Computational Nanophotonics: Band diagrams and Eigenproblems

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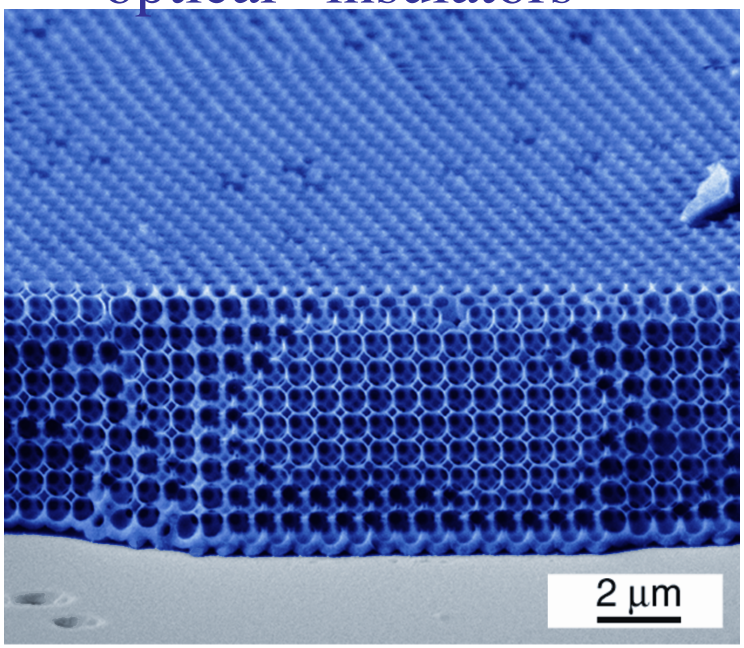
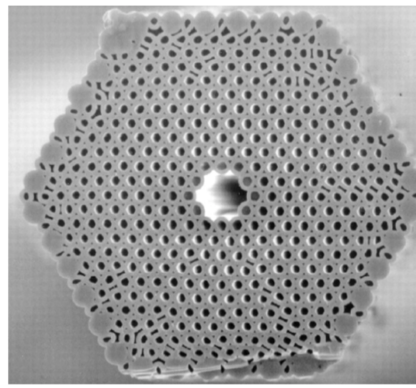
Nanophotonics:

classical electromagnetic effects can be greatly altered by λ-scale structures especially with *many* interacting scatterers

optical "insulators"

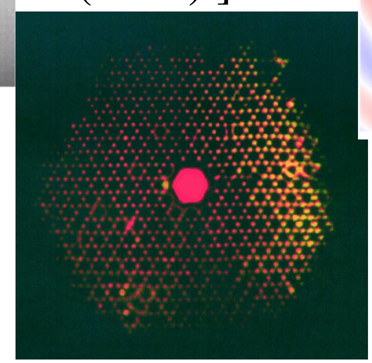


[D. Norris, UMN (2001)]

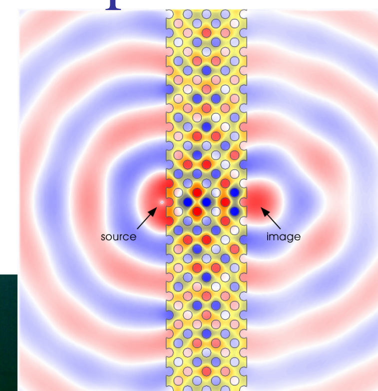


trapping/guiding light in vacuum

[R. F. Cregan (1999)]



flat "superlenses"



[Luo (2003)]

easy to study numerically (methods are "practically exact"), well-developed scalable 3d methods for arbitrary materials

Just solve this:
macroscopic Maxwell's equations

Faraday: $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$

Ampere: $\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$

(nonzero frequency)

Gauss: $\nabla \cdot \mathbf{D} = \rho$

$\nabla \cdot \mathbf{B} = 0$

constitutive equations (here, linear media):

$$\mathbf{D} = \varepsilon * \mathbf{E} \qquad \mathbf{B} = \mu * \mathbf{H}$$

magnetic permeability
…usually $\approx \mu_0$ at infrared/visible ($\lambda \sim \mu$m)

electric permittivity
$\varepsilon_r = \varepsilon / \varepsilon_0$ = relative permittivity or dielectric constant
= n^2 (square of refractive index if $\mu = \mu_0$)

ε, μ depend on frequency (dispersion), i.e. * = convolution
…negligible for transparent media in narrow bandwidth

$c^2 = 1 / \varepsilon_0 \mu_0$

theorists:
often $\varepsilon_0 = \mu_0 = 1$
and/or $\varepsilon_r = \varepsilon$

Limits of validity at the nanoscale?

- Continuum material models (ε etc.) have generally proved very successful down to ~ few nm feature sizes

  [For metal features at < 20nm scale, some predictions of small nonlocal effects (ballistic transport), but this is mostly neglected]

- Phenomena from resonant ~ nm features << λ (e.g. spontaneous emission) usually can be incorporated perturbatively / semiclassically

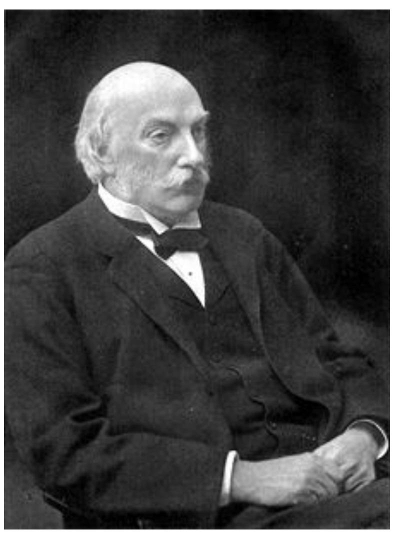
  (e.g. spontaneous emission ~ stochastic dipole source,
  spontaneous emission rate ~ local density of states
  ~ power radiated by dipole)

first, some perspective…

Development of Classical EM Computations

1 Analytical solutions

vacuum, single/double interfaces
various electrostatic problems, …



Lord Rayleigh

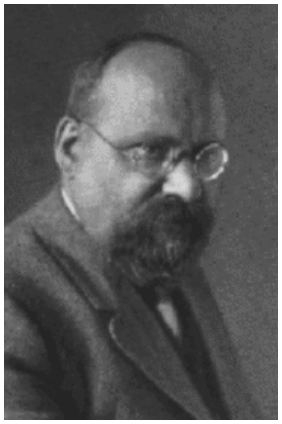
scattering from small particles,
periodic multilayers (Bragg mirrors), …

… & other problems with
very high symmetry
and/or separability
and/or small parameters

Development of Classical EM Computations

1 Analytical solutions

2 Semi-analytical solutions: series expansions



Gustav Mie (1908)

e.g. Mie scattering of light by a sphere

Also called *spectral methods:*

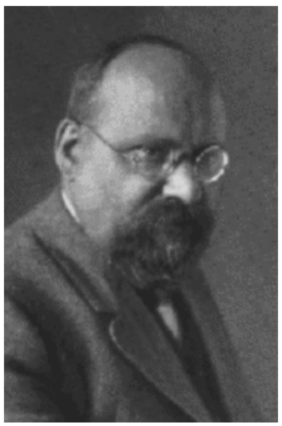
Expand solution in *rapidly converging Fourier-like basis*

- *spectral integral-equation methods:*
  exactly solve homogeneous regions (Green's func.),
  & match boundary conditions via spectral basis
  (e.g. Fourier series, spherical harmonics)
- *spectral PDE methods:*
  spectral basis for unknowns in inhomogeous space
  (e.g. Fourier series, Chebyshev polynomials, …)
  & plug into PDE and solve for coefficients

Development of Classical EM Computations

1. Analytical solutions

2. Semi-analytical solutions & spectral methods



Gustav Mie (1908)

Expand solution in *rapidly converging Fourier-like basis*

e.g. Mie scattering of light by a sphere

Strength: can converge *exponentially fast*

— fast enough for hand calculation

— analytical insights, asymptotics, …

Limitation: fast ("spectral") convergence requires basis to be redesigned for each geometry (to account for any discontinuities/singularities … complicated for complex geometries!)

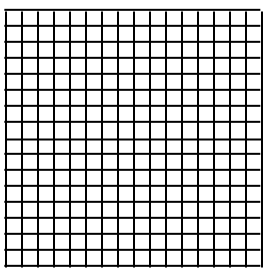
(*Or:* brute-force Fourier series, polynomial convergence)

Development of Classical EM Computations

1. Analytical solutions
2. Semi-analytical solutions & spectral methods
3. Brute force: generic grid/mesh (or generic spectral)

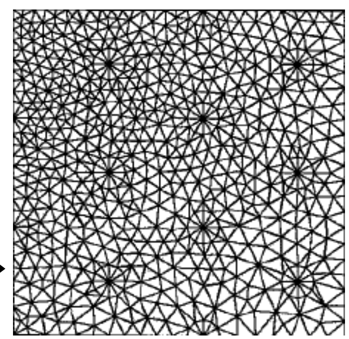
PDEs: discretize space into grid/mesh
— simple (low-degree polynomial) approximations in each pixel/element

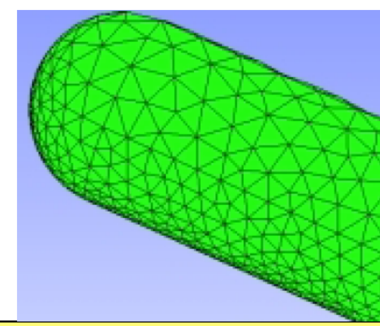
integral equations:
— boundary elements mesh surface unknowns coupled by Green's functions



←finite differences
(or Fourier series)

& finite elements→





lose orders of magnitude in performance … *but* re-usable code
€ computer time << €€€€ programmer time

Computational EM: Three Axes of Comparison

- What *problem* is solved?
  - — eigenproblems: harmonic modes ~ $e^{-i\omega t}$ ($\mathbf{J} = 0$)
  - — frequency-domain response: **E**, **H** from $\mathbf{J}(\mathbf{x})e^{-i\omega t}$
  - — time-domain response: **E**, **H** from $\mathbf{J}(\mathbf{x}, t)$
  - — PDE or integral equation?

- What *discretization*?

  infinitely many unknowns
  ⇒ finitely many unknowns

  - — finite differences (FD)
  - — finite elements (FEM) / boundary elements (BEM)
  - — spectral / Fourier
  - — …

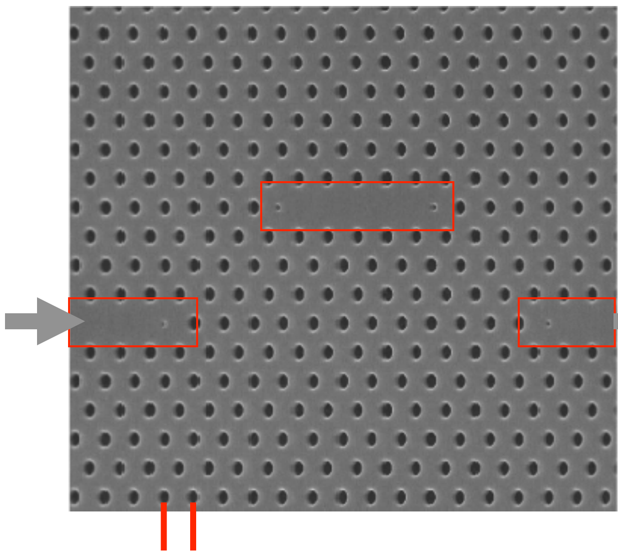
- What *solution method*?
  - — dense linear solvers (LAPACK)
  - — sparse-direct methods
  - — iterative methods

A few lessons of history

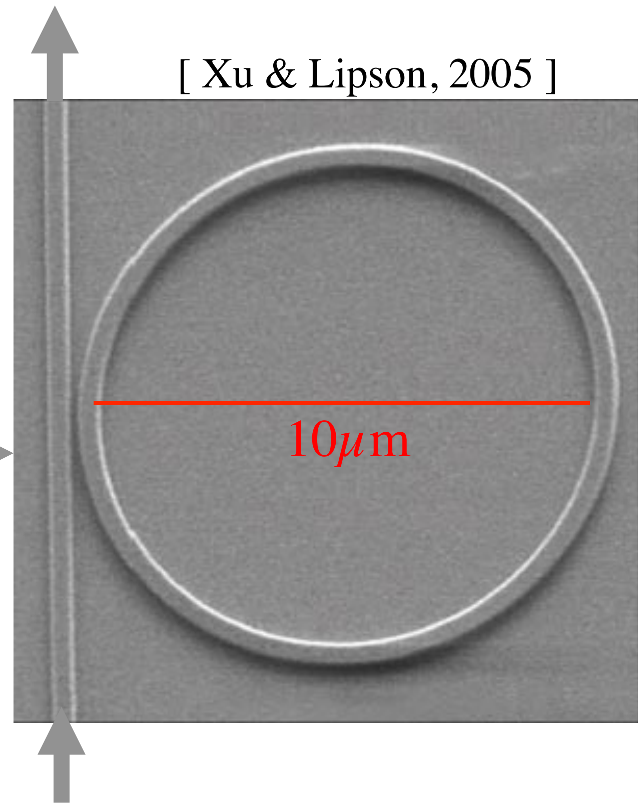
- All approaches still in widespread use
  - brute force methods in 90%+ of papers, typically the first resort to see what happens in a new geometry
  - geometry-specific spectral methods still popular, especially when particular geometry of special interest
  - analytical techniques used less to solve new geometries than to prove theorems, treat small perturbations, etc.
- No single numerical method has "won" in general
  - each has strengths and weaknesses, e.g. tradeoff between simplicity/generalizability and performance/scalability
  - very mature/standardized problems (e.g. capacitance extraction) use increasingly sophisticated methods (e.g. BEM), research fields (e.g. nanophotonics) tend to use simpler methods that are easier to modify (e.g. FDTD)

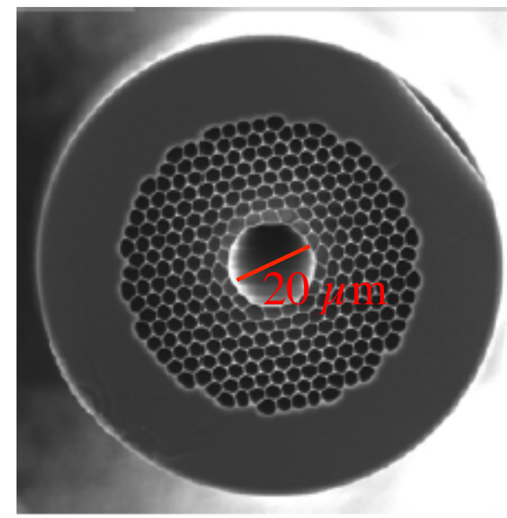
Understanding Photonic Devices

[Notomi *et al*. (2005).]



[Xu & Lipson, 2005]





[Mangan, *et al*., OFC 2004 PDP24]

Model the whole thing at once? Too hard to understand & **design**.

Break it up into pieces first: periodic regions, waveguides, cavities

Building Blocks: "Eigenfunctions"

- Want to know what solutions exist in different regions and how they can interact: look for time-harmonic modes $\sim e^{-i\omega t}$

$$\vec{\nabla} \times \vec{E} = -\cancelto{1}{\mu} \frac{\partial}{\partial t} \vec{H} \rightarrow i\omega \vec{H}$$

$$\vec{\nabla} \times \vec{H} = \varepsilon \frac{\partial}{\partial t} \vec{E} + \cancelto{0}{\vec{J}} \rightarrow -i\omega\varepsilon \vec{E}$$

First task:
get rid of this mess

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \vec{H} = \omega^2 \vec{H}$$

+ constraint

$$\nabla \cdot \vec{H} = 0$$

eigen-operator
(Hermitian for lossless/real e!)

eigen-value

"eigen-field"

Electronic & Photonic Eigenproblems

Electronic

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

nonlinear eigenproblem

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

(+ nasty quantum entanglement)

Photonic

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

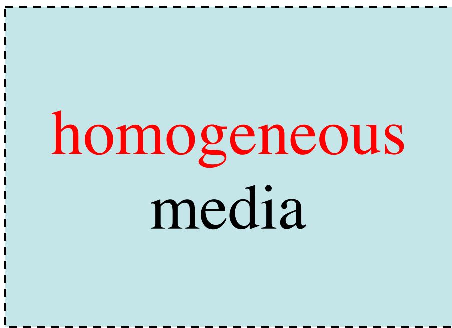
simple linear eigenproblem

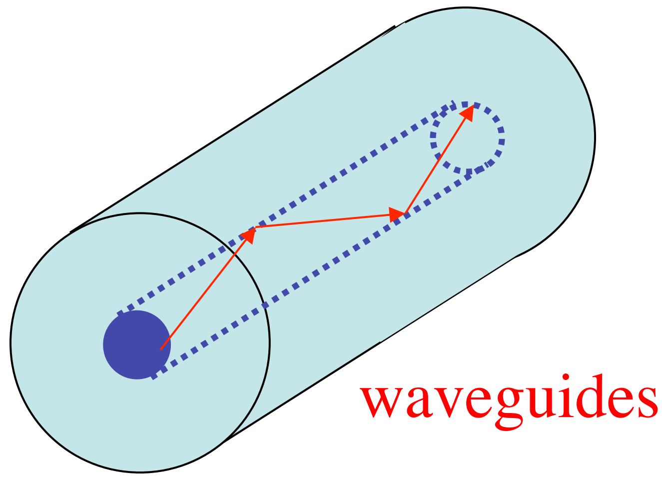
(for linear materials
with negligible dispersion)

— many well-known
computational techniques

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

Building Blocks: Periodic Media

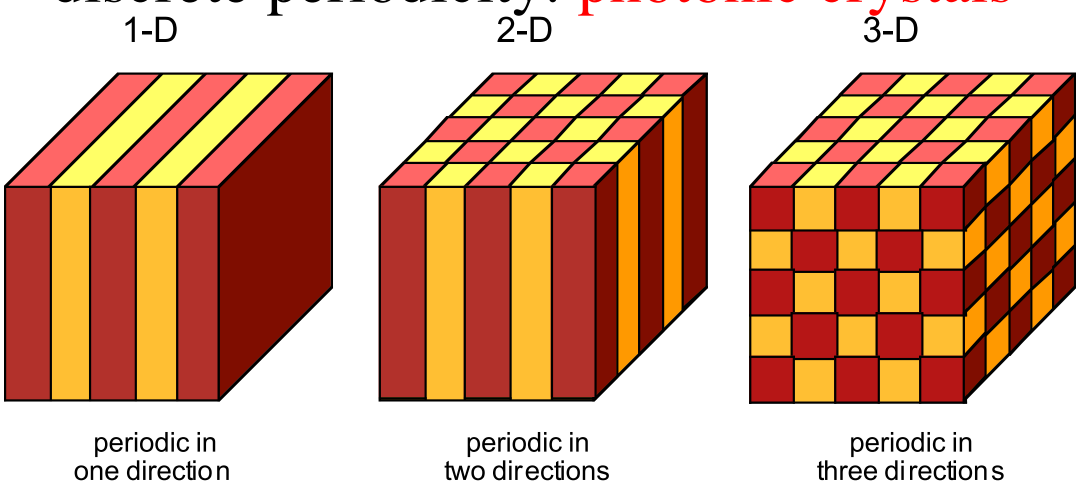




common thread:

translational symmetry

discrete periodicity: photonic crystals



Periodic Hermitian Eigenproblems

[G. Floquet, "Sur les équations différentielles linéaries à coefficients périodiques," *Ann. École Norm. Sup.* **12**, 47–88 (1883).]
[F. Bloch, "Über die quantenmechanik der electronen in kristallgittern," *Z. Physik* **52**, 555–600 (1928).]

if eigen-operator is periodic, then Bloch-Floquet solutions:

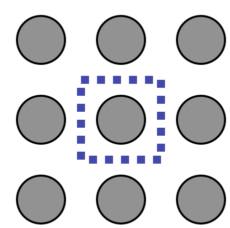
can choose: $$\vec{H}(\vec{x},t) = e^{i\left(\vec{k}\cdot\vec{x}-\omega t\right)}\vec{H}_{\vec{k}}(\vec{x})$$

planewave

periodic "envelope"

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

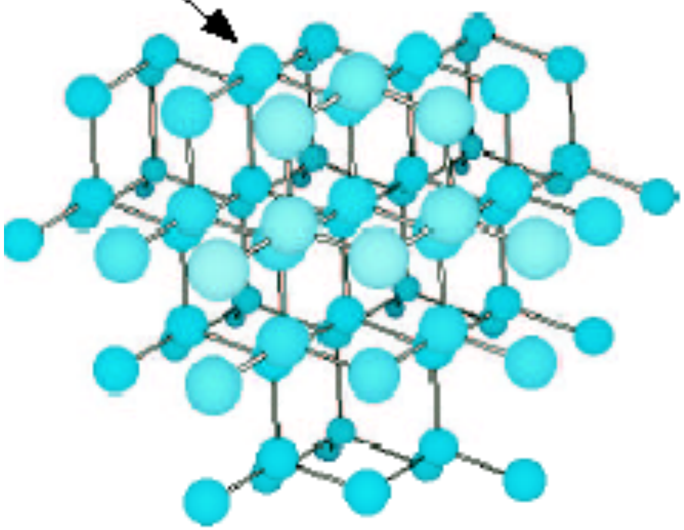
Corollary 2: $\vec{H}_{\vec{k}}$ given by finite unit cell, so w are discrete $\omega_n(\mathbf{k})$



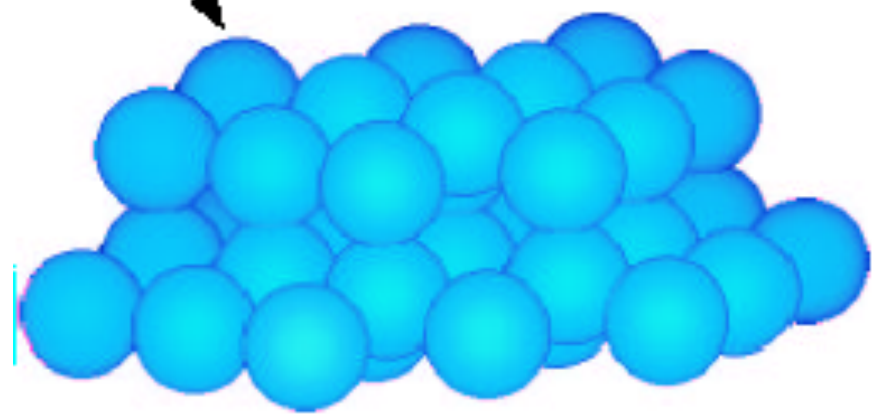
Electronic and Photonic Crystals

Periodic Medium

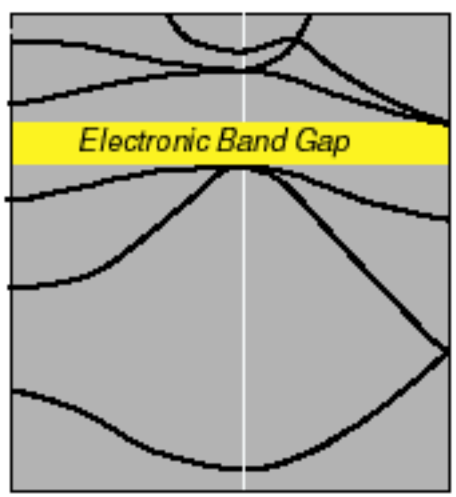
atoms in diamond structure

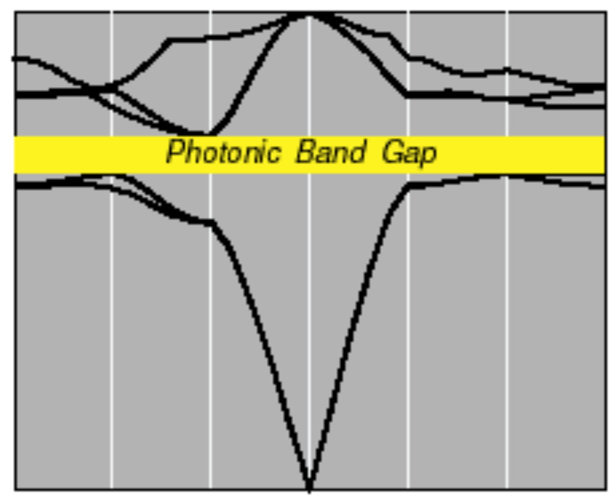


dielectric spheres, diamond lattice



Bloch waves: **Band Diagram**



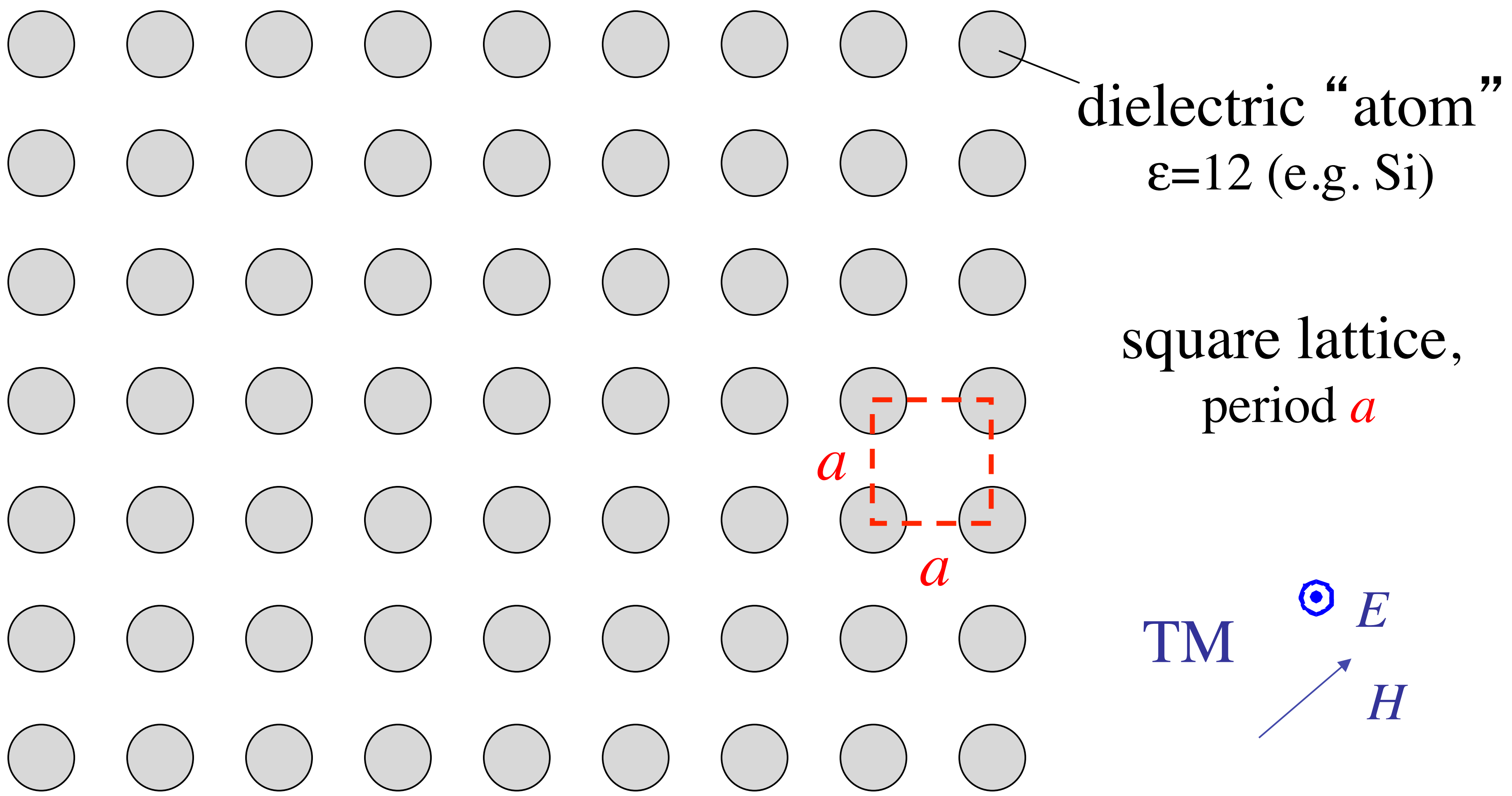


strongly interacting fermions

weakly-interacting bosons

… many design degrees of freedom

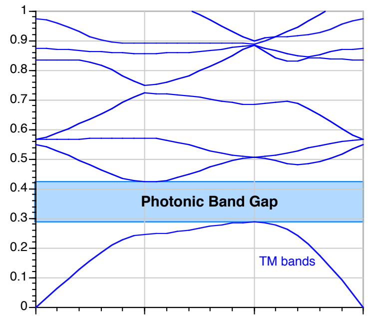
A 2d Model System



Solving the Maxwell Eigenproblem

Finite cell ➔ *discrete* eigenvalues ω_n

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



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

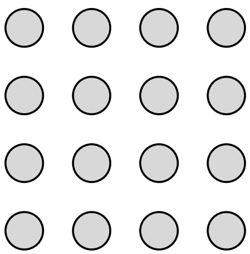
constraint: $(\nabla + i\mathbf{k}) \cdot \mathbf{H}_n = 0$

where field = $\mathbf{H}_n(\mathbf{x})\, e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$

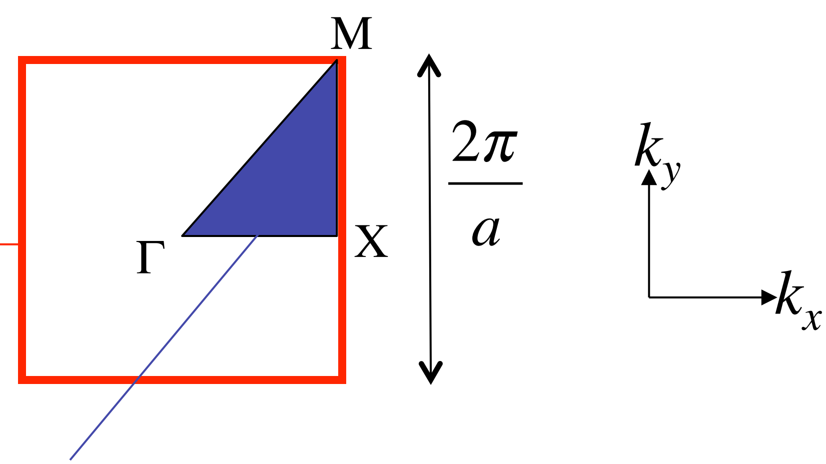
1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis
3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 1

1. Limit range of **k**: irreducible Brillouin zone



—Bloch's theorem: solutions are periodic in **k**



first Brillouin zone
= minimum |**k**| "primitive cell"

irreducible Brillouin zone: reduced by symmetry

2. Limit degrees of freedom: expand **H** in finite basis

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2a

1. Limit range of **k**: irreducible Brillouin zone

2. Limit degrees of freedom: expand **H** in finite basis (N)

$$|\mathbf{H}\rangle = \mathbf{H}(\mathbf{x}_t) = \sum_{m=1}^{N} h_m \mathbf{b}_m(\mathbf{x}_t)$$

solve: $\hat{A}|\mathbf{H}\rangle = \omega^2|\mathbf{H}\rangle$

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

inner product:

$$\langle \mathbf{f}|\mathbf{g}\rangle = \int \mathbf{f}^* \cdot \mathbf{g}$$

Galerkin method:

$$A_{m\ell} = \langle \mathbf{b}_m|\hat{A}|\mathbf{b}_\ell\rangle \quad B_{m\ell} = \langle \mathbf{b}_m|\mathbf{b}_\ell\rangle$$

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2b

1. Limit range of **k**: irreducible Brillouin zone

2. Limit degrees of freedom: expand **H** in finite basis

— must satisfy constraint: $(\nabla + i\mathbf{k}) \cdot \mathbf{H} = 0$

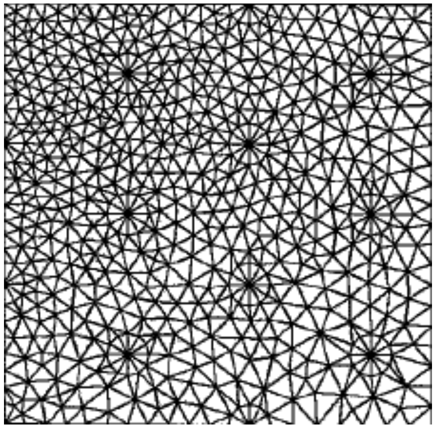
Planewave (FFT) basis

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

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 **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis
3. Efficiently solve eigenproblem: iterative methods

$$Ah = \omega^2 Bh$$

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, ~ $O(Np^2)$ time for p eigenvectors

(p smallest eigenvalues)

Solving the Maxwell Eigenproblem: 3b

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **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

Solving the Maxwell Eigenproblem: 3c

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **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:

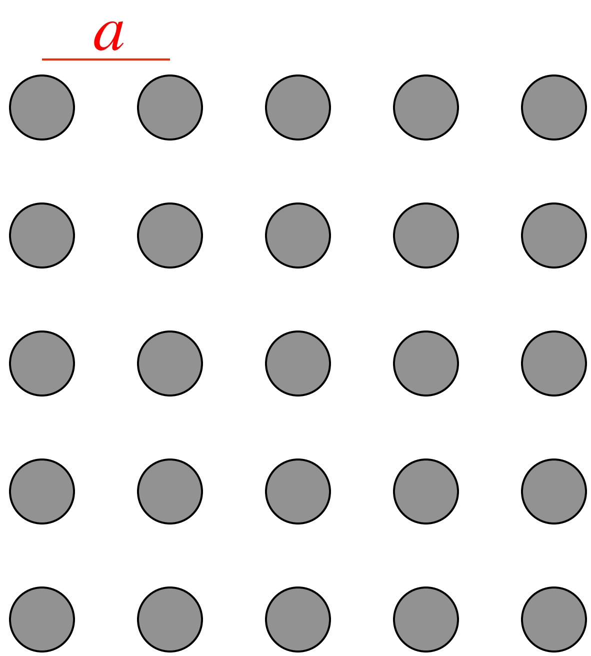
variational / min–max theorem

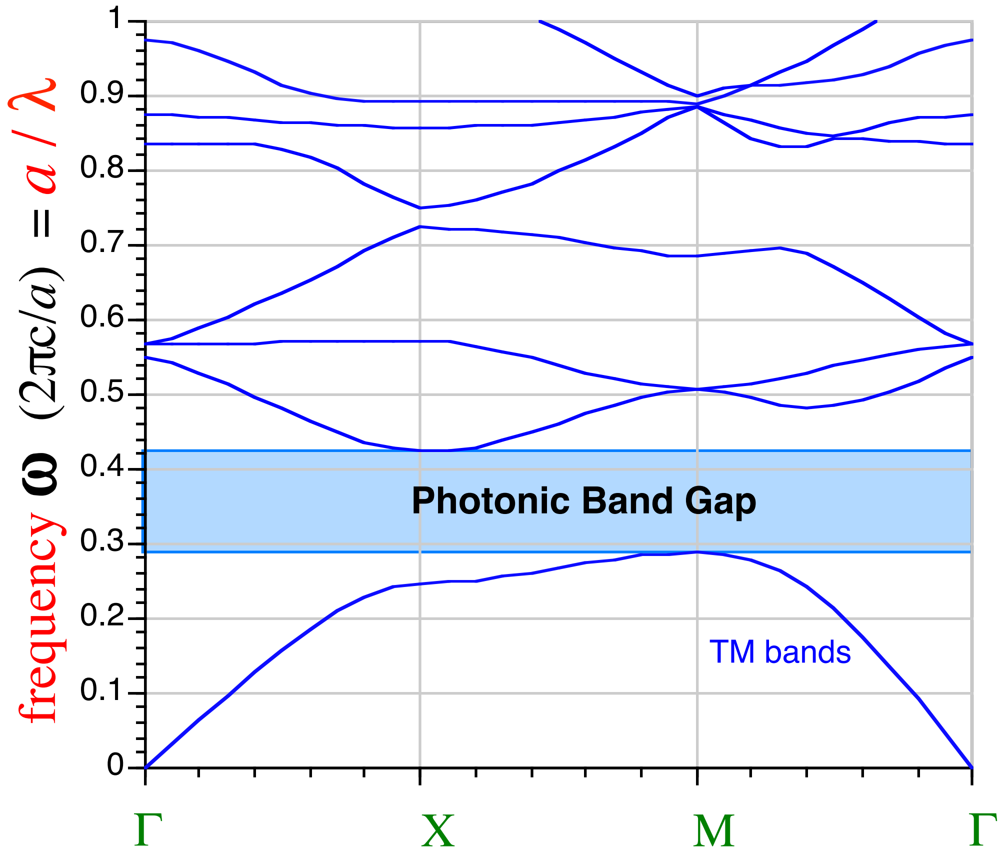
$$\omega_0^2 = \min_h \frac{h^* Ah}{h^* Bh}$$

minimize by preconditioned conjugate-gradient (or…)

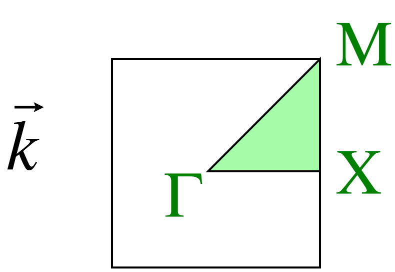
Band Diagram of 2d Model System

(radius 0.2a rods, ε=12)

