Computational EM Overview

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MIT course 18.369/8.315
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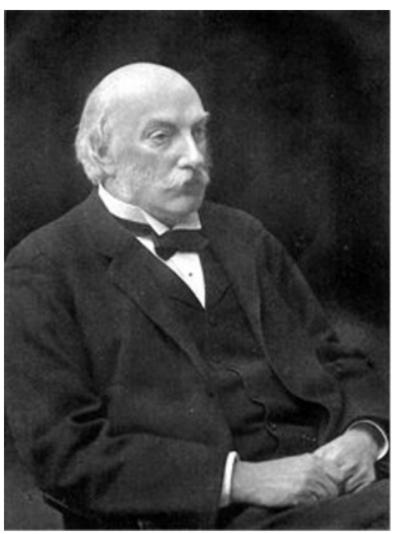
first, some perspective…

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

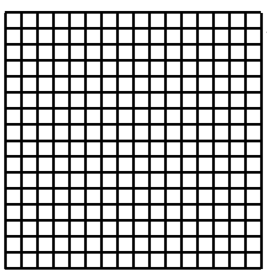
1. Analytical solutions

2. Semi-analytical solutions & spectral methods

3. Brute force: generic grid/mesh (or generic spectral)

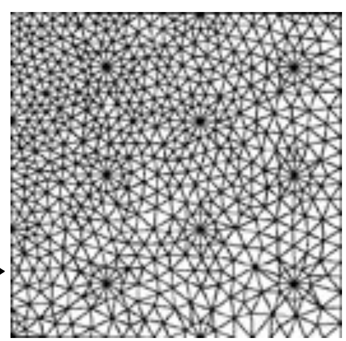
PDEs: discretize space into grid/mesh
— simple (low-degree polynomial) approximations in each pixel/element

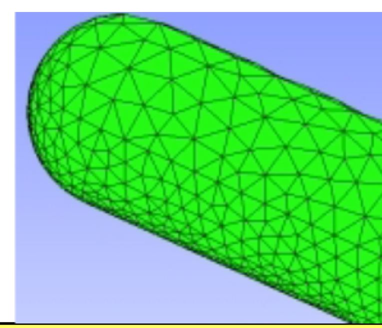
integral equations:
— boundary elements mesh surface unknowns coupled by Green's functions



←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: $\mathbf{E}$, $\mathbf{H}$ from $\mathbf{J}(\mathbf{x})e^{-i\omega t}$
  - — time-domain response: $\mathbf{E}$, $\mathbf{H}$ 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

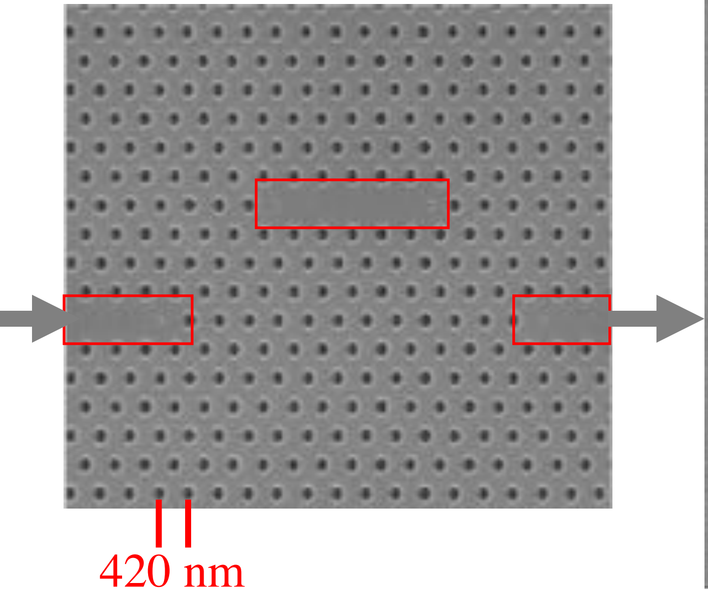
- All approaches still in widespread use
  - brute force methods in 90%+ of papers, typically the first resort to see what happens in a new geometry
  - geometry-specific spectral methods still popular, especially when particular geometry of special interest
  - analytical techniques used less to solve 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)

Computing & Interpreting Band Structures & Dispersion Relations

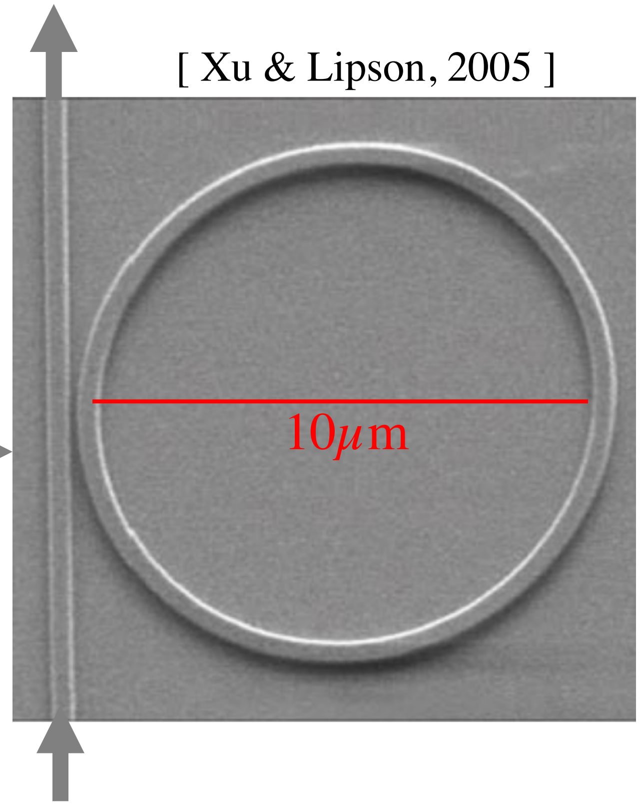
Steven G. Johnson
MIT Applied Mathematics

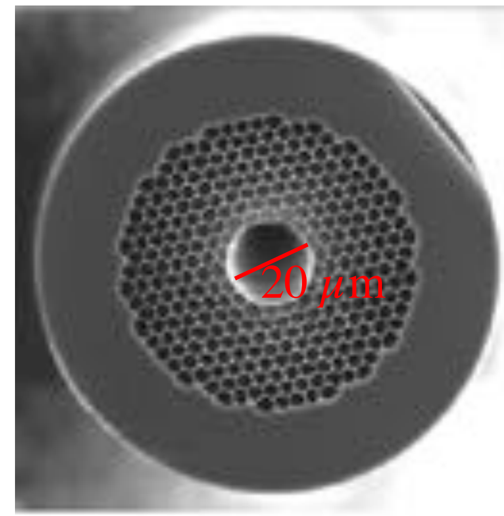
Understanding Photonic Devices

[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

$$\underbrace{\nabla \times \frac{1}{\varepsilon} \nabla \times}_{\text{eigen-operator}} \vec{H} = \underbrace{\omega^2}_{\text{eigen-value}} \vec{H}$$

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

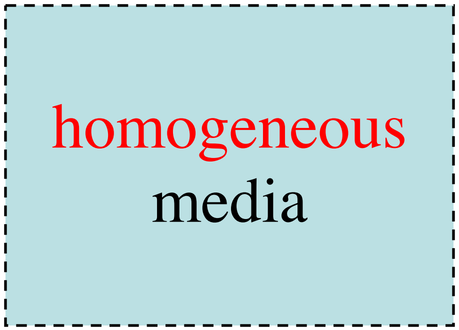
eigen-value

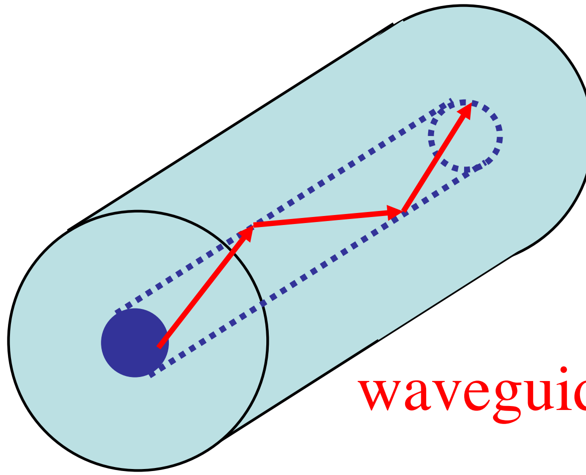
"eigen-field"

