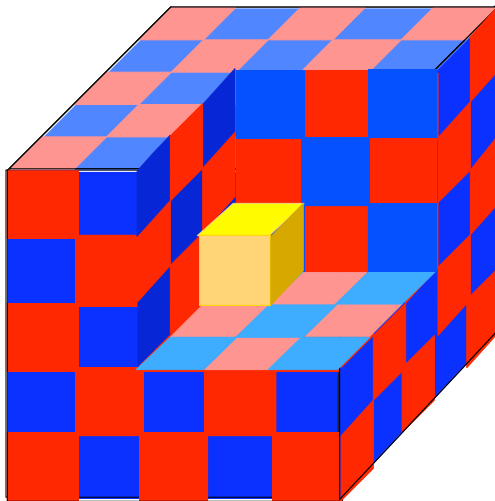
Gap, Schmap?



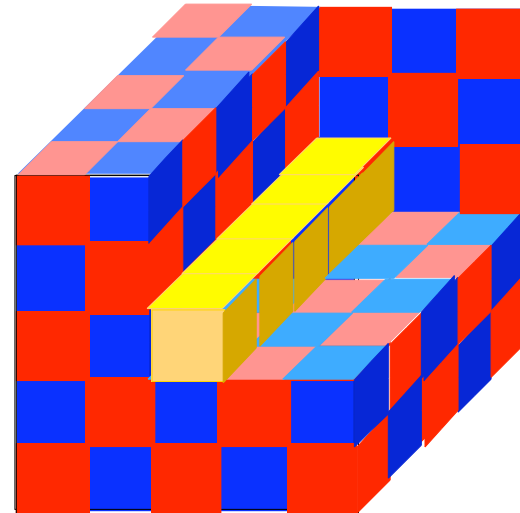
But, what can we *do* with the gap?

Intentional “defects” are good

microcavities

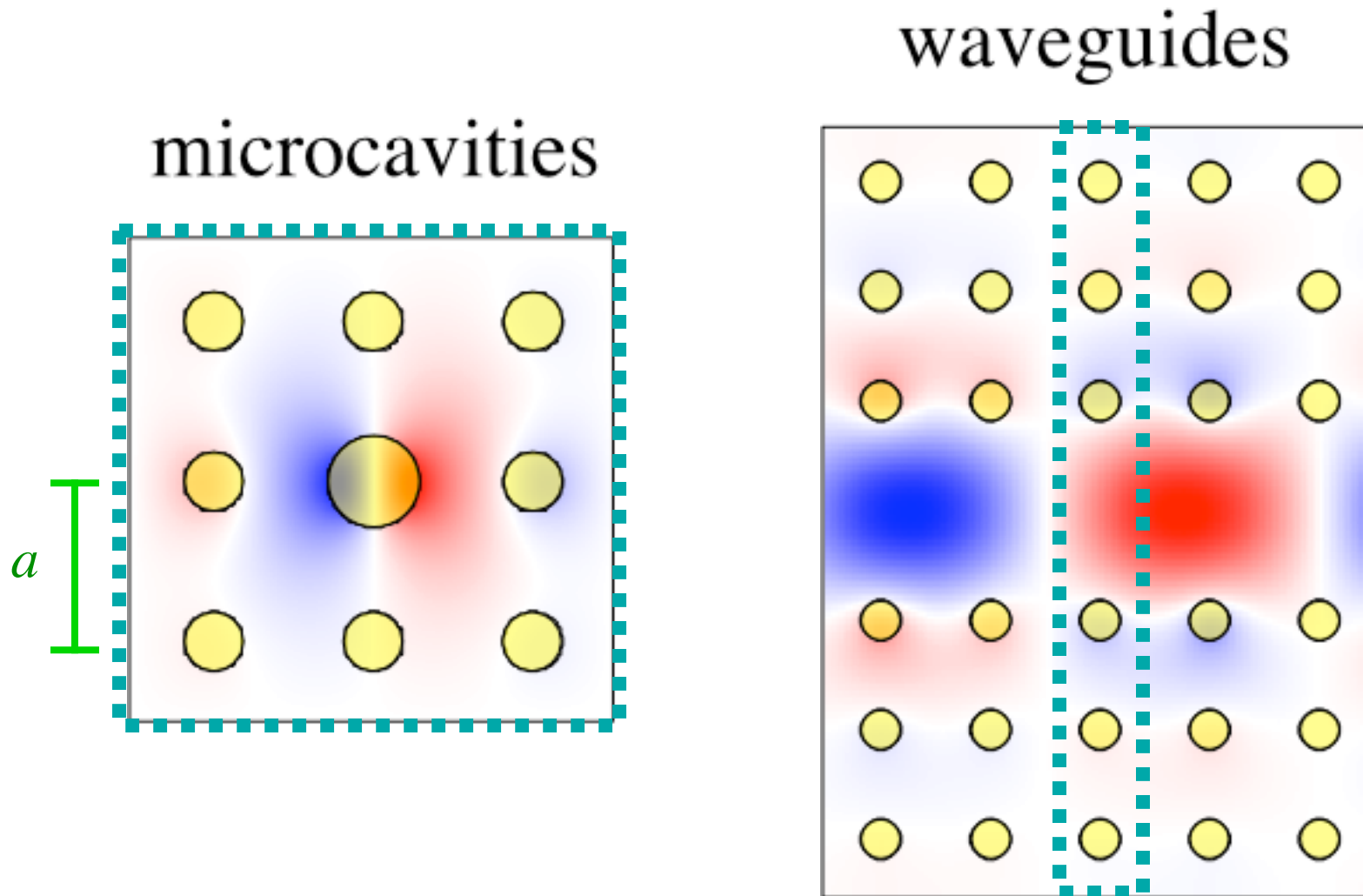


waveguides (“wires”)