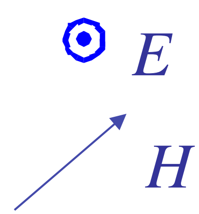




irreducible Brillouin zone



TM



gap for
$n > \sim 1.75:1$

The Iteration Scheme is *Important*

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

$$\omega_0^2 = \min_h \frac{h^* A h}{h^* B h} = f(h)$$

Steepest-descent: minimize ($h + \alpha \nabla f$) over α … repeat

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

— d is ∇f + (stuff): *conjugate* to previous search dirs

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

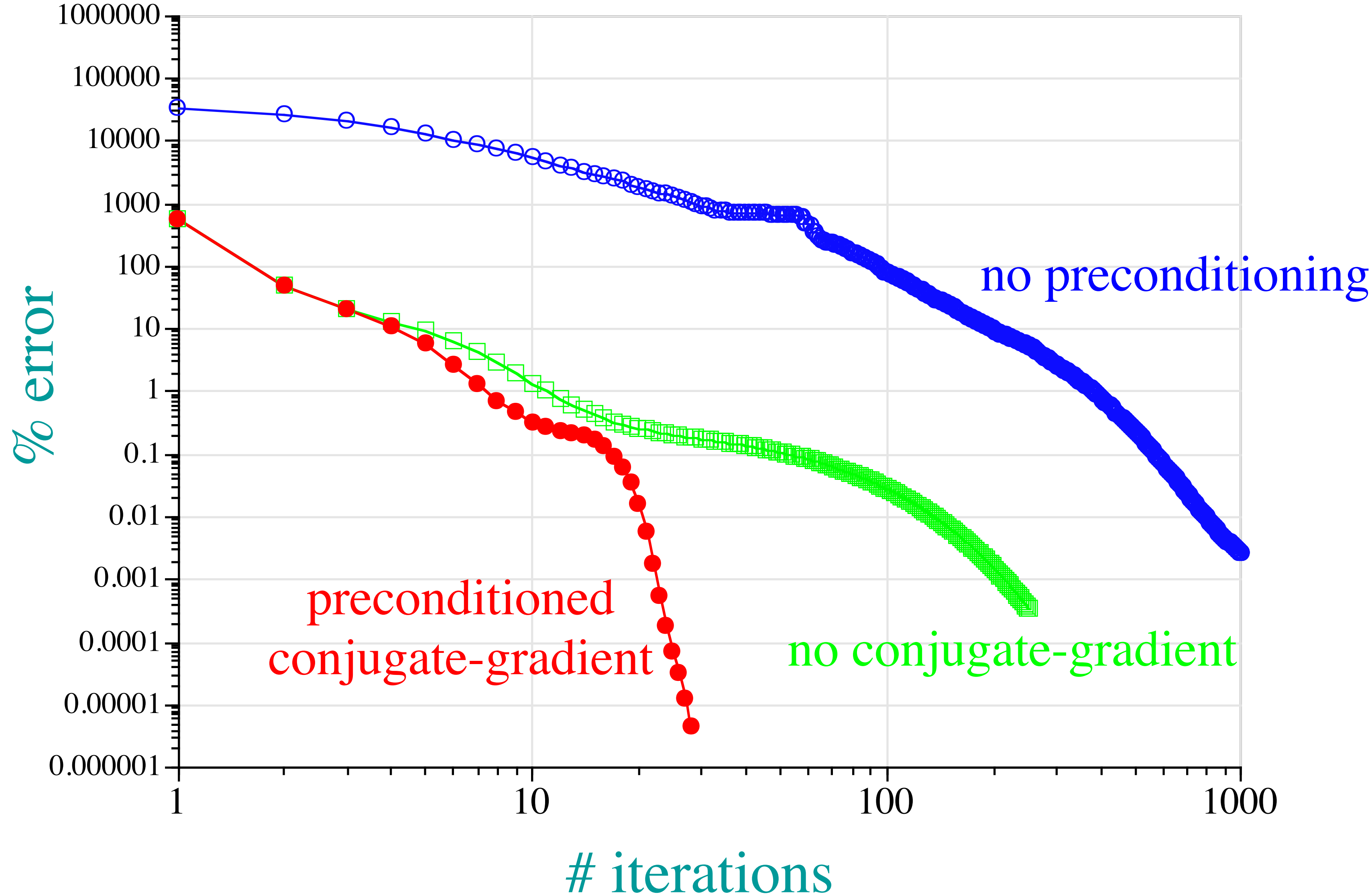
— d = (approximate A^{-1}) ∇f ~ Newton's method

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

— d is (approximate A^{-1}) [∇f + (stuff)]

The Iteration Scheme is *Important*

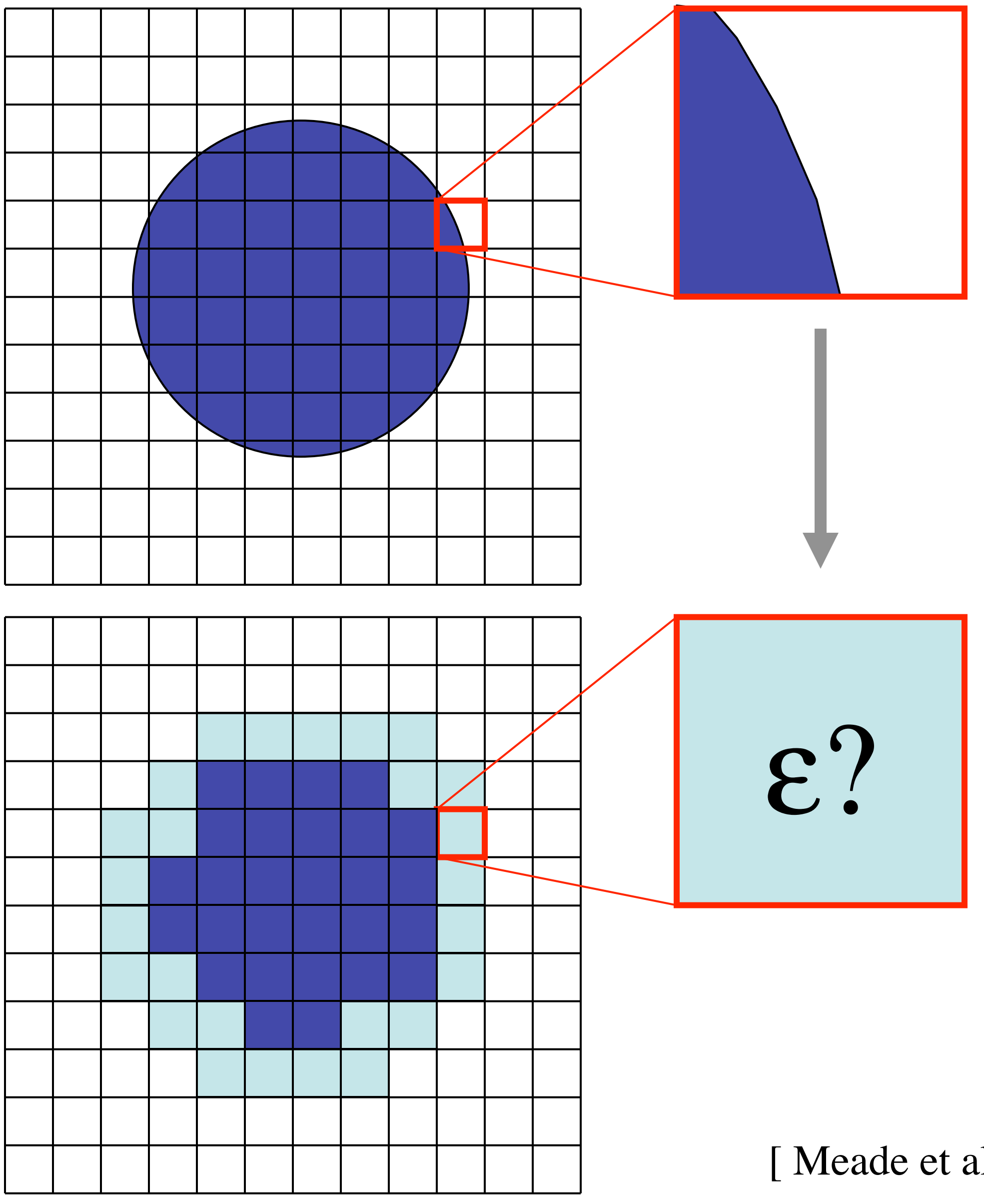
(minimizing function of ~40,000 variables)



Much more on iterative solvers: 18.335 at MIT

See also *Numerical Linear Algebra* (Trefethen & Bau), *Templates for the Solution of Linear Systems*, *Templates for the Solution of Algebraic Eigenproblems,* PETSc and SLEPc libraries, etc.

The Interfaces are Tricky



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

$\mathbf{E}_{\perp}$ is discontinuous

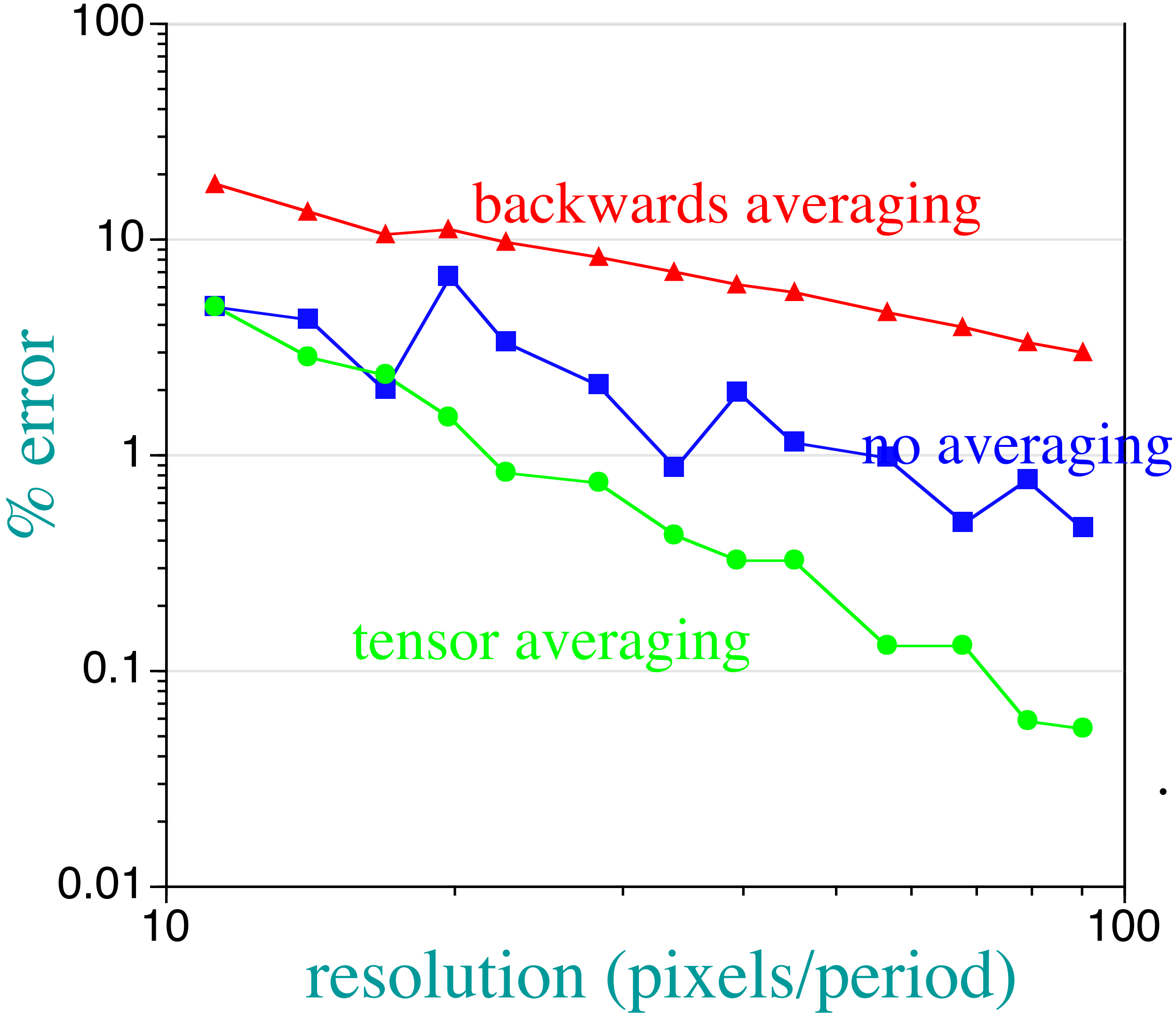
($\mathbf{D}_{\perp} = \varepsilon\mathbf{E}_{\perp}$ is continuous)

Use a tensor ε:

$$\begin{pmatrix} \langle\varepsilon\rangle & & \\ & \langle\varepsilon\rangle & \\ & & \langle\varepsilon^{-1}\rangle^{-1} \end{pmatrix} \begin{matrix} \mathbf{E}_{\parallel} \\ \\ \mathbf{E}_{\perp} \end{matrix}$$

[Meade et al. (1993)]

The ε-averaging is *Important*

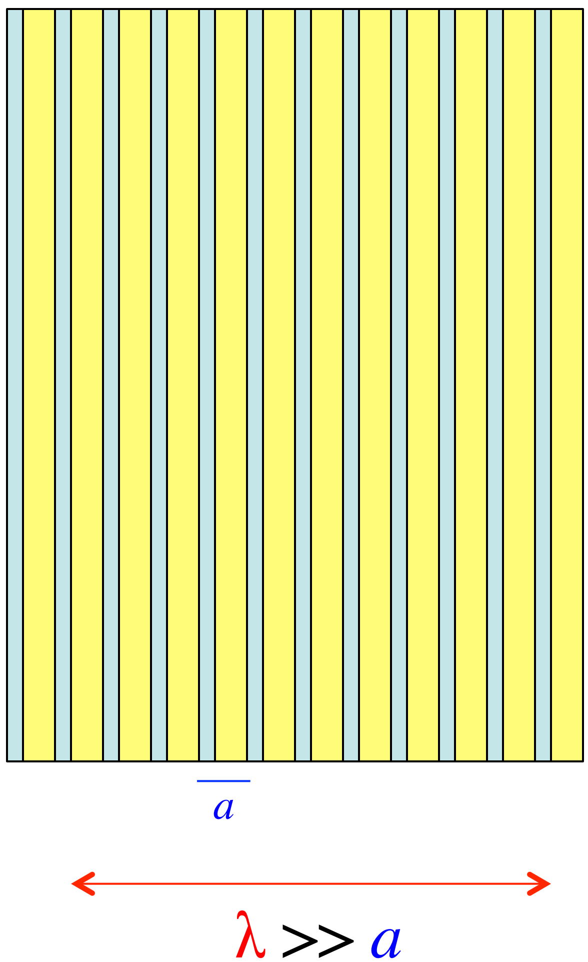


correct averaging changes *order* of convergence from Δx to Δx^2

reason in a nutshell:
averaging
= smoothing ε
= changing structure
… must pick smoothing with zero 1st-order perturbation

[Farjadpour et al. (2006)]

Closely related to anisotropic metamaterial, e.g. multilayer film in large-λ limit



$$\varepsilon_{ij}^{\text{eff}} = \frac{\langle D_i \rangle}{\langle E_j \rangle} = \frac{\langle \varepsilon E_i \rangle}{\langle E_j \rangle} = \frac{\langle D_i \rangle}{\langle \varepsilon^{-1} D_j \rangle}$$

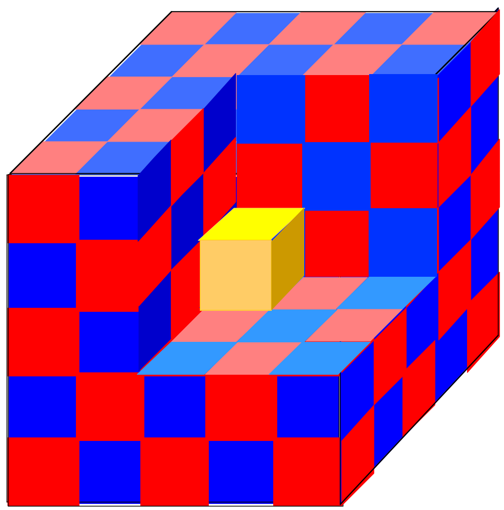
key to anisotropy is differing continuity conditions on **E**:

$E_{\|}$ continuous ⇒ $\varepsilon_{\|} = \langle\varepsilon\rangle$

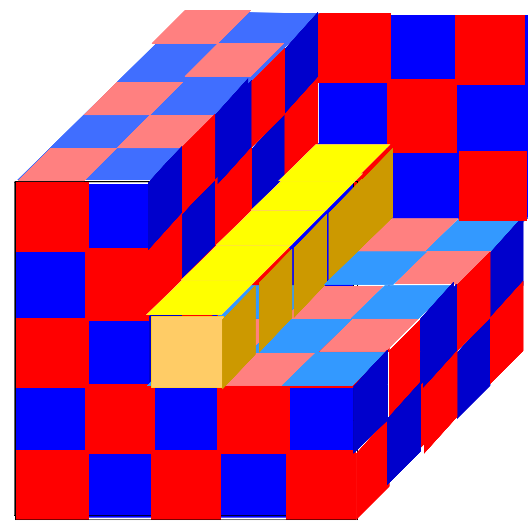
$D_{\perp} = \varepsilon E_{\perp}$ continuous ⇒ $\varepsilon_{\perp} = \langle\varepsilon^{-1}\rangle^{-1}$

Intentional "defects" are good

microcavities

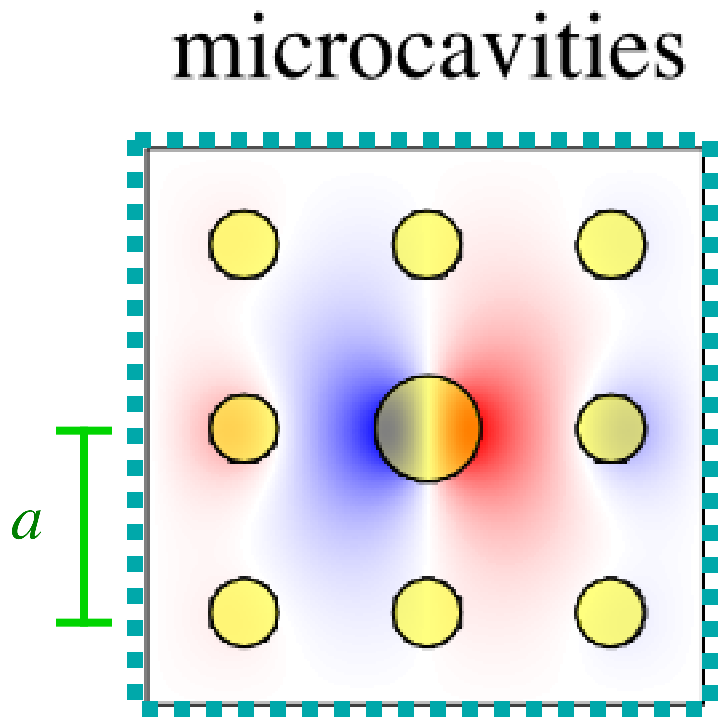


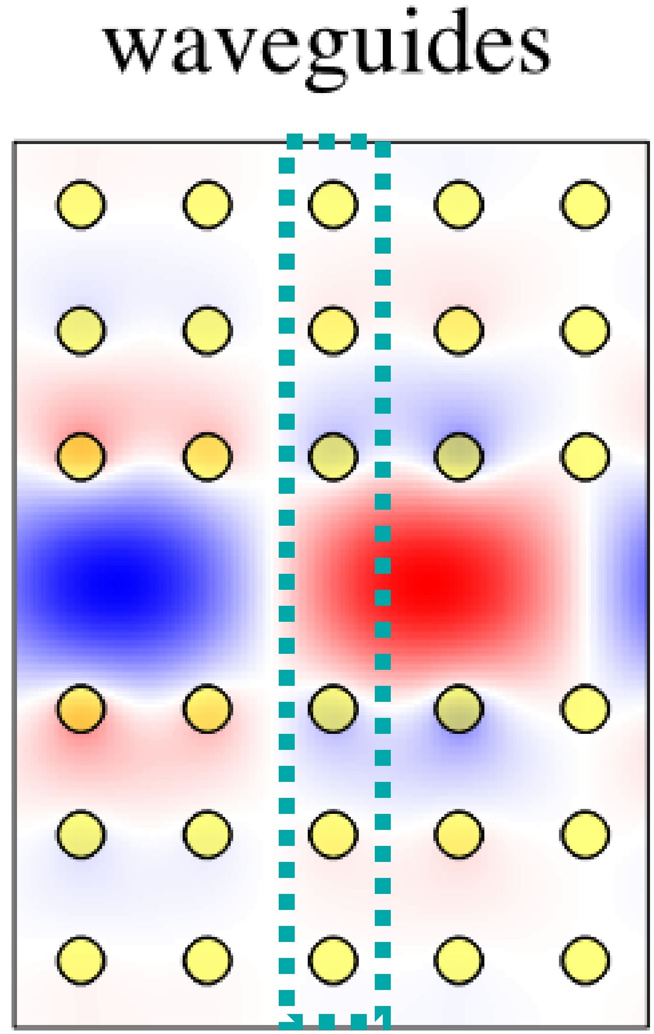
waveguides ("wires")



Intentional "defects" in 2d

(Same computation, with supercell = many primitive cells)





(boundary conditions ~ irrelevant
for exponentially localized modes)

Computational Nanophotonics: Cavities and Resonant Devices

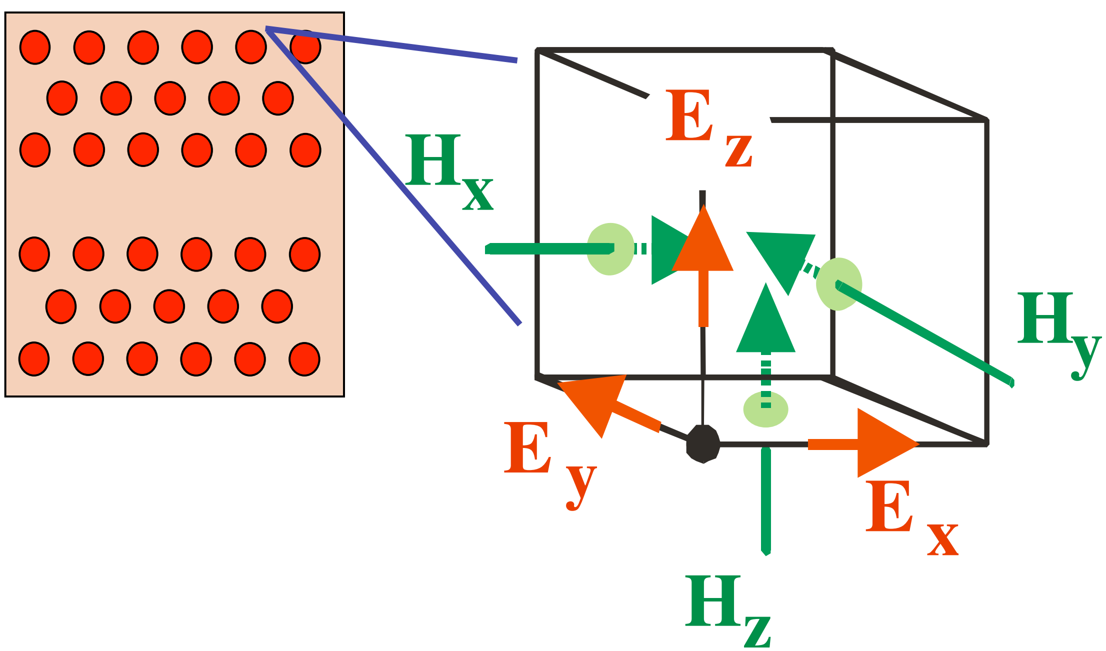
Steven G. Johnson
MIT Applied Mathematics

FDTD: finite difference time domain

Finite-difference-time-domain (FDTD) is a method to model Maxwell's equations on a **discrete time** & **space grid** using finite centered differences

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\mathbf{D} = \varepsilon \mathbf{E} \qquad \mathbf{B} = \mu \mathbf{H}$$



K.S. Yee 1966

A. Taflove & S.C. Hagness 2005

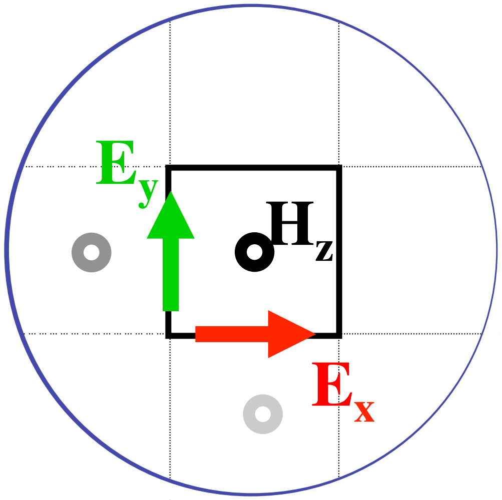
FDTD: Yee leapfrog algorithm

2d example:

1) at time t: Update D fields everywhere using spatial derivatives of H, then find $E=\varepsilon^{-1}D$

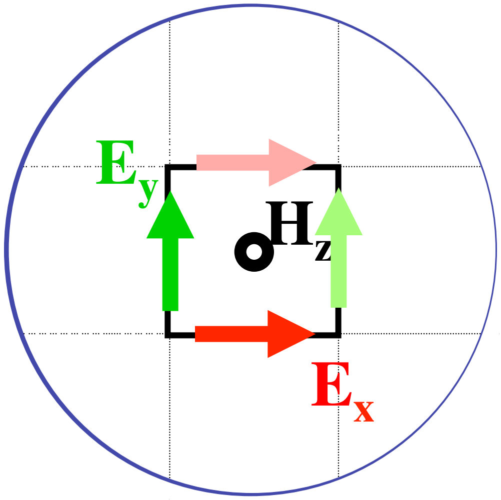
$$E_x \mathrel{+}= \frac{\Delta t}{\varepsilon\, \Delta y}\left(H_z^{\,j+0.5} - H_z^{\,j-0.5} \right)$$

$$E_y \mathrel{-}= \frac{\Delta t}{\varepsilon\, \Delta x}\left(H_z^{\,i+0.5} - H_z^{\,i-0.5} \right)$$



2) at time t+0.5: Update H fields everywhere using spatial derivatives of E

$$H_z \mathrel{+}= \frac{\Delta t}{\mu}\left(\frac{E_x^{\,j+1} - E_x^{\,j}}{\Delta y} + \frac{E_y^{\,i} - E_y^{\,i+1}}{\Delta x} \right)$$

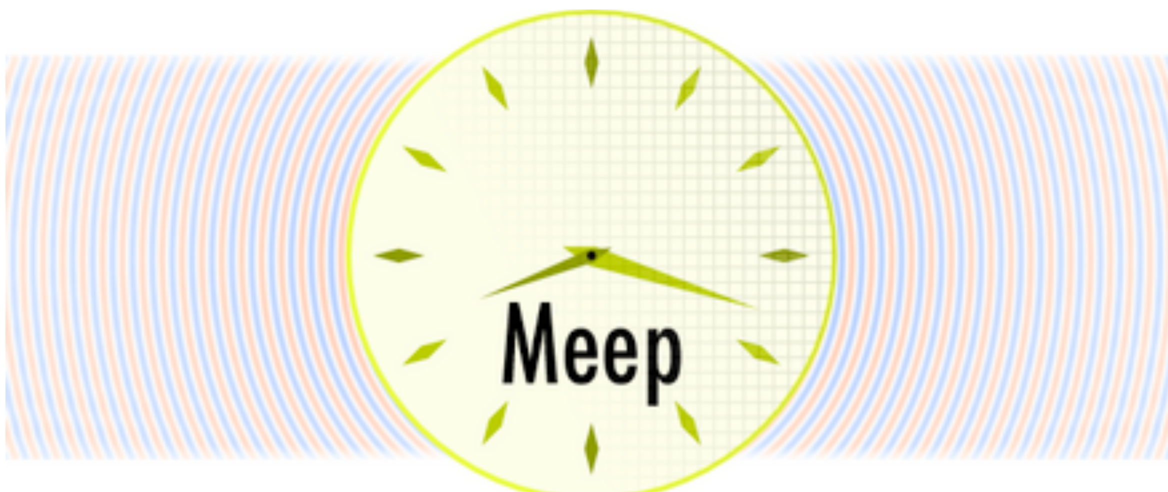


CFL/Von Neumann stability: $c\Delta t < 1 / \sqrt{\Delta x^{-2}+\Delta y^{-2}}$

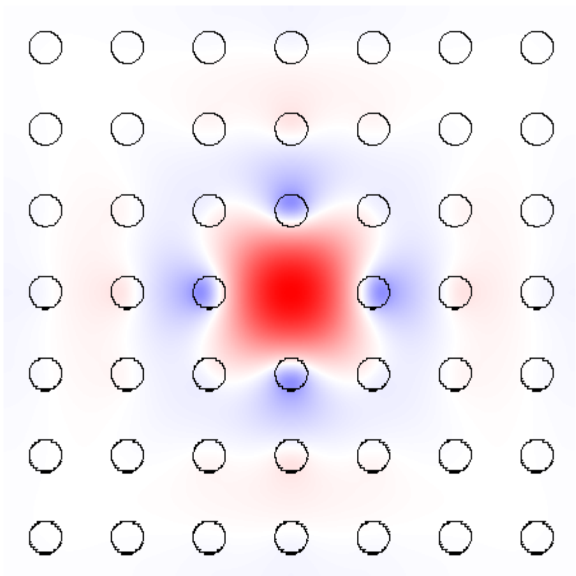
Free software: MEEP

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

- FDTD Maxwell solver: 1d/2d/3d/cylindrical
- Parallel, scriptable, integrated optimization, signal processing
- Arbitrary geometries, anisotropy, dispersion, nonlinearity
- Bloch-periodic boundaries, symmetry boundary conditions,
  + PML absorbing boundary layers…



Microcavity Blues



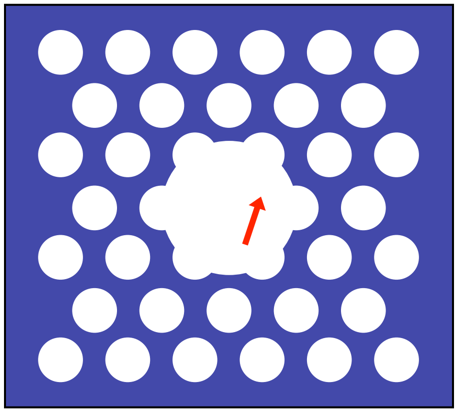
For cavities (*point defects*)
frequency-domain has its drawbacks:

• Best methods compute lowest-ω eigenvals,
but N^d supercells have N^d modes
below the cavity mode — *expensive*

• Best methods are for Hermitian operators,
but losses requires non-Hermitian

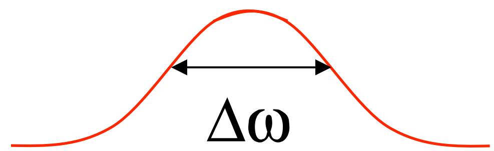
Time-Domain Eigensolvers

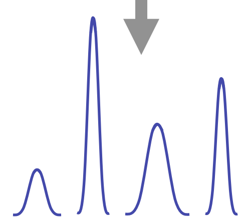
(finite-difference time-domain = FDTD)



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

tricky signal processing

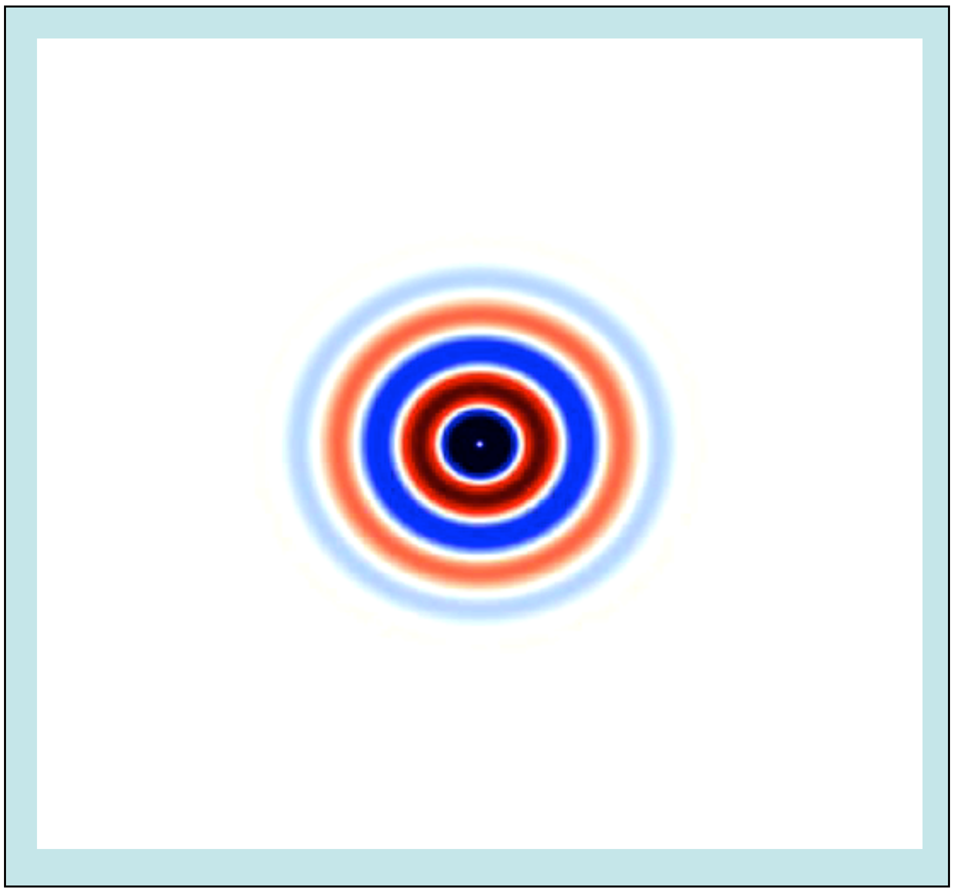
[Mandelshtam, *J. Chem. Phys.* **107**, 6756 (1997)]

complex ω_n

decay rate in time gives loss

Absorbing boundaries?

Finite-difference/finite-element volume discretizations need to artificially truncate space for a computer simulation.



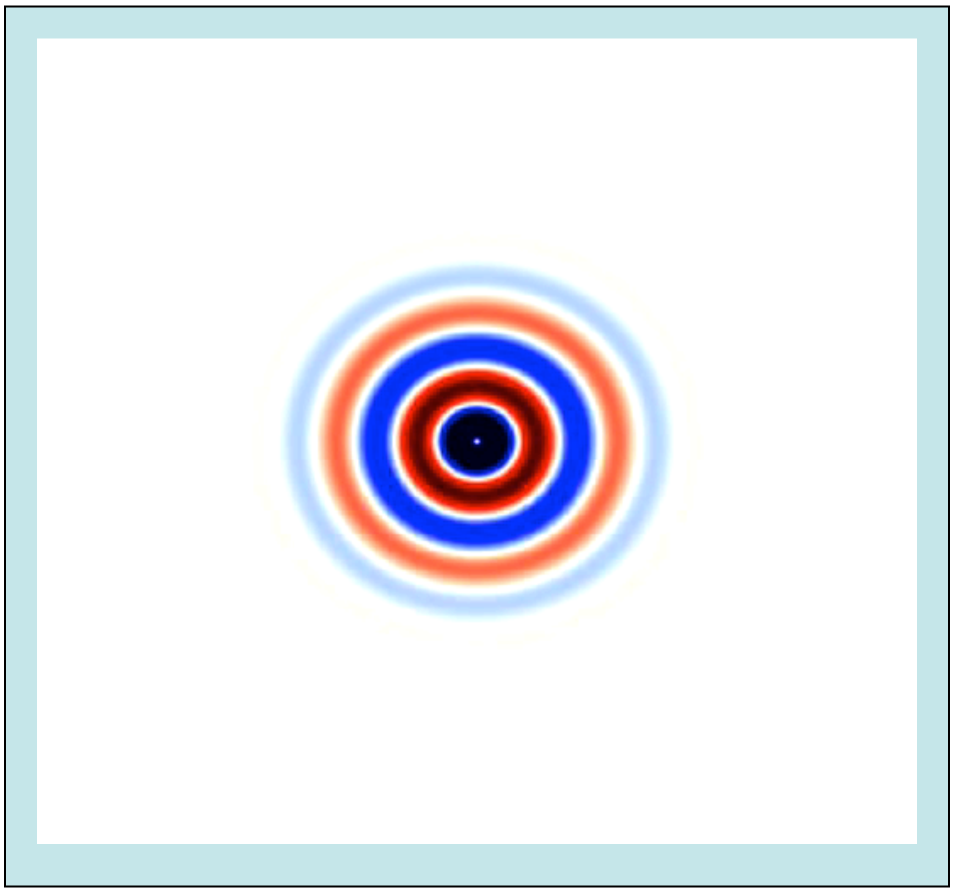
In a wave equation, a hard-wall truncation gives reflection artifacts.

An old goal: "absorbing boundary condition" (ABC) that absorbs outgoing waves.

Problem: good ABCs are hard to find in > 1d.

Perfectly Matched Layers (PMLs)

Bérenger, 1994: design an *artificial* absorbing layer that is analytically reflectionless



Works *remarkably well*.

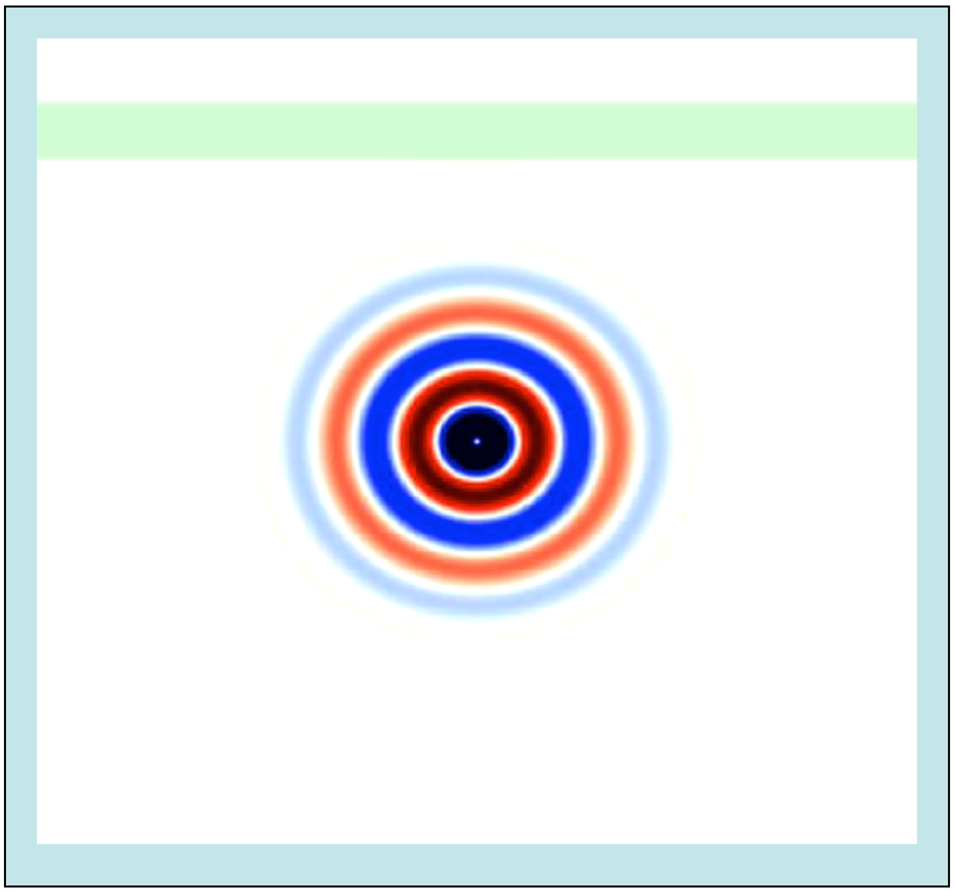
Now ubiquitous in FD/FEM wave-equation solvers.

Several derivations, cleanest & most general via "complex coordinate stretching"

[Chew & Weedon (1994)]

Perfectly Matched Layers (PMLs)

Bérenger, 1994: design an *artificial* absorbing layer that is analytically reflectionless



Even works in inhomogeneous media (e.g. waveguides).