+ constraint

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

Building Blocks: Periodic Media



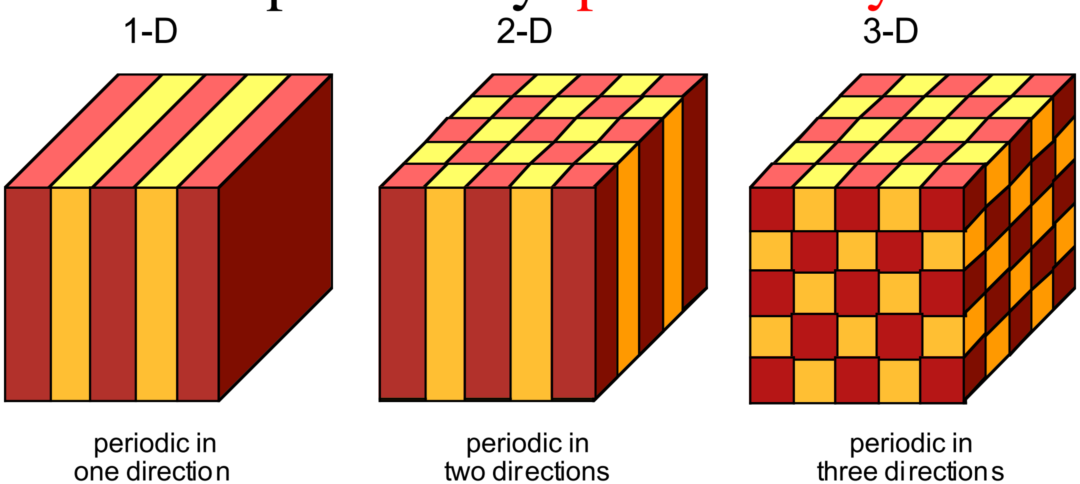


waveguides

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:

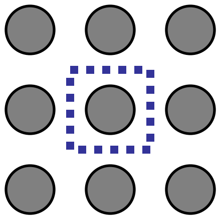
can choose: $$\vec{H}(\vec{x},t) = e^{i\left(\vec{k}\cdot\vec{x}-\omega t\right)}\vec{H}_{\vec{k}}(\vec{x})$$

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 ω are discrete $\omega_n(\mathbf{k})$

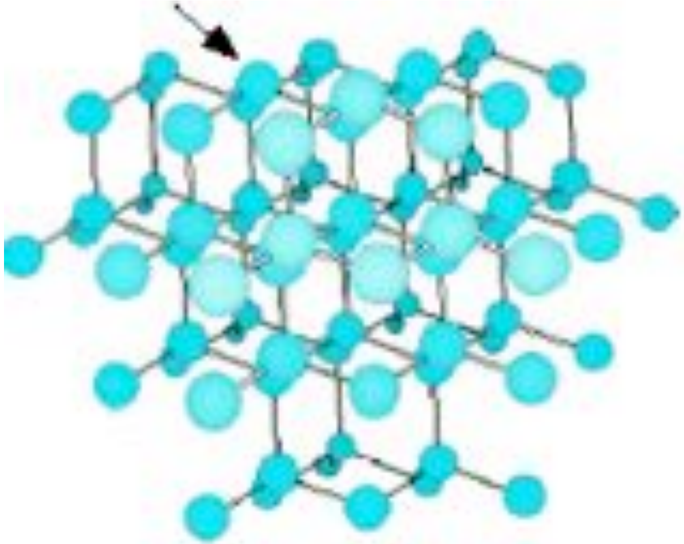


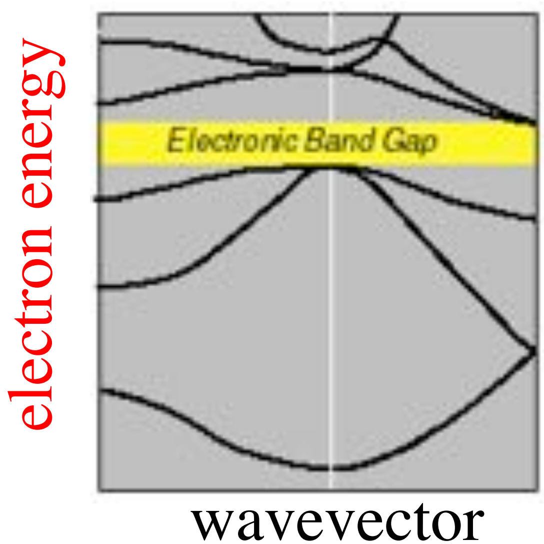
Electronic and Photonic Crystals

Periodic Medium

Bloch waves: **Band Diagram**

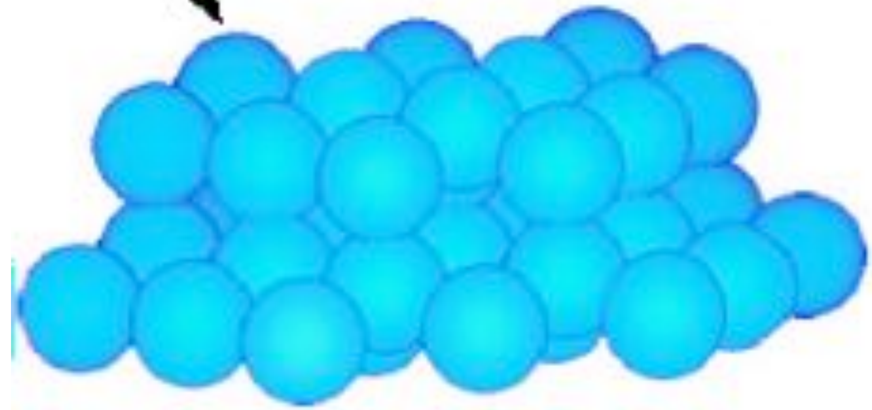
atoms in diamond structure

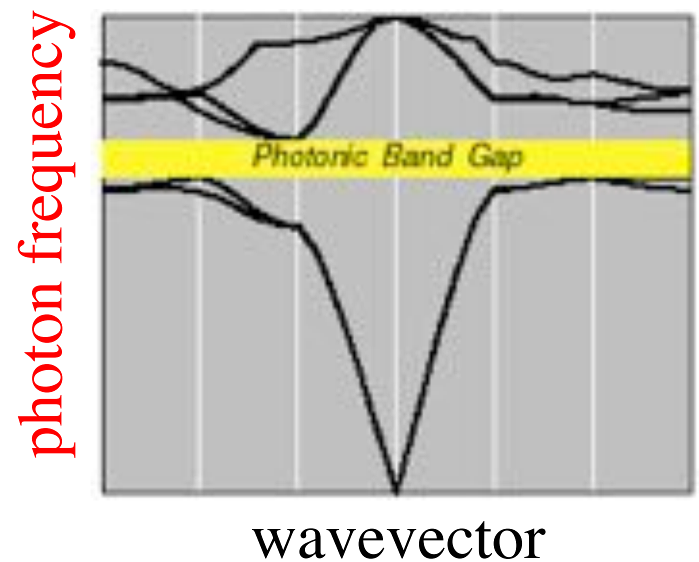




strongly interacting fermions

dielectric spheres, diamond lattice





weakly-interacting bosons

… many design degrees of freedom

Solving the Maxwell Eigenproblem

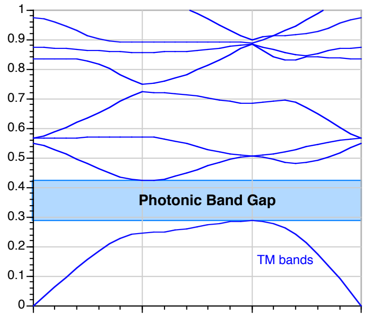
Finite cell ➔ *discrete* eigenvalues ω_n

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

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

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

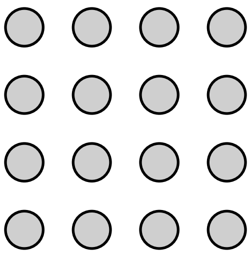
where field = $\mathbf{H}_n(\mathbf{x})\, e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$



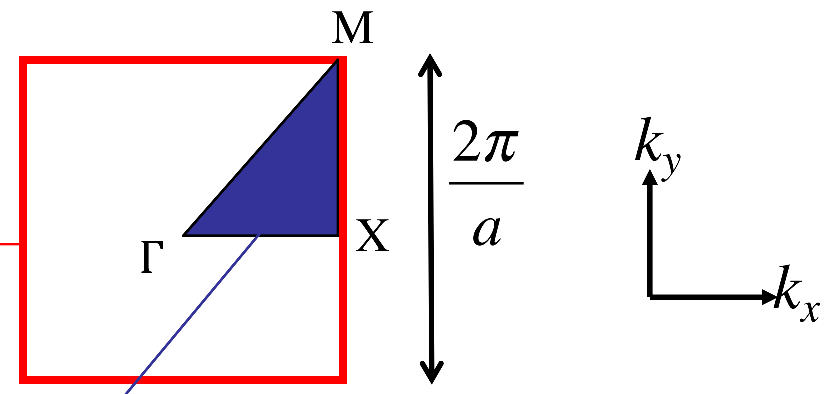
1. Limit range of $\mathbf{k}$: irreducible Brillouin zone
2. Limit degrees of freedom: expand $\mathbf{H}$ in finite basis
3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 1

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

2. Limit degrees of freedom: expand $\mathbf{H}$ in finite basis (N)

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

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

inner product:

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

Galerkin method:

$$A_{ml} = \langle \mathbf{b}_m | \hat{A} | \mathbf{b}_l \rangle \qquad B_{ml} = \langle \mathbf{b}_m | \mathbf{b}_l \rangle$$

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2b

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

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

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

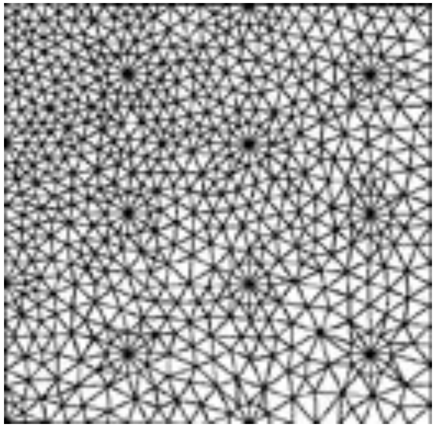
Planewave (FFT) basis

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

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

$$Ah = \omega^2 Bh$$

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:

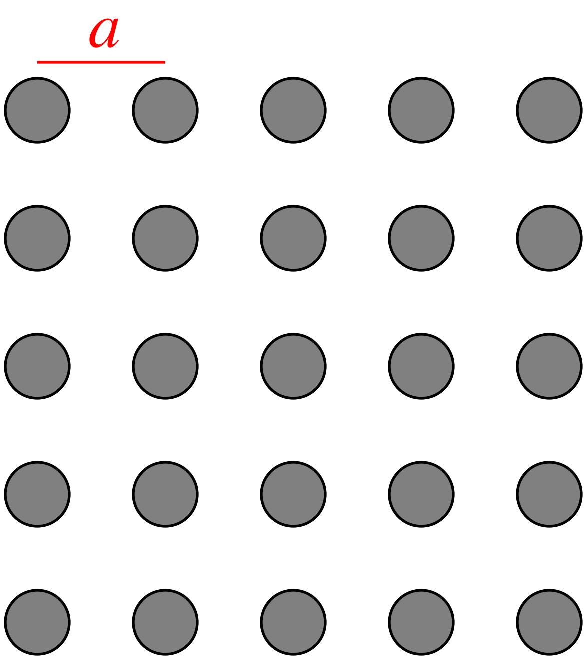
variational / min–max theorem

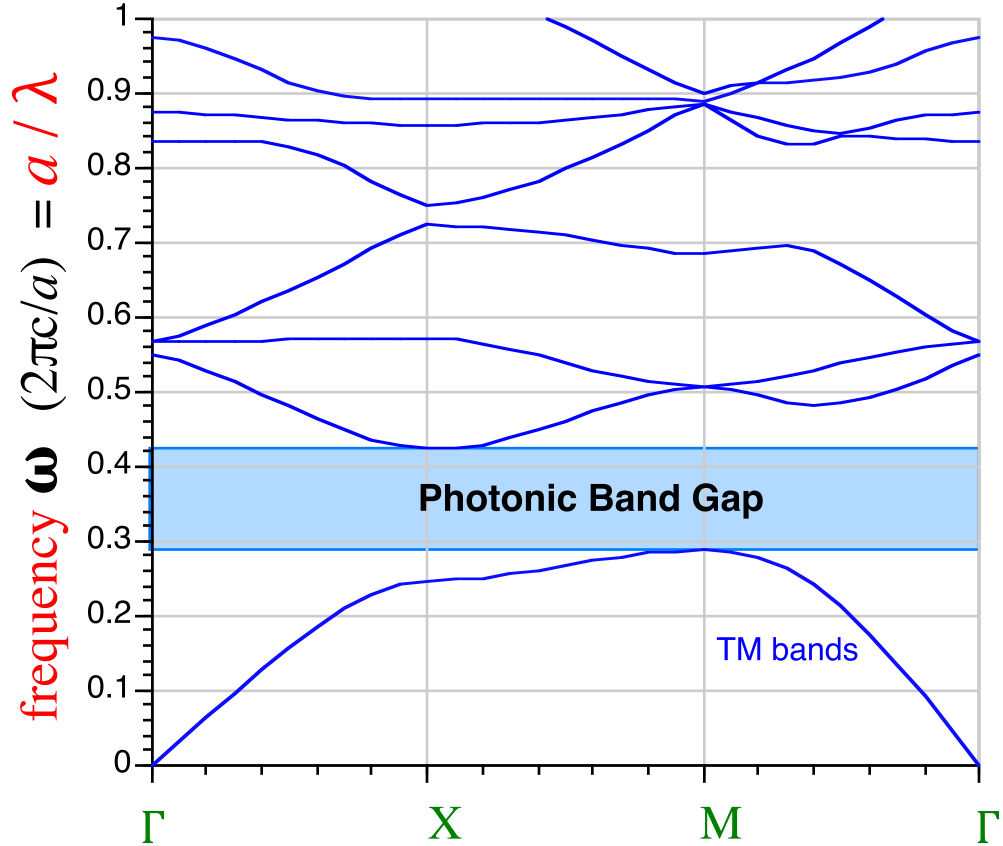
$$\omega_0^2 = \min_h \frac{h^* A h}{h^* B h}$$

minimize by preconditioned conjugate-gradient (or…)

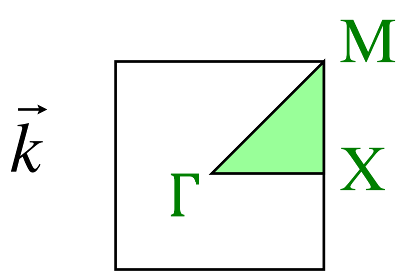
Band Diagram of 2d Model System

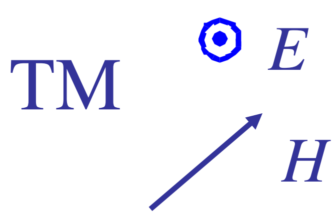
(radius 0.2a rods, ε=12)





irreducible Brillouin zone





gap for
n > ~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 ($h + \alpha\, d$)

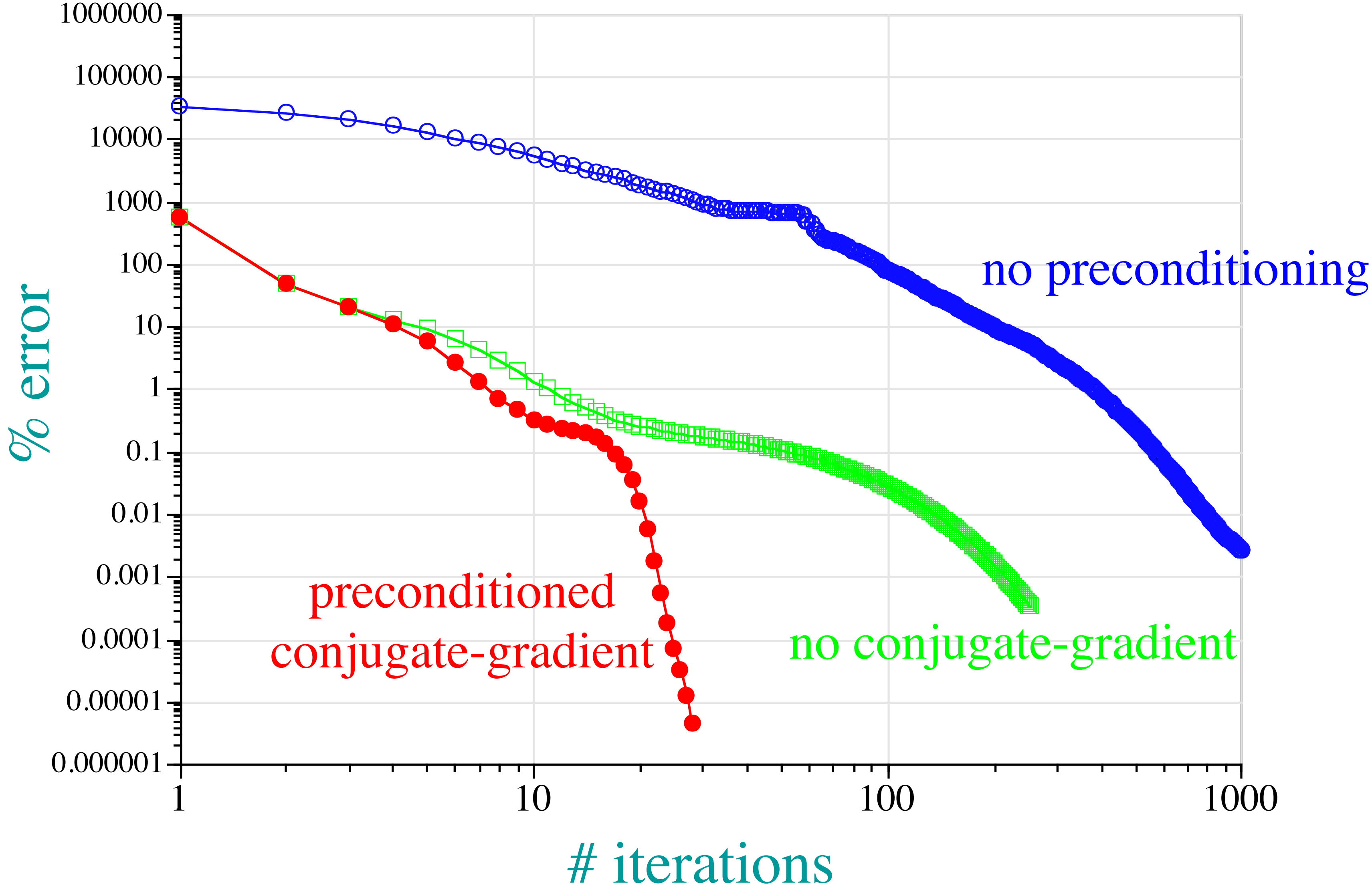
— d = (approximate A^{-1}) ∇f ~ Newton's method