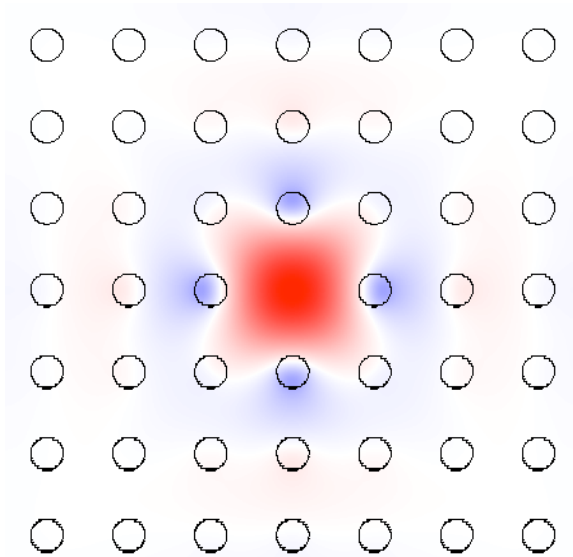


Intentional “defects” in 2d

(Same computation, with supercell = many primitive cells)



Microcavity Blues

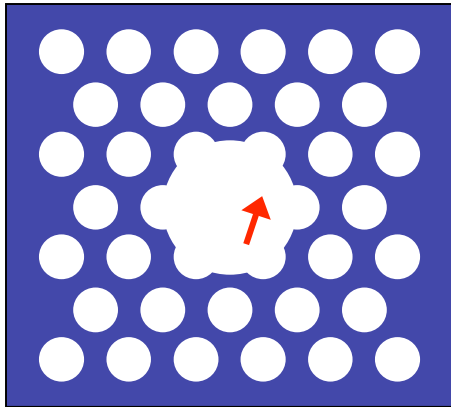


For cavities (*point defects*)
frequency-domain has its drawbacks:

- Best methods compute lowest- ω bands,
but N^d supercells have N^d modes
below the cavity mode — *expensive*
- Best methods are for Hermitian operators,
but losses requires non-Hermitian

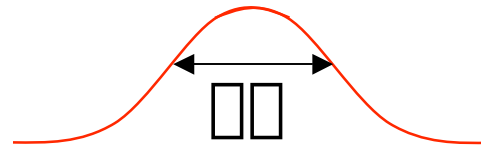
Time-Domain Eigensolvers

(finite-difference time-domain = FDTD)

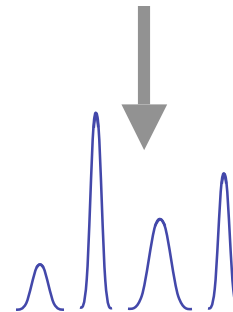


Simulate Maxwell's equations on a **discrete grid**,
+ **absorbing** boundaries (**leakage loss**)

- Excite with broad-spectrum **dipole** (↑) source



Response is many
sharp peaks,
one peak per mode



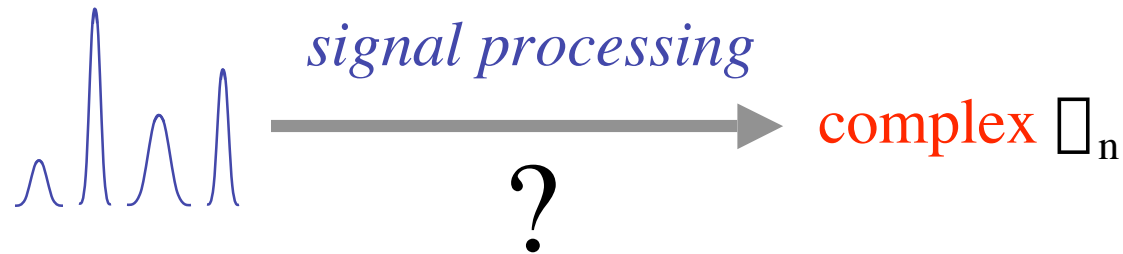
signal processing

complex \square_n

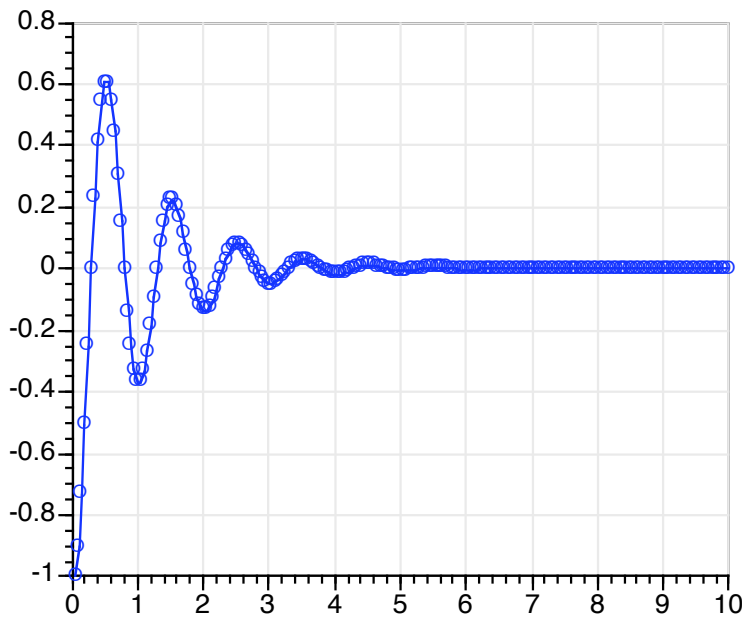
[Mandelshtam,
J. Chem. Phys. **107**, 6756 (1997)]