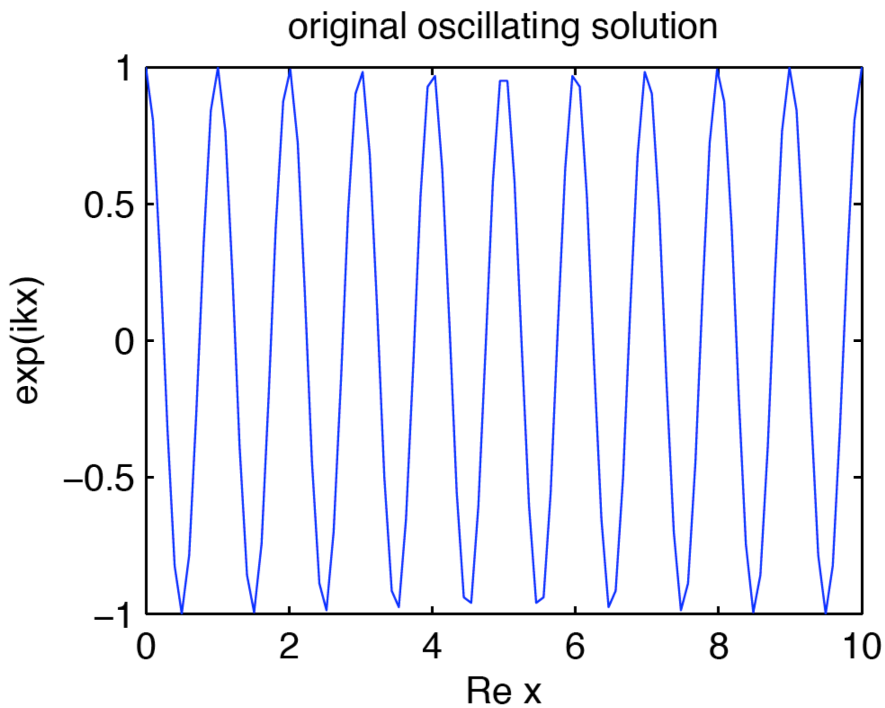
PML Starting point: propagating wave

- Say we want to absorb wave traveling in $+x$ direction in an x-invariant medium at a frequency $\omega>0$.

$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)}$$

$(usually, k > 0)$

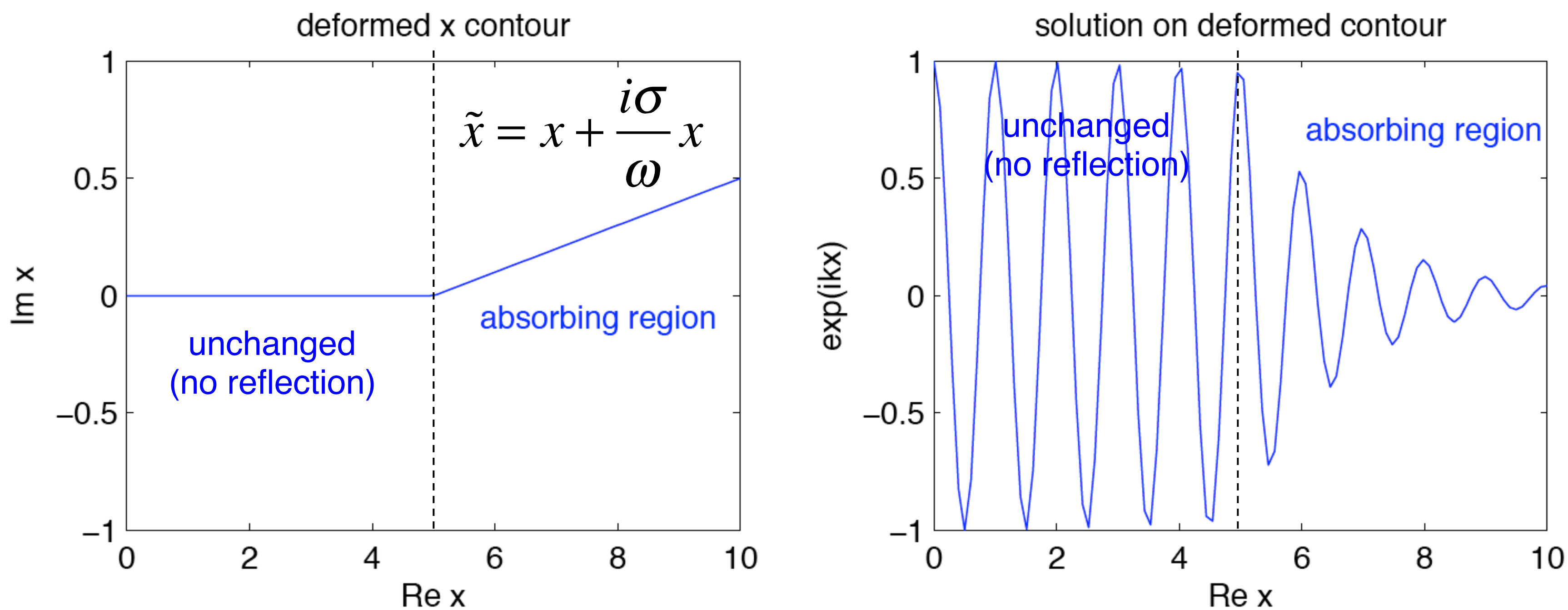
[rare "backward-wave" cases defeat PML (Loh, 2009)]



(only x in wave equation is via $\partial / \partial x$ terms.)

PML step 1: Analytically continue

Electromagnetic fields & equations are *analytic* in x,
so we can evaluate at complex x & still solve same equations



$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \rightarrow f(y,z)e^{i(kx-\omega t)-\frac{k}{\omega}\sigma x}$$

PML step 2: Coordinate transformation

Weird to solve equations for complex coordinates $\tilde{x}$,
so do coordinate transformation back to real x.

$$\tilde{x}(x) = x + \int^{x} \frac{i\sigma(x')}{\omega} dx'$$

(allow x-dependent PML strength σ)

$$\frac{\partial}{\partial x} \overset{①}{\rightarrow} \frac{\partial}{\partial \tilde{x}} \overset{②}{\rightarrow} \left[\frac{1}{1 + \frac{i\sigma(x)}{\omega}} \right] \frac{\partial}{\partial x}$$

$$\text{fields} \sim f(y,z) e^{i(kx - \omega t)} \rightarrow f(y,z) e^{i(kx - \omega t) - \frac{k}{\omega} \int^{x} \sigma(x') dx'}$$

nondispersive materials: $k/\omega \sim$ constant
so decay rate independent of ω
(at a given incidence angle)

PML Step 3: Effective materials

In Maxwell's equations, $\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E} + \mathbf{J}$,
coordinate transformations are *equivalent* to transformed *materials*
(Ward & Pendry, 1996: "transformational optics")

$$\{\varepsilon, \mu\} \to \frac{J\{\varepsilon, \mu\}J^T}{\det J}$$

x PML Jacobian

$$J = \begin{pmatrix} (1 + i\sigma/\omega)^{-1} & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$\left(\frac{\partial x}{\partial \tilde{x}}\right)$$

for isotropic starting materials:

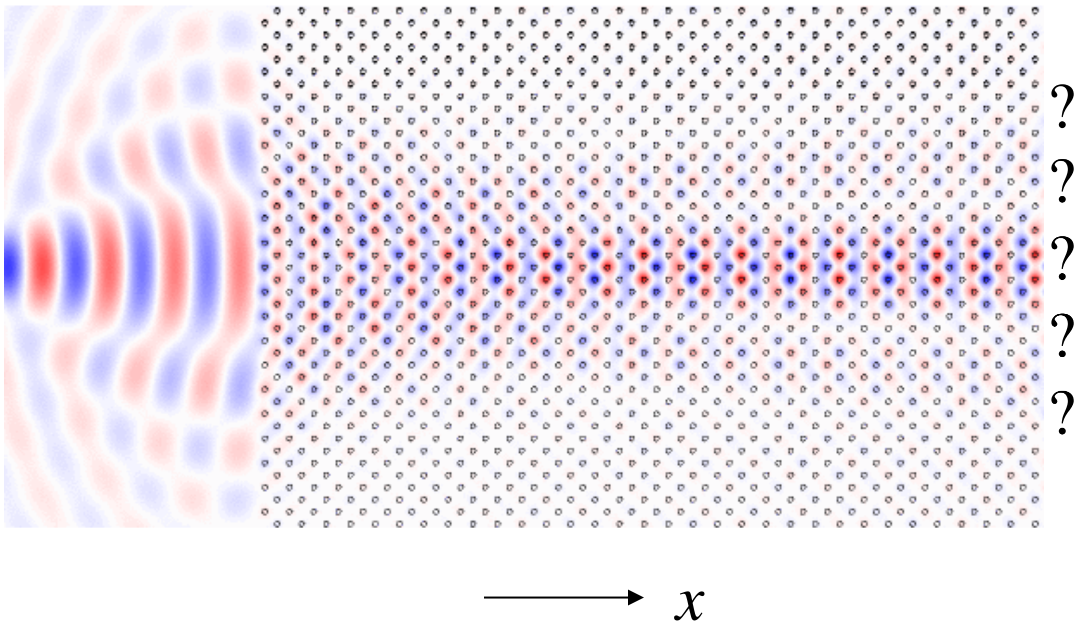
effective *conductivity*

$$\{\varepsilon, \mu\} \to \{\varepsilon, \mu\} \begin{pmatrix} (1 + i\sigma/\omega)^{-1} & & \\ & 1 + i\sigma/\omega & \\ & & 1 + i\sigma/\omega \end{pmatrix}$$

PML = effective anisotropic "absorbing" ε, μ

Photonic-crystal PML?

FDTD (Meep) simulation:

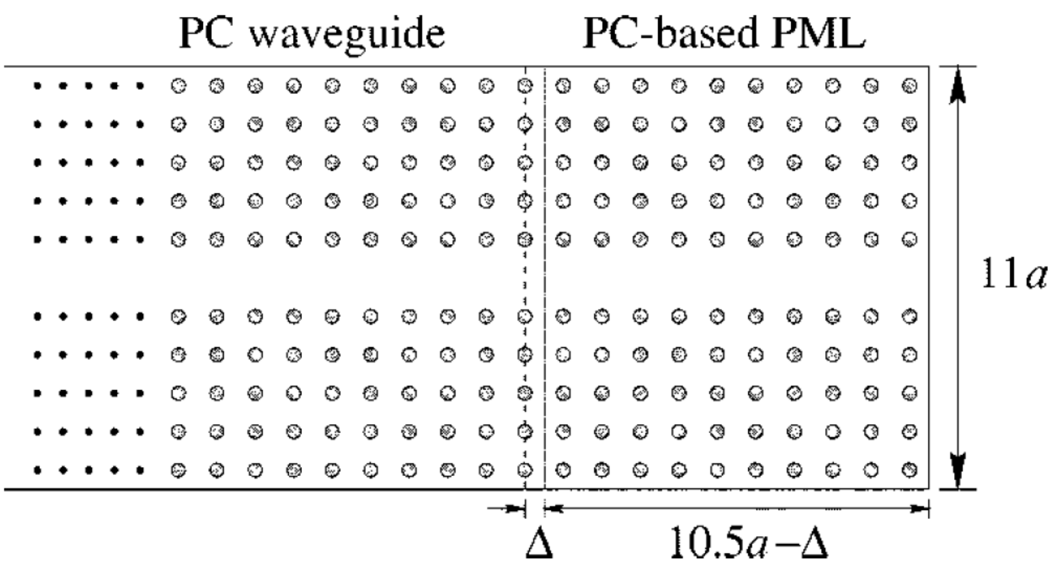


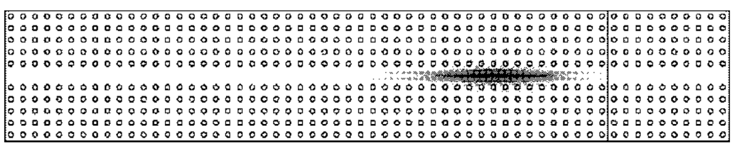
ε not even *continuous*
in x direction,
much less analytic!

Analytic continuation of Maxwell's equations is hopeless
— no reason to think that PML technique should work

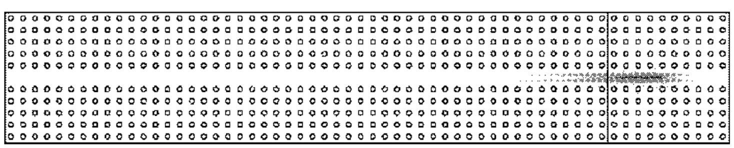
Photonic-crystal PMLs: Magic?

[Koshiba, Tsuji, & Sasaki (2001)]

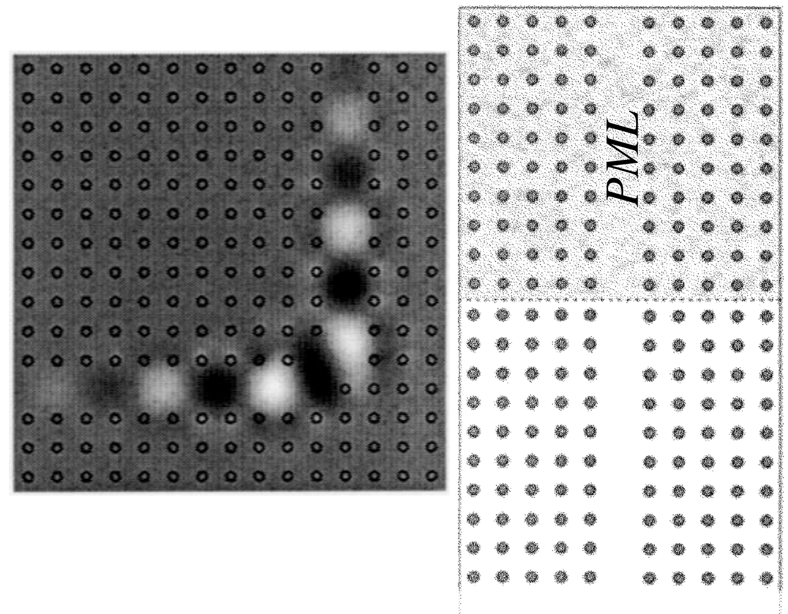




(b)



[Kosmidou *et al* (2003)]



… & several other authors …

Low reflections claimed

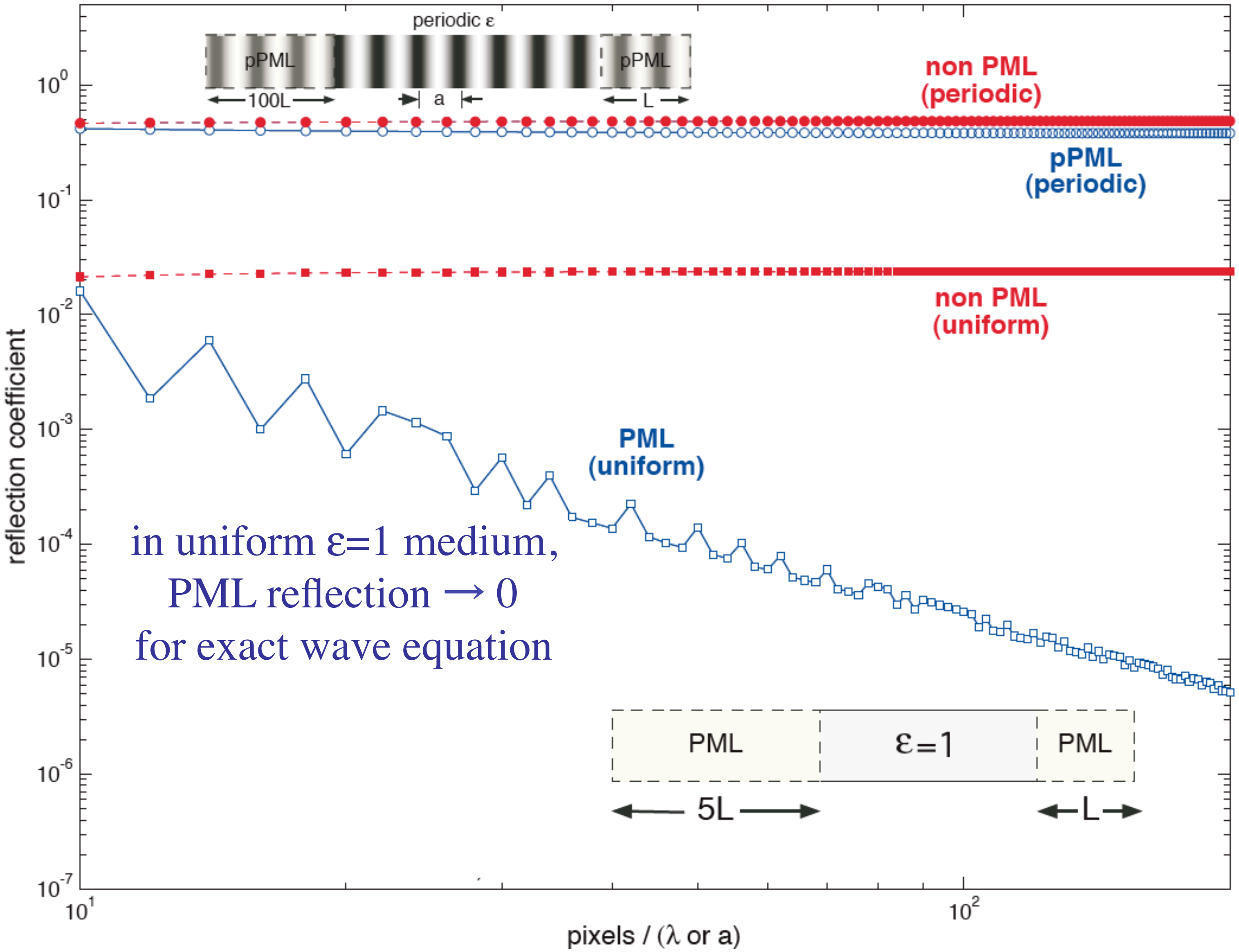
— is PML working?

Something suspicious:

very thick absorbers.

Failure of Photonic-crystal "pseudo-PML"

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]



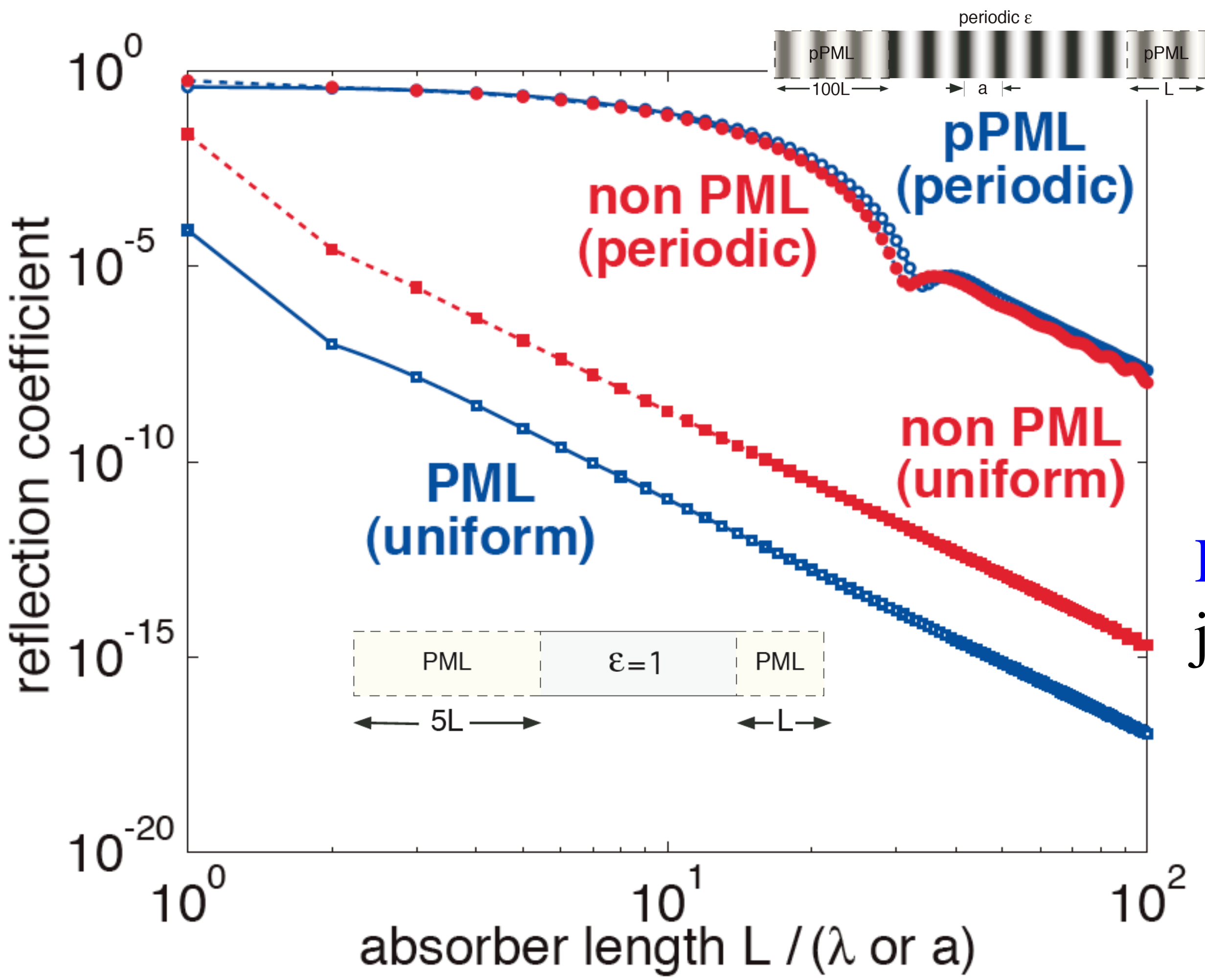
1d test case:

(pseudo-) PML in periodic ε reflection doesn't → 0 as Δx → 0

… similar to non-PML scalar σ

Redemption of the pseudo-PML: *slow ("adiabatic") absorption turn-on*

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]



Any absorber, turned on gradually enough, will have reflections → 0!

PML (when it works) just helps coefficient.

Back to absorption tapers

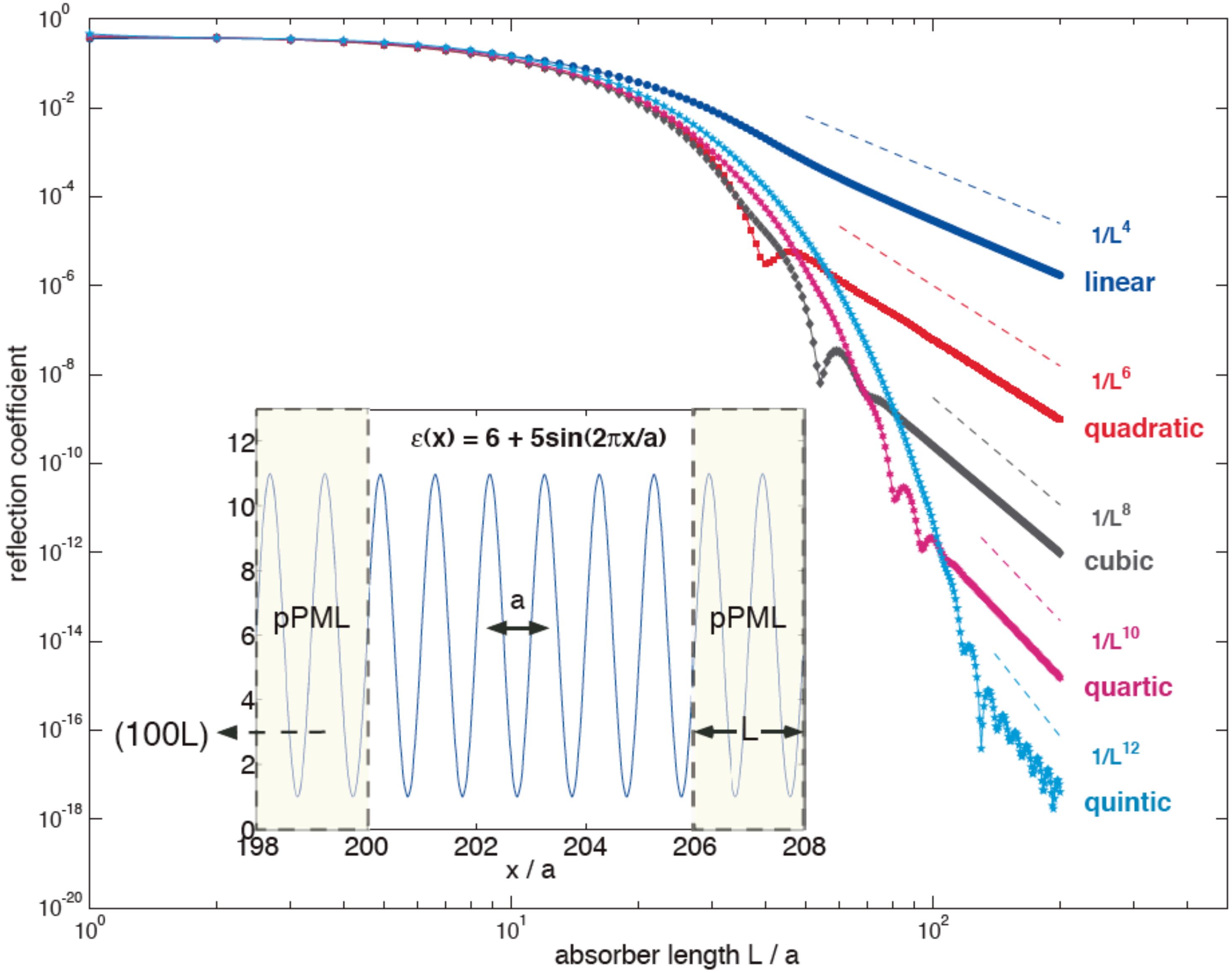
- Suppose absorption is: $\sigma(x) = \sigma_0\, s(x/L)$, say $s(u) = u^d$
- Fix the round-trip reflection: $R_{\text{round-trip}} = e^{-\#\, L\sigma_0 \int_0^1 s(u)\,du} \Rightarrow \sigma_0 \sim \frac{1}{L}$

$\Rightarrow \ldots \Rightarrow$ transition reflections $\sim O(L^{-2d-2})$

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]

Reflection vs. Absorber Thickness

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]



$s = u^1$

$s = u^2$

$s = u^3$

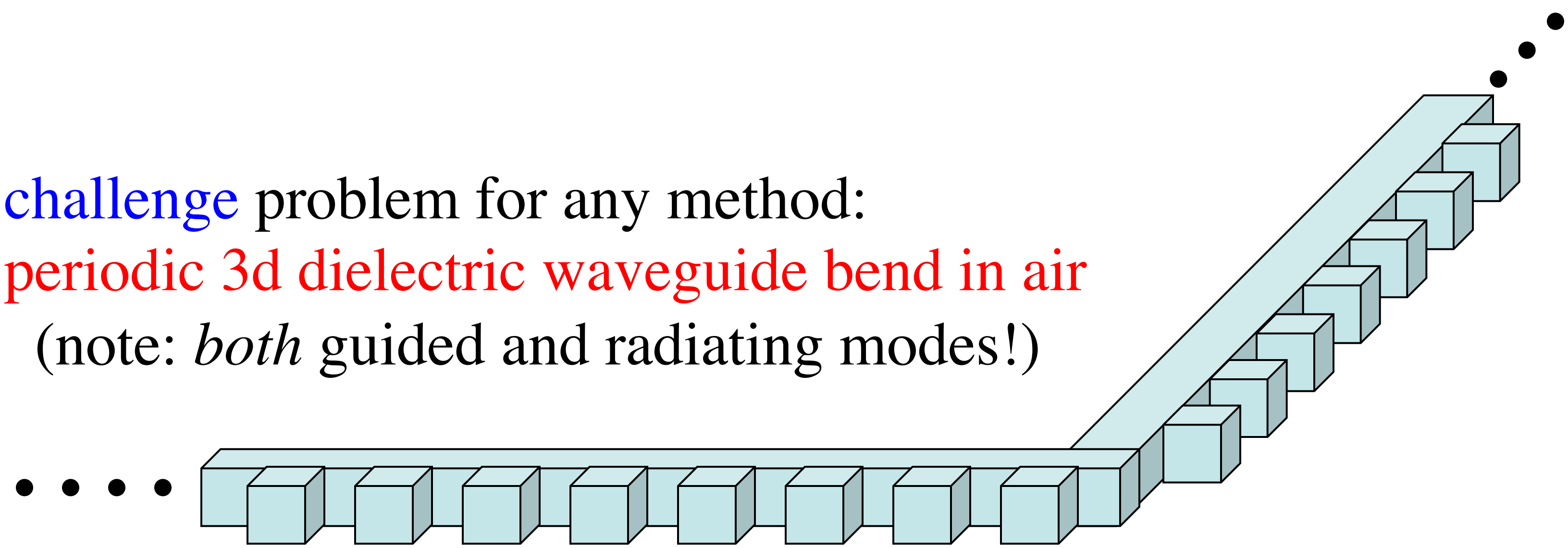
$s = u^4$

$s = u^5$

What about DtN / RCWA / Bloch-mode-expansion / SIE methods?

— useful, nice methods that can impose outgoing boundary conditions exactly, once the Green's function / Bloch modes computed

challenge problem for any method:
periodic 3d dielectric waveguide bend in air
(note: *both* guided and radiating modes!)

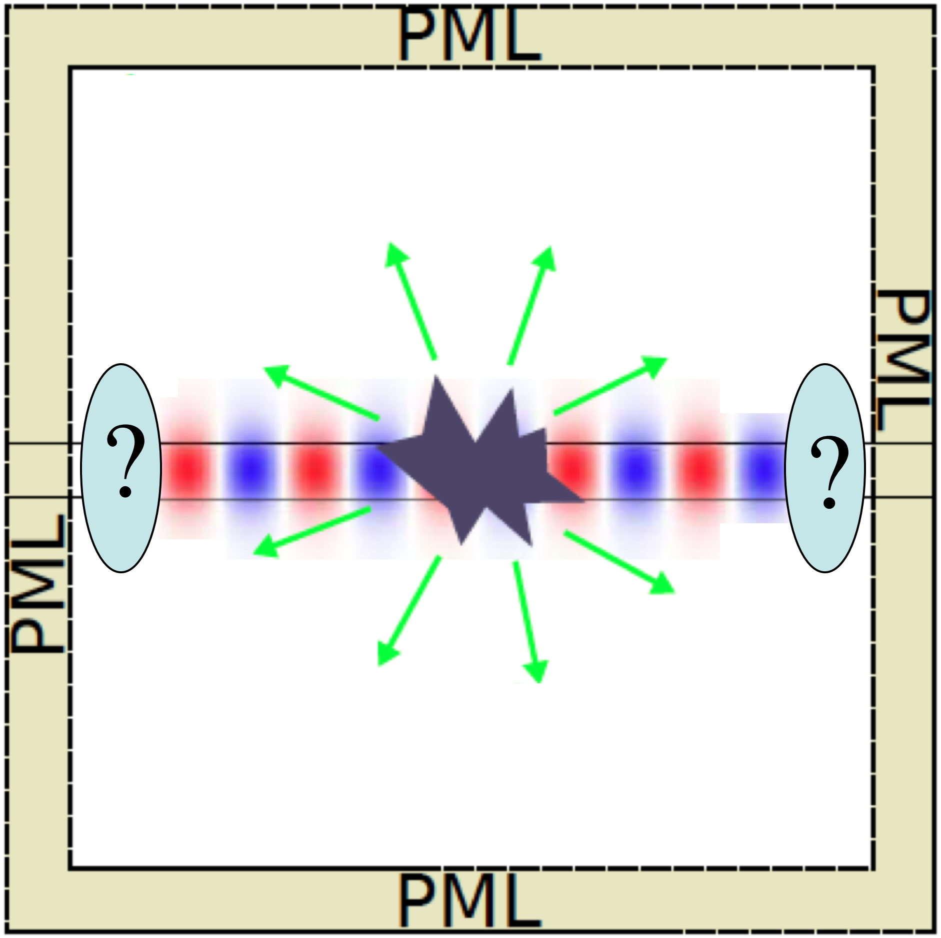


… DtN / Green's function / Bloch modes (incl. radiation!) expensive

Computational Nanophotonics: Sources & Integral Equations

Steven G. Johnson
MIT Applied Mathematics

How can we excite a desired incident wave?



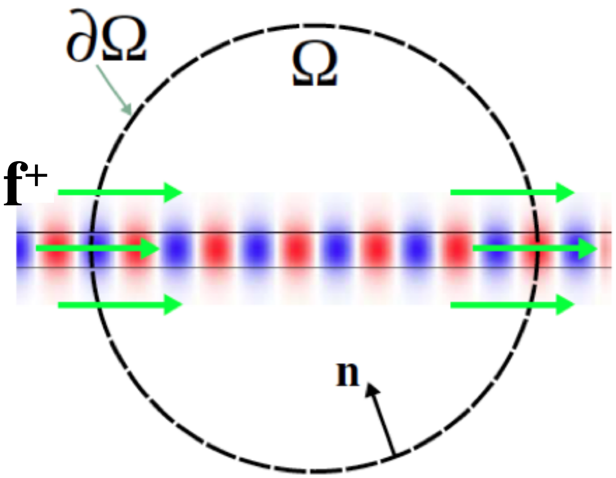
Want some current source to excite incident waveguide mode, planewave, etc…

— also called transparent source since waves do not scatter from it (thanks to linearity)

— vs. hard source = Dirichlet field condition

Equivalent currents ("total-field/scattered-field" approach)

[review article: arXiv:1301.5366]

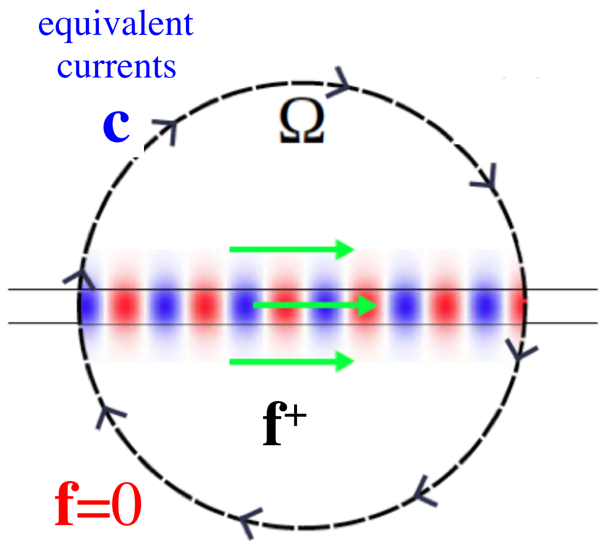


known incident fields

$$\mathbf{f}^{+} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$$

in ambient medium

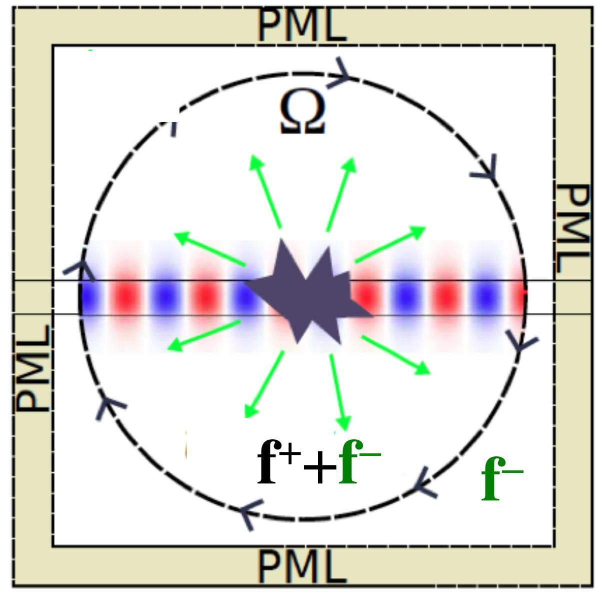
(possibly inhomogeneous, e.g. waveguide or photonic crystal)



want to construct surface currents

$$\mathbf{c} = \begin{pmatrix} \mathbf{J} \\ \mathbf{K} \end{pmatrix}$$

giving same $\mathbf{f}^{+}$ in Ω



do simulations in finite domain + inhomogeneities / interactions = scattered field $\mathbf{f}^{-}$

The *Principle of Equivalence* in classical EM

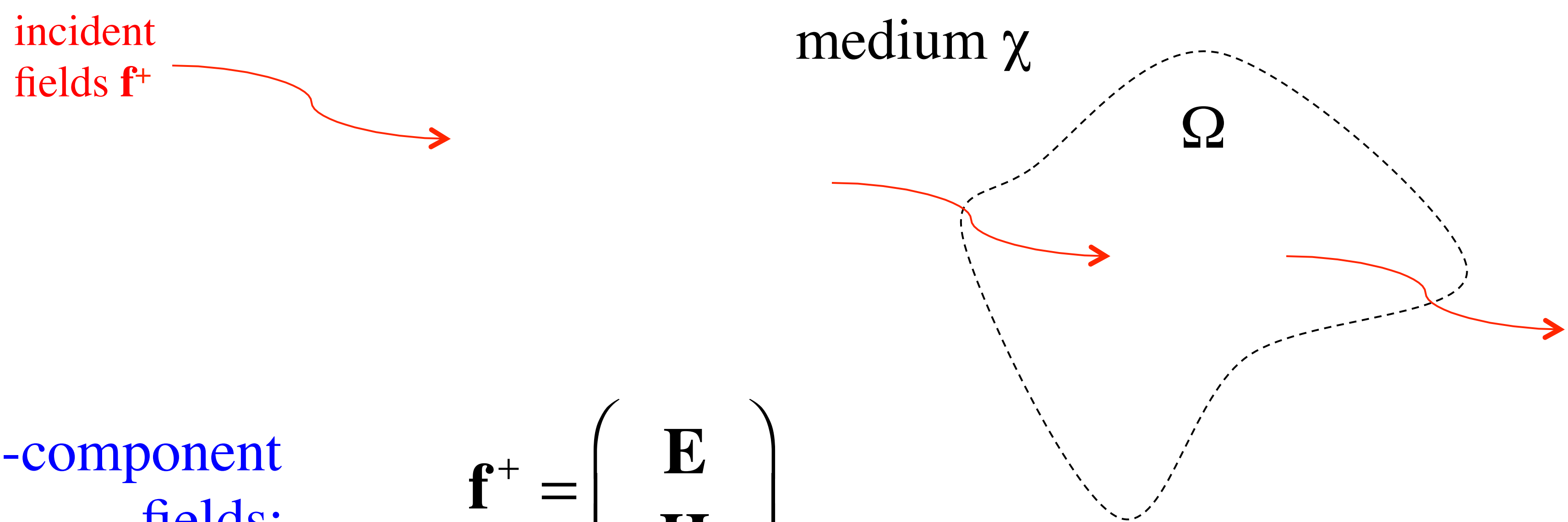
(or Stratton–Chu equivalence principle)
(formalizes Huygens' Principle)
(or total-field/scattered-field, TFSF)

(close connection to Schur complement [Kuchment])