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

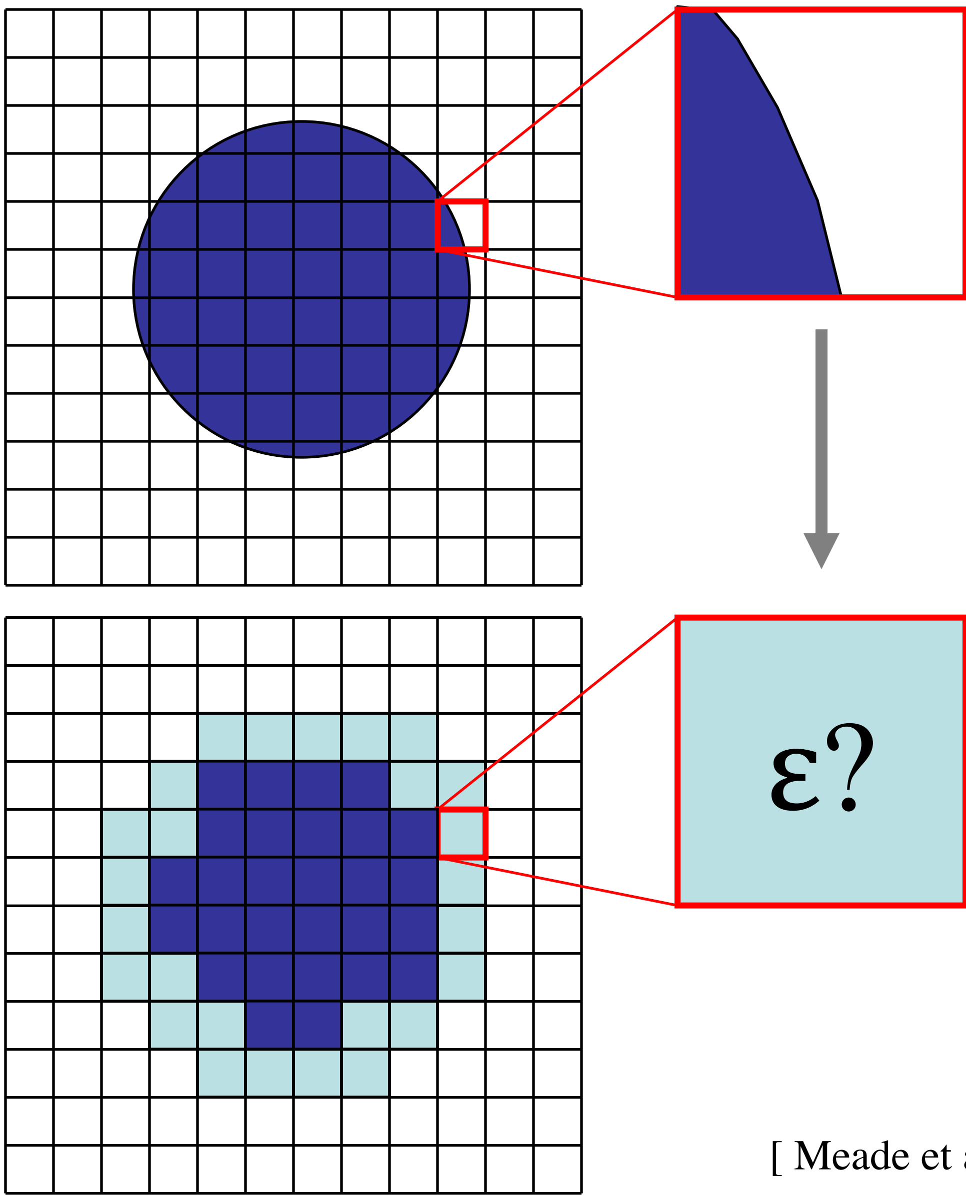
— d is (approximate A^{-1}) [∇f + (stuff)]

The Iteration Scheme is *Important*

(minimizing function of ~40,000 variables)



The Boundary Conditions are Tricky



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

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

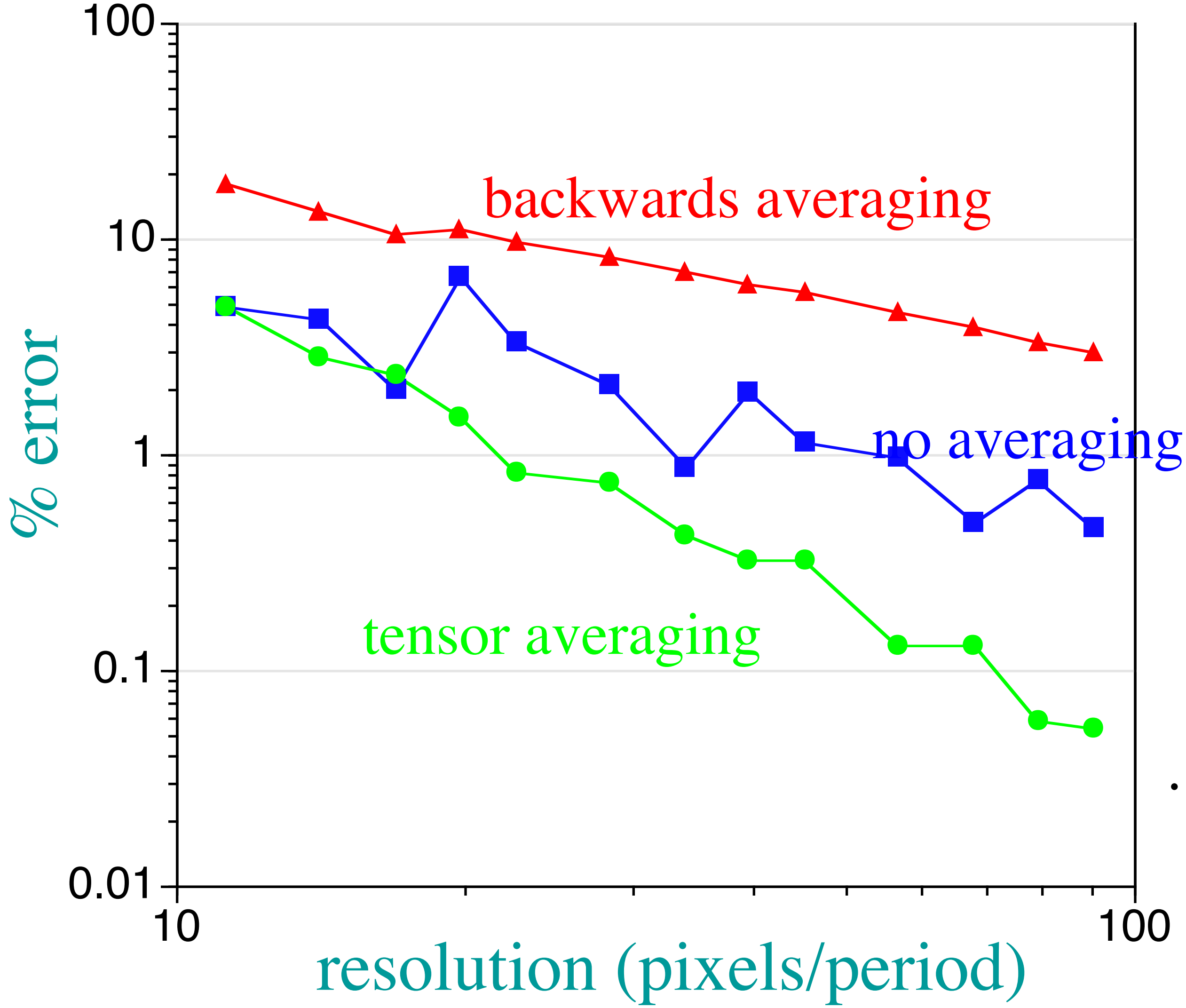
($\mathbf{D}_{\perp} = \varepsilon\mathbf{E}_{\perp}$ is continuous)

Use a tensor ε:

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

[Meade et al. (1993)]