decay rate in time gives **loss**

Signal Processing is Tricky

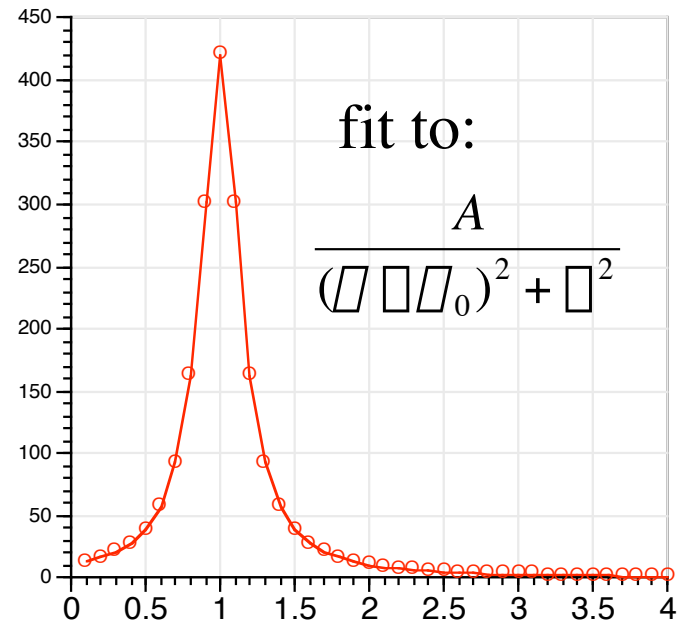


a common approach: least-squares fit of spectrum



Decaying signal (t)

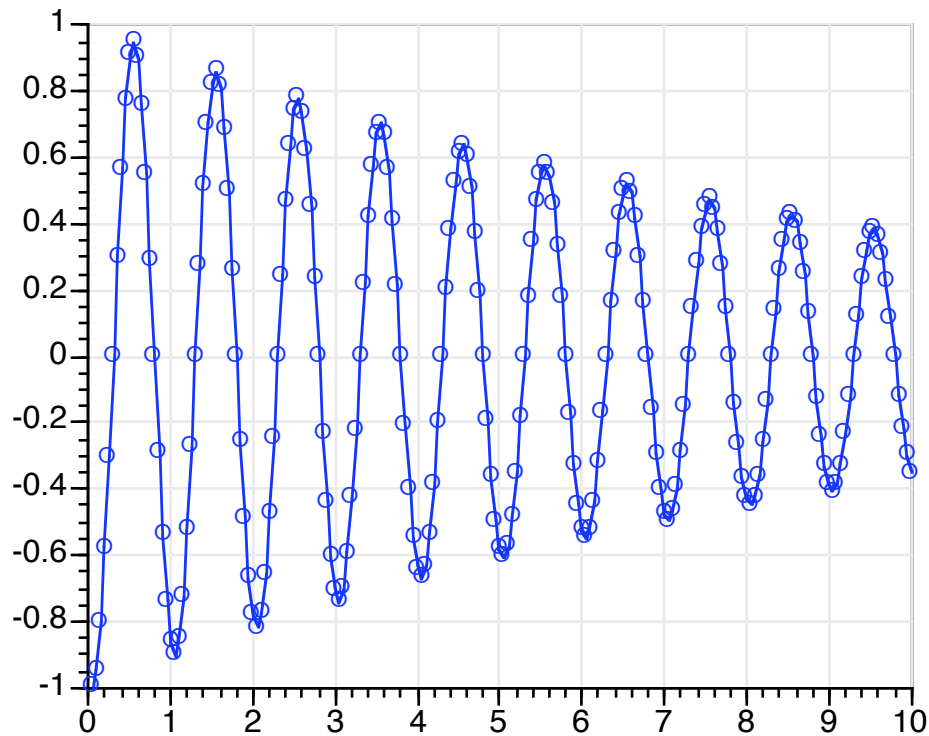
FFT



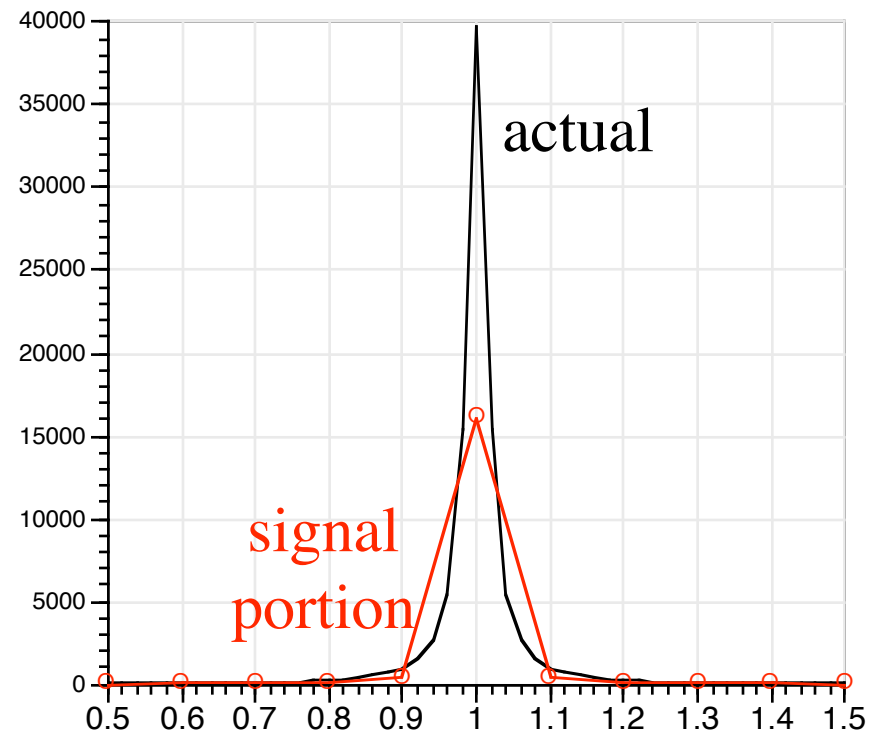
Lorentzian peak (\square)