[see e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

[review article: arXiv:1301.5366]

starting point: solution in all space



6-component fields:

$$\mathbf{f}^{+} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$$

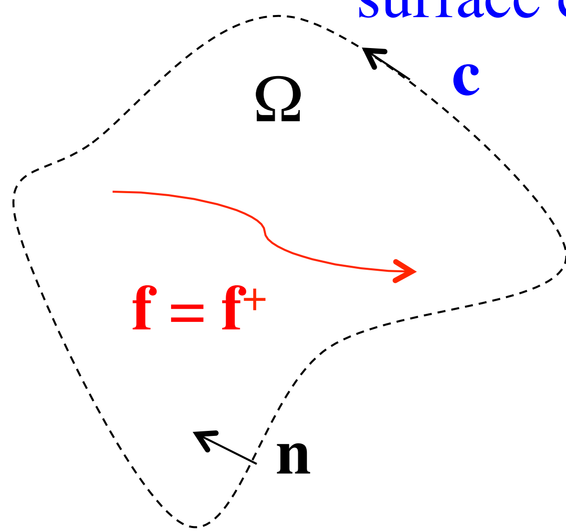
solve (source-free) Maxwell PDE (in frequency domain):

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix}\mathbf{f}^{+} = -i\omega\begin{pmatrix} \varepsilon & \\ & \mu \end{pmatrix}\mathbf{f}^{+} = -i\omega\chi\mathbf{f}^{+}$$

constructing solution in Ω

equivalent
"6"-component
surface currents

$\mathbf{f} = 0$



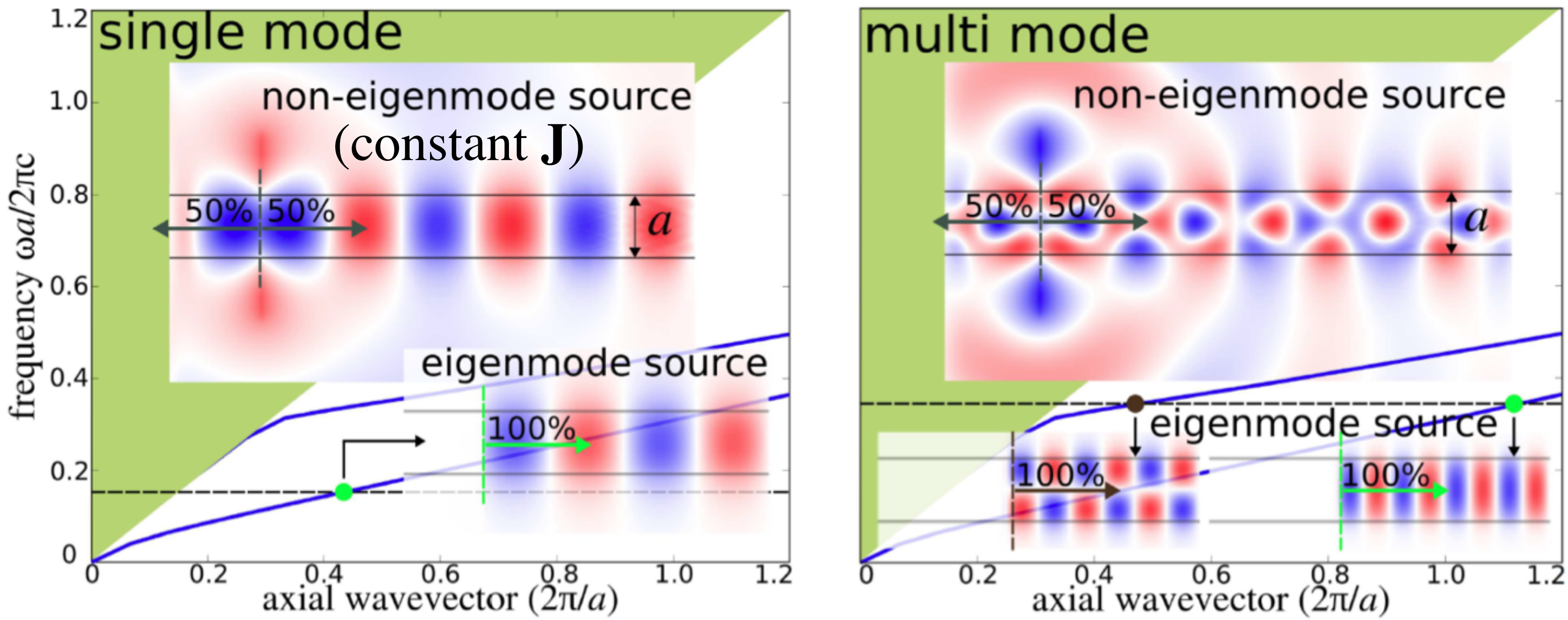
construct **c** so that **f** is a new solution:

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix}\mathbf{f} = -i\omega\chi\mathbf{f} + \underbrace{\delta(\partial\Omega)\begin{pmatrix} \mathbf{n}\times\mathbf{H} \\ -\mathbf{n}\times\mathbf{E} \end{pmatrix}}_{\mathbf{c}}$$

$$= -i\omega\chi\mathbf{f} + \mathbf{c}$$

Exciting a waveguide mode in FDTD

— compute mode in MPB, then use as source in MEEP



[review article: arXiv:1301.5366]

Problems with equivalent sources

(if not solved, undesired excitation of other waves)

[review article: arXiv:1301.5366]

- Discretization mismatch: at finite resolution, solutions from one technique (MPB) don't exactly match discrete modes in another technique (Meep) — leads to small imperfections

  — solvable by using the same discretization to find modes

time domain only

- Dispersion: mode profile varies with ω, so injecting a pulse $p(t)$ requires a convolution with $\hat{\mathbf{c}}(\mathbf{x},\omega) \underset{\text{Fourier}}{\leftrightarrow} \mathbf{c}(\mathbf{x},t)$

$$\text{currents}(\mathbf{x},\mathrm{t}) = p(t) * \mathbf{c}(\mathbf{x},t) \approx p(t)\, \hat{\mathbf{c}}(\mathbf{x},\omega)$$

narrow-bandwidth

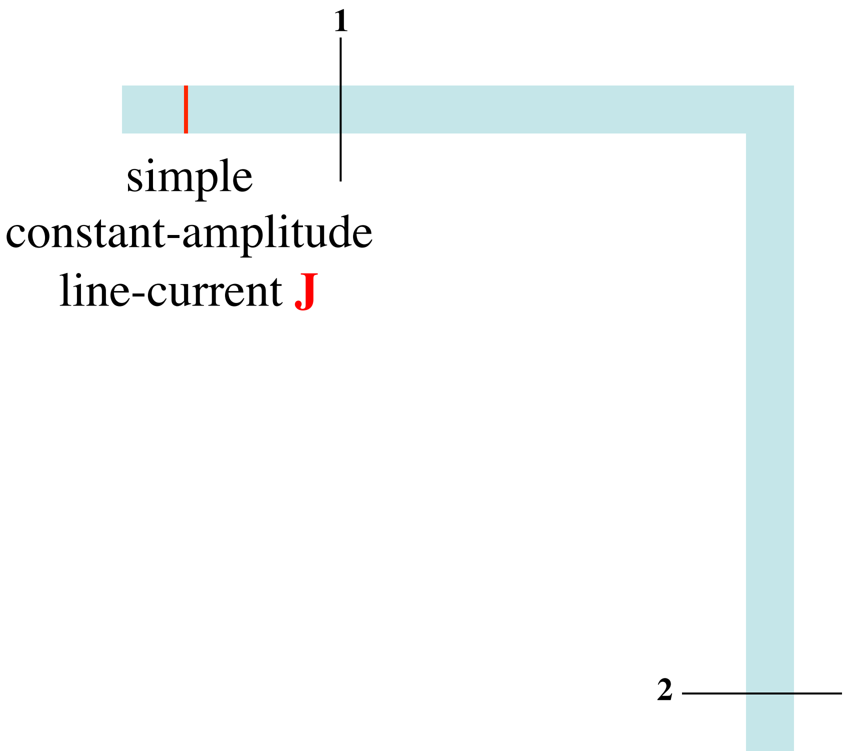
  – convolutions expensive, can be approximated by finite-time (FIR/IIR) calculations using DSP techniques

  – specialized methods are known for planewave sources

(have numerical dispersion!)

Shortcut: Subtract two simulations

example: 90° bend of single-mode dielectric waveguide



want incident, transmitted, and reflected energy-flux spectra:

incident: Poynting flux of $\hat{\mathbf{f}}^{2}_{\text{straight}}$

transmitted: flux of $\hat{\mathbf{f}}^{2}_{\text{bend}}$

reflected: flux of $\hat{\mathbf{f}}^{1}_{\text{bend}} - \hat{\mathbf{f}}^{1}_{\text{straight}}$

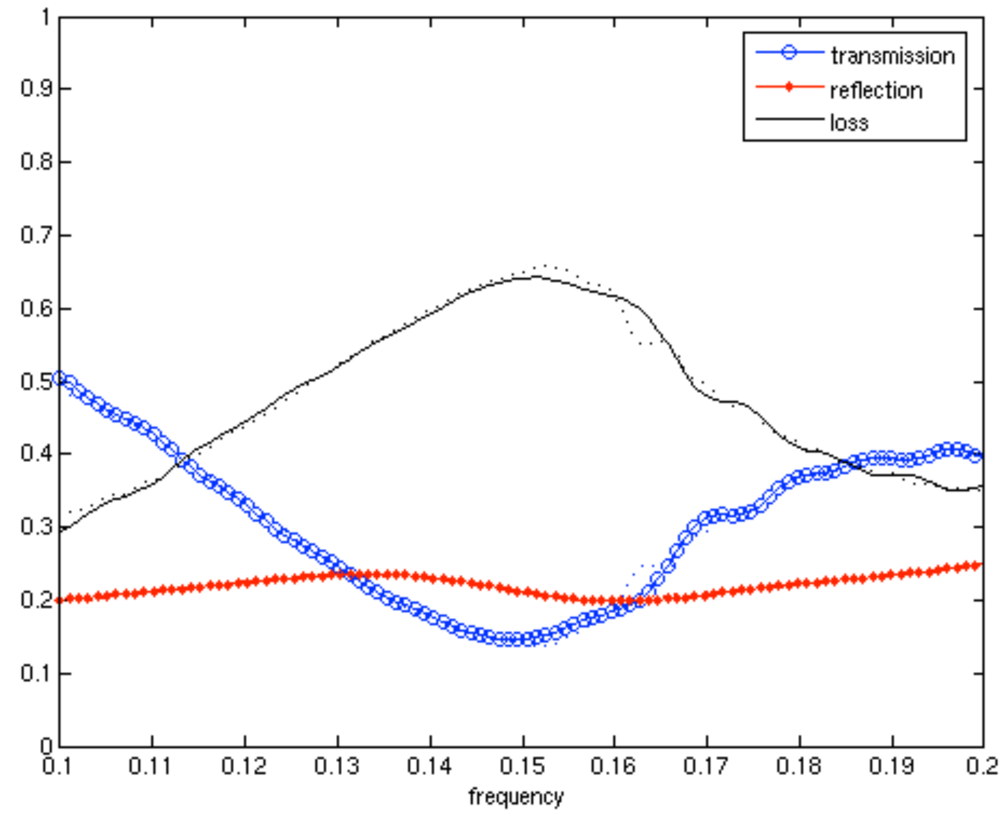
accumulate (discrete-time) Fourier transforms of fields:

$$\hat{\mathbf{f}}^{1,2}_{\text{bend,straight}}(\mathbf{x},\omega) = \sum_{n} \mathbf{f}(\mathbf{x}, n\Delta t)\, e^{i\omega n\Delta t}$$

at desired frequencies ω

Shortcut: Subtract two simulations

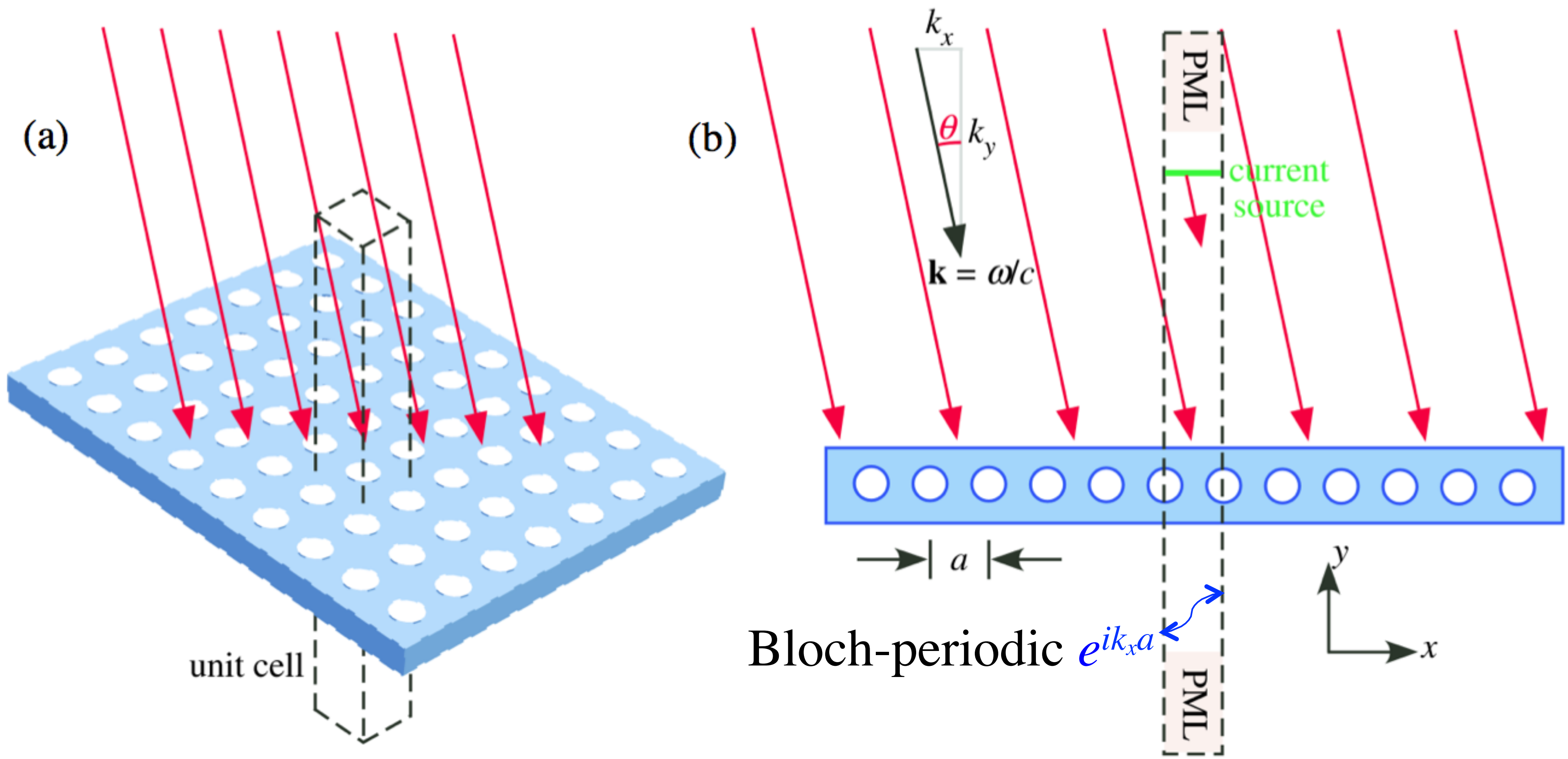
example: 90° bend of single-mode dielectric waveguide



(waveguide width) / λ

Shortcut: Planewave sources for periodic media

[review article: arXiv:1301.5366]

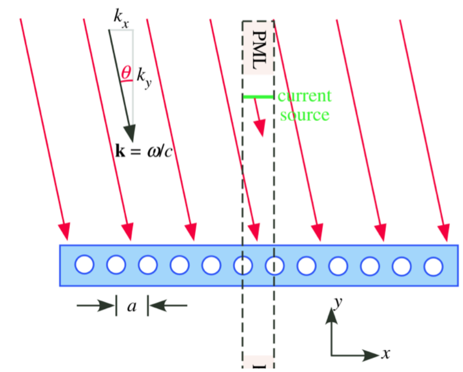


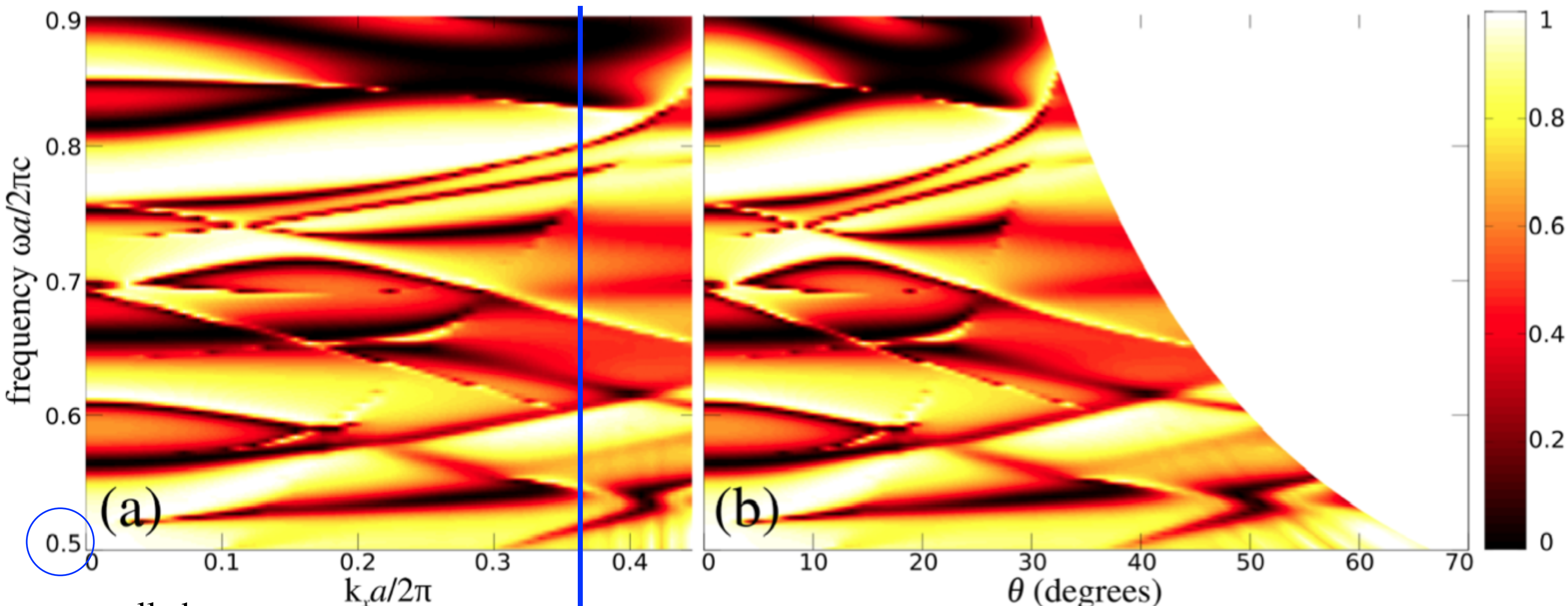
trick #1: incident & scattered fields are Bloch-periodic/quasiperiodic

trick #2: $e^{ik_x x}$ current source produces planewave

Reflection spectra example for periodic media

(Fano resonance lineshapes)





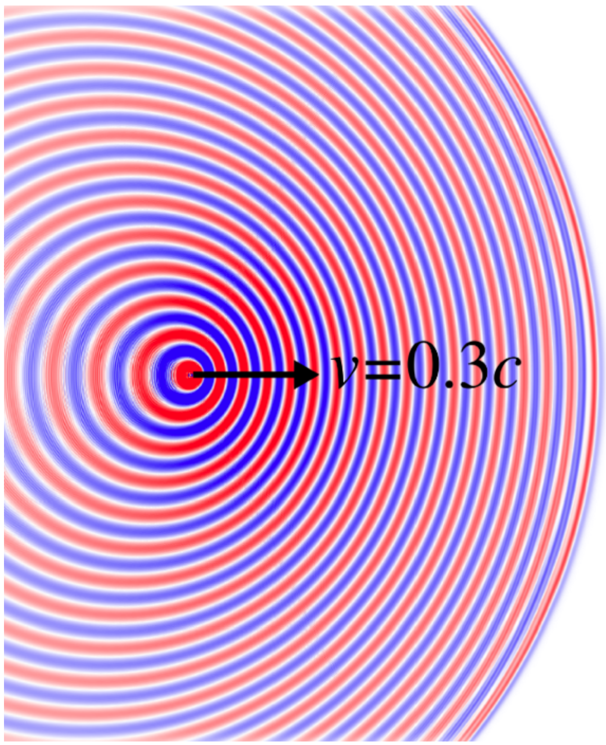
note: ω all above light line
(req. for incident planewave)

entire spectrum at fixed k_x from single FDTD simulation (Fourier transform of pulse)

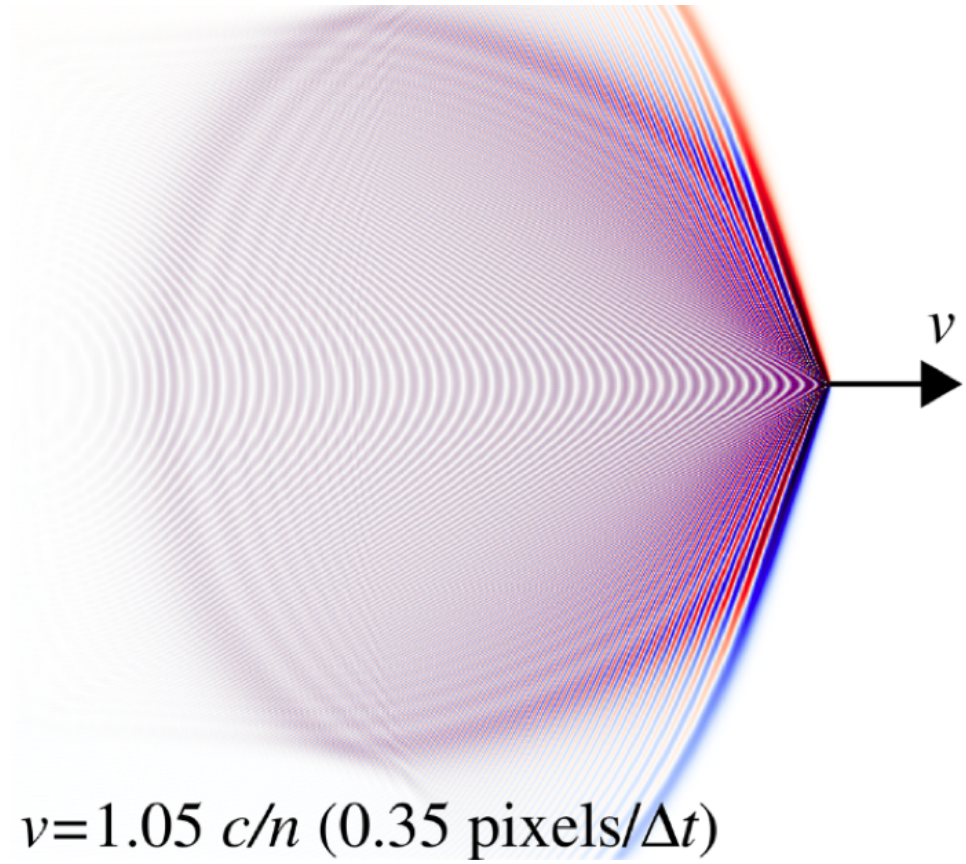
⇔ curved line $\theta = \text{asec}(ck_x/\omega)$ in (ω,θ) plot

Fun possibilities in FDTD:

moving sources [= just some currents $J(x,t)$]

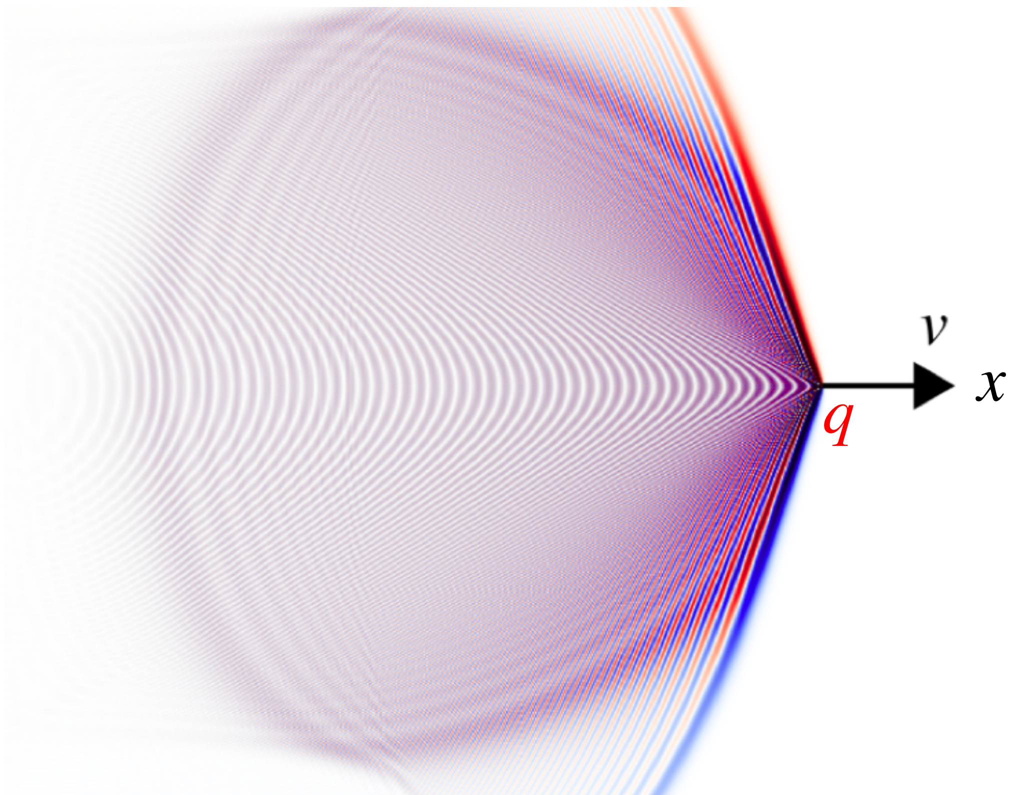


Doppler shift from moving oscillating dipole



Cerenkov radiation from moving point charge in dielectric medium

Cerenkov radiation



v=1.05 c/n (0.35 pixels/Δt)

charge density $\rho = q\delta(x - vt)$

$\Rightarrow$ current density

$$J_x = qv\delta(x - vt)$$

$$= \frac{qv}{2\pi} \int_{-\infty}^{+\infty} e^{ik(x-vt)}\, dk$$

$= e^{i(kx-\omega t)}$

if $\omega(k)=kv$

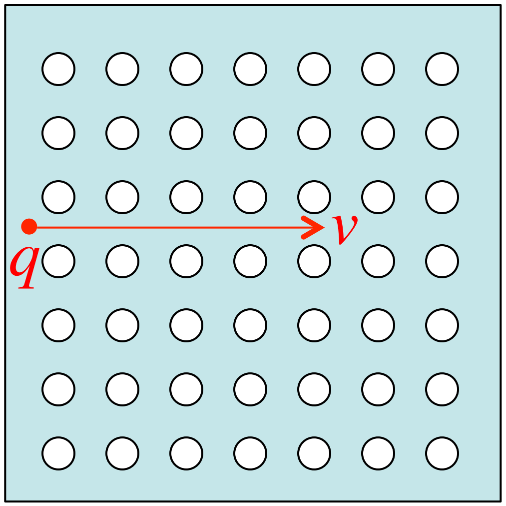
excites radiating mode $\omega(k_x,k_y)$

if $v = \omega(k_x,k_y)/k_x$

= phase velocity in x direction

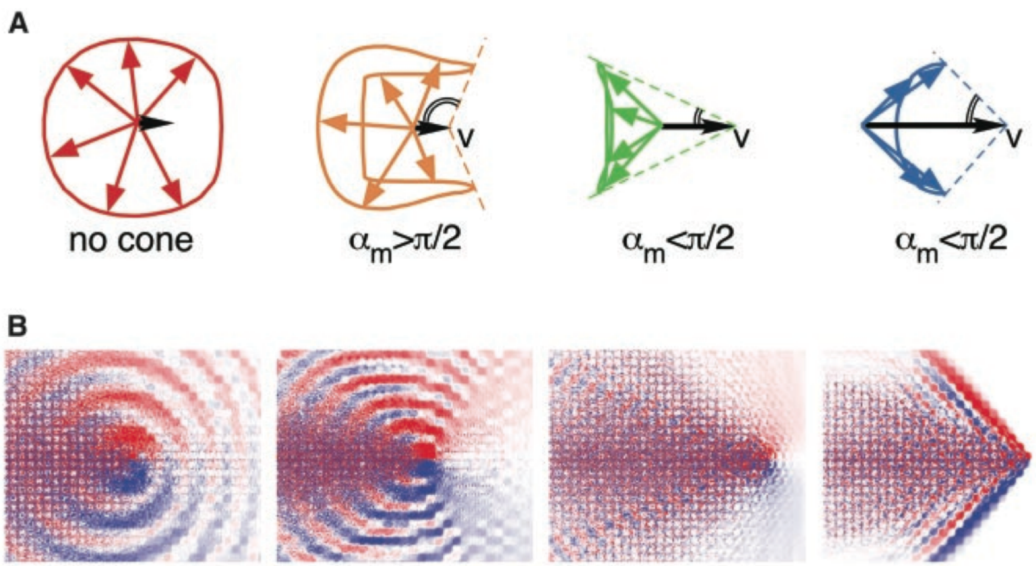
$\geq c/n$ in index-n medium

Cerenkov radiation in photonic crystal



excites radiating mode $\omega(k_x,k_y)$
if $v = \omega(k_x,k_y)/(k_x + 2\pi m/a)$
for any integer m

⇒ no minimum v
[Smith–Purcell effect]



very different radiation patterns & directions depending on v, due to interactions with 2d PhC dispersion curves

[Luo, Ibanescu, Johnson, & Joannopoulos (Science, 2002)]

Surface-integral equations (SIEs) and boundary-element methods (BEMs)

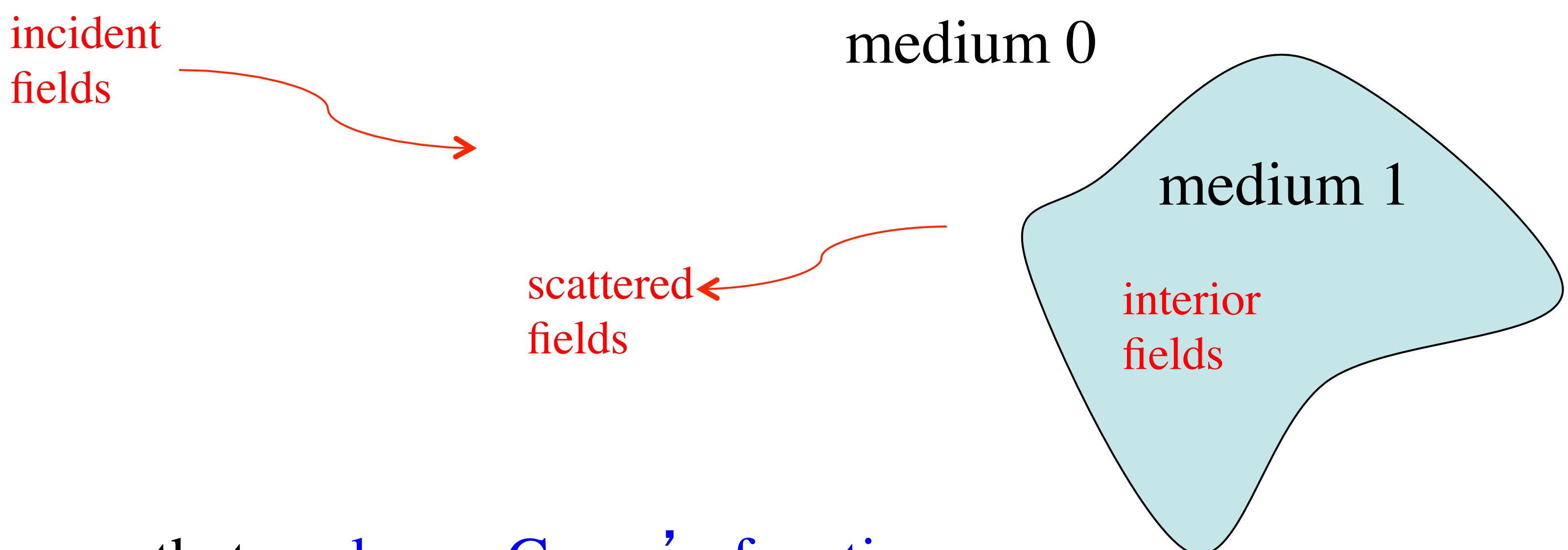
[see e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

Harrington, "Boundary integral formulations for homogeneous material bodies," *J. Electromagnetic Waves Appl.* **3**, 1–15 (1989)

Chew *et al.*, *Fast and Efficient Algorithms in Computational Electromagnetics* (2001)].

Exploiting partial knowledge of Green's functions

a typical scattering problem:



suppose that we know Green's functions in infinite medium 0 or medium 1

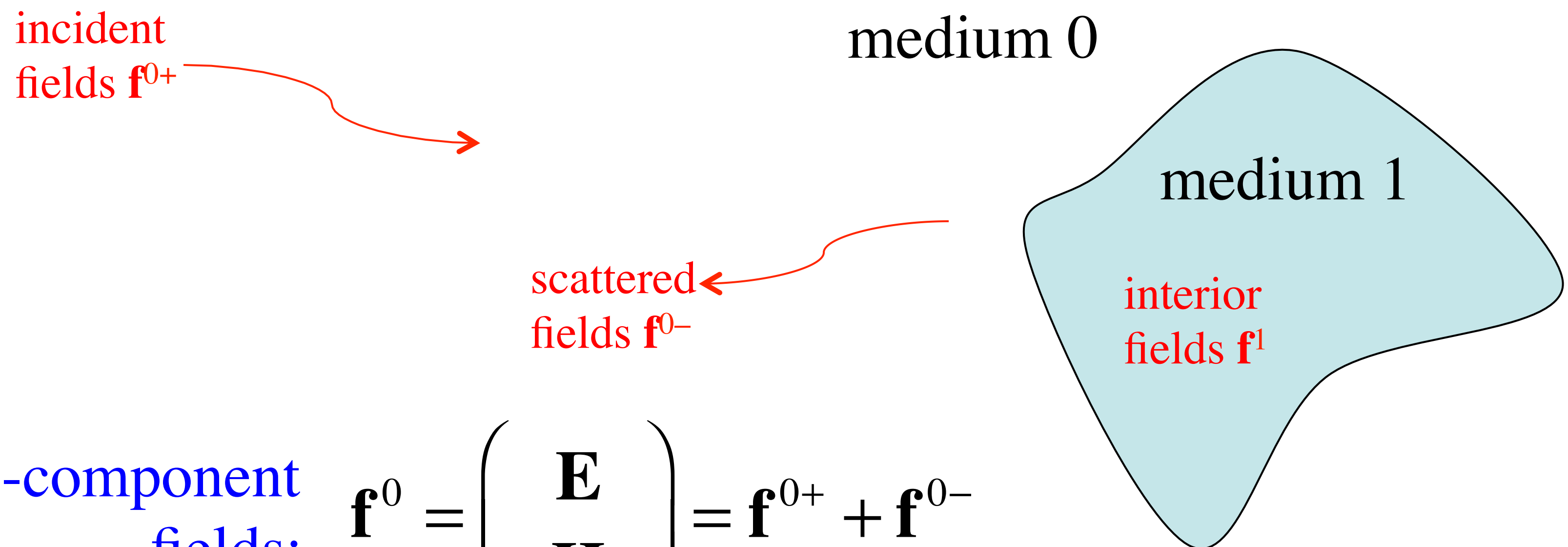
— known analytically for homogeneous media

— computable by *much smaller* calculation in periodic medium

Can exploit this to derive *integral equation* for *surface unknowns* only.