The ε-averaging is *Important*

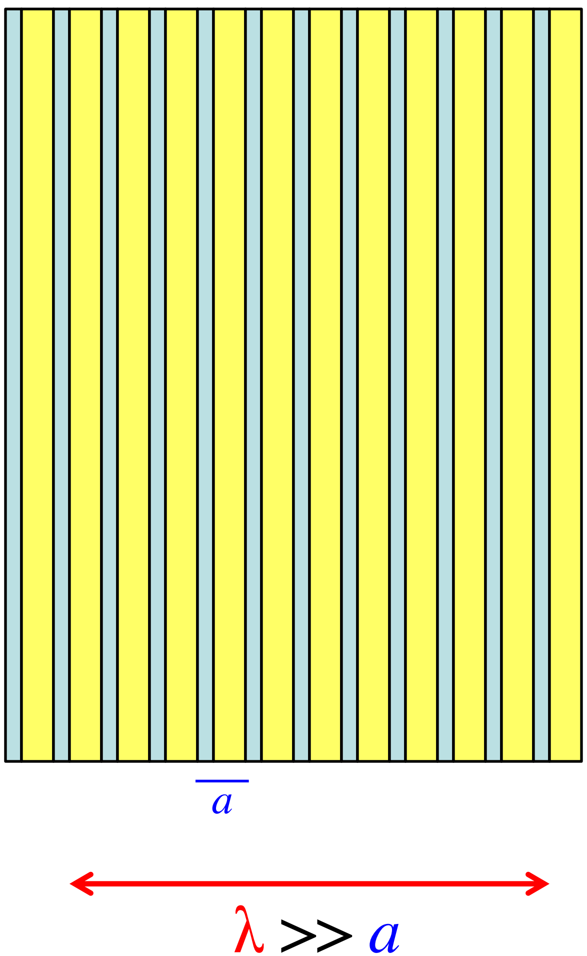


correct averaging
changes *order*
of convergence
from Δx to Δx^2

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



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

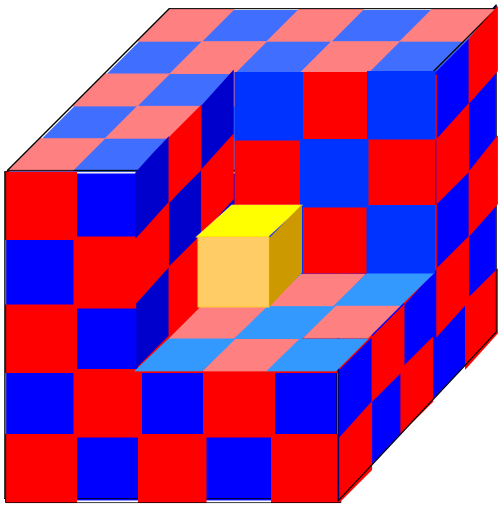
key to anisotropy is differing continuity conditions on **E**:

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

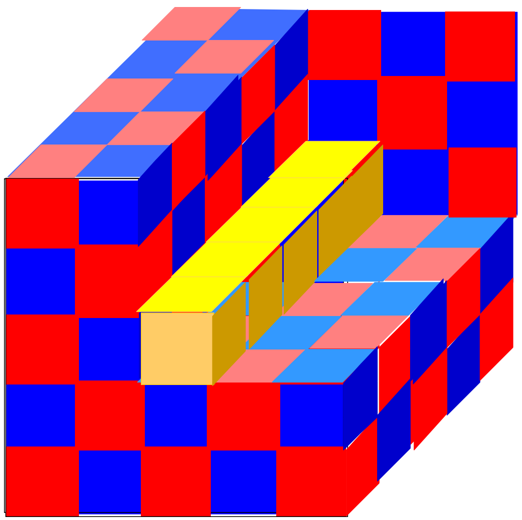
$D_{\perp} = \varepsilon E_{\perp}$ continuous $\Rightarrow$ $\varepsilon_{\perp} = \langle \varepsilon^{-1} \rangle^{-1}$

Intentional “defects” are good

microcavities

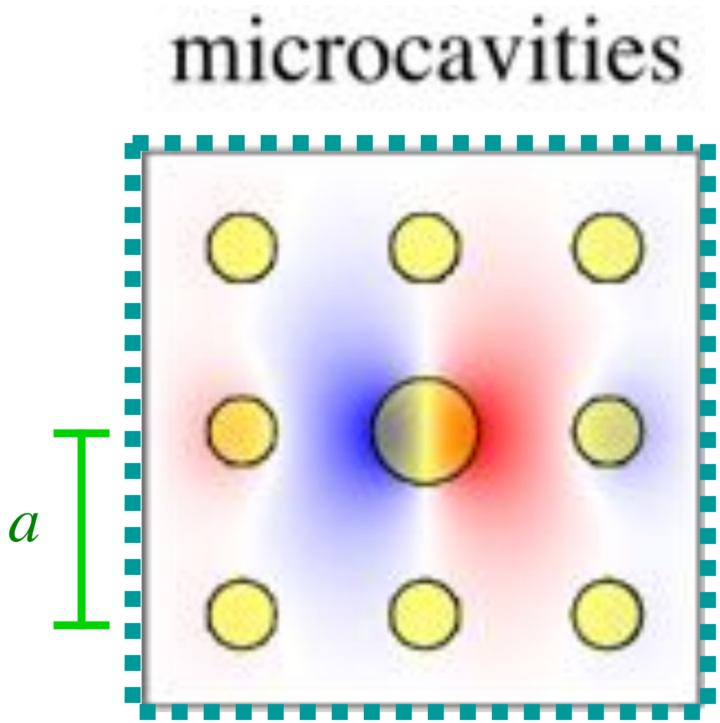


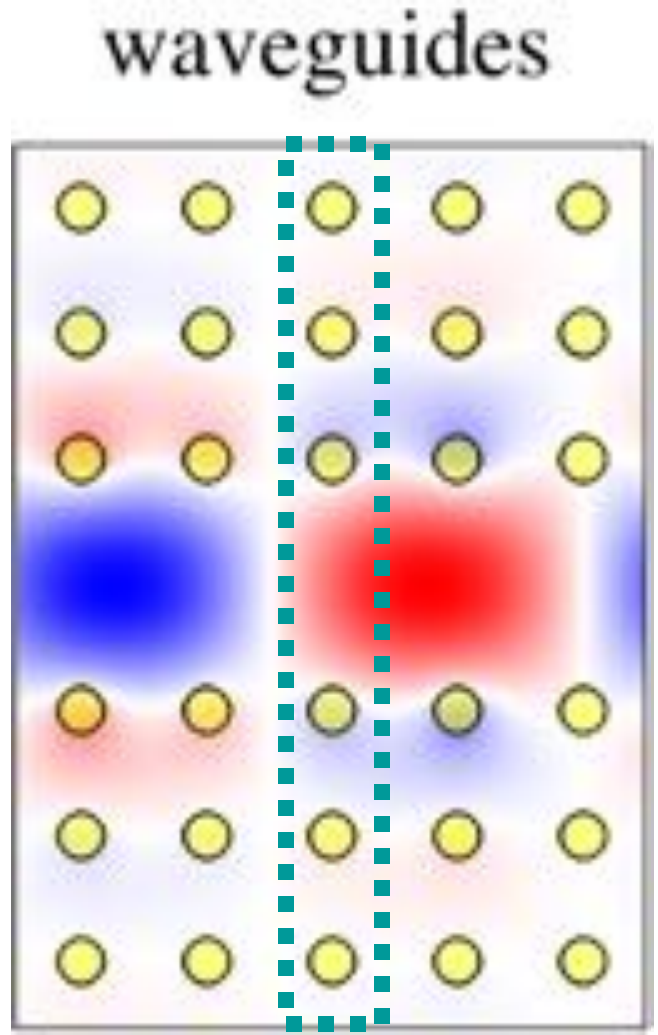
waveguides (“wires”)