Fits and Uncertainty

problem: have to run long enough to *completely* decay



Portion of decaying signal (t)

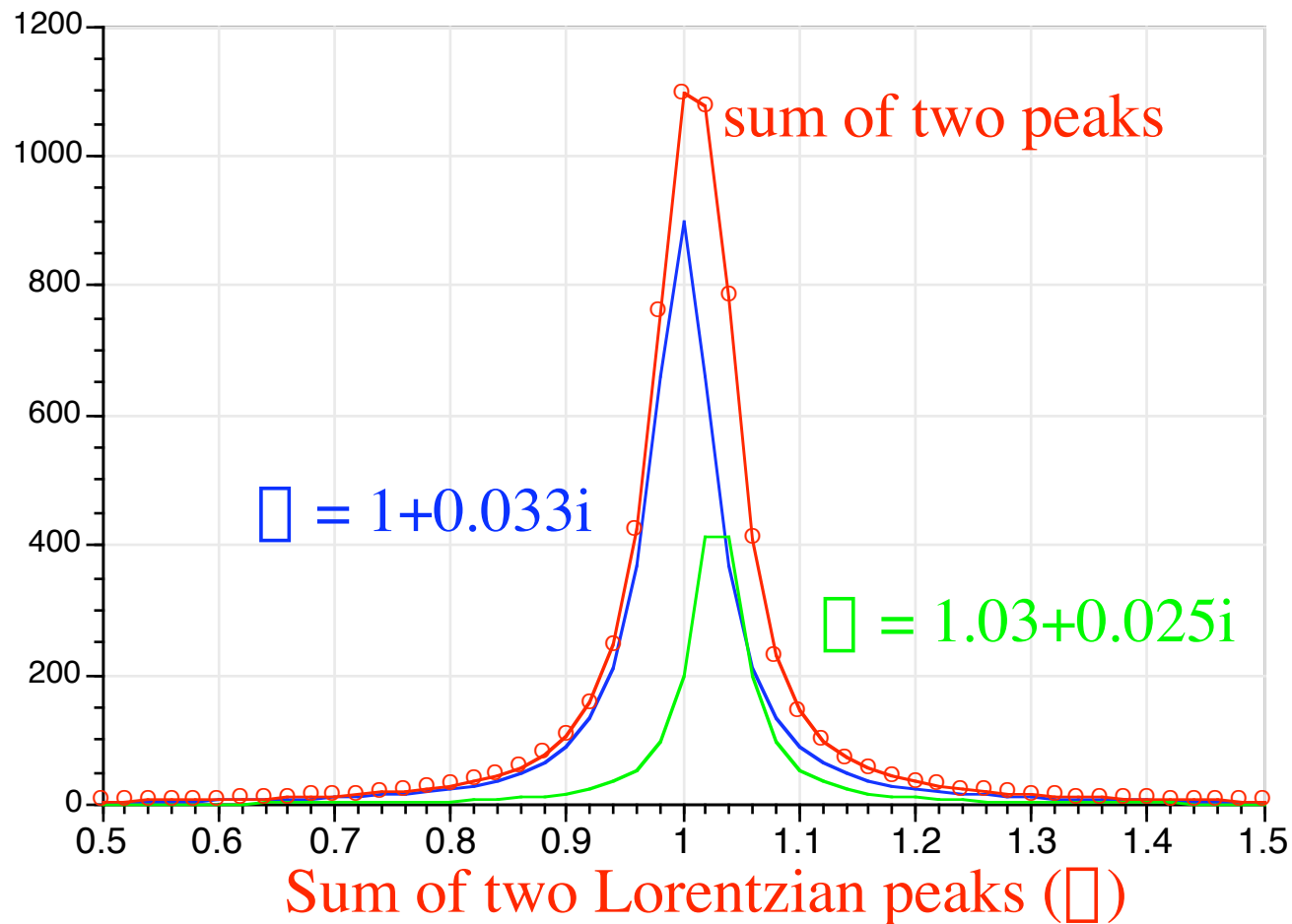


Unresolved Lorentzian peak (\square)

There is a better way, which gets complex \square to > 10 digits

Unreliability of Fitting Process

Resolving **two overlapping peaks** is
near-impossible 6-parameter nonlinear fit
(too many local minima to converge reliably)



There is a better way, which gets
complex \square
for *both* peaks
to > 10 digits

Quantum-inspired signal processing (NMR spectroscopy): Filter-Diagonalization Method (FDM)

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

Given **time series** y_n , write: $y_n = y(n\Delta t) = \sum_k a_k e^{i\omega_k n\Delta t}$

...find *complex amplitudes* a_k & *frequencies* ω_k
by a simple linear-algebra problem!