The *Principle of Equivalence* in classical EM

[see e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]



6-component fields:

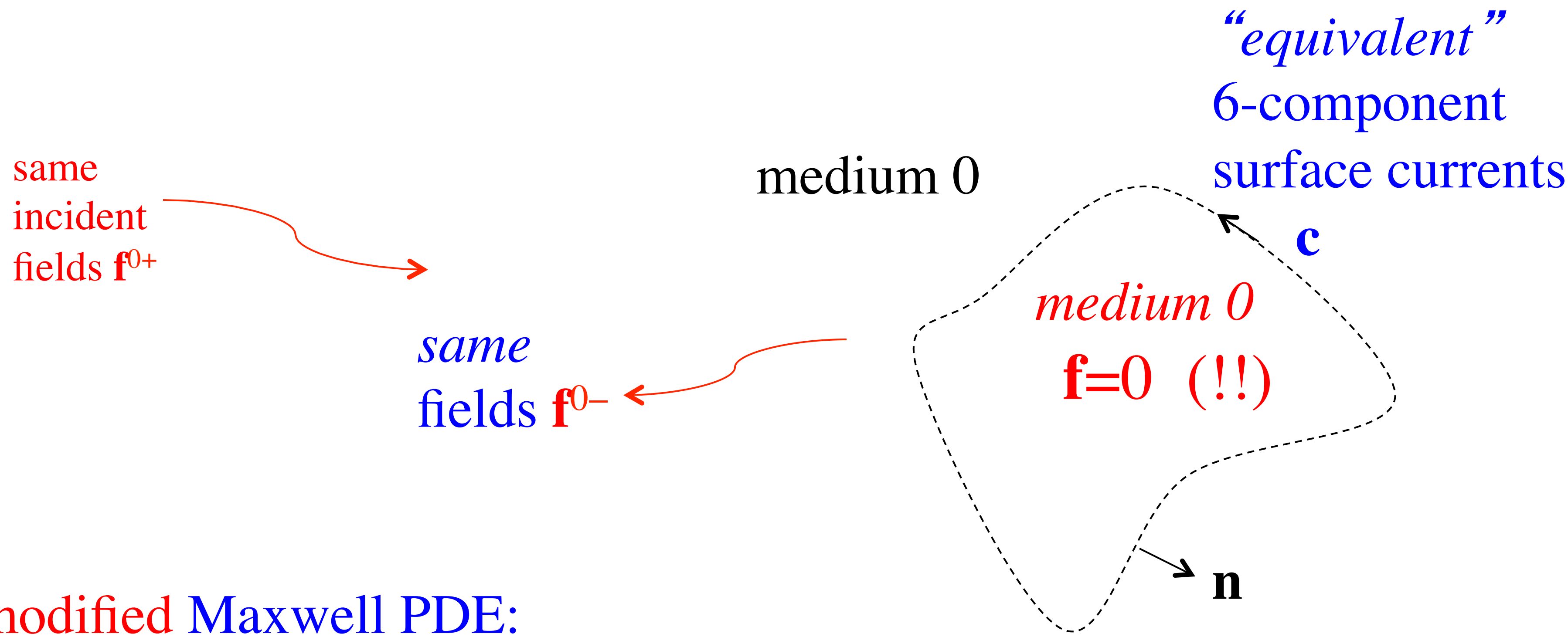
$$\mathbf{f}^{0} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathbf{f}^{0+} + \mathbf{f}^{0-}$$

Maxwell PDE:

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix} \mathbf{f} = -i\omega\chi^{(0,1)}\mathbf{f}$$

… we want to partition *into* separate *medium* 0/1 *problems &* enforce continuity…

Constructing a medium-0 solution

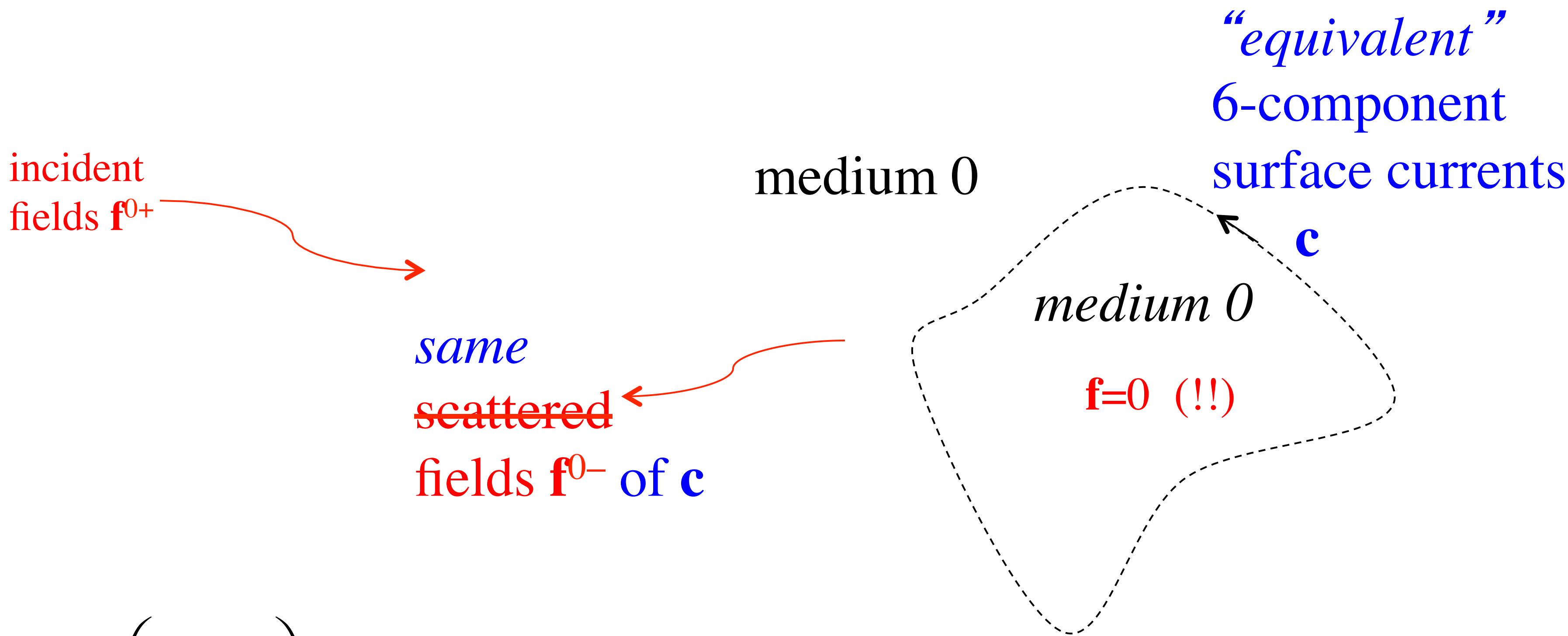


modified Maxwell PDE:

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix}\mathbf{f} = -i\omega\chi^0\mathbf{f} + \delta(\text{surface})\underbrace{\begin{pmatrix} -\mathbf{n}\times\mathbf{H} \\ \mathbf{n}\times\mathbf{E} \end{pmatrix}}_{\mathbf{c}}$$

$$= -i\omega\chi^0\mathbf{f} + \mathbf{c}$$

The *Principle of Equivalence* I

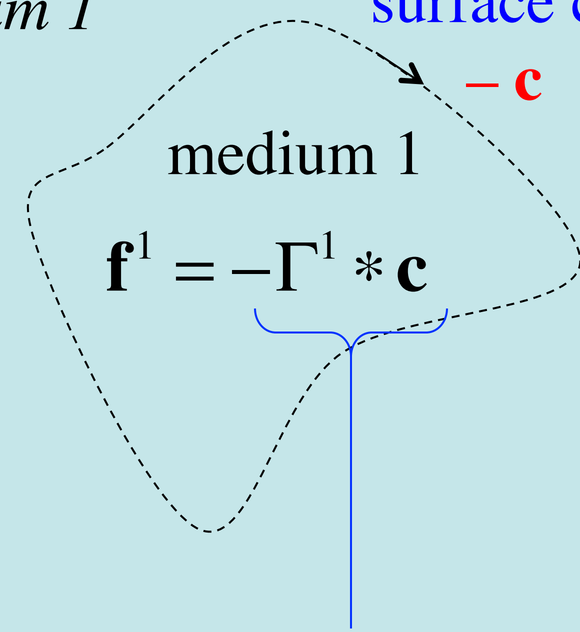


$$\mathbf{f}^0 = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathbf{f}^{0+} + \mathbf{f}^{0-} = \mathbf{f}^{0+} + \underbrace{\Gamma^0 * \mathbf{c}}$$

convolution with
6x6 Green's function Γ^0
of *homogenous* medium 0

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

The *Principle of Equivalence* II



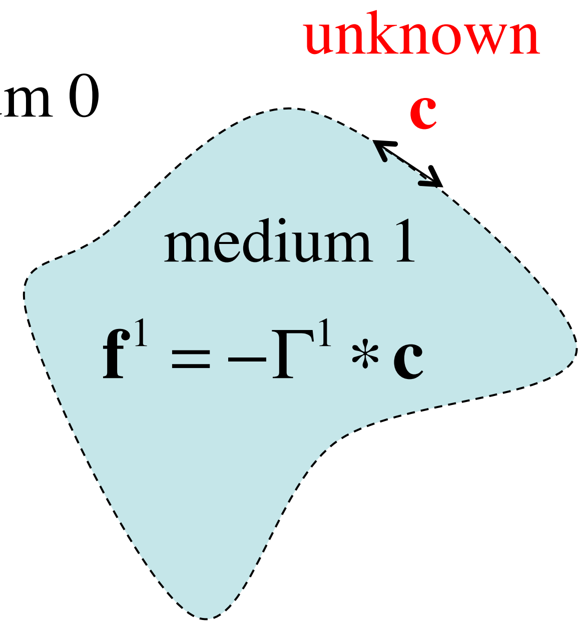
convolution with
6x6 Green's function Γ^1
of *homogenous* medium 1

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

Surface-Integral Equations (SIE)

medium 0

$$\mathbf{f}^{0} = \mathbf{f}^{0+} + \Gamma^{0} * \mathbf{c}$$



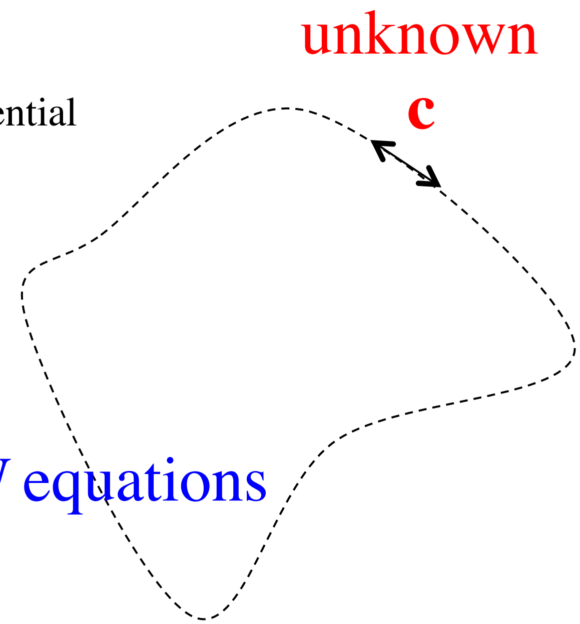
c determined by
continuity of tangential fields
at 0/1 interface:

$$\left(\Gamma^{0} + \Gamma^{1}\right) * \mathbf{c}\Big|_{\text{tangential}} = -\mathbf{f}^{0+}\Big|_{\text{tangential}}$$

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

Discretizing the Maxwell SIE

$$\left(\Gamma^{0}+\Gamma^{1}\right)*\mathbf{c}\Big|_{\text{tangential}}=-\mathbf{f}^{0+}\Big|_{\text{tangential}}$$



pick some **basis** $\mathbf{b}_{\mathrm{n}}$ (n=1,…,$N\rightarrow\infty$)
for surface-tangential vector fields

$$\mathbf{c}=\sum_{n}x_{n}\mathbf{b}_{n}$$

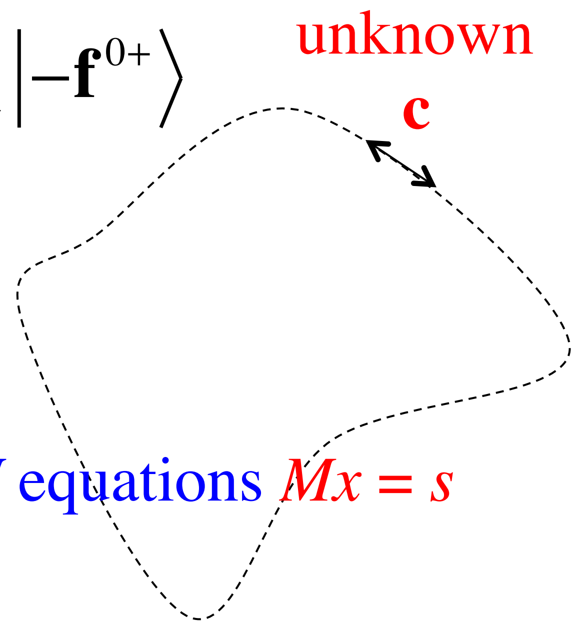
N discrete unknowns x_n ⇒ N equations

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

Discretizing the Maxwell SIE

Galerkin method — require error ⊥ basis:

$$\left\langle \mathbf{b}_m \middle| \left(\Gamma^0 + \Gamma^1\right) * \left(\sum_n x_n \mathbf{b}_n\right) \right\rangle = \left\langle \mathbf{b}_m \middle| -\mathbf{f}^{0+} \right\rangle$$



pick some **basis b**$_n$ (n=1,…,N→∞)
for surface-tangential vector fields

$$\mathbf{c} = \sum_n x_n \mathbf{b}_n$$

N discrete
unknowns x_n

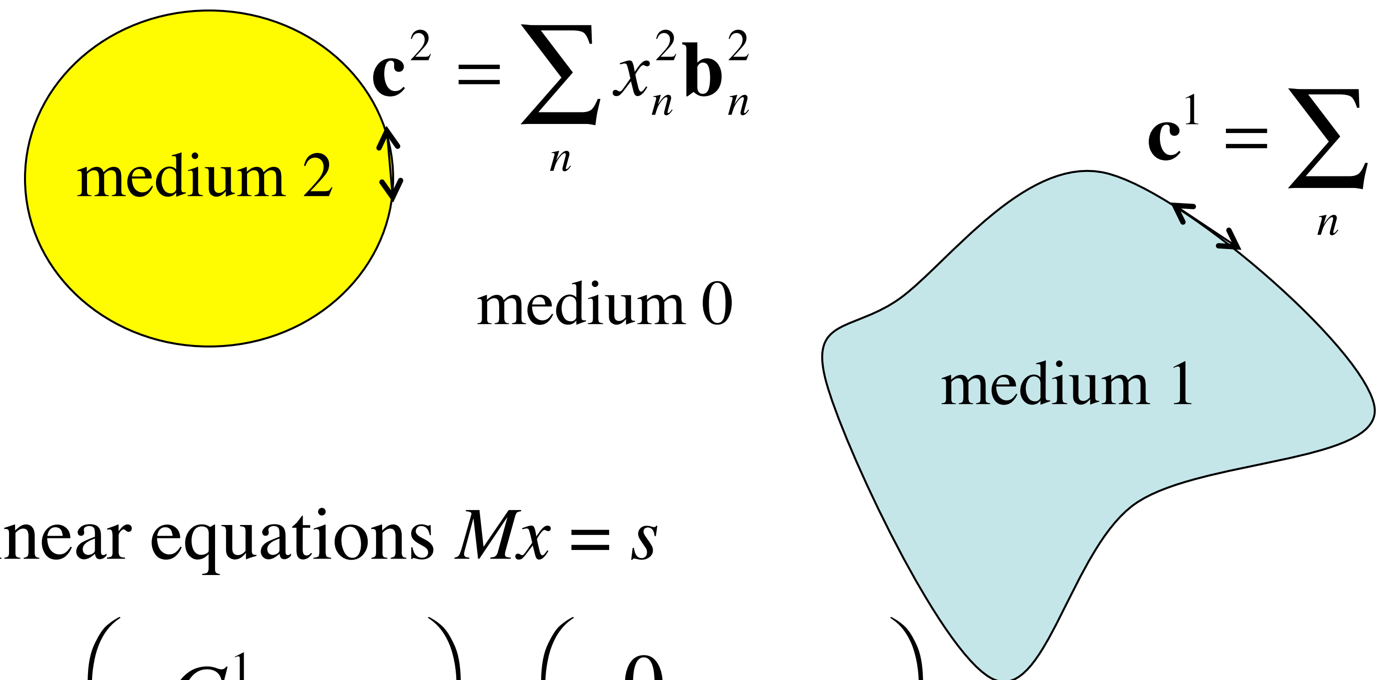
⇒ N equations $Mx = s$

$$M_{mn} = \left\langle \mathbf{b}_m \middle| \left(\Gamma^0 + \Gamma^1\right) * \mathbf{b}_n \right\rangle = G^0_{mn} + G^1_{mn}$$

$$s_m = \left\langle \mathbf{b}_m \middle| -\mathbf{f}^{0+} \right\rangle$$

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

Discretized SIE: Two Objects



$\Rightarrow$ linear equations $Mx = s$

$$M = G^0 + \begin{pmatrix} G^1 & \\ & 0 \end{pmatrix} + \begin{pmatrix} 0 & \\ & G^2 \end{pmatrix}$$

… + straightforward generalizations to more objects, nested objects, etcetera

SIE basis choices

- Can use *any* basis for **c** = any basis of surface functions

  … basis is *not* incoming/outgoing waves

  & need *not* satisfy *any wave equation*

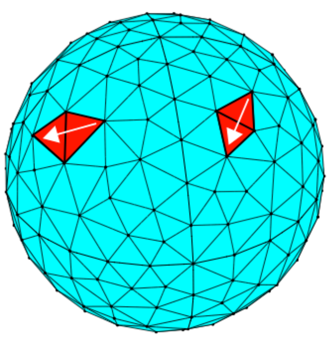
- Spectral bases: spherical harmonics, Fourier series, …

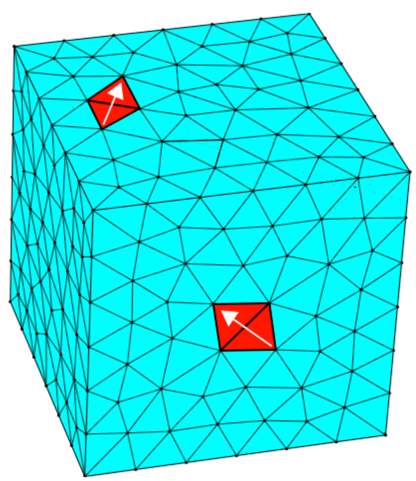
  … nice for high symmetry

  ~ uniform spatial resolution

- Boundary Element Methods (BEM):

  localized basis functions defined on **irregular mesh**





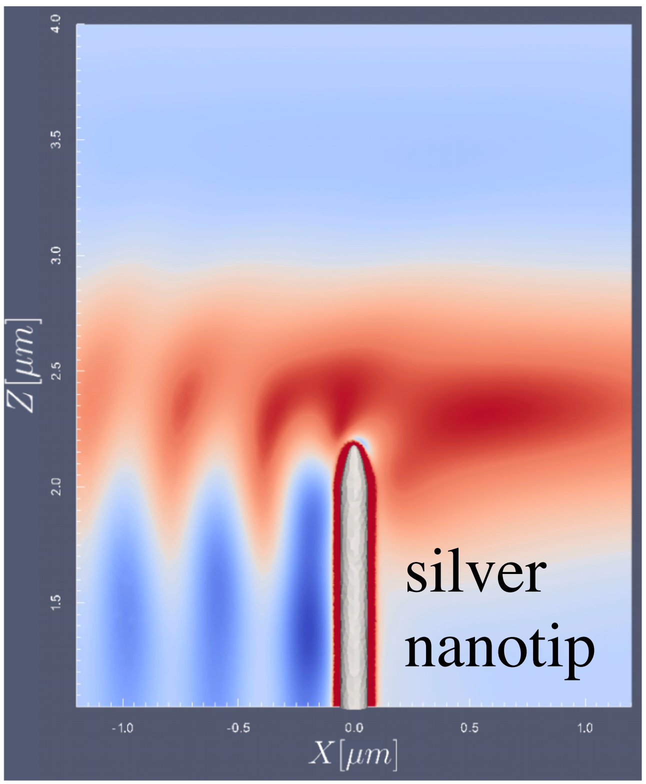
"RWG" basis (1982):

vector-valued $\mathbf{b}_n$ defined
on *pairs* of adjacent triangles
via degree-1 polynomials

BEM strengths

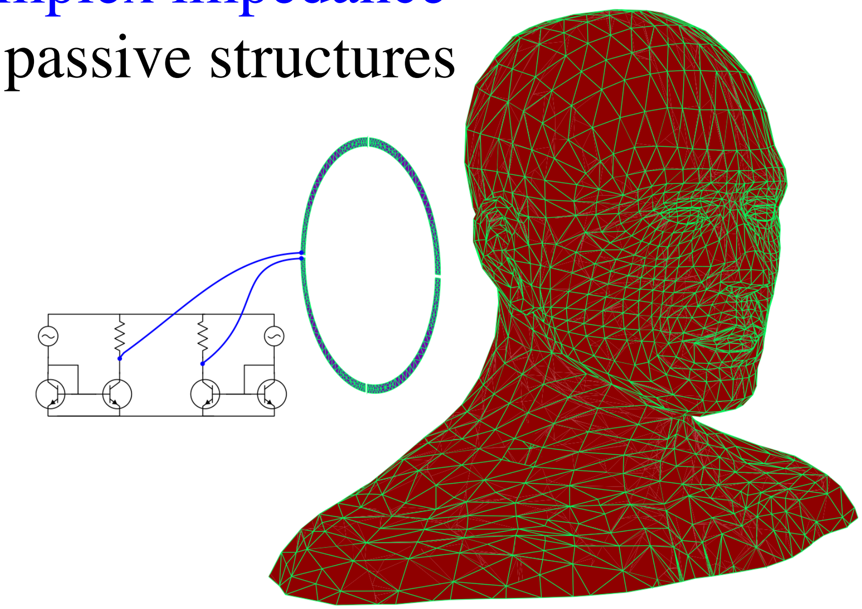
especially small surface areas in a large (many-λ) volume, e.g.:

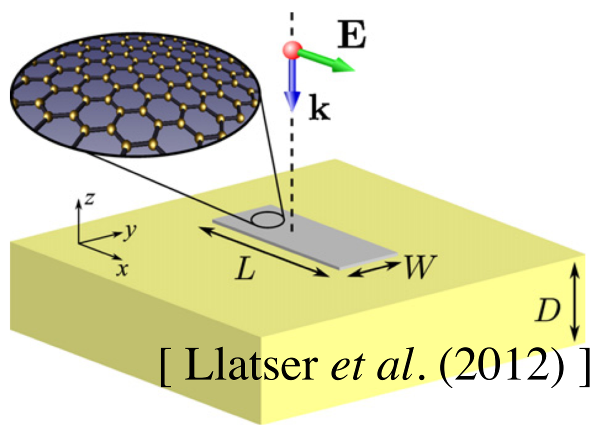
surface plasmons (metals):
extremely sub-λ fields



[Johannes Feist, Harvard]

complex impedance
of passive structures





[Llatser *et al*. (2012)]

Graphene
~ delta-function
surface conductivity
= jump discontinuity
(~ **E**) in **H** field

The bad news of BEM

- Not well-suited for nonlinear, time-varying, or non-piecewise-constant media

- BEM system matrix $M_{mn} = \left\langle \mathbf{b}_m \middle| \left(\Gamma^0 + \Gamma^1\right) * \mathbf{b}_n \right\rangle = G^0_{mn} + G^1_{mn}$

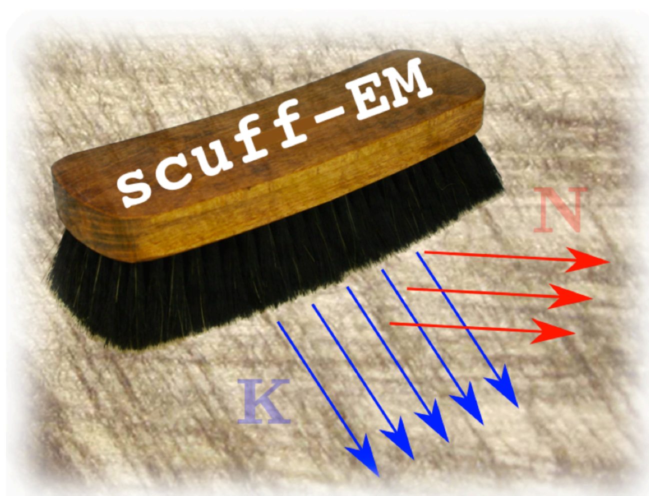
  — *singular* integrals for overlapping $\mathbf{b}_m$, $\mathbf{b}_n$
  …special numerical integration techniques

  — M is *not sparse*, but:
  often small enough for dense solvers ($\lesssim 10^4 \times 10^4$)
  + "fast solvers:" approximate sparse factorizations
  (fast multipole method, etc.)

  — lots of work every time you change Γ
  (e.g. 3d vs. 2d, periodic boundaries, anisotropic, …)
  … but independent of geometry

The good news of BEM:
You don't have to write it yourself

Free software developed by Dr. Homer Reid
(collaboration with Prof. Jacob White @ MIT)



SCUFF-EM

[http://homerreid.ath.cx/scuff-EM]

Surface-
CUrrent /
Field
Formulation
| of
Electro-
Magnetism

SCUFF-EM is a free, open-source software implementation of the boundary-element method of electromagnetic scattering.

SCUFF-EM supports a wide range of geometries, including compact scatterers, infinitely extended scatterers, and multi-material junctions.

The SCUFF-EM suite includes 8 standalone application codes for specialized problems in EM scattering, fluctuation physics, and RF engineering.

The SCUFF-EM suite also includes a core library with C++ and PYTHON APIs for designing homemade applications.

http://homerreid.com/scuff-EM

** to be released by end of October-ish*

SCUFF usage outline

The steps involved in solving any BEM scattering problem:

1. Mesh object surfaces into triangles.

   Not done by SCUFF-EM; high-quality free meshing packages exist (e.g. GMSH).

2. Assemble the BEM matrix $\mathbf{M}$ and RHS vector $\mathbf{v}$.

   SCUFF-EM **does this.**

3. Solve the linear system $\mathbf{M}\mathbf{k} = \mathbf{v}$ for the surface currents $\mathbf{k}$.

   SCUFF-EM uses LAPACK for this.

4. Post-process to compute scattered fields $\{\mathbf{E}, \mathbf{H}\}^{\text{scat}}$ from $\mathbf{k}$.

   SCUFF-EM **does this.**

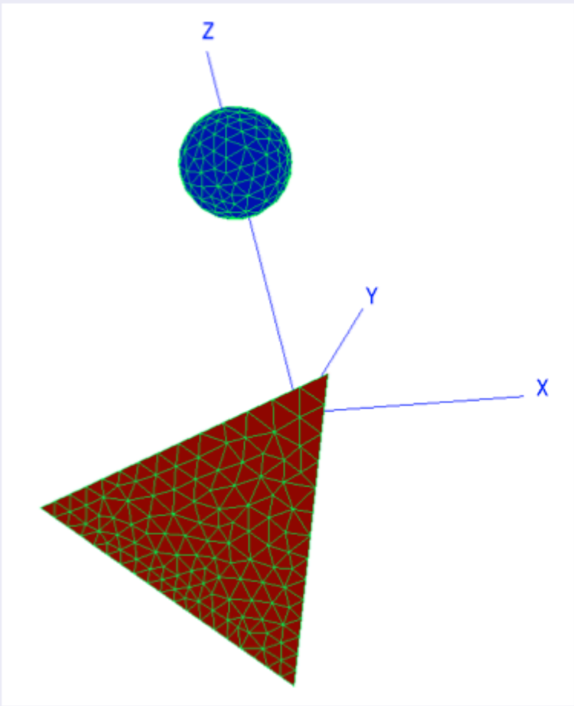
Innovations unique to SCUFF-EM:

- Bypass step 4: Compute scattered/absorbed power, force, and torque **directly from $\mathbf{k}$**
- Bypass steps 3 and 4: Compute Casimir forces and heat transfer **directly from $\mathbf{M}$**

Geometries in SCUFF

A gold sphere and a displaced and rotated SiO2 tetrahedron:

The geometry:



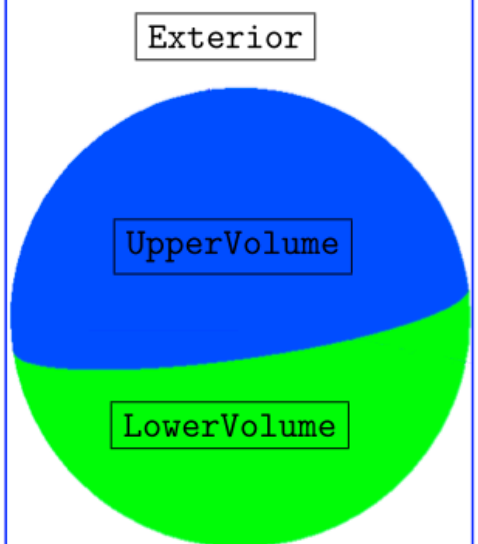
The .scuffgeo file:

```
OBJECT TheSphere
   MESHFILE Sphere.msh
   MATERIAL Gold
ENDOBJECT

OBJECT ThePyramid
   MESHFILE Pyramid.msh
   MATERIAL SiO2
   DISPLACED 0 0 -1
   ROTATED 45 ABOUT 0 1 0
ENDOBJECT
```

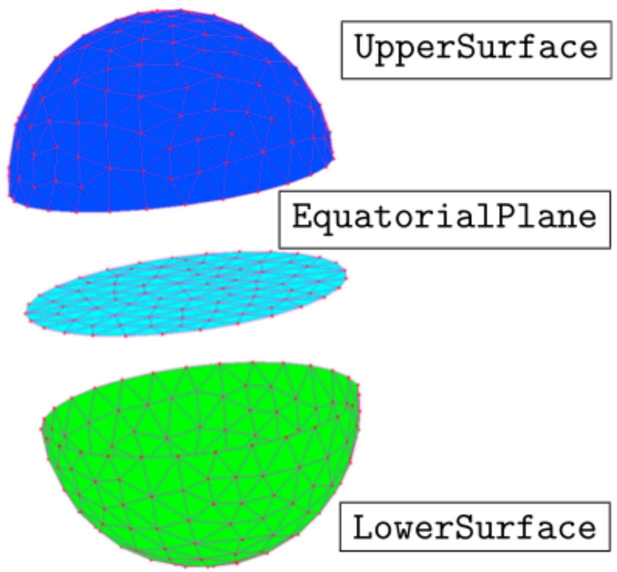
⟹ Handle displacements and rotations without re-meshing.

Geometries in SCUFF

Regions



Surfaces



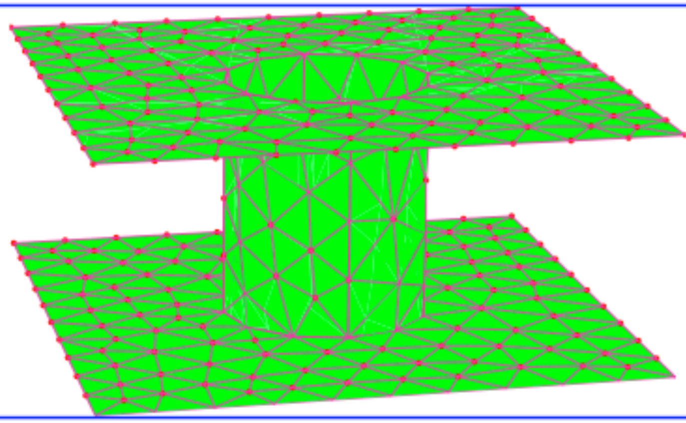
.scuffgeo File

```
REGION Exterior    MATERIAL Vacuum
REGION UpperVolume MATERIAL Gold
REGION LowerVolume MATERIAL Silicon

SURFACE UpperSurface
     MESHFILE UpperSurface.msh
     REGIONS Exterior UpperVolume
ENDSURFACE

SURFACE LowerSurface
     MESHFILE LowerSurface.msh
     REGIONS Exterior LowerVolume
ENDSURFACE

SURFACE EquatorialPlane
     MESHFILE EquatorialPlane.msh
     REGIONS UpperVolume LowerVolume
ENDSURFACE
```

(discretization of SIE at junctions of 3+ materials is a bit tricky)

Periodic geometries in SCUFF

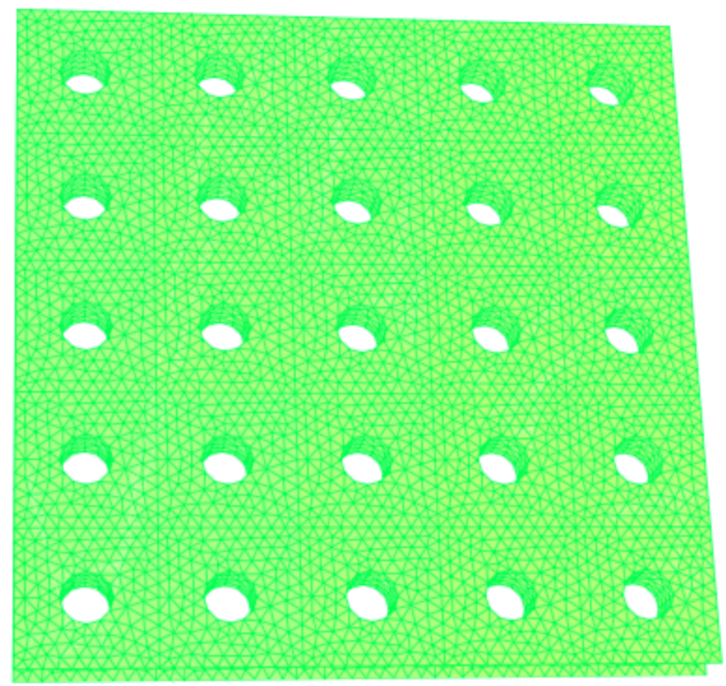
Unit cell mesh



.scuffgeo file

```
LATTICE
        VECTOR 0.75 0
        VECTOR 0    0.75
ENDLATTICE

OBJECT UnitCell
        MESHFILE UnitCellMesh.msh
        MATERIAL Silver
ENDOBJECT
```

First 25 lattice cells



(implementing periodicity is nontrivial: changes Green's function!
SCUFF: periodic $\Gamma = \Sigma$(nearest neighbors) + Ewald summation)

Using SIE/BEM solutions

Solving the SIE gives the surface currents **c**, and
from these (via $\Gamma^*\mathbf{c}$) one can obtain any desired fields, but…

It is much more efficient to compute as much as possible
directly from **c** (~ **n** × surface fields). Examples:

- Scattering matrices (e.g. spherical-harmonic waves in → out):
  obtain directly from multipole moments of "currents"
- Any bilinear function of the surface fields can be computed
  directly from bilinear functions of **c**:
  — scattered/absorbed power, force, torque, …
- Net effects of quantum/thermal fluctuations in matter can
  be computed from norm/det/trace of M or M^{-1}:
  — thermal radiation, Casimir (van der Waals) forces, …

Resonant modes (and eigenvalues)

- BEM scattering problems are of the form $M(\omega)x = s$. Resonances (and eigenvalues) are ω where this system is singular, i.e. the **nonlinear eigenproblem**

$$\det M(\omega) = 0$$

For passive (⇒causal) systems, solutions can only occur for $\mathrm{Im}\,\omega \leq 0$.

- Various algorithms exist, including an intriguing algorithm using contour integrals of $M(\omega)$ [Beyn (2012)].

Computational Nanophotonics: Optimization and "Inverse Design"

Steven G. Johnson
MIT Applied Mathematics

Many, many papers that parameterize
by a *few* degrees of freedom and optimize…

Today, focus is on *large-scale optimization*,
also called *inverse design*:
so many degrees of freedom (10^2–10^6)
that computer is "discovering" new designs.

Outline

- Brief overview/examples of large-scale optimization work in photonics

- Overview of optimization terminology, problem types, and techniques.

- Some more detailed photonics examples.

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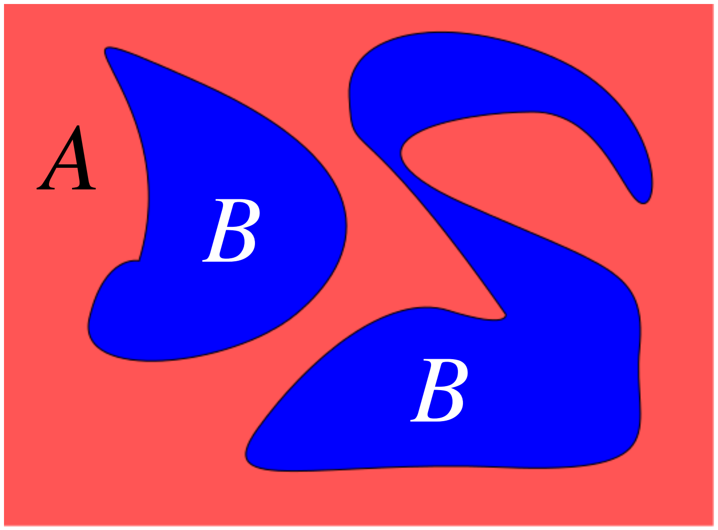
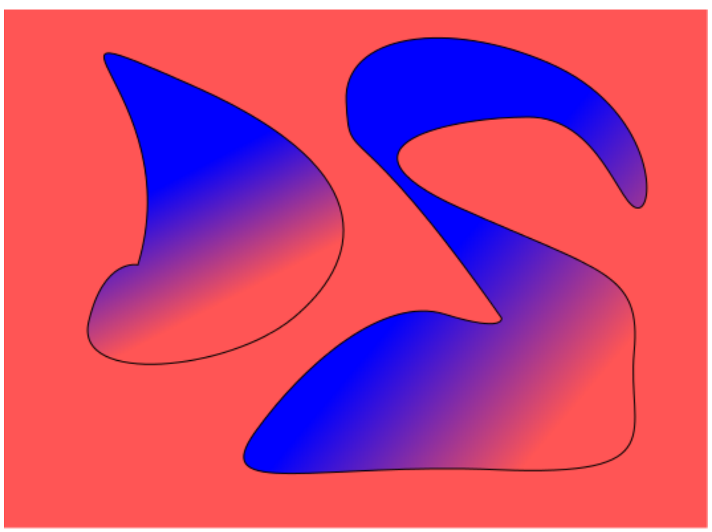
- Brief overview/examples of large-scale optimization work in photonics
- Overview of optimization terminology, problem types, and techniques.
- Some more detailed photonics examples.

Topology optimization



Given two (or more) materials *A* and *B*, determine what arrangement — including what topology — optimizes some objective/constraints.



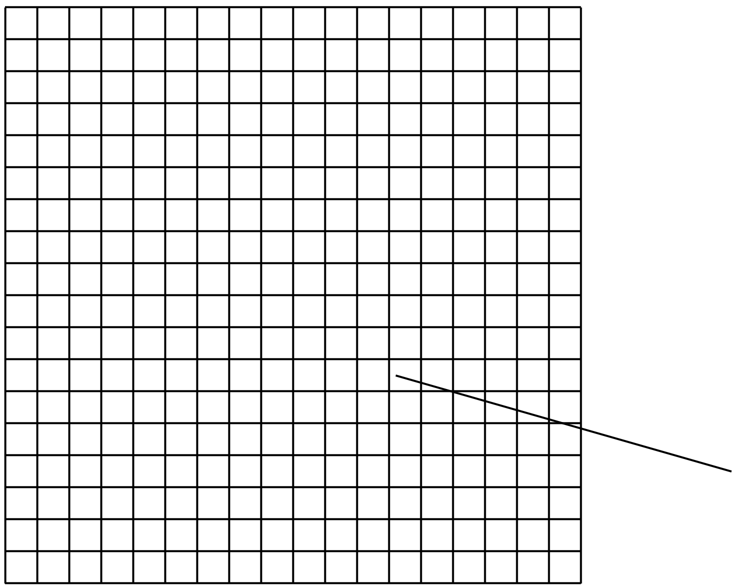
Continuous relaxation:
allow material to vary in [*A*,*B*] continously at every point

- Not uncommon for optimum to yield *A* or *B* almost everywhere
- Possible to add "penalty" to objective for intermediate values

Discretizing Topology Optimization

for computer, need finite-dimensional parameter space

some computational grid



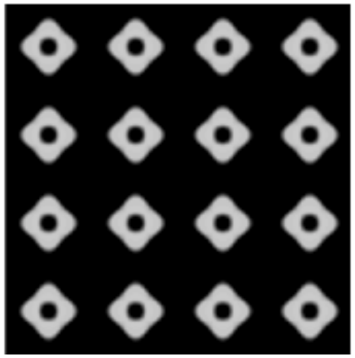
Level-set method: value of "level-set" function $\phi(\mathbf{x})$ varies continuously at each pixel
$\Rightarrow$ material A or B if $\phi > 0$ or < 0

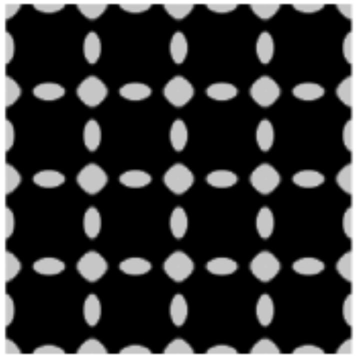
…or…

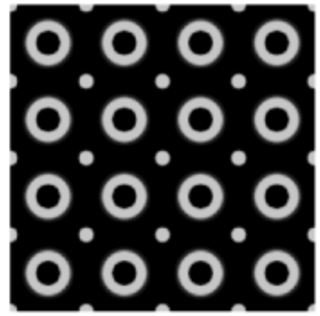
Continuous relaxation: material varies in [A,B] at each pixel

e.g. in electromagnetism, let ε at each pixel vary in [A,B].