Intentional "defects" in 2d

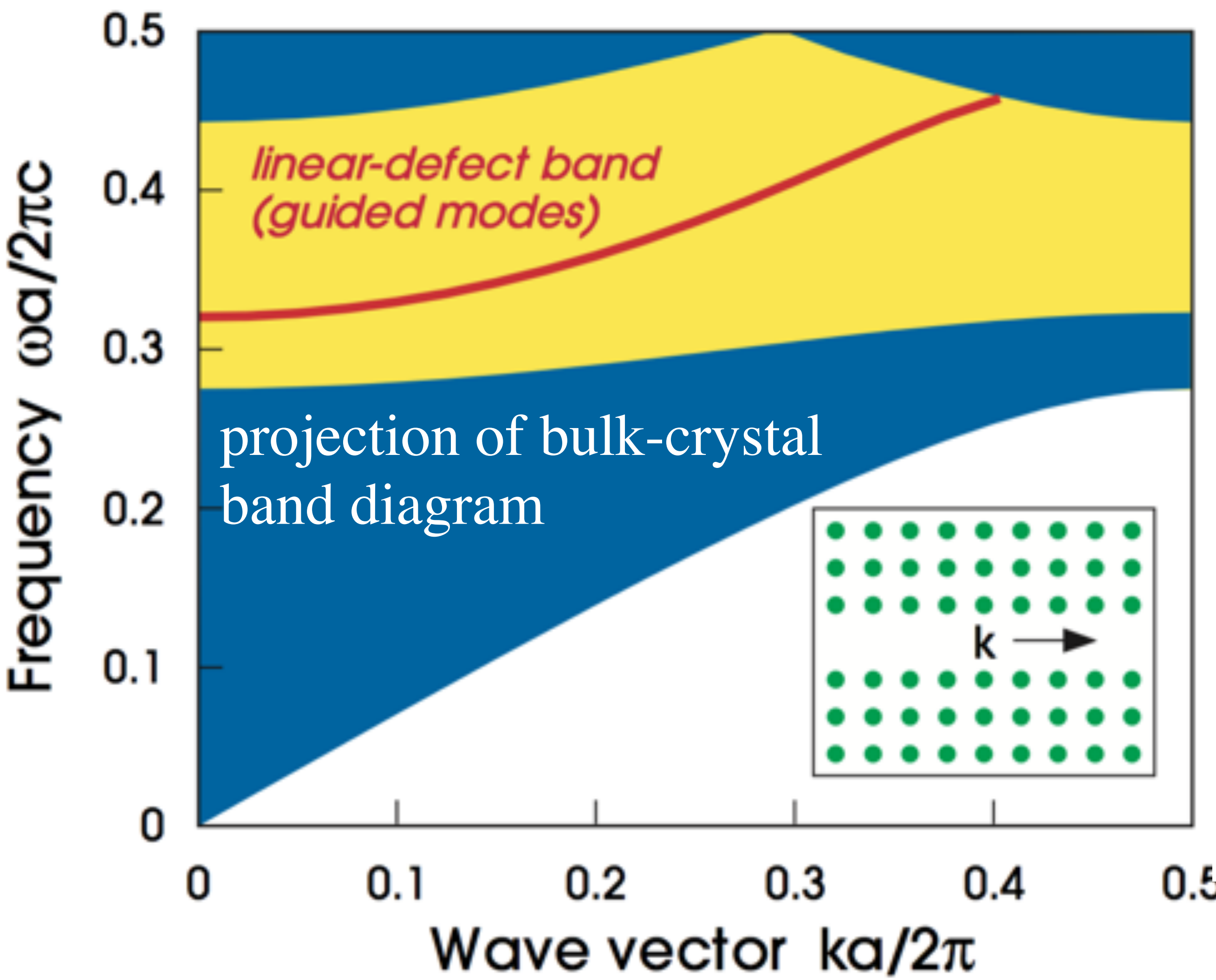
(Same computation, with supercell = many primitive cells)

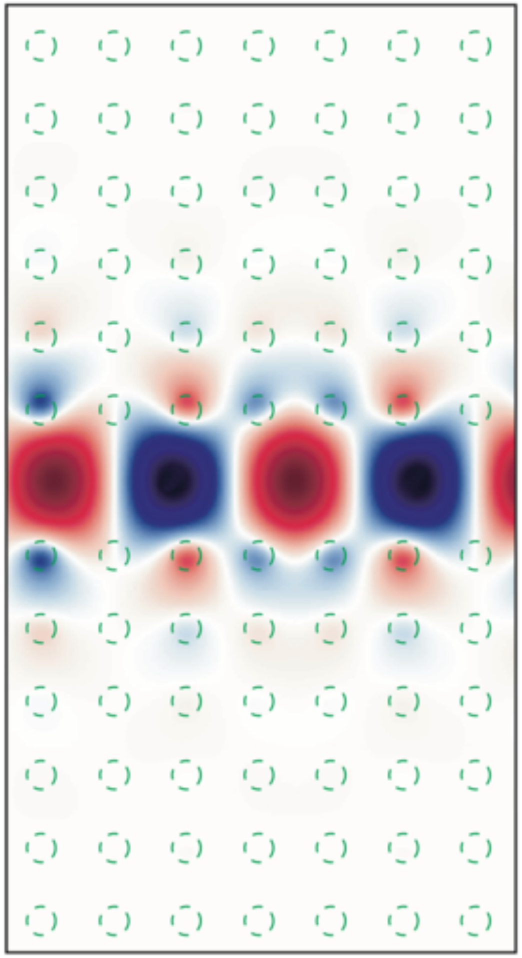




(boundary conditions ~ irrelevant
for exponentially localized modes)

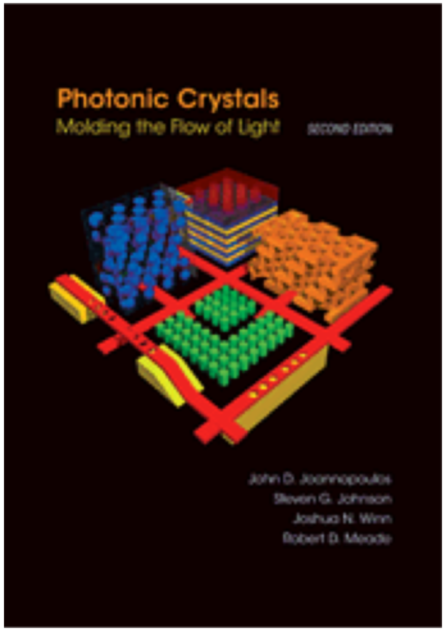
Air-waveguide Band Diagram





any state in the gap cannot couple to bulk crystal –> localized

to be continued…



Further reading:

Photonic Crystals book: http://jdj.mit.edu/book

Bloch-mode eigensolver: http://jdj.mit.edu/mpb

Computational Nanophotonics: Cavities and Resonant Devices

Steven G. Johnson
MIT Applied Mathematics

Resonance

an oscillating mode trapped for a long time in some volume

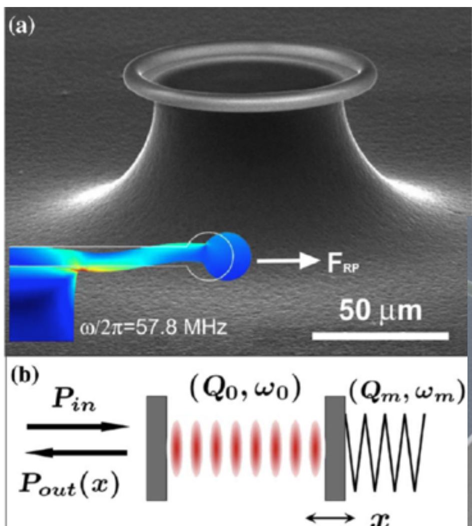
(of light, sound, …) lifetime $\tau >> 2\pi/\omega_0$

frequency ω_0

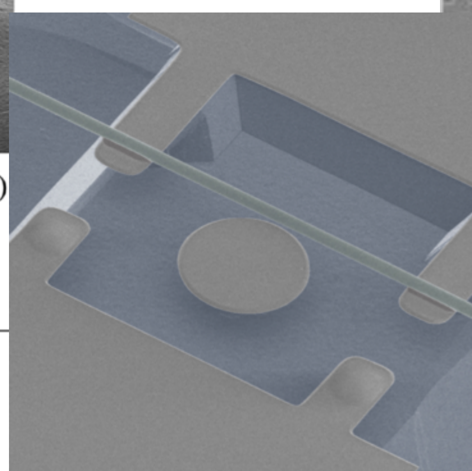
quality factor $Q = \omega_0\tau/2$

energy in cavity $\sim e^{-\omega_0 t/Q}$

modal volume V

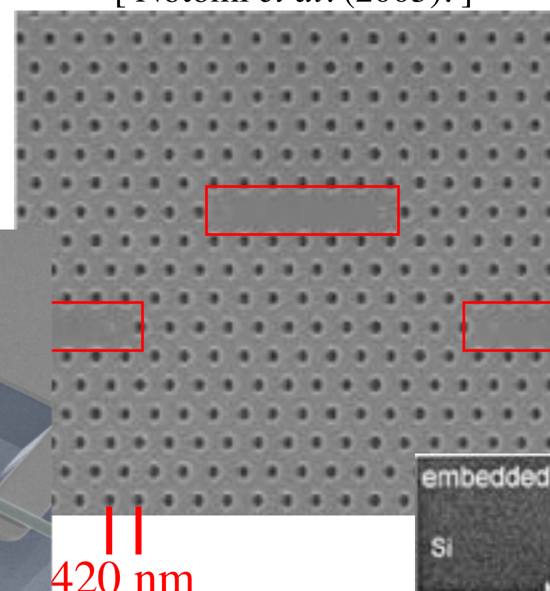


[Schliesser et al., *PRL* **97**, 243905 (2006)]

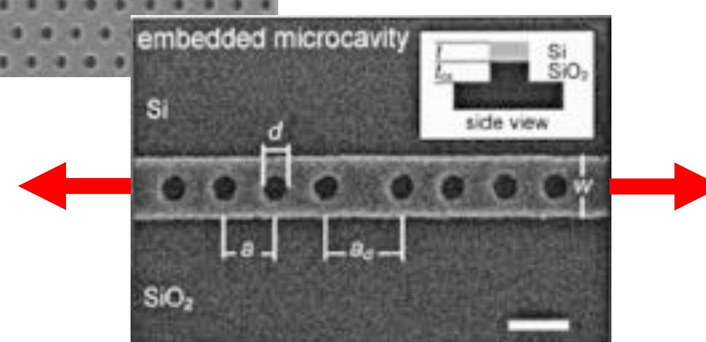


[Eichenfield et al. *Nature Photonics* **1**, 416 (2007)]

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



[C.-W. Wong, *APL* **84**, 1242 (2004).]