Idea: pretend $y(t)$ is autocorrelation of a quantum system:

$$\hat{H}|\square\rangle = i\hbar \frac{\partial}{\partial t} |\square\rangle \quad \text{time-}\Delta t \text{ evolution-operator: } \hat{U} = e^{i\hat{H}\Delta t/\hbar}$$

$$\text{say: } y_n = \langle \square(0) | \square(n\Delta t) \rangle = \langle \square(0) | \hat{U}^n | \square(0) \rangle$$

Filter-Diagonalization Method (FDM)

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

$$y_n = \langle \square(0) | \square(n\Delta t) \rangle = \langle \square(0) | \hat{U}^n | \square(0) \rangle \quad \hat{U} = e^{i\hat{H}\Delta t/\hbar}$$

We want to diagonalize U : eigenvalues of U are $e^{i\epsilon\Delta t}$
...expand U in basis of $|\square(n\Delta t)\rangle$:

$$U_{m,n} = \langle \square(m\Delta t) | \hat{U} | \square(n\Delta t) \rangle = \langle \square(0) | \hat{U}^m \hat{U} \hat{U}^n | \square(0) \rangle = y_{m+n+1}$$

U_{mn} given by y_n 's — just diagonalize known matrix!

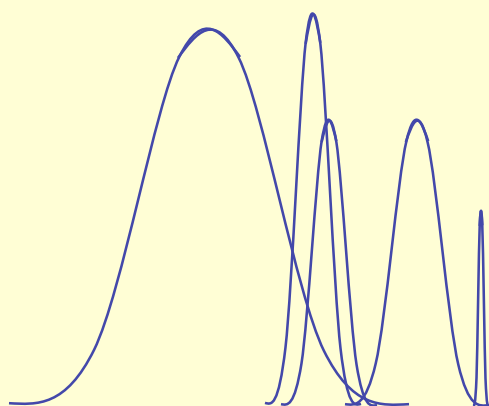
Filter-Diagonalization Summary

[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

U_{mn} given by y_n 's — just diagonalize known matrix!

A few omitted steps:

- Generalized eigenvalue problem (basis not orthogonal)
- **Filter** y_n 's (Fourier transform):
small bandwidth = **smaller matrix** (less singular)



- resolves **many peaks** at once
- **# peaks not known** *a priori*
- resolve **overlapping peaks**
- **resolution** \gg **Fourier** uncertainty

Do try this at home

FDTD simulation:

`http://ab-initio.mit.edu/meep/`

Bloch-mode eigensolver:

`http://ab-initio.mit.edu/mpb/`

Filter-diagonalization:

`http://ab-initio.mit.edu/harminv/`

Photonic-crystal tutorials (+ THIS TALK):

`http://ab-initio.mit.edu/
/photons/tutorial/`

Meep (FDTD)

- Arbitrary $\epsilon(\mathbf{x})$ — including dispersive, loss/gain, and nonlinear [$\epsilon^{(2)}$ and $\epsilon^{(3)}$]
- Arbitrary $\mathbf{J}(\mathbf{x}, t)$
- PML/periodic/metal bound.
- 1d/2d/3d/cylindrical
- power spectra • eigenmodes

MPB (Eigensolver)

- Arbitrary periodic $\epsilon(\mathbf{x})$ — anisotropic, magneto-optic, ... (lossless, linear materials)
 - 1d/2d/3d
- band diagrams, group velocities
perturbation theory, ...



Free/open-source
software (GNU)

- MPI parallelism
- exploit mirror symmetries
- fully scriptable interface
- built-in multivariate optimization, integration, root-finding, ...
- field output (standard HDF5 format)

Unix Philosophy

combine small, well-designed tools, via files

Input text file → **MPB/Meep** → standard formats
(text + HDF5)

Disadvantage:

- have to learn several programs

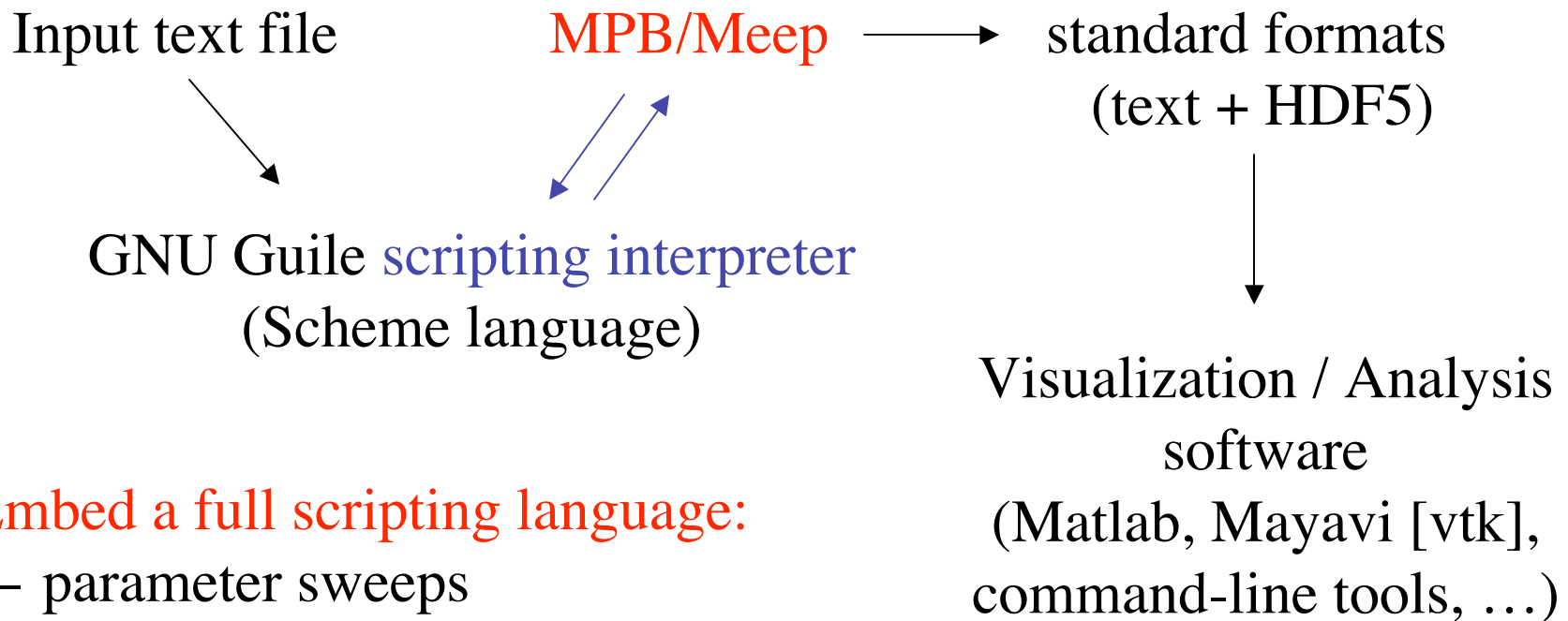
Advantages:

- flexibility
- batch processing, shell scripting
- ease of development

↓
Visualization / Analysis
software
(Matlab, Mayavi [vtk],
command-line tools, ...)

Unix Philosophy

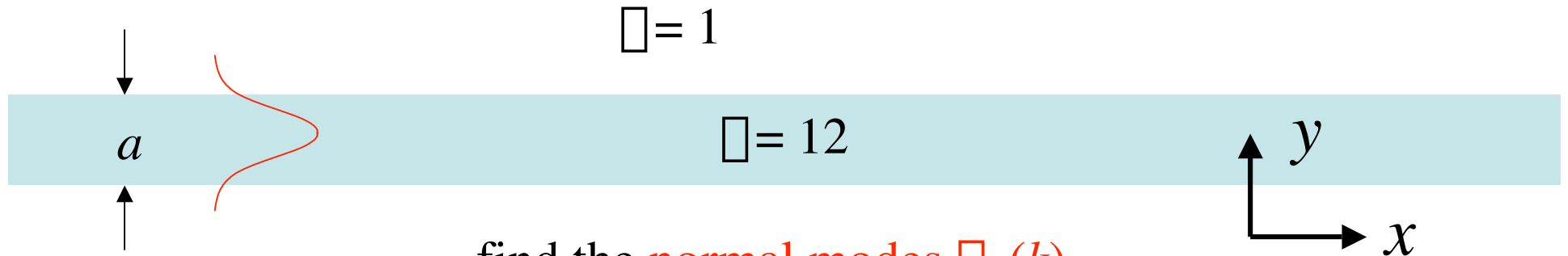
combine small, well-designed tools, via files



Embed a full scripting language:

- parameter sweeps
- complex parameterized geometries
- optimization, integration, etc.
- programmable $\mathbf{J}(\mathbf{x}, t)$, etc.
- ... Turing complete

A Simple Example (MPB)



find the **normal modes** $\Delta_n(k)$
of the waveguide:

$$\mathbf{H}(y, t) = \mathbf{H}_k(y) e^{i(kx - \Delta t)}$$

Need to specify:

- **computational cell** size/resolution
- **geometry**, i.e. $\Delta(y)$
- what k values
- how **many modes** ($n = 1, 2, \dots$?)

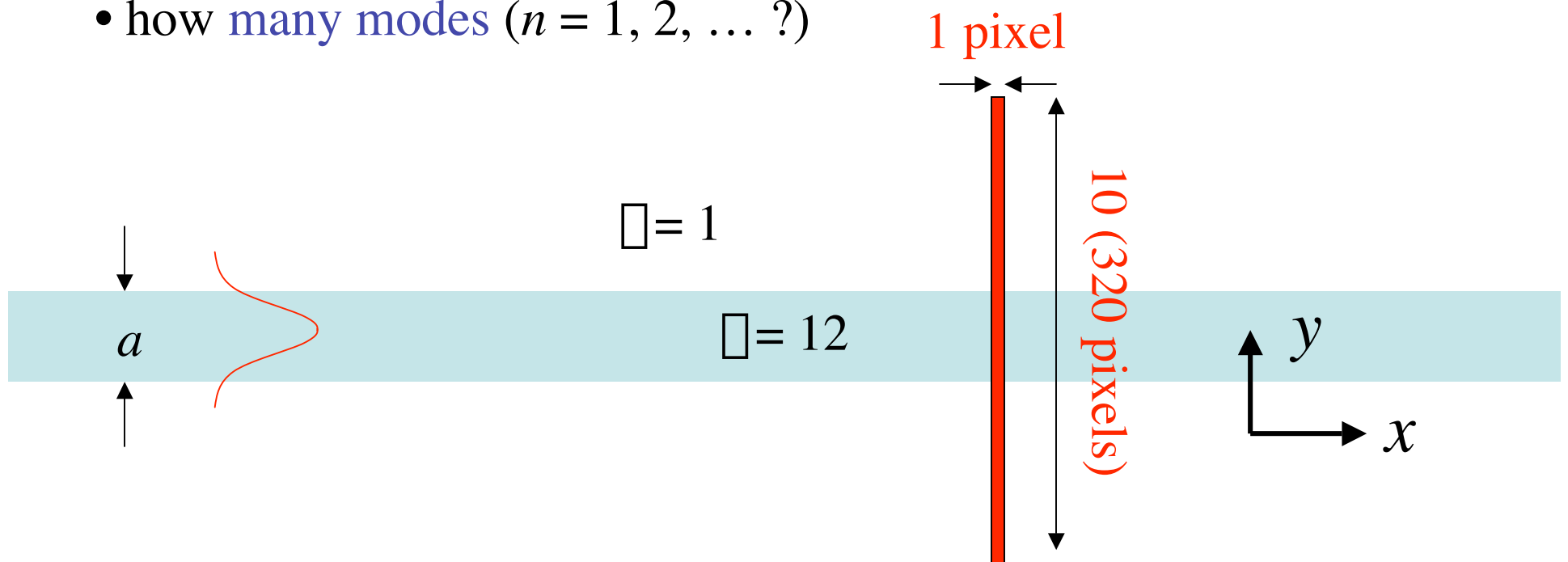
A File Format Made of Parentheses

Need to specify:

- computational cell size/resolution

```
(set! geometry-lattice (make lattice (size no-size 10 no-size)  
(set! resolution 32)
```

- geometry, i.e. $\epsilon(y)$
- what k values
- how many modes ($n = 1, 2, \dots$?)