Dobson et al. (Texas A&M)







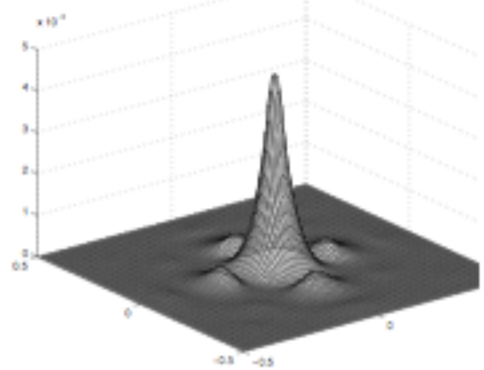
(maximizes ~$\Delta\omega$, not fractional gap!)

(square lattices only)

TM gap, bands 3 & 4

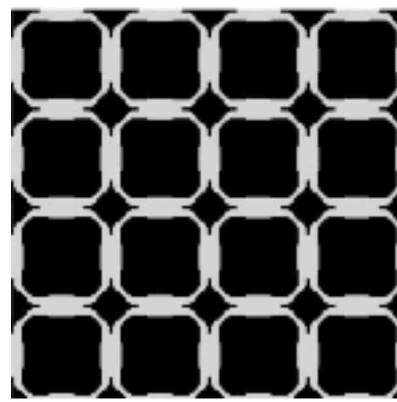
TM bands 6 & 7

SIAM J. Appl. Math. **59**, 2108 (1999)



optimize TM localization in supercell

SIAM J. Appl. Math **64**, 762 (2004)

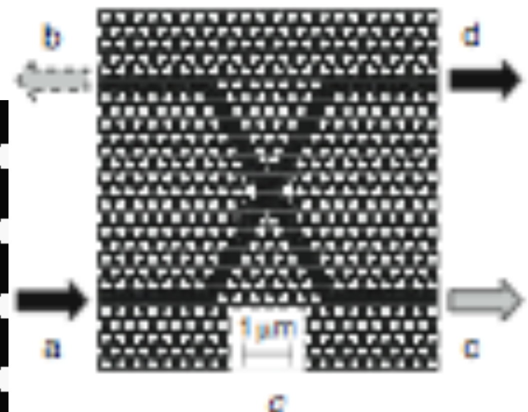


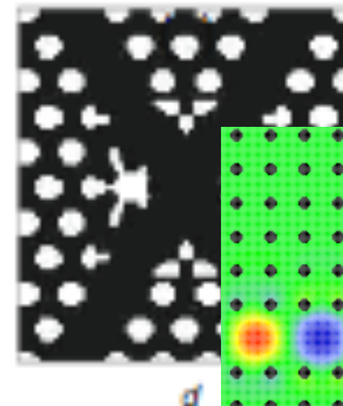
optimized TE gaps
square lattice
thousands of iterations
& still not optimal!

J. Comput. Phys **158**, 214 (2000)

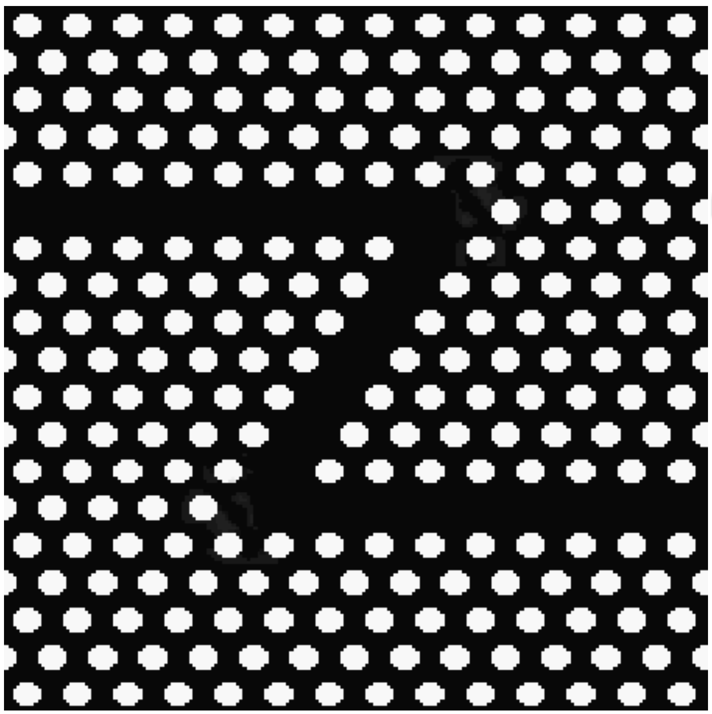
2d (TE or TM) transmission optimization
Sigmund, Jensen, Pederson et al. [www.topopt.dtu.dk]

crossings (2d TE) *Elec. Lett.* **42**, 1031 (2006)

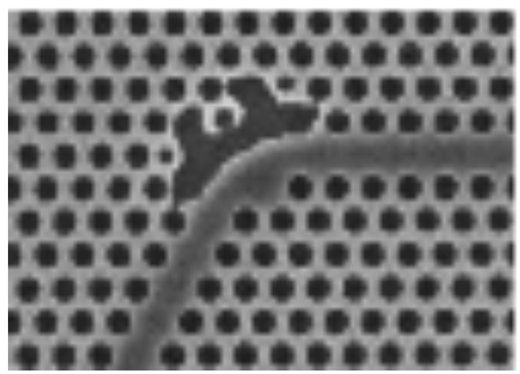




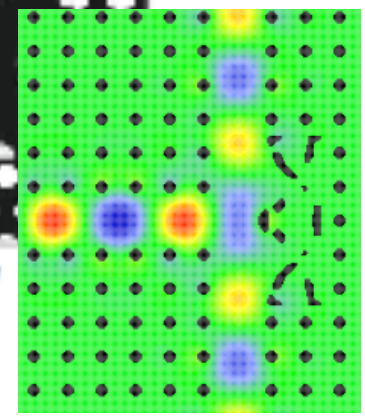
bend optimization



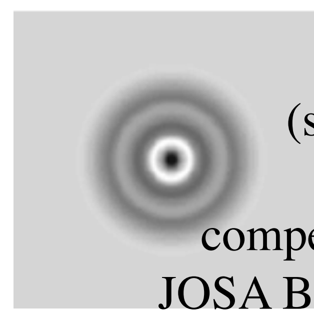
Opt. Express **12**, 1996 (2004)



OE **12**, 5916 (2004)



T-junctions
JOSA B **22**, 1191 (200

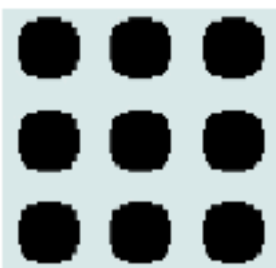


low-index
(scalar approx.)
dispersion-
compensating fibers
JOSA B **25**, 88 (2008)

Dispersion optimization

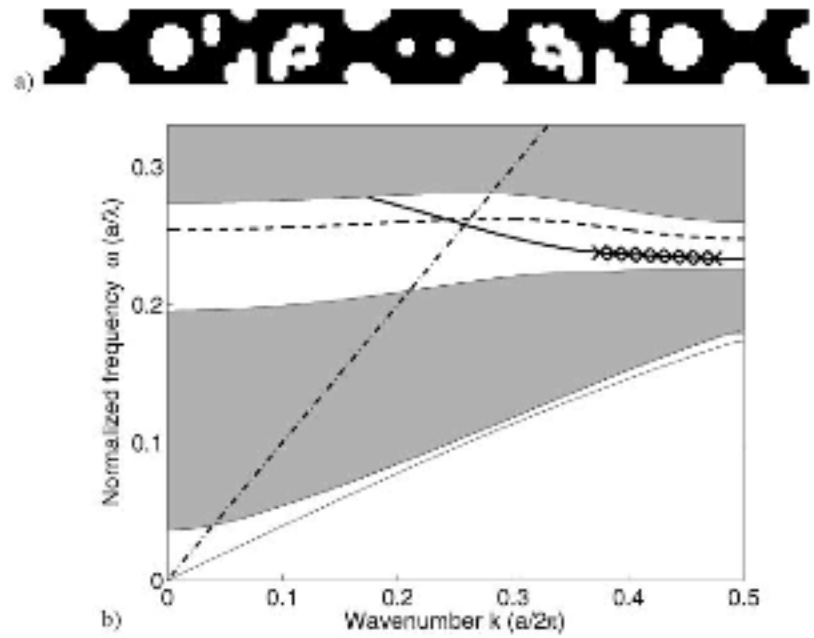
Sigmund, Jensen, Pederson et al. [www.topopt.dtu.dk]

low-index
(scalar approx.)
dispersion-
compensating fibers
JOSA B **25**, 88 (2008)



optimized
phononic gap Δω
bands 1 & 2

optimized 2d scalar
phononic crystals
[Phil. Trans. Roy. Soc.
London A **361**, 1001 (2003)]

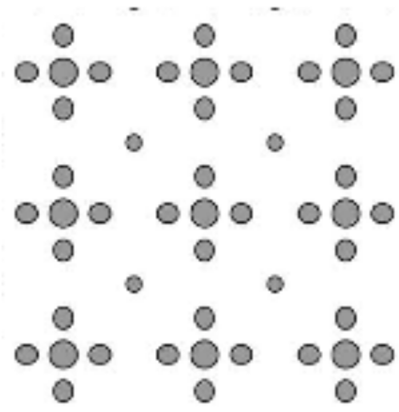


constant group-velocity
band in 2d TE line-defect

… also band gaps for 2d (scalar) phononic crystals…

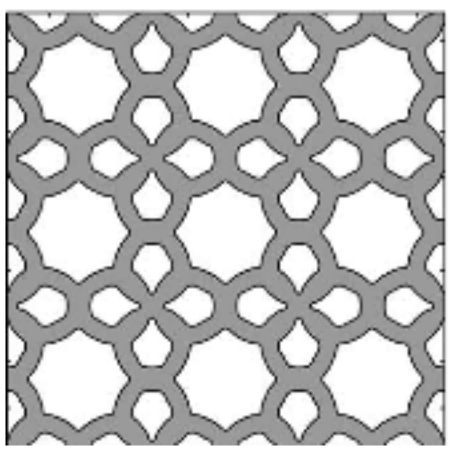
Kao, Osher, and Yablonovitch
2d TM and TE square-lattice gaps via level sets

Appl. Phys. B **81**, 235 (2005)



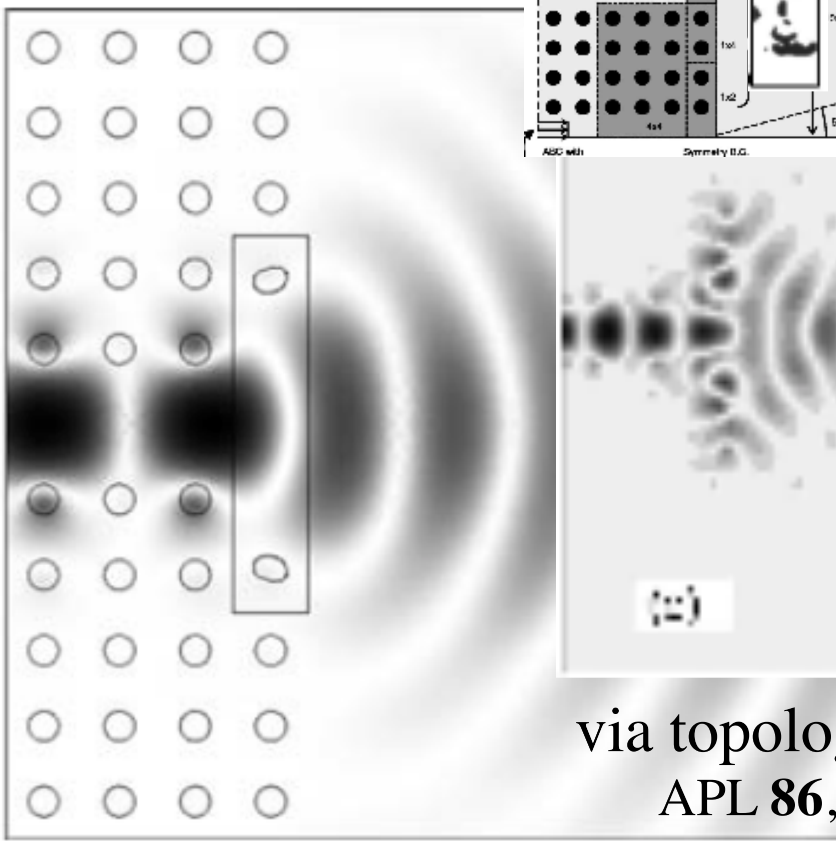
TM gap,
bands 6 & 7

(maximizes $\Delta\omega$,
not fractional gap!)

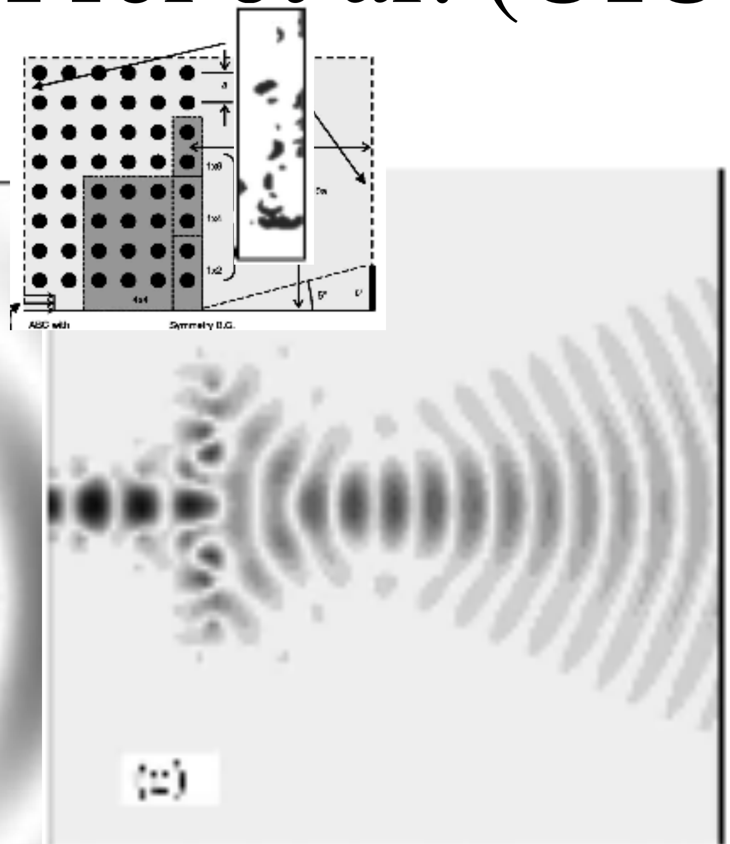


TE gap,
bands 5 & 6

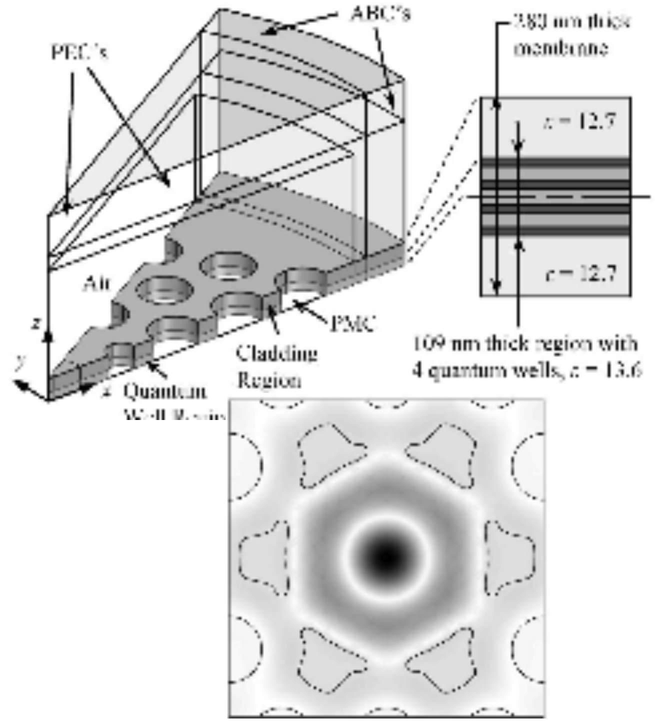
Frei et al. (UIUC)



2d TM “directional” emission
via level-set method
Frei, Opt. Lett. **32**, 77 (2007)

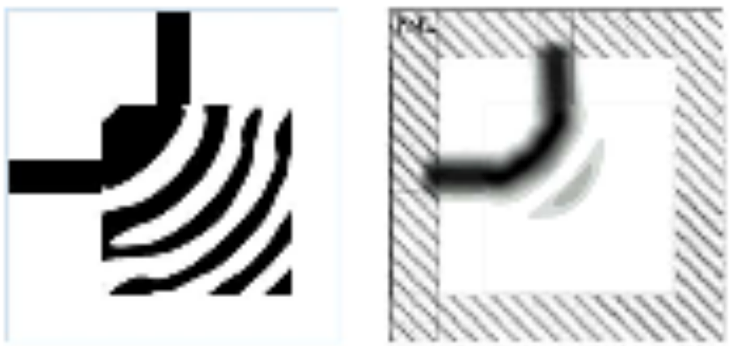


via topology optimization
APL **86**, 111114 (2005)



optimizing 3d Q
J. Appl. Phys **103**, 033102 (2008)
(level-set + MMA)

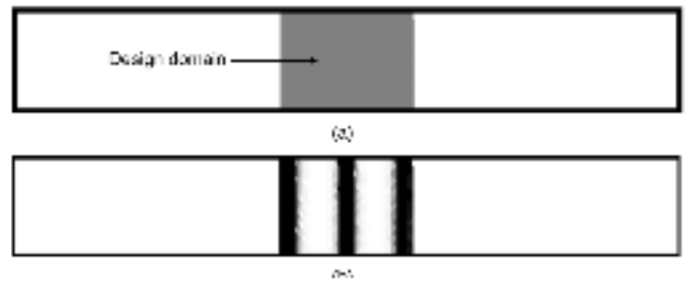
Other Topology Optimizers



(a) (b)

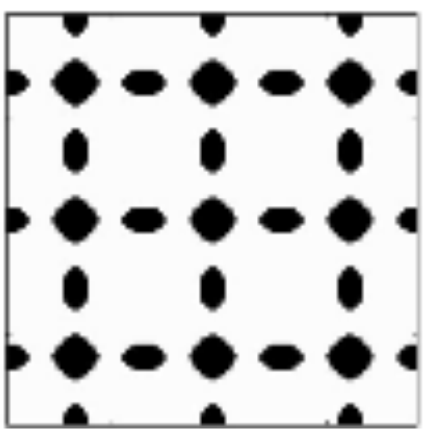
2d TM bend

[Tsuji, Phot. Tech. Lett. 20, 982 (2008)]



"2d" (really 1d) TE filter

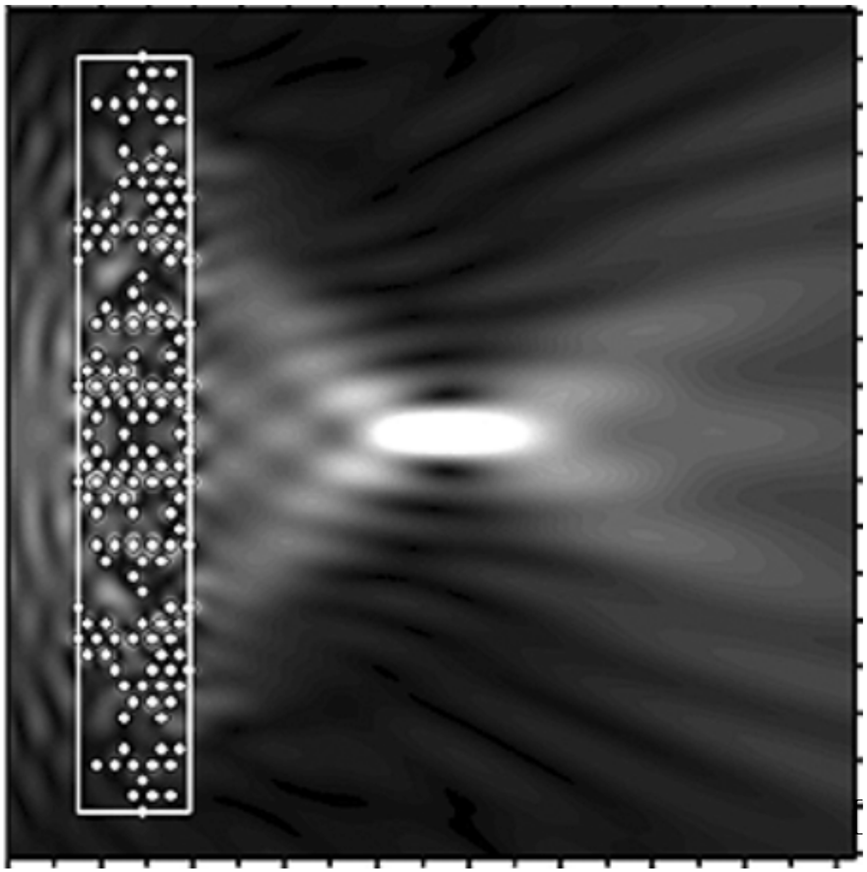
Byun, IEEE Trans. Magnetics 43, 1573 (2007)



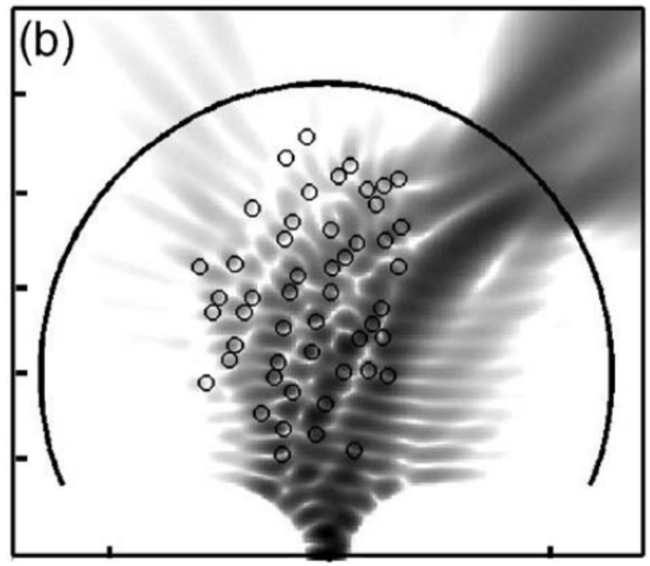
2d TM gap (Δw)
bands 3 & 4

He et al.,
J. Comput. Phys. **225**, 891 (2007)

Optimization with many discrete degrees of freedom



2d TM “lens” design
genetic algorithms: moving cylinders around
[Håkansson, IEEE J. Sel. Ar. Commun. **23**, 1365 (2005)



2d TM “bender”
moving cylinders around
(steepest-descent)
[Seliger, J. Appl. Phys. **100**, 034310 (2006)]

Outline

- Brief overview/examples of large-scale optimization work in photonics
- Overview of optimization terminology, problem types, and techniques.
- Some more detailed photonics examples.

A general optimization problem

$$\min_{x \in \mathbb{R}^n} f_0(x)$$

subject to m constraints

$$f_i(x) \leq 0$$

$$i = 1, 2, \ldots, m$$

x is a *feasible point* if it satisfies all the constraints

feasible region = set of all feasible x

minimize an objective function f_0 with respect to n design parameters x
(also called *decision parameters*, *optimization variables*, etc.)

— note that *maximizing* $g(x)$ corresponds to $f_0(x) = -g(x)$

note that an *equality constraint*

$$h(x) = 0$$

yields two inequality constraints

$$f_i(x) = h(x) \text{ and } f_{i+1}(x) = -h(x)$$

(although, in practical algorithms, equality constraints typically require special handling)

Important considerations

- *Global* versus *local* optimization
- *Convex* vs. non-convex optimization
- Unconstrained or box-constrained optimization, and other special-case constraints
- Special classes of functions (linear, etc.)
- Differentiable vs. non-differentiable functions
- Gradient-based vs. derivative-free algorithms
- …
- Zillions of different algorithms, usually restricted to various special cases, each with strengths/weaknesses

Global vs. Local Optimization

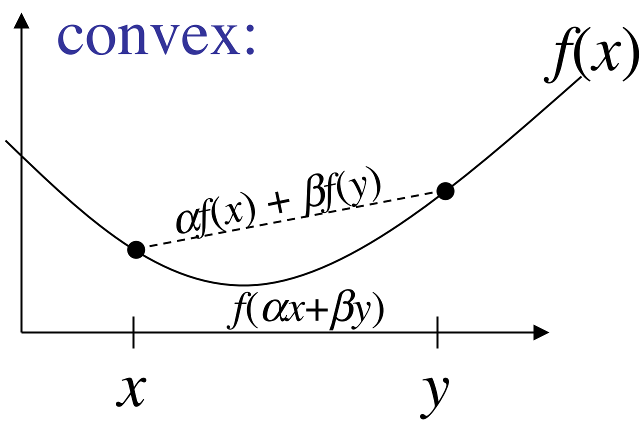
- For *general nonlinear* functions, *most* algorithms only guarantee a local optimum
  - that is, a feasible x_o such that $f_0(x_o) \leq f_0(\mathrm{x})$ for all feasible x within some neighborhood $\|x - x_o\| < R$ (for some small R)
- A *much harder* problem is to find a global optimum: the minimum of f_0 for *all* feasible x
  - exponentially increasing difficulty with increasing n, practically impossible to *guarantee* that you have found global minimum without knowing some special property of f_0
  - many available algorithms, problem-dependent efficiencies
    - *not* just genetic algorithms or simulated annealing (which are popular, easy to implement, and thought-provoking, but usually *very slow*!)
    - for example, non-random systematic search algorithms (e.g. DIRECT), partially randomized searches (e.g. CRS2), repeated local searches from different starting points ("multistart" algorithms, e.g. MLSL), …

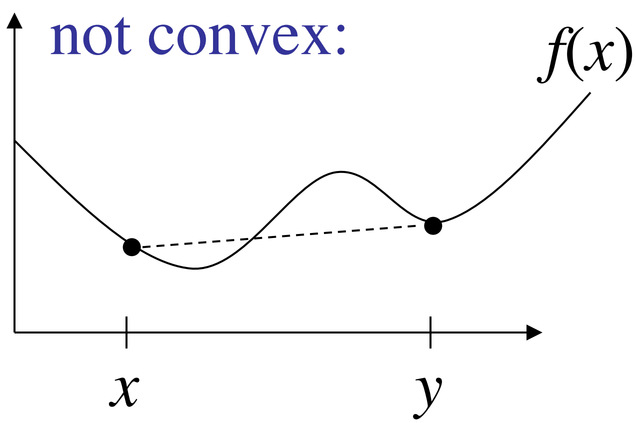
Convex Optimization

[good reference: *Convex Optimization* by Boyd and Vandenberghe, free online at www.stanford.edu/~boyd/cvxbook]

All the functions f_i (i=0…m) are *convex*:

$$f_i(\alpha x + \beta y) \leq \alpha f_i(x) + \beta f_i(y) \quad \text{where} \quad \begin{array}{c} \alpha + \beta = 1 \\ \alpha, \beta \in [0,1] \end{array}$$





For a convex problem (convex objective & constraints)
any local optimum *must* be a global optimum
⇒ efficient, robust solution methods available

Important Convex Problems

- LP (linear programming): the objective and constraints are *affine*: $f_i(x) = a_i^T x + \alpha_i$
- QP (quadratic programming): affine constraints + convexquadratic objective $x^T Ax+b^T x$
- SOCP (second-order cone program): LP + *cone* constraints $\|Ax+b\|_2 \leq a^T x + \alpha$
- SDP (semidefinite programming): constraints are that $\Sigma A_k x_k$ is positive-semidefinite

all of these have very efficient, specialized solution methods

Non-convex local optimization: a typical generic outline

[many, many variations in details !!!]

1 At current **x**, construct approximate model of f_i
—e.g. affine, quadratic, … often convex

2 Optimize the model problem ⇒ new **x**
— use a *trust region* to prevent large steps

3 Evaluate new **x**:
— if "acceptable," go to **1**
— if bad step (or bad model), update trust region / model and go to **2**

Important special constraints

- Simplest case is the *unconstrained* optimization problem: m=0
  - e.g., line-search methods like steepest-descent, nonlinear conjugate gradients, Newton methods …
- Next-simplest are *box constraints* (also called *bound constraints*): $x_k^{\min} \leq x_k \leq x_k^{\max}$
  - easily incorporated into line-search methods and many other algorithms
  - many algorithms/software *only* handle box constraints
- …
- Linear equality constraints $Ax=b$
  - for example, can be explicitly eliminated from the problem by writing $x=Ny+x$, where x is a solution to $Ax=b$ and N is a basis for the nullspace of A

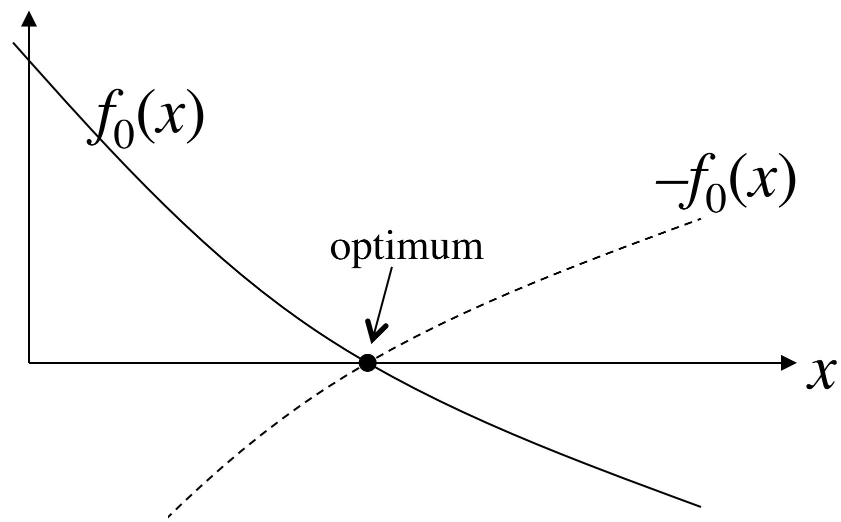
Derivatives of f_i

- Most-efficient algorithms typically require user to supply the gradients $\nabla_x f_i$ of objective/constraints
  - you should *always* compute these analytically
    - rather than use finite-difference approximations, better to just use a derivative-free optimization algorithm
    - in principle, one can always compute $\nabla_x f_i$ with about the same cost as f_i, using adjoint methods
  - gradient-based methods can find (local) optima of problems with millions of design parameters
- Derivative-free methods: only require f_i values
  - easier to use, can work with complicated "black-box" functions where computing gradients is inconvenient
  - *may* be only possibility for nondifferentiable problems
  - need $> n$ function evaluations, bad for large n

Removable non-differentiability

consider the *non*-differentiable *unconstrained* problem:

$$\min_{x \in \mathbb{R}^n} \left| f_0(x) \right|$$



equivalent to *minimax* problem:

$$\min_{x \in \mathbb{R}^n} \left(\max \left\{ f_0(x), -f_0(x) \right\} \right)$$

…still nondifferentiable…

…equivalent to *constrained* problem with a "temporary" variable *t*:

differentiable!

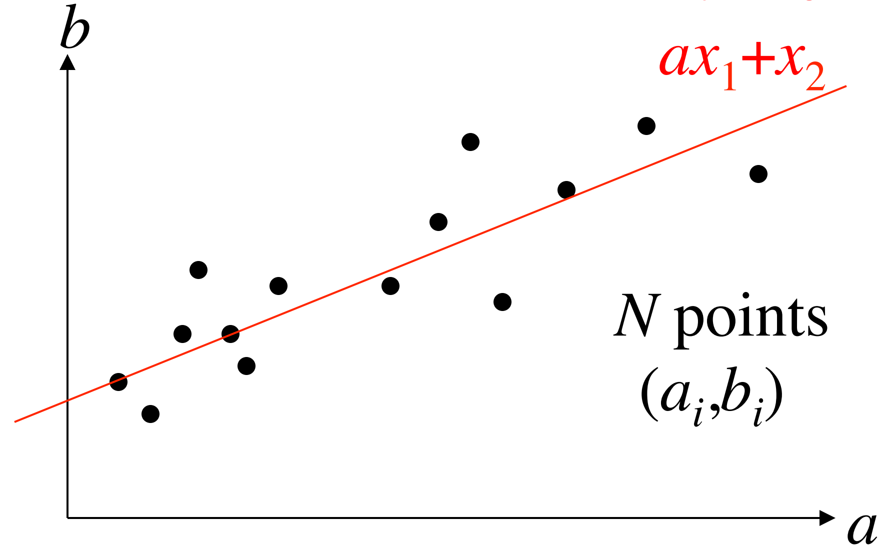
$$\min_{x \in \mathbb{R}^n, t \in \mathbb{R}} t \quad \text{subject to:} \quad \begin{array}{ll} t \geq f_0(x) & \left(f_1(x) = f_0(x) - t \right) \\ t \geq -f_0(x) & \left(f_2(x) = -f_0(x) - t \right) \end{array}$$

Example: Chebyshev linear fitting

find the fit that minimizes
the *maximum error*:

$$\min_{x_1, x_2} \left(\max_i \left| x_1 a_i + x_2 - b_i \right| \right)$$

… nondifferentiable minimax problem



equivalent to a *linear programming* problem (LP):

$$\min_{x_1, x_2, t} t$$

subject to $2N$ constraints:

$$x_1 a_i + x_2 - b_i - t \leq 0$$

$$b_i - x_1 a_i - x_2 - t \leq 0$$

Gap Optimization via nonlinear constraints

we want:

$$\max_{\varepsilon}\left(2\frac{\left[\min_{\mathbf{k}}\omega_{n+1}(\mathbf{k})\right]-\left[\max_{\mathbf{k}}\omega_{n}(\mathbf{k})\right]}{\left[\min_{\mathbf{k}}\omega_{n+1}(\mathbf{k})\right]+\left[\max_{\mathbf{k}}\omega_{n}(\mathbf{k})\right]}\right)$$

not differentiable at accidental degeneracies

an equivalent problem:

$$\max_{\varepsilon}\left(2\frac{f_2-f_1}{f_2+f_1}\right)$$

subject to:

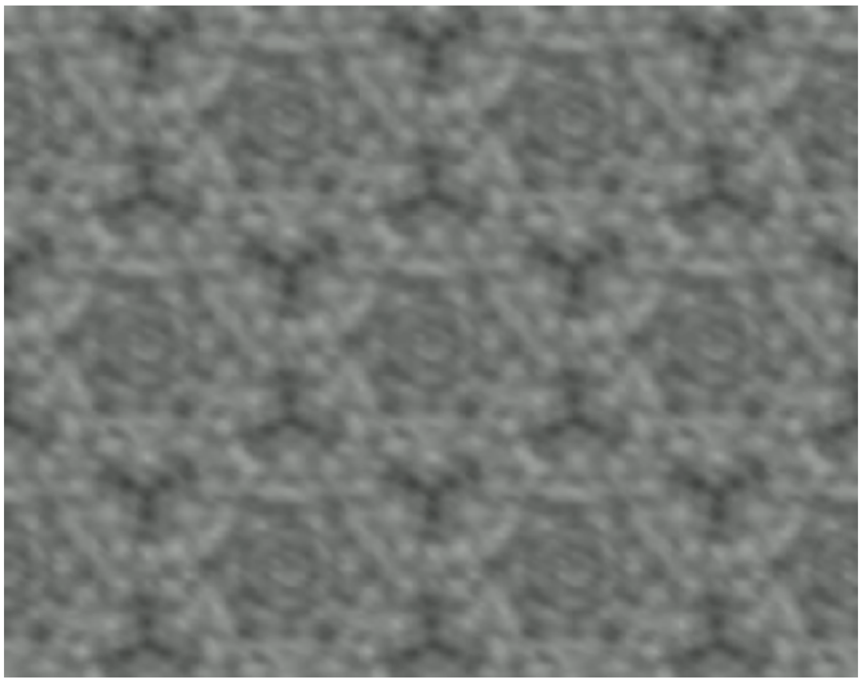
…with (mostly) differentiable nonlinear constraints:

$$f_1 \geq \omega_n(\mathbf{k})$$

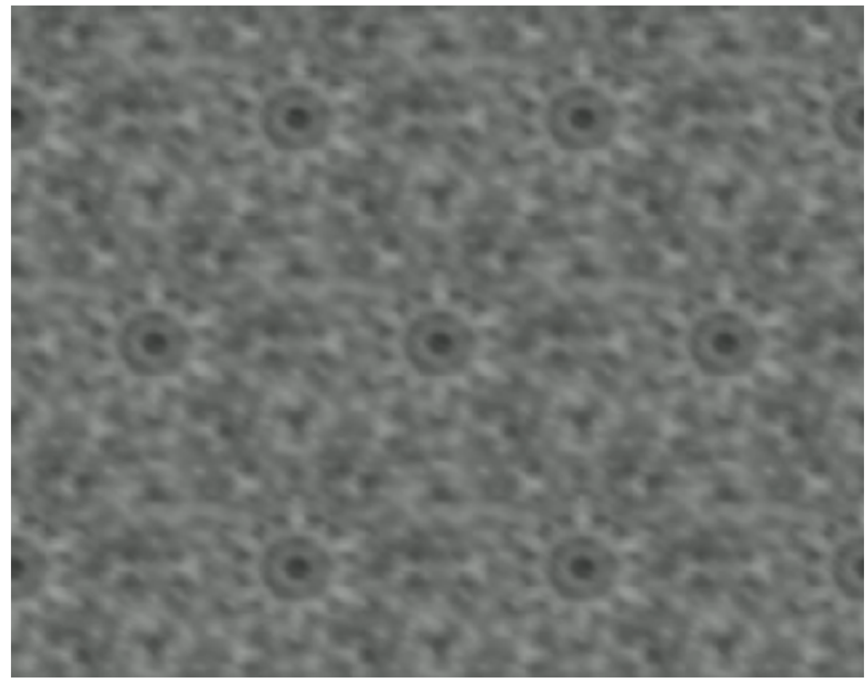
$$f_2 \leq \omega_{n+1}(\mathbf{k})$$

Optimizing 1st TM and TE gaps

for a triangular lattice with 6-fold symmetry (between bands 1 & 2)



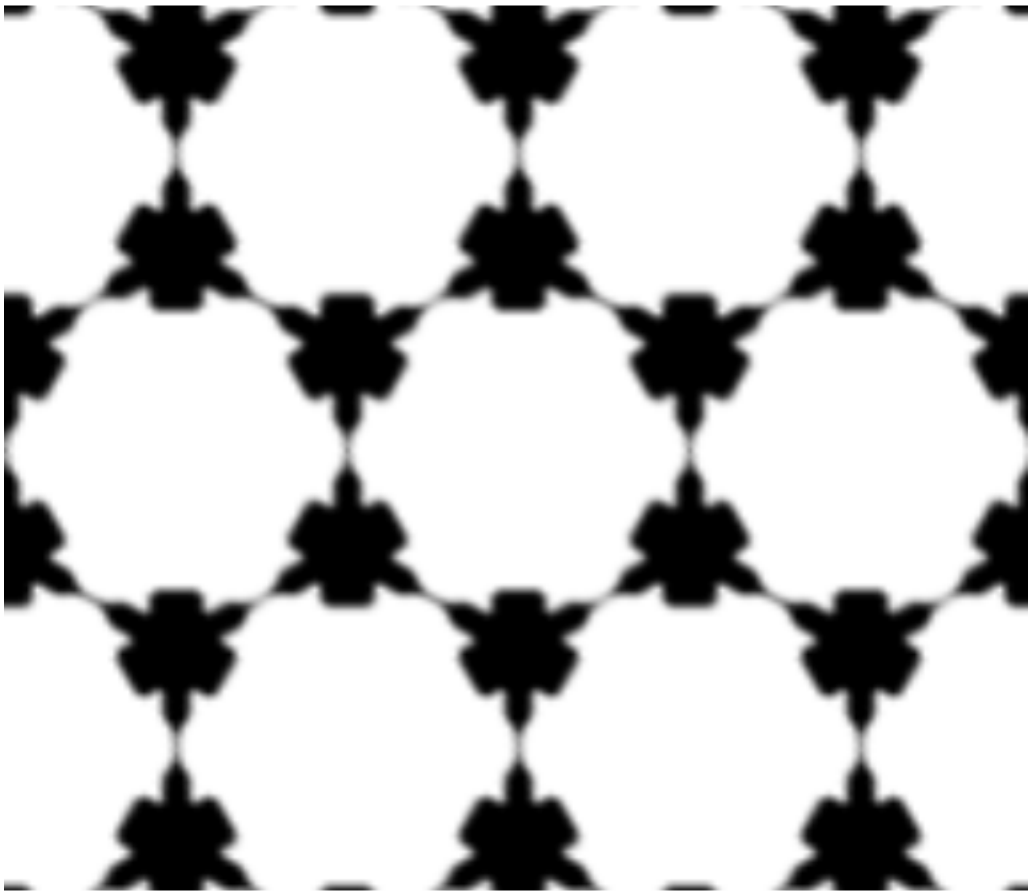
48.3% TM gap (ϵ = 12:1)



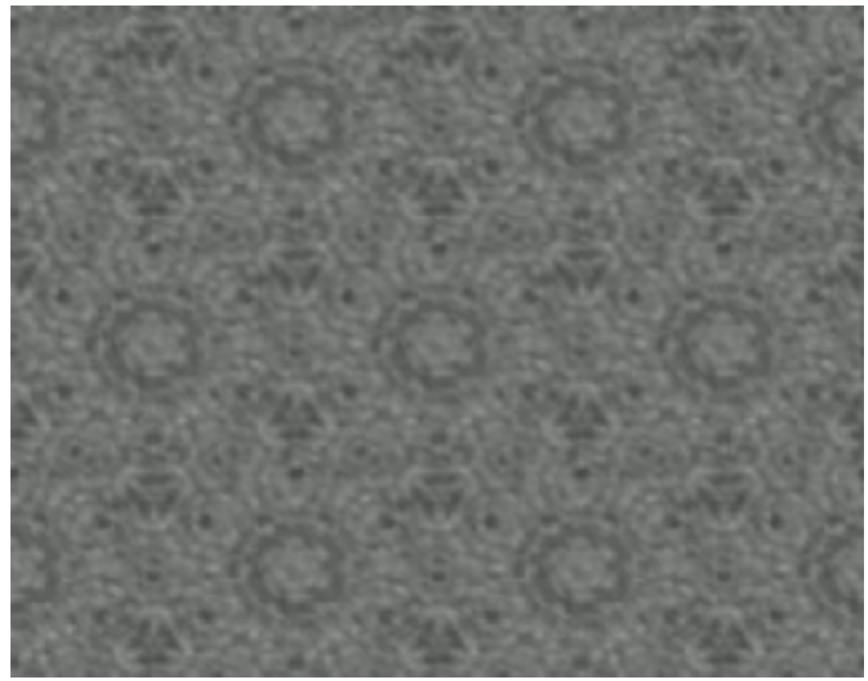
51.4% TE gap (ϵ = 12:1)

30 iterations of optimizer

Optimizing 1st complete (TE +TM) 2d gap

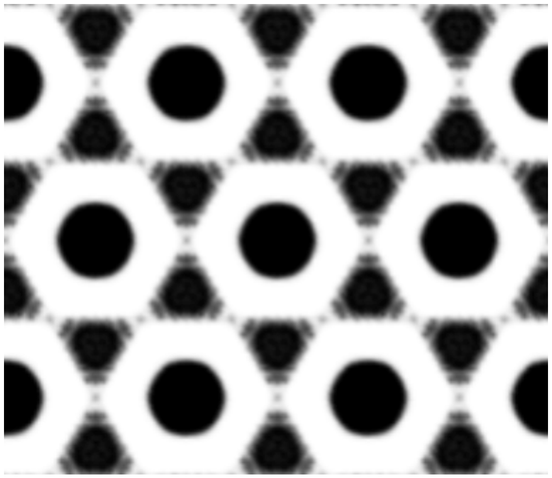


21.1% gap (e = 12:1)



20.7% gap (e = 12:1)

+ some local minima



–0.5% gap

–2% gap

–10% gap

good news: only a handful of minima (in 10^3-dimensional space!)