Resonance = Pole in Green's Function

an oscillating mode trapped for a long time in some volume

(of light, sound, …)

lifetime $\tau \gg 2\pi/\omega_0$

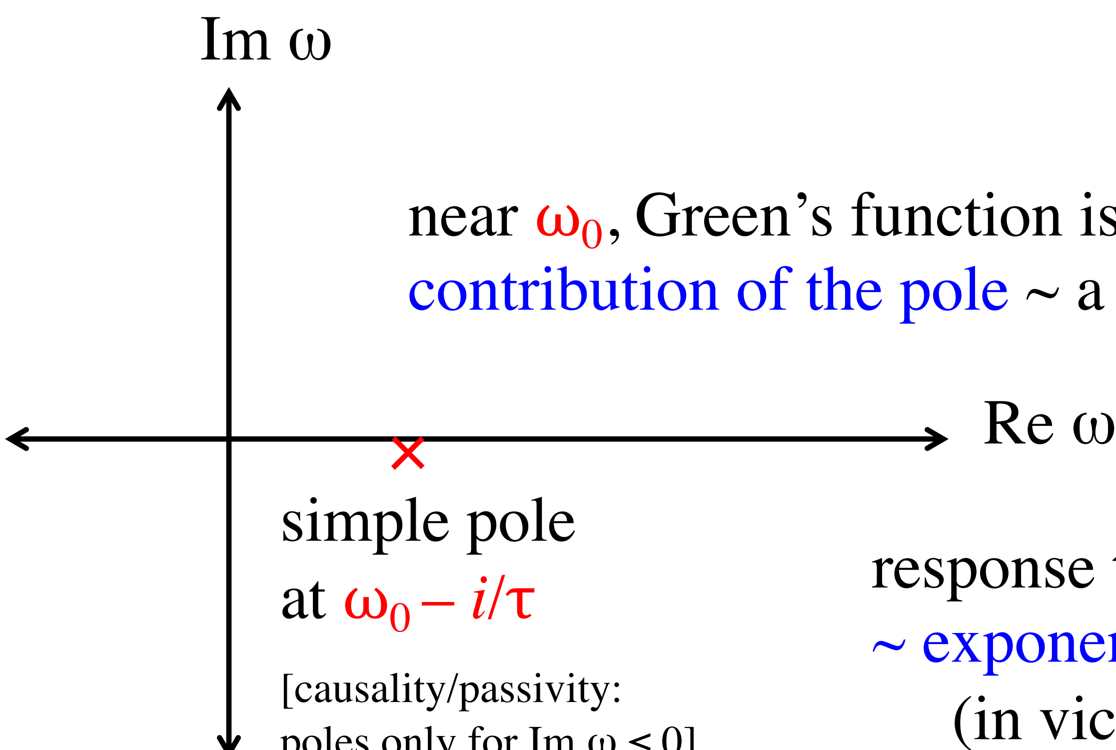
frequency ω_0

quality factor $Q = \omega_0\tau/2$

energy in cavity $\sim e^{-\omega_0 t/Q}$

modal volume V

~ volume where residue is large



near ω_0, Green's function is dominated by contribution of the pole ~ a "resonant mode" profile

simple pole at $\omega_0 - i/\tau$

[causality/passivity: poles only for $\mathrm{Im}\,\omega \leq 0$]

response to a narrowband pulse
~ exponential decay in time
(in vicinity of the cavity)

Green's functions, briefly

Green's function = field(s) at **x** from dipole at **y**
at a frequency ω

$$(\nabla\times\mu^{-1}\nabla\times-\omega^2\varepsilon)\mathbf{E}^{(j)}(\mathbf{x}) = i\omega\delta(\mathbf{x}-\mathbf{y})\times(\text{unit vector in } j)$$

$\Longrightarrow$ electric "*dyadic*" Green's function $\mathrm{G}_\omega(\boldsymbol{x},\boldsymbol{y}) = [\mathbf{E}^{(1)} \quad \mathbf{E}^{(2)} \quad \mathbf{E}^{(3)}]$

… any electric current $\mathbf{J}(\boldsymbol{x})e^{-i\omega t}$ then gives the "convolution" $\mathbf{E}(\mathbf{x}) = \mathrm{G}_\omega * \mathbf{J} = \int \mathrm{G}_\omega(\mathbf{x},\mathbf{y})\mathbf{J}(\mathbf{y})d^3\mathbf{y}$

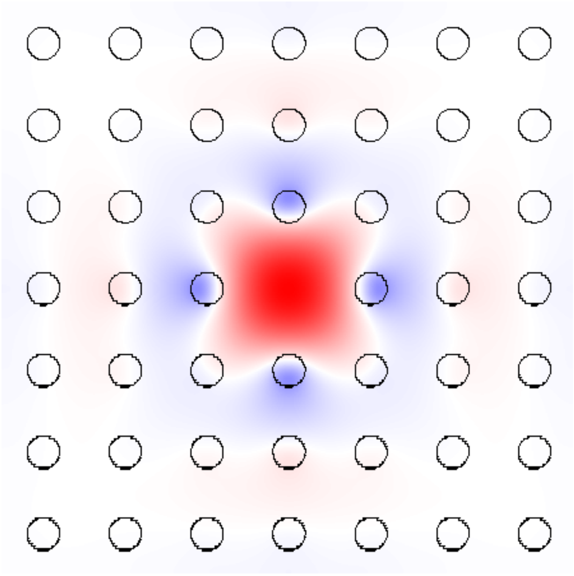
At eigenvalue/resonance frequency ω_0 ($\nabla\times\mu^{-1}\nabla\times\mathbf{E}_0 = \omega_0^2\varepsilon\mathbf{E}_0$), the operator $(\nabla\times\mu^{-1}\nabla\times-\omega_0^2\varepsilon)$ becomes singular.

G_ω blows up = "pole" at ω_0^2

Similarly, 6×6 Green's function $\Gamma_\omega(\mathbf{x},\mathbf{y})$ gives $\begin{bmatrix}\mathbf{E}\\\mathbf{H}\end{bmatrix} = \psi$

fields from 6-component currents $\xi = \begin{bmatrix}\mathbf{J}\\\mathbf{K}\end{bmatrix}$ at via $\psi = \Gamma_\omega * \xi$.

Microcavity Blues



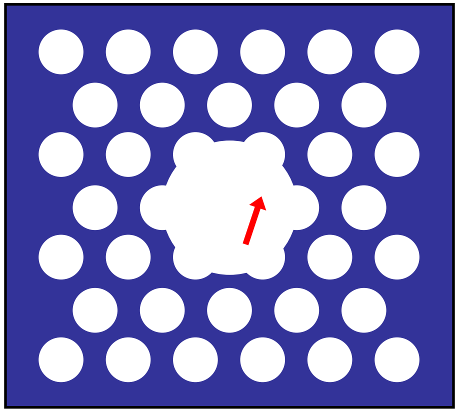
For cavities (*point defects*)
frequency-domain has its drawbacks:

- 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

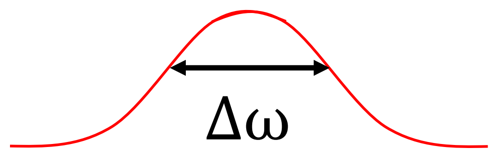
Time-Domain Eigensolvers

(finite-difference time-domain = FDTD)