A File Format Made of Parentheses

Need to specify:

- computational cell size/resolution
- geometry, i.e. $\square(y)$

(set! geometry

(list

(make block (size infinity 1 infinity)

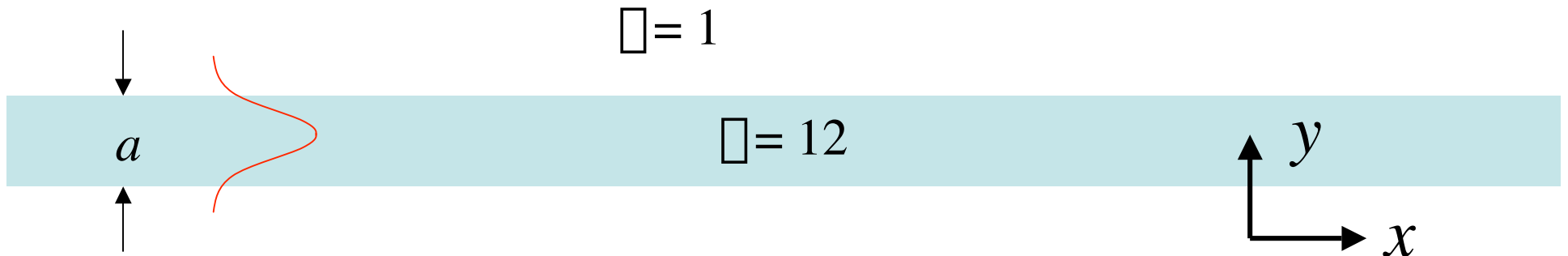
(center 0 0 0)

(material (make dielectric (epsilon 12))))))

(choose units of a)



- what k values
- how many modes ($n = 1, 2, \dots$?)



A File Format Made of Parentheses

Need to specify:

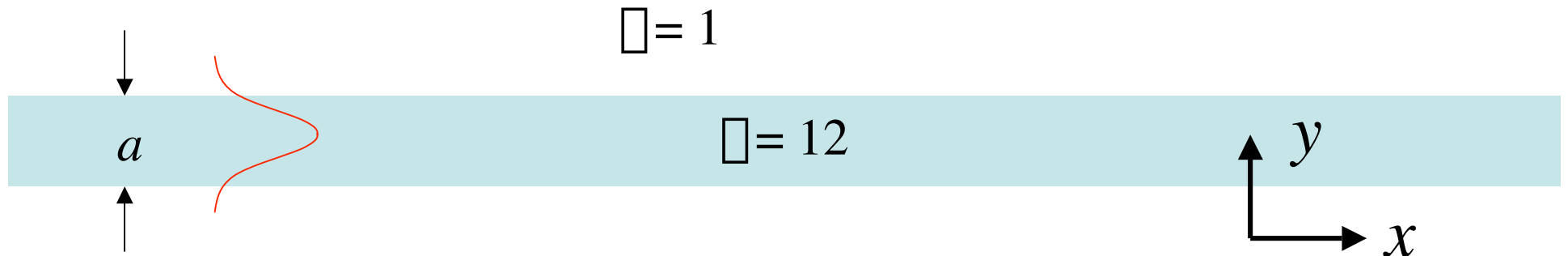
- computational cell size/resolution
- geometry, i.e. $\epsilon(y)$
- what k values

(units of $2\pi/a$)

```
(set! k-points  
  (interpolate 10 (list (vector3 0 0 0) (vector3 2 0 0))))
```

(built-in function)

- how many modes ($n = 1, 2, \dots$?)



A File Format Made of Parentheses

Need to specify:

- computational cell size/resolution
- geometry, i.e. $\epsilon(y)$
- what k values
- how many modes ($n = 1, 2, \dots$?)

`(set! num-bands 5)`

...Then run:

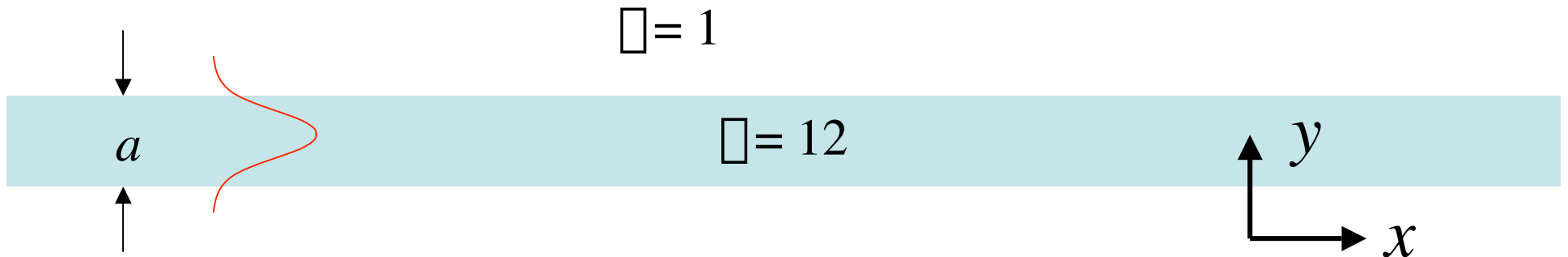
`(run)`

or only TM polarization:

`(run-tm)`

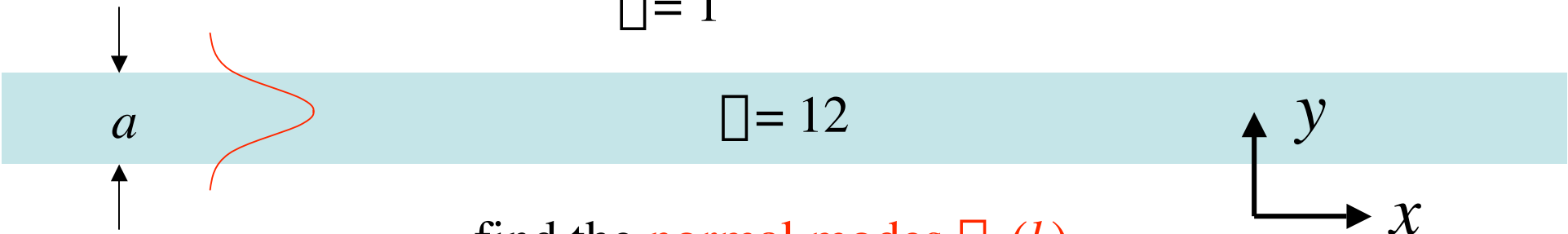
or only TM, even modes:

`(run-tm-yeven)`

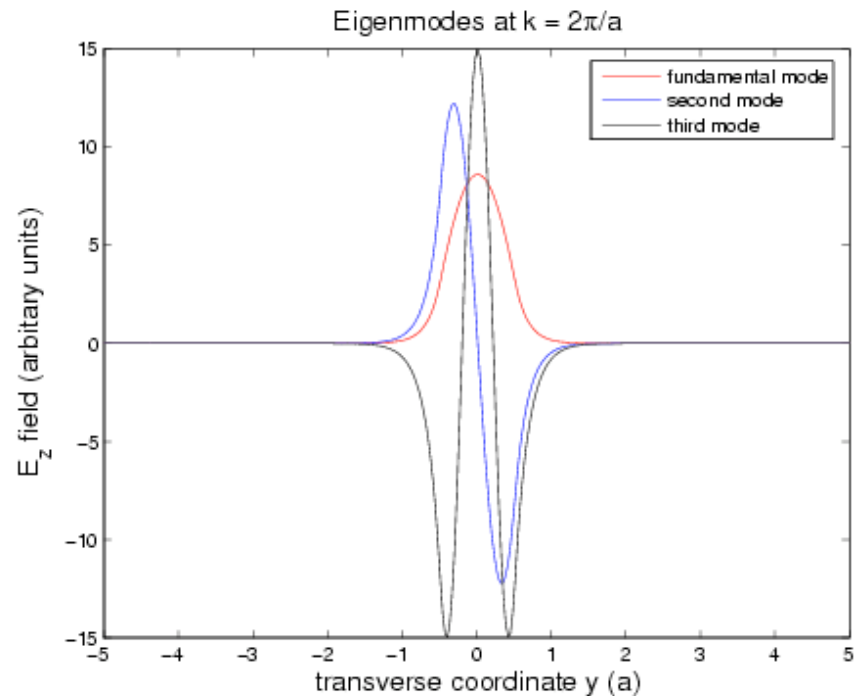
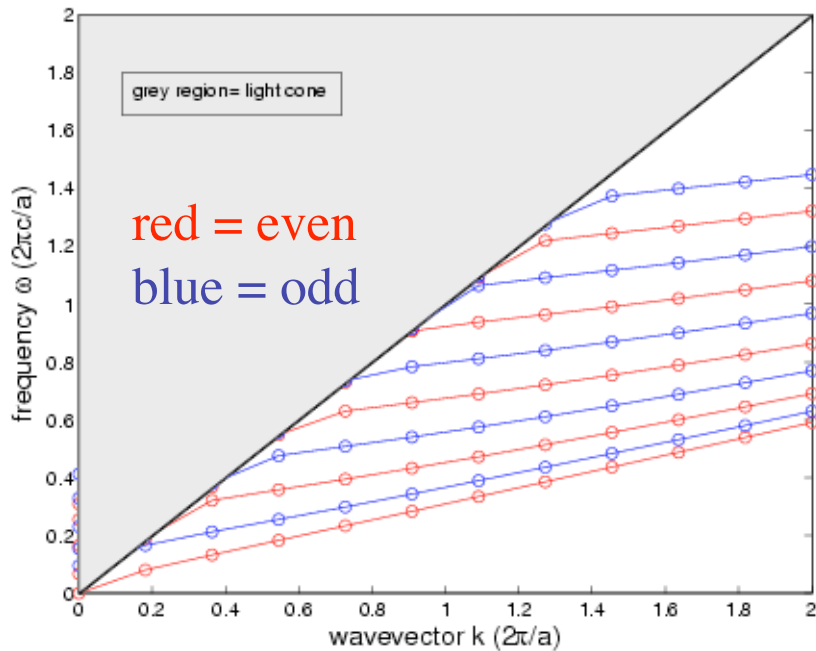


Simple Example (MPB) Results

$$\epsilon = 1$$



find the **normal modes** $\epsilon_n(k)$
of the waveguide:



Do try this at home

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`http://ab-initio.mit.edu/mpb/`

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