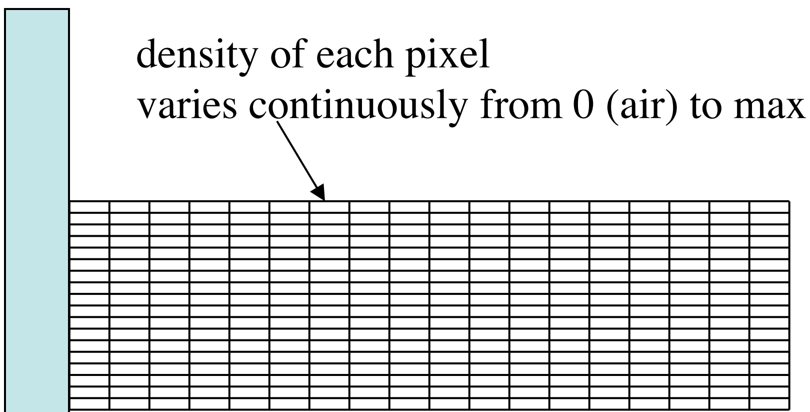
Relaxations of Integer Programming

If x is integer-valued rather than real-valued (e.g. $x \in \{0,1\}^n$), the resulting *integer programming* or *combinatorial optimization* problem becomes *much harder* in general (often NP-complete).

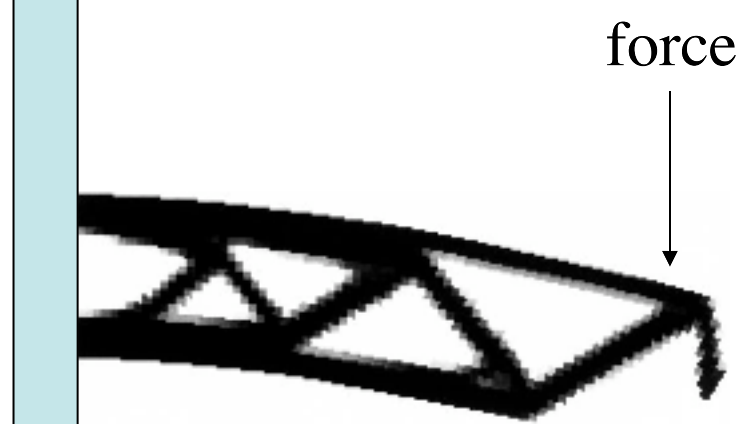
However, useful results can often be obtained by a *continuous relaxation* of the problem — e.g., going from $x \in \{0,1\}^n$ to $x \in [0,1]^n$
… at the very least, this gives an lower bound on the optimum f_0
… and penalty methods (e.g. SIMP) can be used to gradually eliminate intermediate x values.

Early Topology Optimization

design a structure to do something, made of material A or B…
let *every pixel* of discretized structure vary *continuously* from A to B



ex: design a cantilever
to support maximum weight
with a fixed amount of material



optimized structure,
deformed under load

[Buhl *et al*, *Struct. Multidisc. Optim.* **19**, 93–104 (2000)]

Some Sources of Software

- Decision tree for optimization software:
  http://plato.asu.edu/guide.html
  — lists many packages for many problems

- CVX: general convex-optimization package
  http://www.stanford.edu/~boyd/cvx

- NLopt: implements many nonlinear optimization algorithms
  (global/local, constrained/unconstrained, derivative/no-derivative)
  http://ab-initio.mit.edu/nlopt

Outline

- Brief overview/examples of large-scale optimization work in photonics

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Key questions occur *before* choosing optimization algorithm:

- How to parameterize the degrees of freedom
  — how much knowledge of solution to build in?

- Which objective function & constraints?
  — many choices for a given design goal,

… can make an enormous difference in the
computational feasibility
& the robustness of the result.

Today: Three Examples

- Optimizing photonics without solving Maxwell's equations
  — transformational inverse design

- Ensuring manufacturability of narrow-band devices
  — robust optimization in photonics design

- Optimizing eigenvalues without eigensolvers
  — microcavity design and the
  frequency-averaged local density of states

Today: Three Examples

- Optimizing photonics without solving Maxwell's equations
  — transformational inverse design

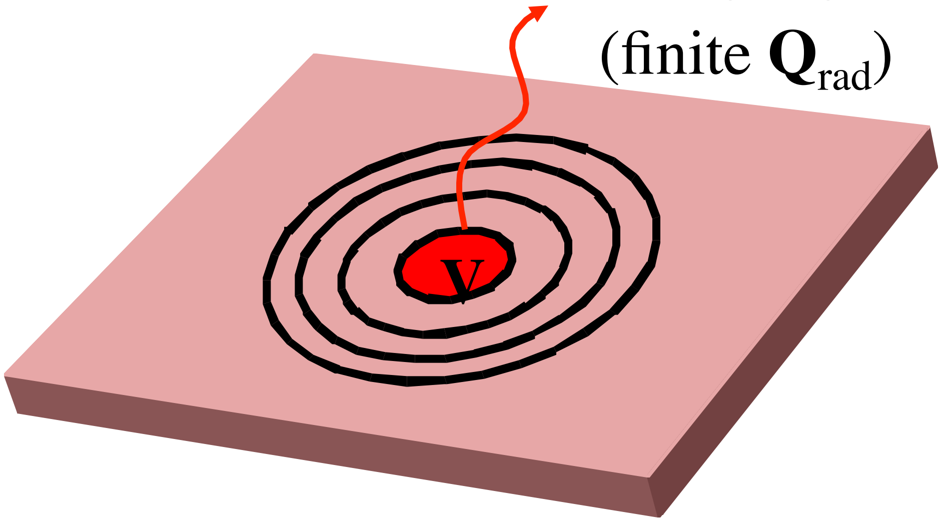
- Ensuring manufacturability of narrow-band devices
  — robust optimization in photonics design

- Optimizing eigenvalues without eigensolvers
  — microcavity design and the
  frequency-averaged local density of states

[X. Liang *et al*., manuscript in preparation]

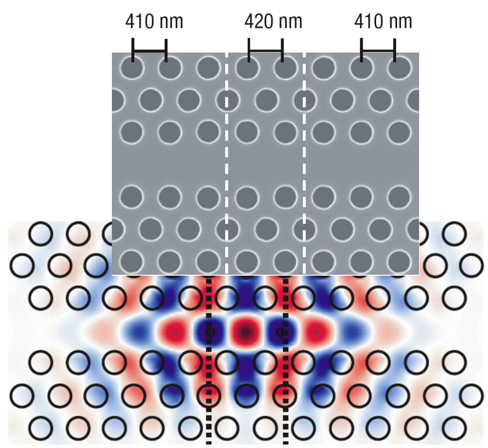
3d Microcavity Design Problem

radiation loss
(finite $\mathbf{Q}_{rad}$)



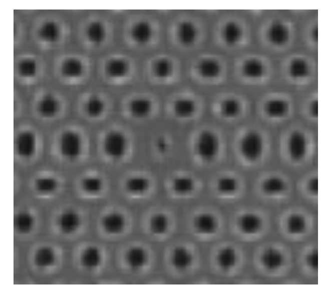
Want some 2d pattern
that will confine light in 3d
with maximal lifetime (“Q_{rad}”)
and minimal modal volume (“V”)

Many *ad hoc* designs,
trading off Q_{rad} and V…

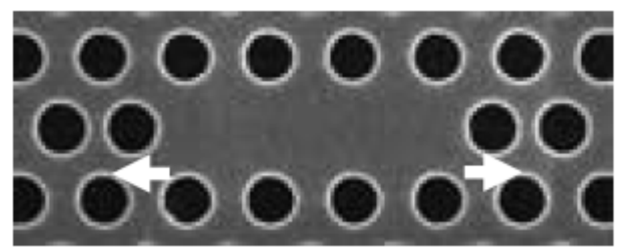


[Song, (2005)]

[Loncar, 2002]



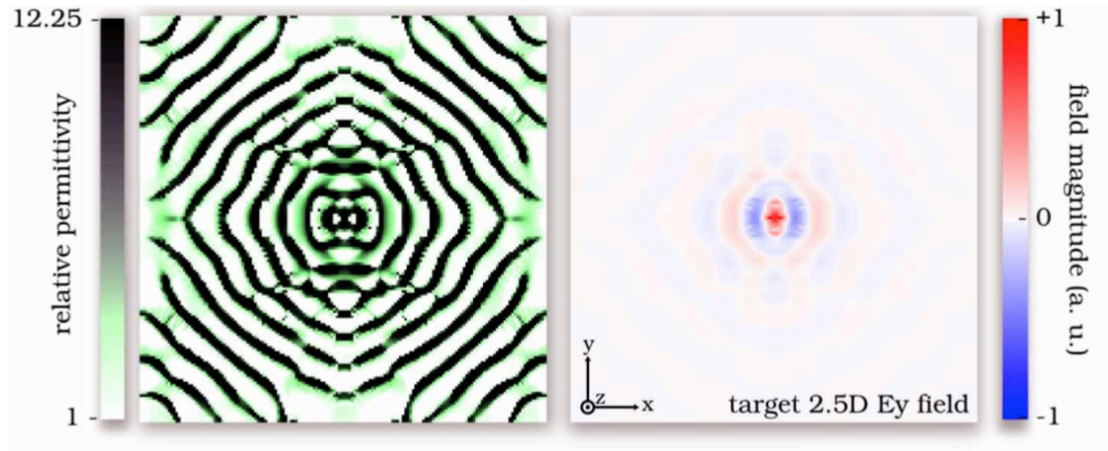
(“defects”
in periodic
structures)



[Akahane, 2003]

Topology optimization? Mostly 2d…

[Kao and Santosa, 2008]
in-plane *Q*, no *V*



Vuckovic (2011): ~ min *V*
2d heuristic for the radiation loss

Can we formulate a *practical* approach to solve the *full* problem, computing the *true* 3d radiation loss?

Goals: understand ultimate limits on cavity performance,
& eventually push cavity design into new regimes

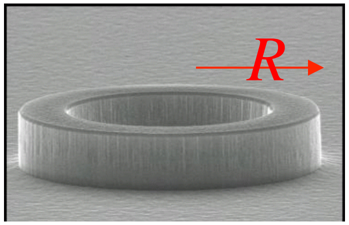
Not just maximizing Q or Q/V!

Typical figure of merit is "Purcell factor" Q/V
(~ enhancement of light-matter coupling)

$$V = \frac{\int \varepsilon |\mathbf{E}|^2}{\max \varepsilon |\mathbf{E}|^2}$$

Naively, should we maximize Q/V?

☹ Trivial design problem: maximum $Q/V = \infty$
[e.g. perfect ring resonator of ∞ radius]



$V \sim R$

$Q_{\text{rad}} \sim \exp(\# R)$

Real design problem:

maximize Q
such that $V \leq V_0$

or

minimize V
such that $Q \geq Q_0$

set by bandwidth, loss tolerance,
& fabrication capabilities

Transforming the problem…

a series of nonobvious transformations makes the problem *much easier*

minimize modal volume V
subject to $Q \geq Q_0$

↓

Maximize mean LDOS (local density of states)
(= power of dipole)
over bandwidth ω_0/Q_0

↓

Maximize LDOS at complex $\omega=\omega_0(1+i/2Q_0)$

↓

Minimize 1/LDOS at $\omega_0(1+i/2Q_0)$

turn difficult eigenproblem into easier scattering problem: Q/V is really just LDOS

complex analysis: contour integration + causality

technical issue: avoid optimizing along "narrow ridge" (avoid ill-conditioned Hessian)

LDOS: Local Density of States

[review: arXiv:1301.5366]

Maxwell eigenproblem:

$$\frac{1}{\varepsilon}\nabla\times\frac{1}{\mu}\nabla\times\boldsymbol{E} \triangleq \Theta\boldsymbol{E} = \omega^2\boldsymbol{E}$$

$$\langle\boldsymbol{E},\boldsymbol{E}'\rangle = \int\boldsymbol{E}^*\cdot\varepsilon\boldsymbol{E}'$$

Maxwell vector-Helmholtz:

$$\boldsymbol{E} = i\omega(\Theta-\omega^2)^{-1}\varepsilon^{-1}\boldsymbol{J}$$

Power radiated by a current **J** (Poynting's theorem)

$$P = -\frac{1}{2}\mathrm{Re}\int\boldsymbol{E}^*\cdot\boldsymbol{J}\,d^3\boldsymbol{x} = -\frac{1}{2}\mathrm{Re}\langle\boldsymbol{E},\varepsilon^{-1}\boldsymbol{J}\rangle$$

special case of a dipole source: LDOS

$$\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{e}_\ell\,\delta(\boldsymbol{x}-\boldsymbol{x}_0)$$

$$\mathrm{LDOS}_\ell(\boldsymbol{x}_0,\omega) = \frac{4}{\pi}\varepsilon(\boldsymbol{x}_0)P_\ell(\boldsymbol{x}_0,\omega)$$

Why a "density of states"

[review: arXiv:1301.5366]

consider a
finite domain
(periodic/Dirichlet)
+ small absorption

$$\frac{1}{\varepsilon}\nabla\times\frac{1}{\mu}\nabla\times\boldsymbol{E} \triangleq \Theta\boldsymbol{E} = \omega^2\boldsymbol{E}$$

$$\langle\boldsymbol{E},\boldsymbol{E}'\rangle = \int\boldsymbol{E}\cdot\varepsilon\boldsymbol{E}'$$

countable eigenfunctions
$\mathbf{E}^{(n)}$ and frequencies $\omega^{(n)}$ $+\, i\gamma^{(n)}$

$$\boldsymbol{E} = i\omega(\Theta-\omega^2)^{-1}\varepsilon^{-1}\boldsymbol{J}$$

$$P = -\frac{1}{2}\mathrm{Re}\langle\boldsymbol{E},\varepsilon^{-1}\boldsymbol{J}\rangle$$

$$\varepsilon^{-1}\boldsymbol{J} = \sum_n \boldsymbol{E}^{(n)}\langle\boldsymbol{E}^{(n)},\varepsilon^{-1}\boldsymbol{J}\rangle$$

loss → 0: a localized measure of spectral density

$$\mathrm{LDOS}_\ell(\boldsymbol{x},\omega) = \sum_n \delta\left(\omega-\omega^{(n)}\right)\varepsilon(\boldsymbol{x})\left|E_\ell^{(n)}(\boldsymbol{x})\right|^2$$

$$\mathrm{DOS}(\omega) = \sum_n \delta\left(\omega-\omega^{(n)}\right)$$

Minimize 1/LDOS at $\omega_0(1+i/2Q_0)$

…Let every pixel be a degree of freedom (ε in [1,12])

~ 10^5 degrees of freedom

…Solve with (mostly) standard methods:

FDFD solver (sparse-direct + GMRES)

adjoint sensitivity analysis

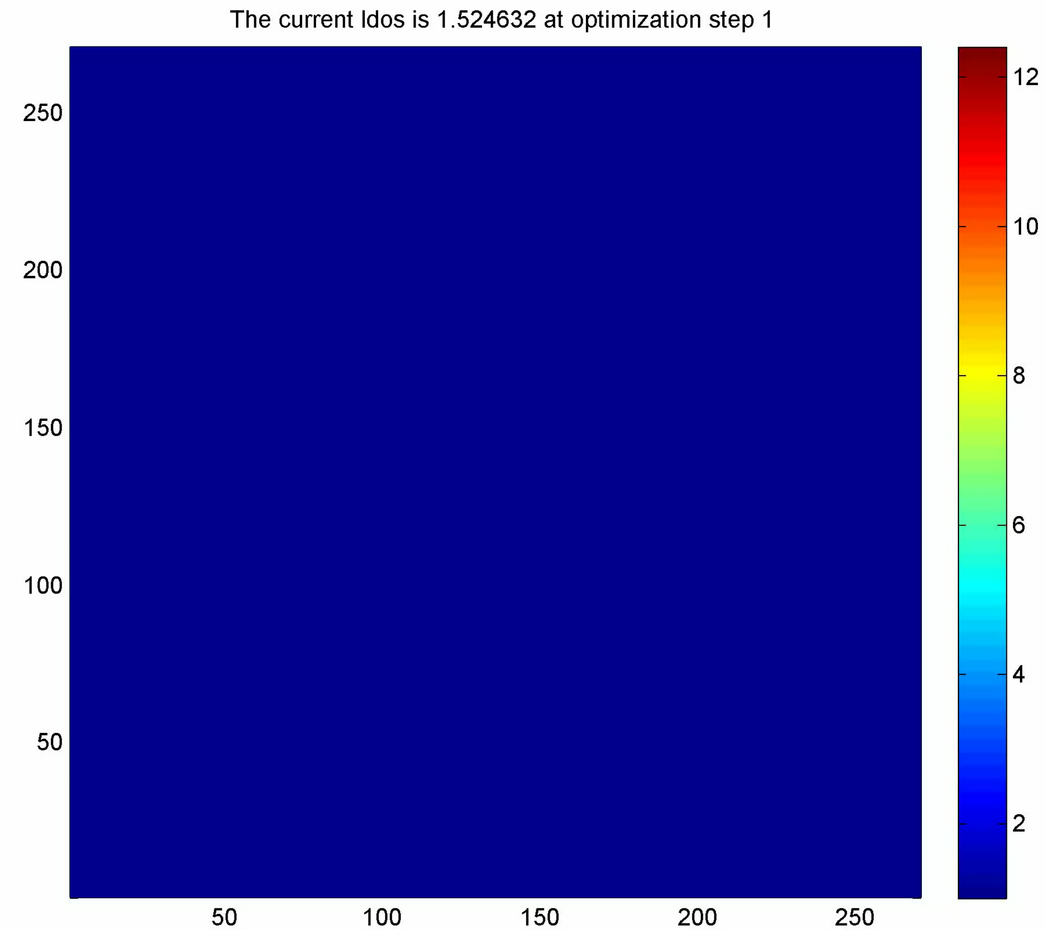
quasi-Newton optimization (L-BFGS)

Now, a few results…

2d test case: Out-of-plane **J**, starting from vacuum initial guess

finds
"Bragg onio
structure

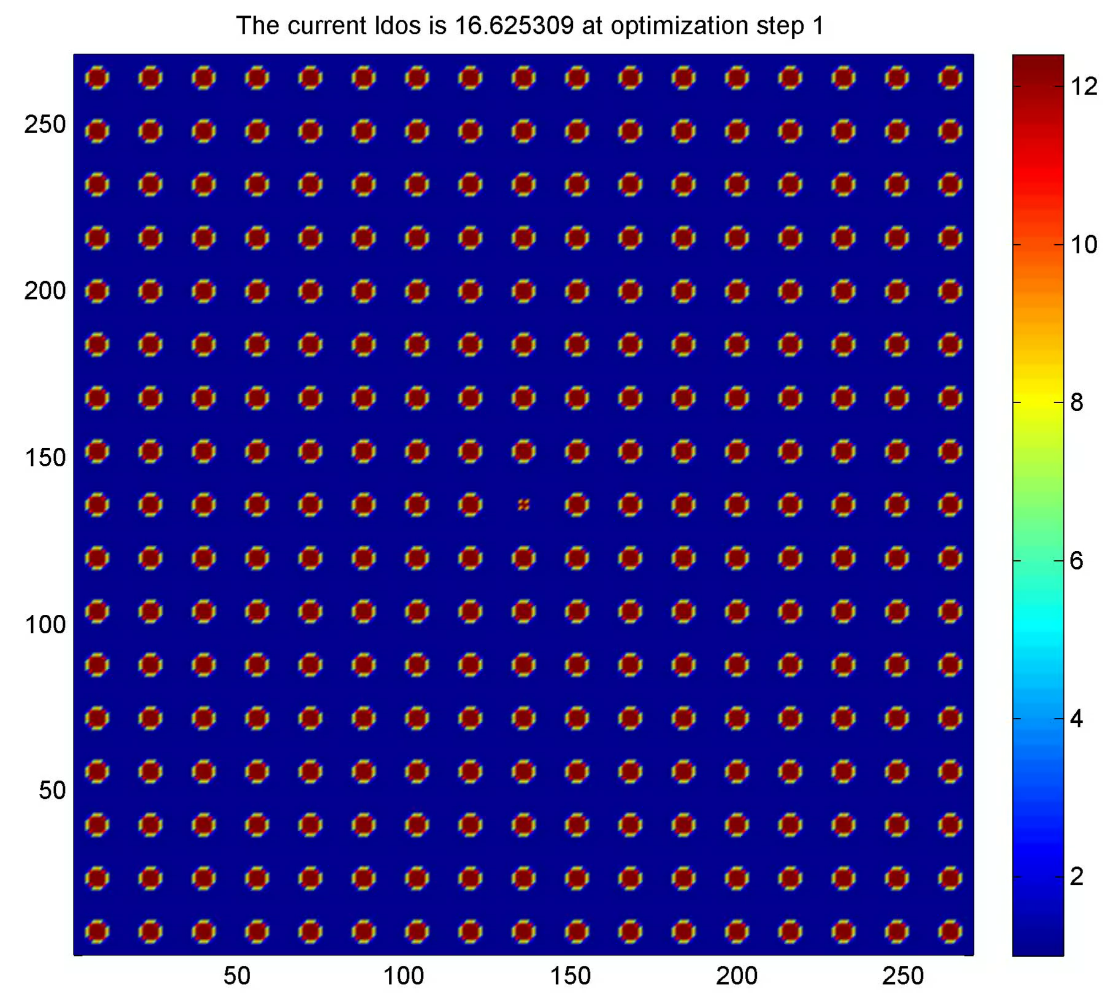
(No *Q* vs. *V*
tradeoff)



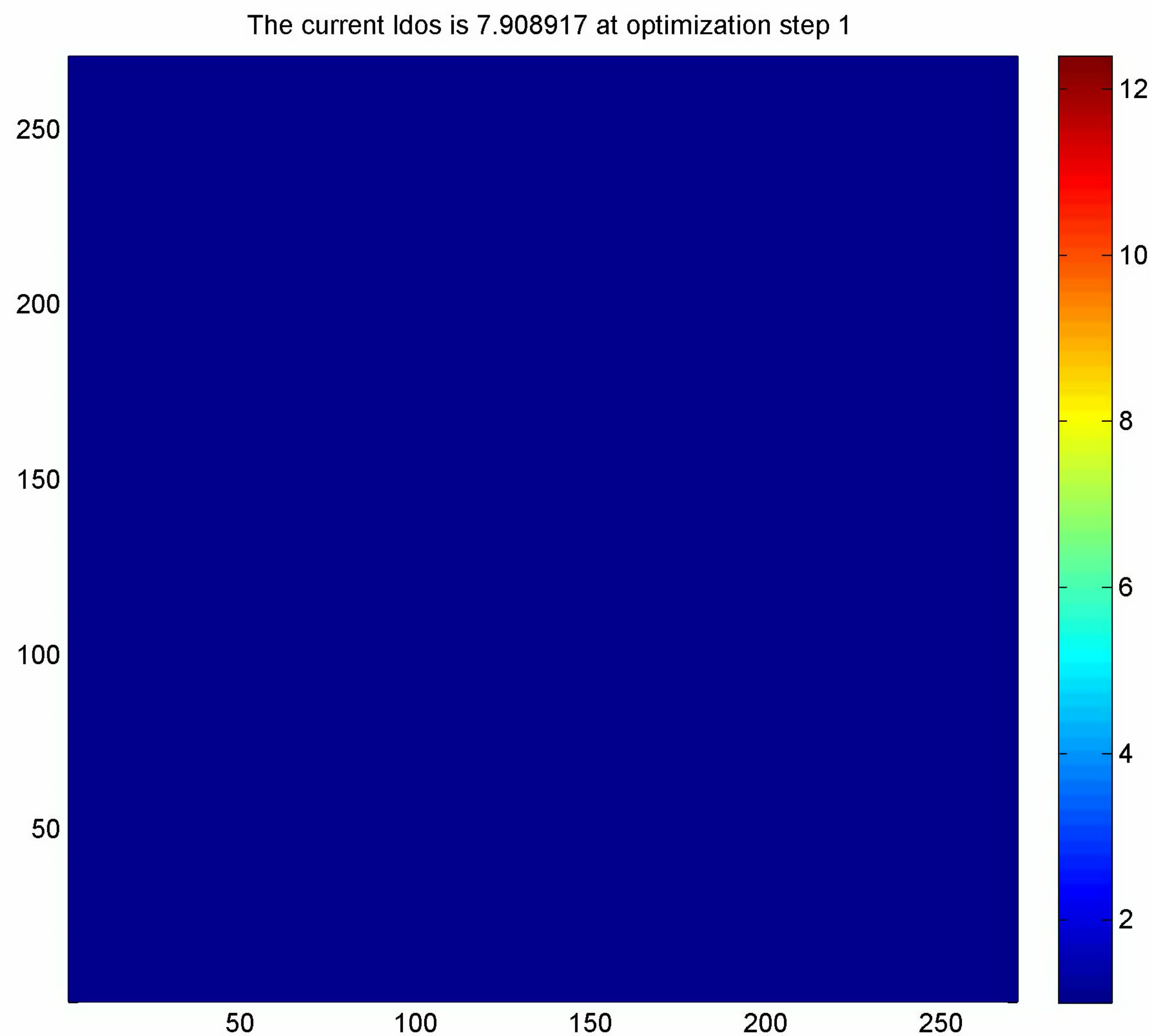
pixels
vary
[1,12]

2d test case: Out-of-plane **J**, starting from PhC initial guess

starting guess
has PhC resona
mode already,
but optimizatic
converts back
to Bragg onion

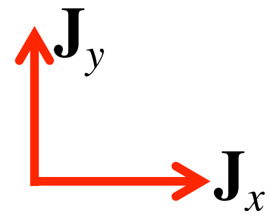


2d test case: In-plane J (breaks symmetry), starting from vacuum initial guess



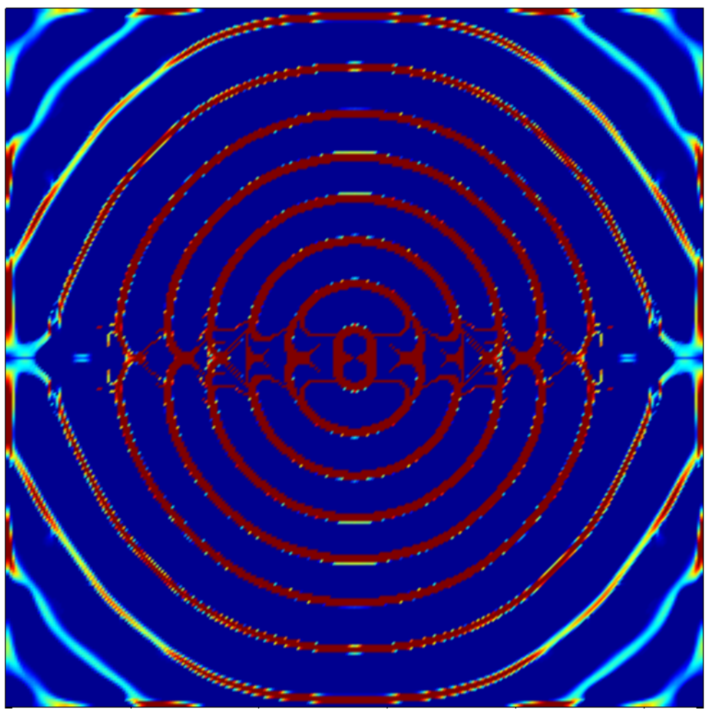
n-plane **J**

in-plane **J**

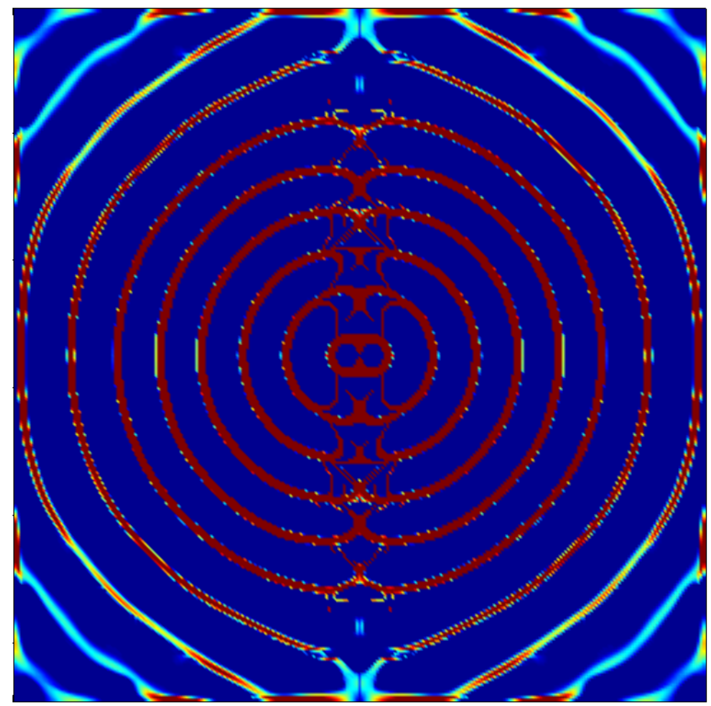


Maximizing LDOS for random in-plane J

$$= \max[\mathrm{LDOS}(\omega,\mathbf{J}_x)+\mathrm{LDOS}(\omega,\mathbf{J}_x)]/2$$



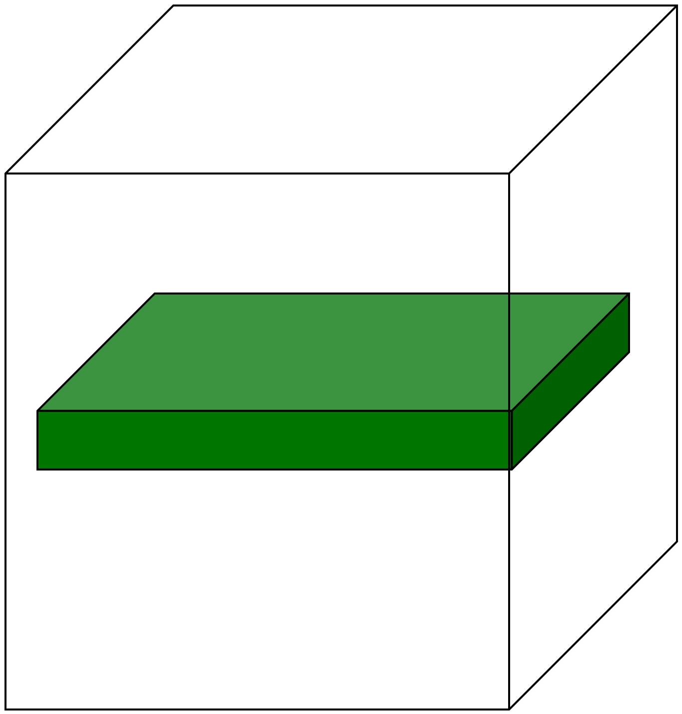
4 out of 10



6 out of 10

Spontaneous symmetry breaking! "Picks" one polarization randomly

3d results: Photonic-crystal slab



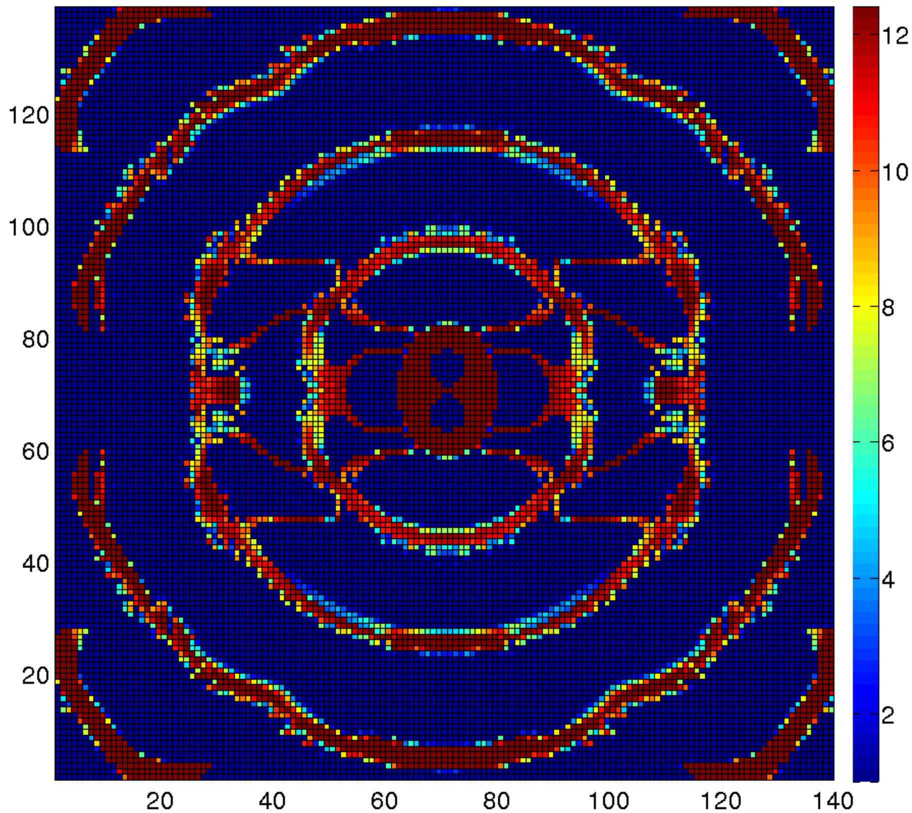
Optimize with $Q_0 = 10^4$

i.e. prefer $Q \geq 10^4$ but after that mainly minimize V

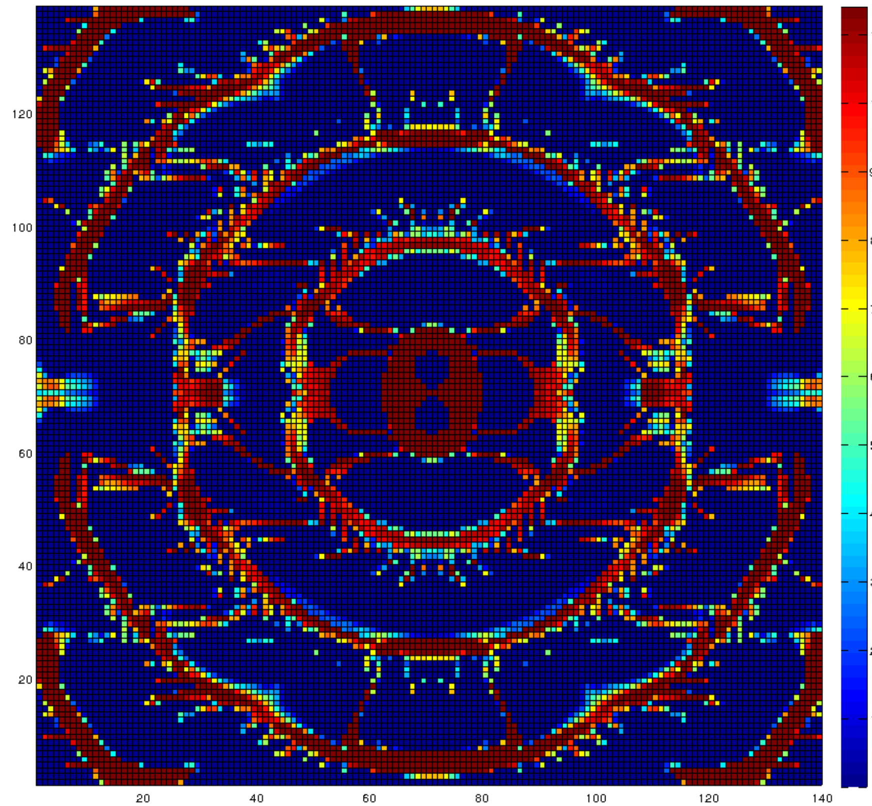
Next: 2d pattern in 3d slab

(including radiation loss via PML absorbing boundaries)

3d Slab Results



after deleting "hairs":
$Q \sim 10{,}000$
(without re-optimizing)



$Q \sim 30{,}000$, $V \sim 0.06(\lambda/\mathrm{n})^3$

vs. hand-optimized:

$Q \sim 100{,}000$, $V \sim 0.7(\lambda/\mathrm{n})^3$
$Q \sim 300{,}000$, $V \sim 0.2(\lambda/\mathrm{n})^3$
and others…

Today: Three Examples

- Optimizing photonics without solving Maxwell's equations
  — transformational inverse design

- Ensuring manufacturability of narrow-band devices
  — robust optimization in photonics design

[Oskooi *et al.*, *Optics Express* **20**, 21558 (2012).]
[Mutapcic *et al.*, *Engineering Optim*. (2009)]

- Optimizing eigenvalues without eigensolvers
  — microcavity design and the
  frequency-averaged local density of states

Robustness of optimized designs

a "nominal" optimization problem: $\underset{\textit{design parameters } \mathbf{p}}{\text{minimize}} \; \text{objective}(\mathbf{p})$

Robustness of optimized designs

a "nominal" optimization problem: $\underset{\textit{design parameters } \mathbf{p}}{\text{minimize}}$ objective($\mathbf{p}$,**0**)

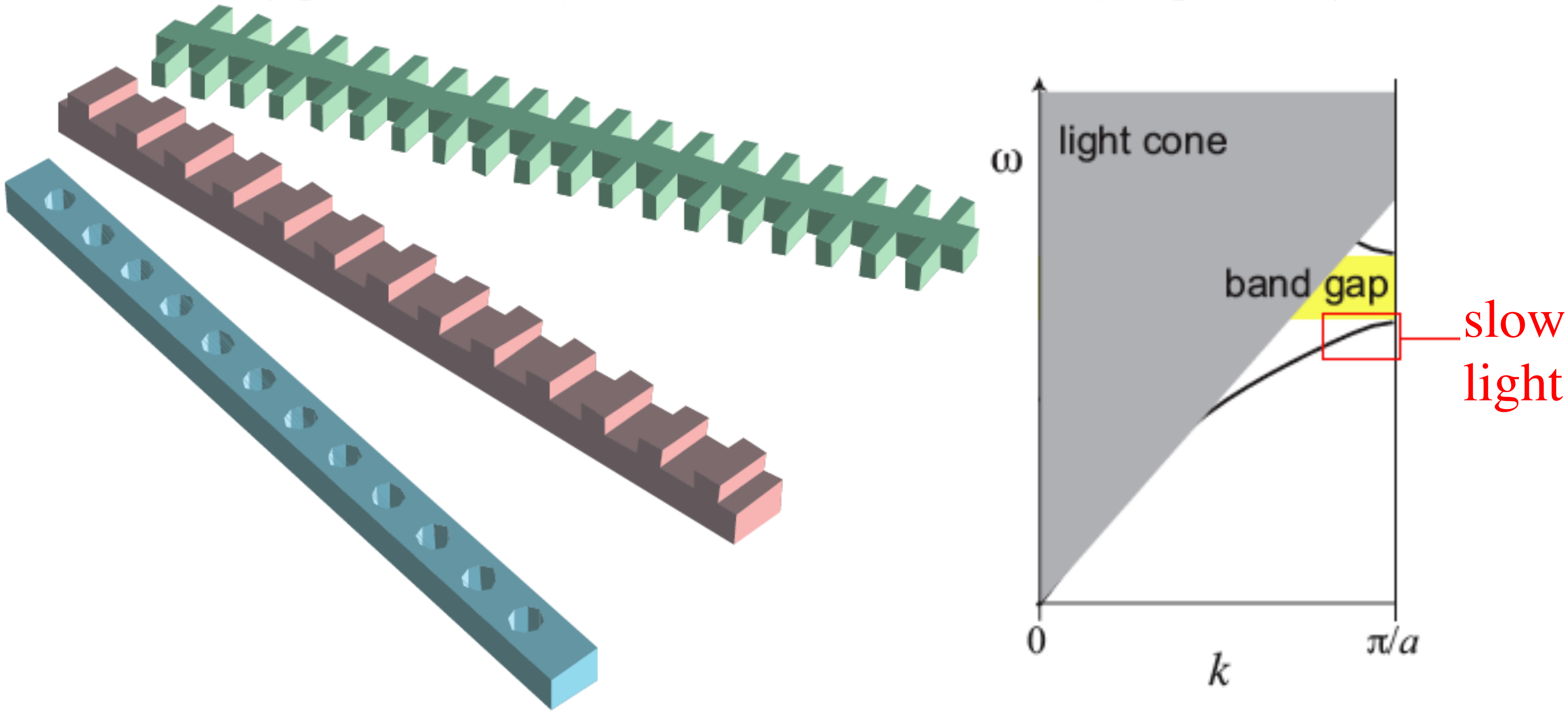
Problem: real objective is inexact, due to uncertainties
in modeling, fabrication, materials, etcetera
… is a function objective($\mathbf{p}$,$\mathbf{u}$) of $\mathbf{p}$
and unknown/uncertain parameters $\mathbf{u} \in U$

Problem: optimization sometimes finds solutions
that are "delicate" and destroyed by uncertainty
… i.e. objective($\mathbf{p}$, actual $\mathbf{u}$) >> objective($\mathbf{p}$,**0**)

… can easily happen in single-frequency wave-optics designs
where optimization finds a delicate interference effect…

Slow light

Any periodic waveguide has a band edge where group velocity → 0



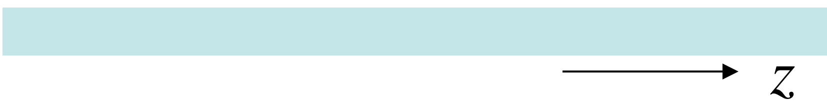
Enhances light-matter interactions, dispersion phenomena, tunable time delays
… but hard to couple to ordinary waveguide: large “impedance mismatch”

A slow-light optimization problem

[Povinelli, Johnson, Joannopoulos (2005)]

[Mutapcic, Boyd, Farjadpour, Johnson, Avniel (2009)]
[Oskooi *et al*., *Optics Express* **20**, 21558 (2012).]

going from uniform waveguide … to periodic waveguide



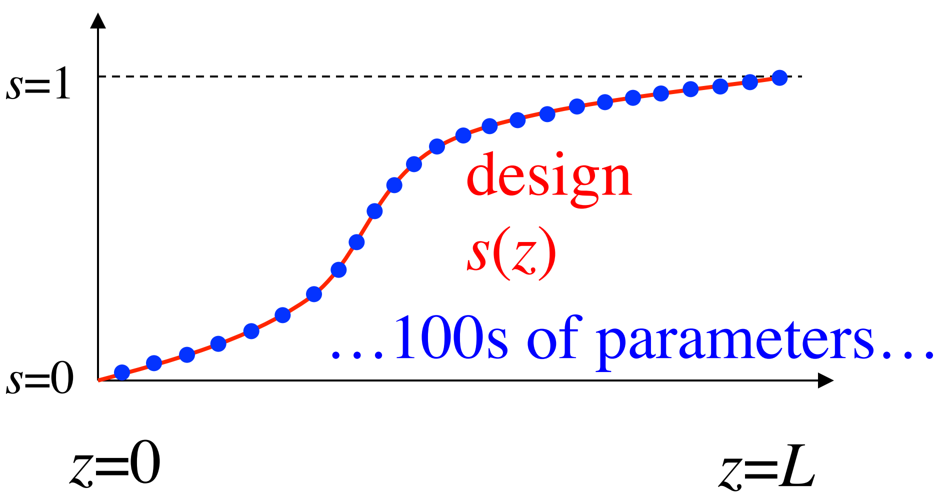
parameter $s = 0$

or

or

or…

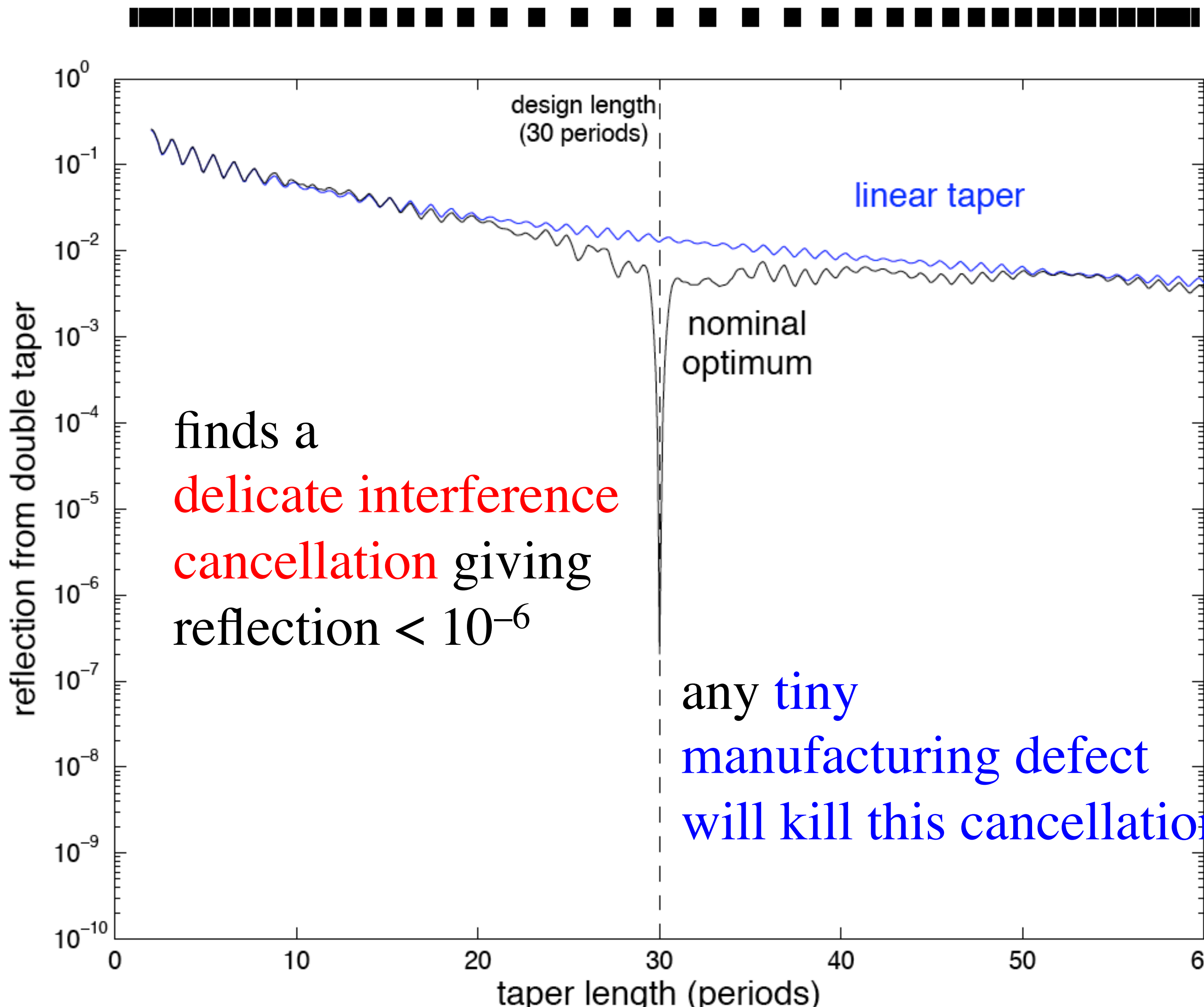
parameter $s = 1$
(e.g. s ~ flange width,
hole radius,
block width, …)



nominal problem:

Find $s(z)$ minimizing loss...

A nominal optimum

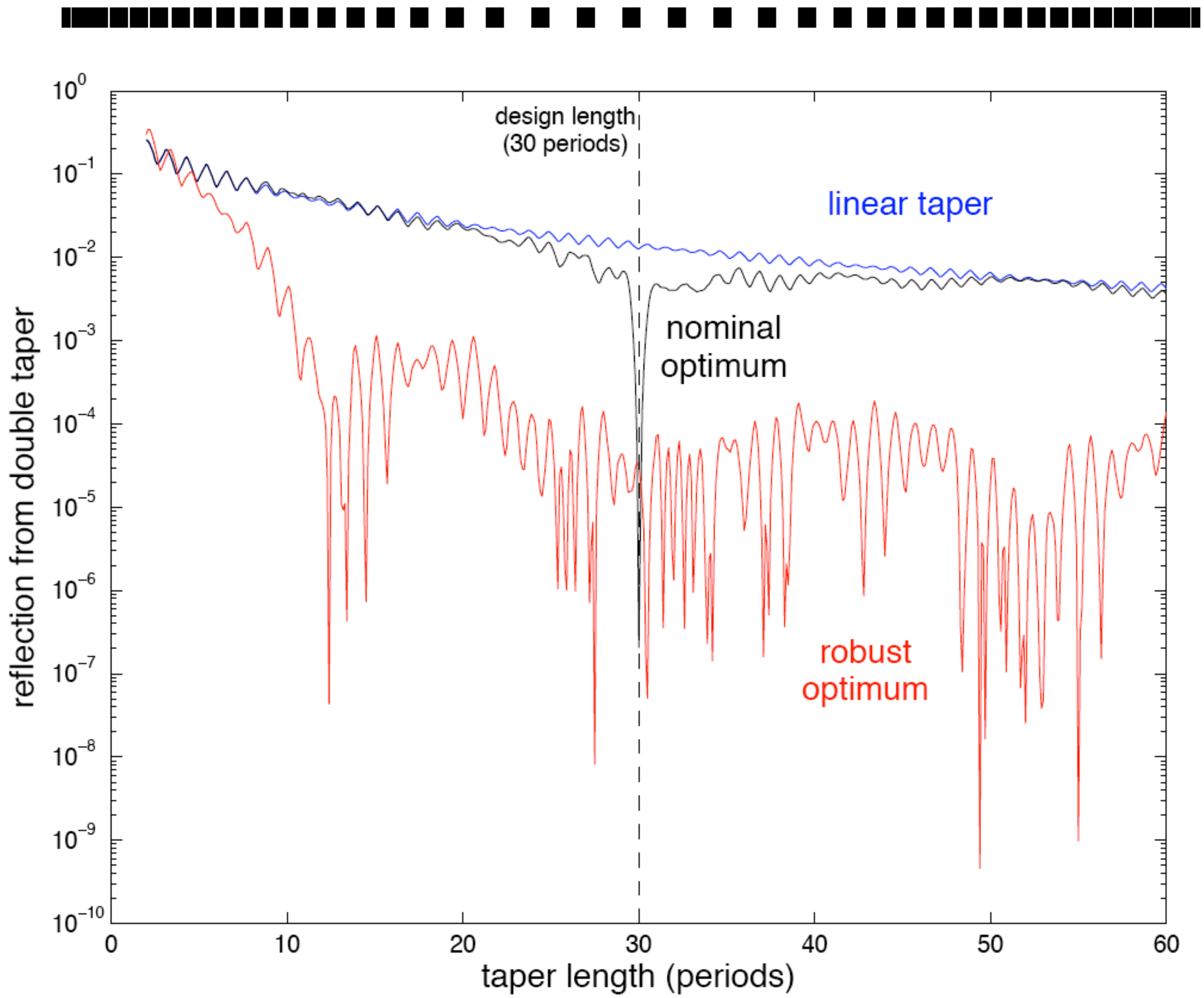


finds a delicate interference cancellation giving reflection < 10^{-6}

any tiny manufacturing defect will kill this cancellation

(stretching design taper — a simple perturbation)

The solution: Robust optimization
(worst-case minimax)



[Mutapcic, Boyd, Farjadpour, Johnson, Avniel (2009)]

- Minimize worst-case reflection:

$$\min_{s} \max_{u} R(s,u)$$

(manufacturing variation)

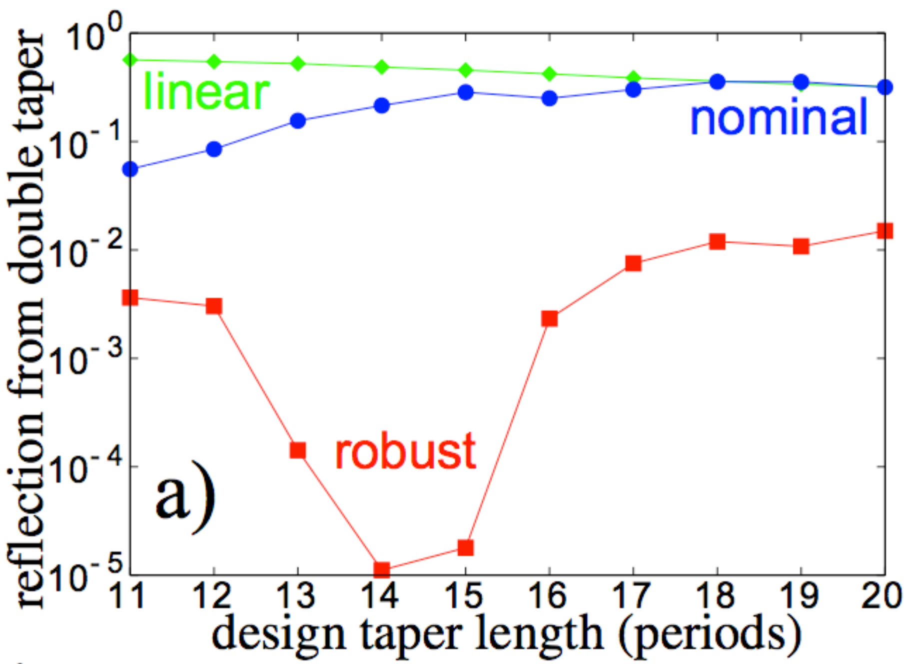
- Robust design still works when random disorder introduced:

brute-force results = 40× better than nominal optimum with surface roughness

A more realistic, slow-light structure

[Oskooi *et al*., *Optics Express* **20**, 21558 (2012).]

Slow-light waveguide for TE (in-plane polarization), tapers contain no narrow gaps, corresponds to contiguous, low-aspect ratio structure in 3d.
… Operate close to band edge, group velocity c/34.



(different design for each length)

In the presence of disorder, robust is orders of magnitude better than nominal optimum.

Nominal optimum is worthless: reflections > 10%.

Making taper too long makes things worse: disorder kills you.

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[Gabrielli, Liu, Johnson & Lipson, *Nature Commun*. (2012)]
[Liu *et al*., manuscript in preparation.]

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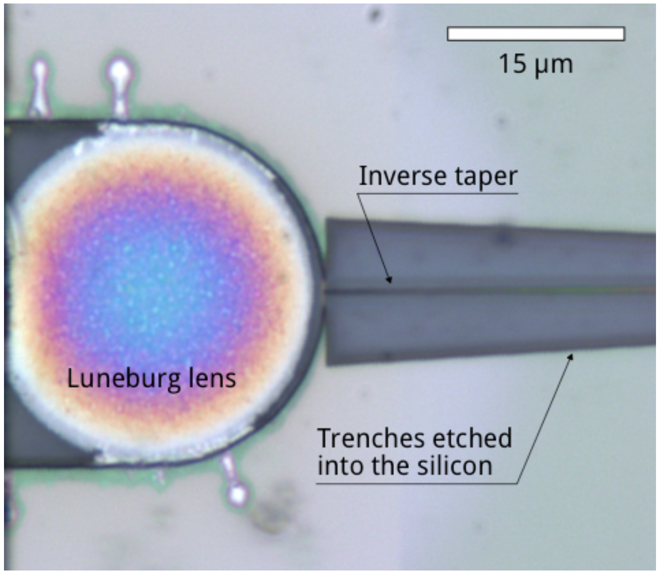
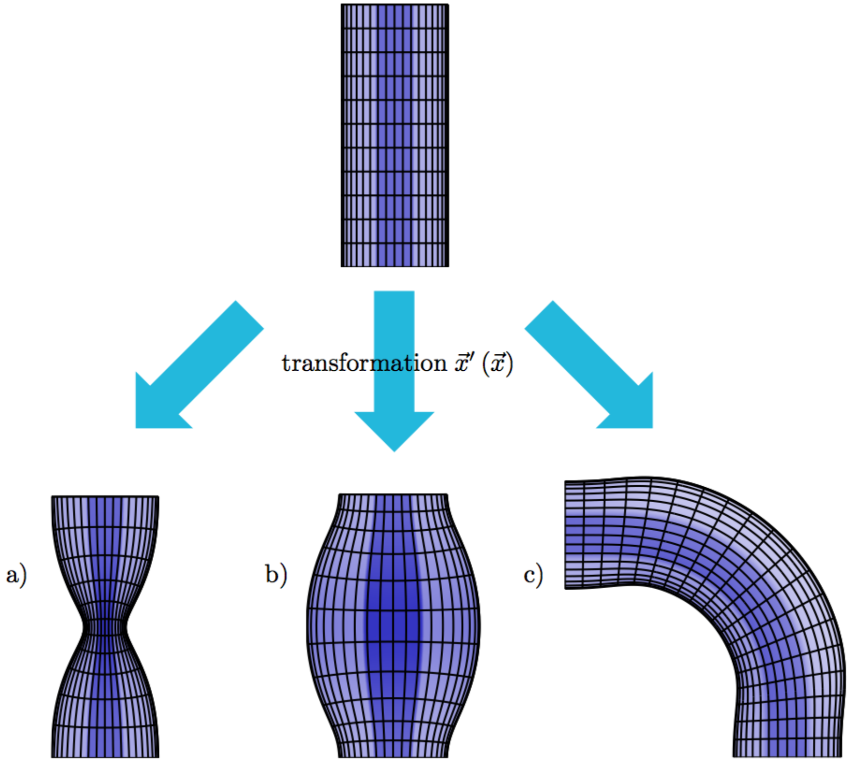
Gradient-index Multimode Optics

Lipson group @ Cornell

can make smoothly varying "gradient-index" structures by grayscale lithography

(variable-thickness waveguide = gradient effective index)



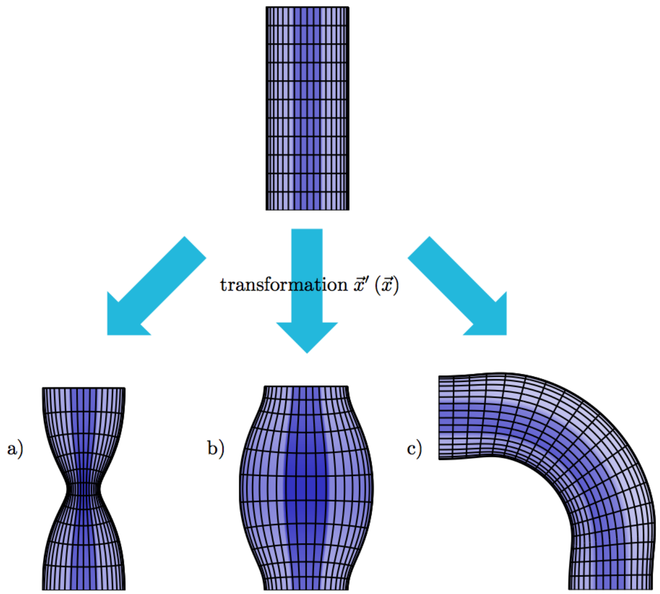


Transformation optics:
design materials that mathematically mimic coordinate transformations

Transformational Optics

[Ward & Pendry (1996)]

Idea: warping light with **x**'(**x**)



= material transformations

$$\varepsilon' = \varepsilon \frac{JJ^T}{\det J} \qquad \mu' = \mu \frac{JJ^T}{\det J}$$

(J = Jacobian matrix)

Pro: exact transformation of Maxwell solutions, so no reflections or scattering

- transforms all modes same way, preserving relative phase → multimode optics

Cons: most transformations give difficult-to-achieve ε , μ:

- anisotropy; $\mu \neq \mu_0$,

… "round" to isotropic index

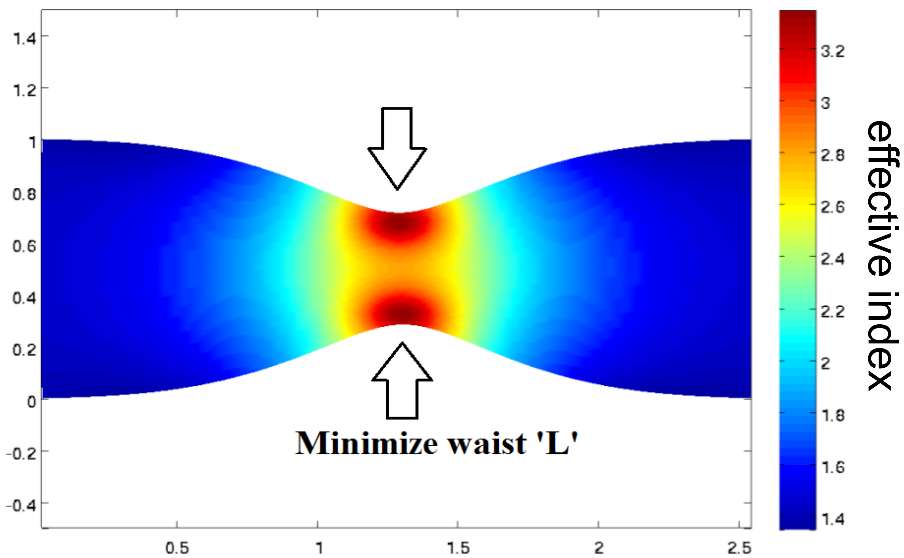
$$n \approx \sqrt{\varepsilon\mu / \varepsilon_0\mu_0}$$

- n may be too big / small

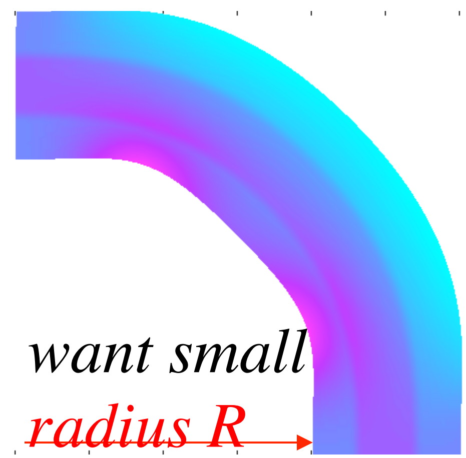
Transformational Inverse Design

Given a transformation **x**'(**x**), we can evaluate its manufacturability
(need minimal anisotropy, attainable indices)
quickly, without solving Maxwell's equations

… so optimization can rapidly search many transformations
to find the "best" manufacturable design

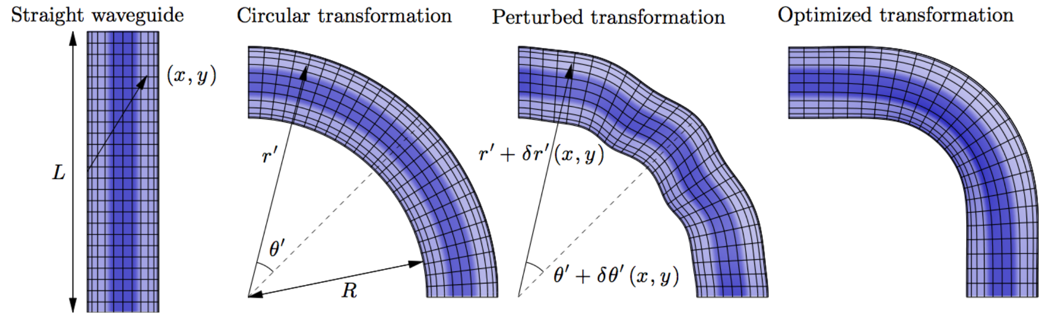


"mode squeezer"



multimode bend

Technical outline



For a given radius R, minimize the maximum anisotropy, subject to index constraints, over "all" transformations $\mathbf{x}'(\mathbf{x})$:

$$\min_{\mathbf{x}'(\mathbf{x})}\left[\max_{\mathbf{x}} \text{anisotropy}(\mathbf{x})\right] \qquad = \min_{\mathbf{x}'(\mathbf{x}),t} t$$

subject to: $1.6 \le n(\mathbf{x}) \le 3.2$ at all $\mathbf{x}$

$t \ge$ anisotropy$(\mathbf{x})$ (= "Distortion"−1)

$-1 + \text{tr } J^T J / 2 \det J \ge 0$

(J = Jacobian)

~ 30,000 constraints (100×100 **x** grid)

where smooth transformations $\mathbf{x}'(\mathbf{x})$ are parameterized by exponentially convergent Chebyshev/sine series

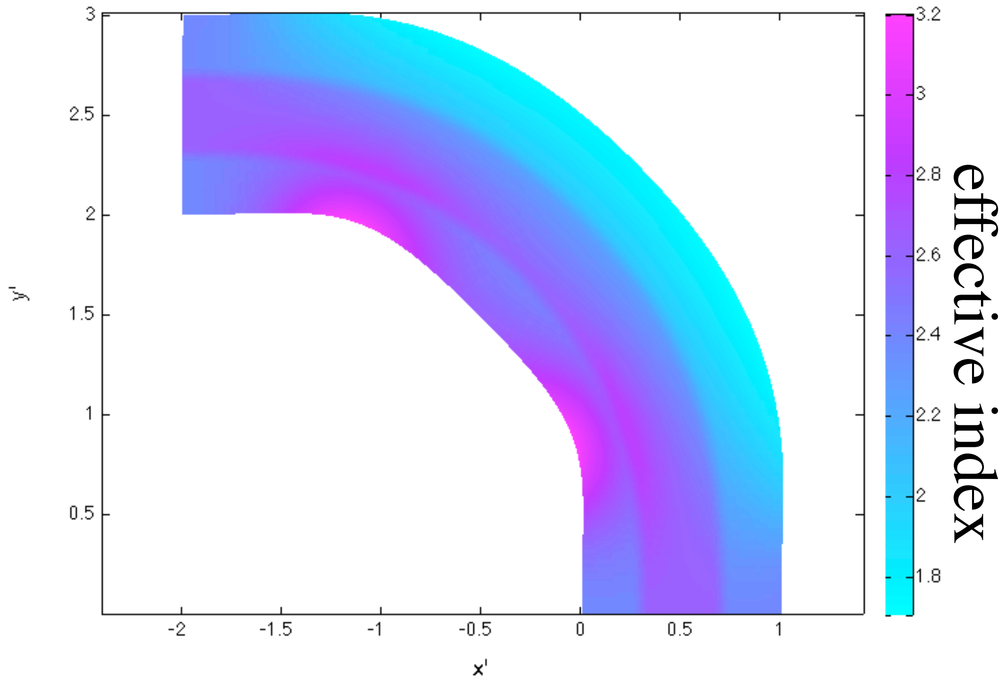
~ 100 parameters

… so cheap that almost any (local) optimization algorithm is okay …

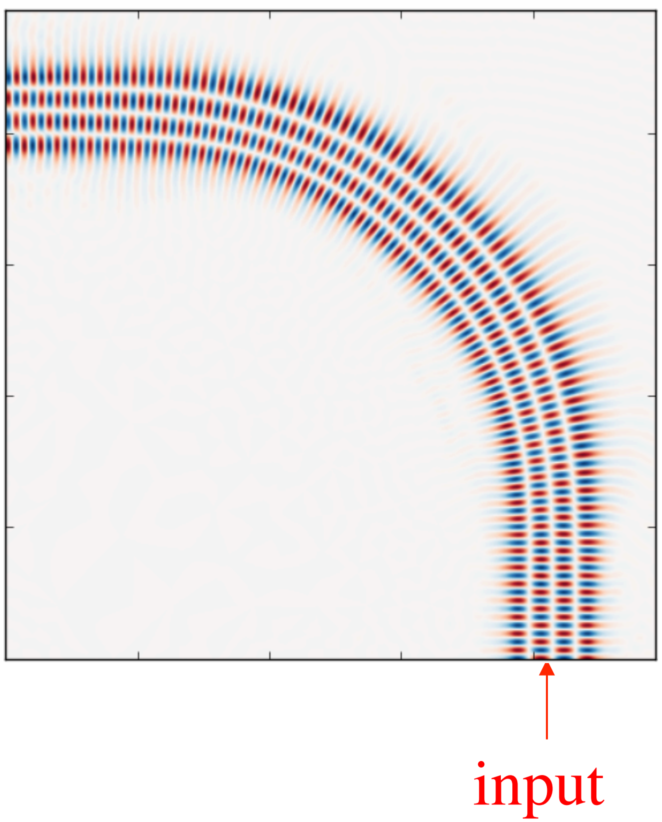
[use COBYLA derivative-free sequential LP algorithm of Powell (1994)]

An optimized multimode bend

optimized index profile



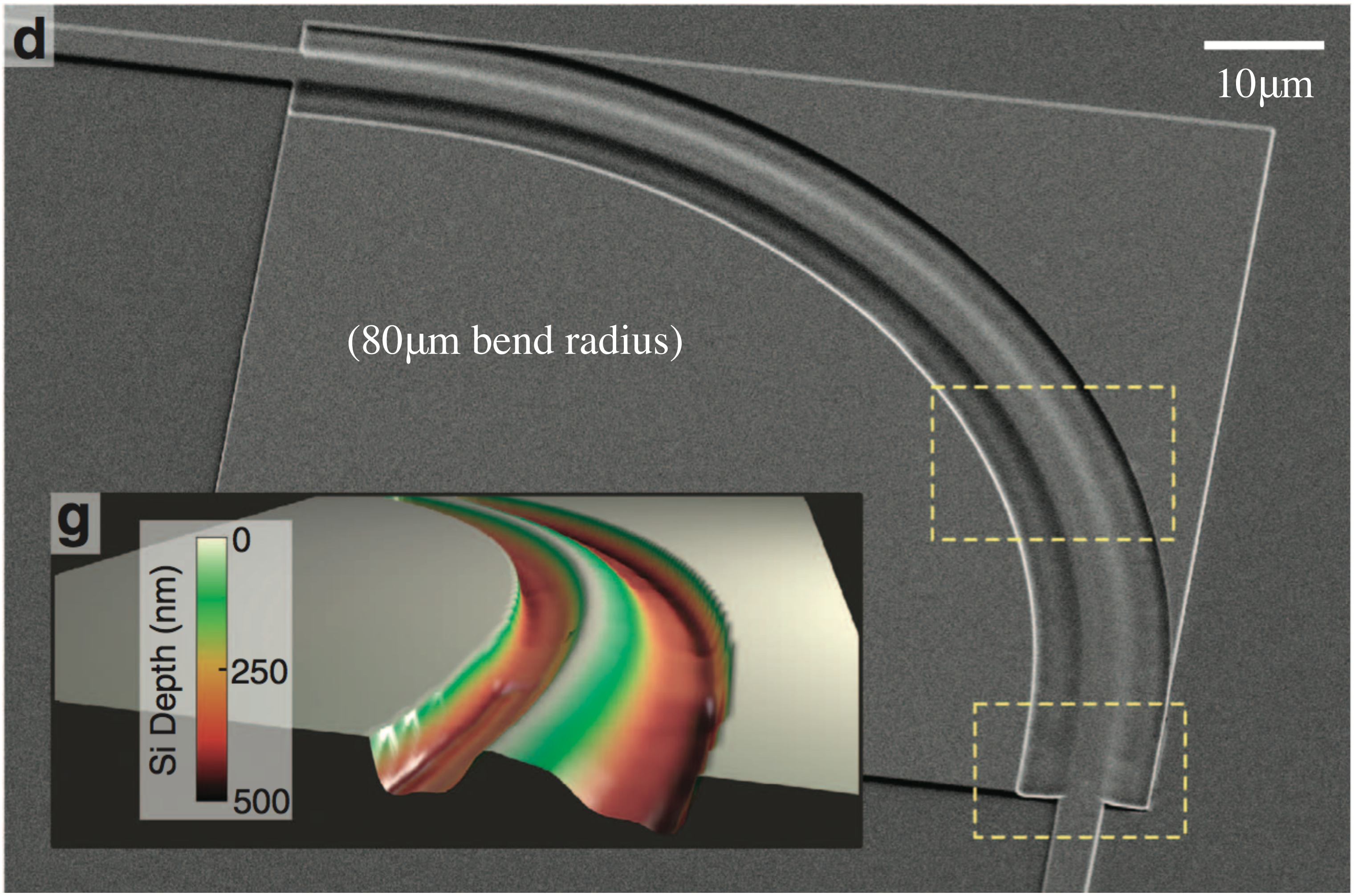
FEM simulation



[arXiv:1304.1553]

Experimental (Si/SiO_2) Realization

[Gabrielli, Liu, Johnson & Lipson, *Nature Commun*. (2012)]



measured 14dB reduction in loss (conversion) of the fundamental mode (λ=1.55μm) vs. circular bend