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

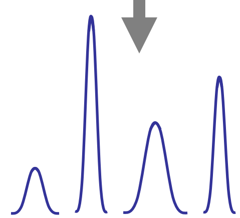
• Excite with broad-spectrum dipole (↑) source



tricky
signal processing

complex ω_n

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



Response is many
sharp peaks,
one peak per mode

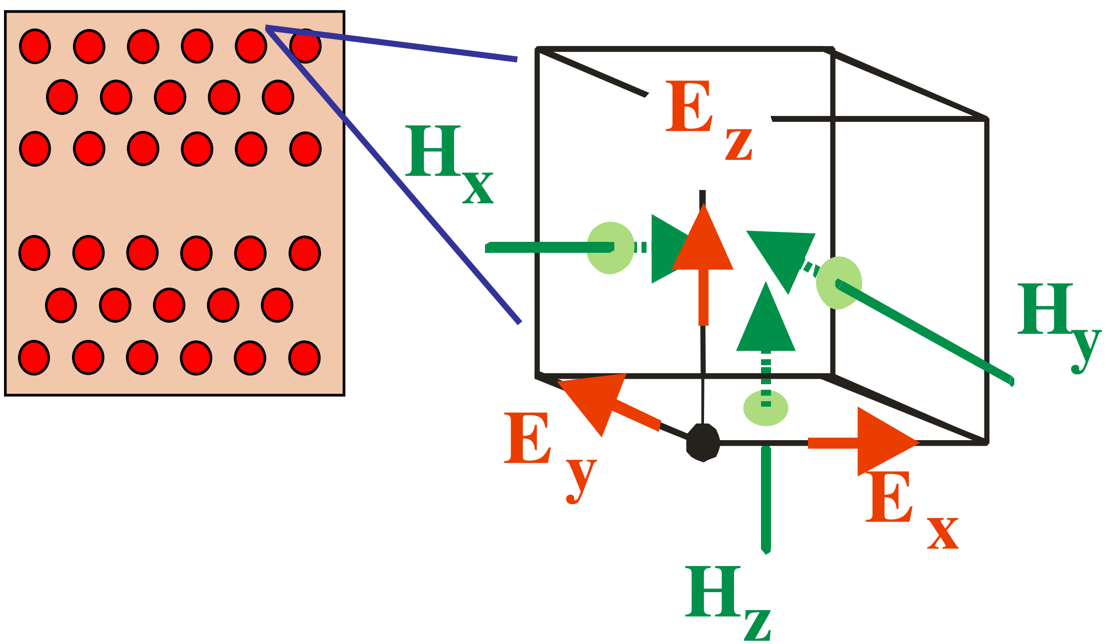
decay rate in time gives loss

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

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

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



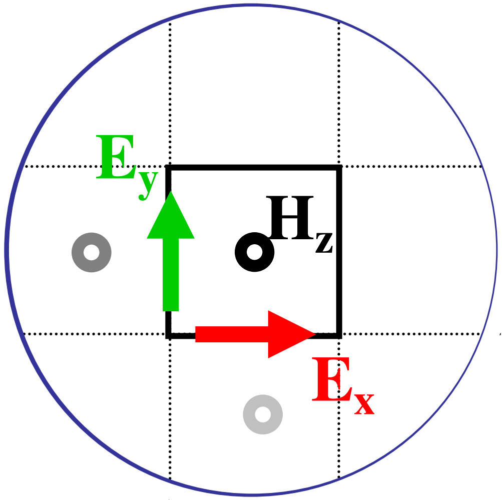
K.S. Yee 1966

A. Taflove & S.C. Hagness 2005

FDTD: Yee leapfrog algorithm

2d example:

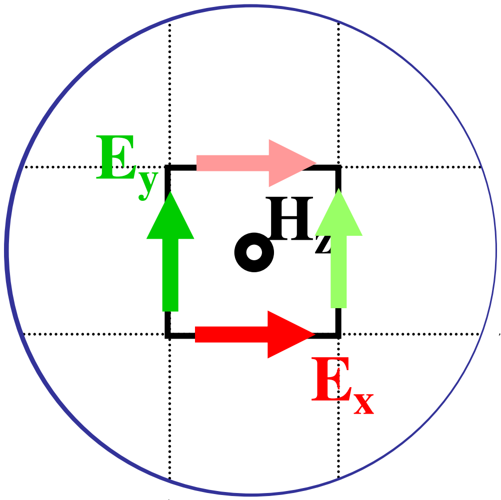
1) **at time t: Update D fields everywhere using spatial derivatives of H, then find $E = \varepsilon^{-1} D$**



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

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

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

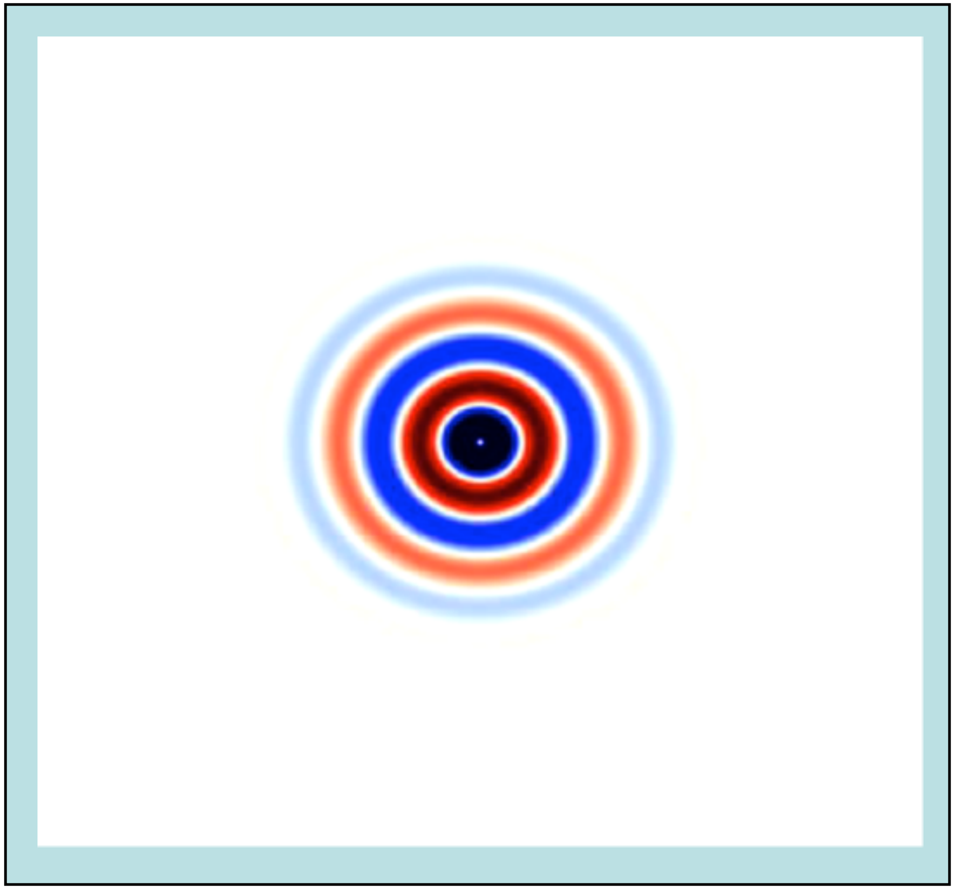
Free software: Meep

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…

Absorbing boundaries?

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



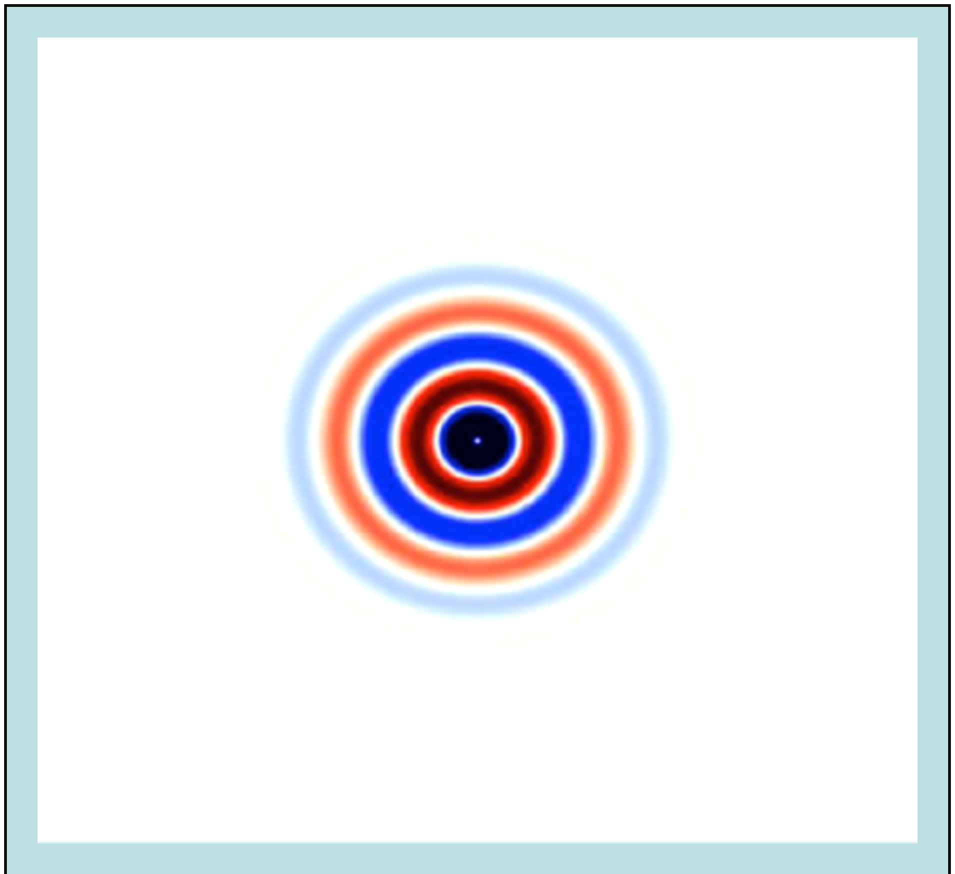
In a wave equation, a hard-wall truncation gives reflection artifacts.

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



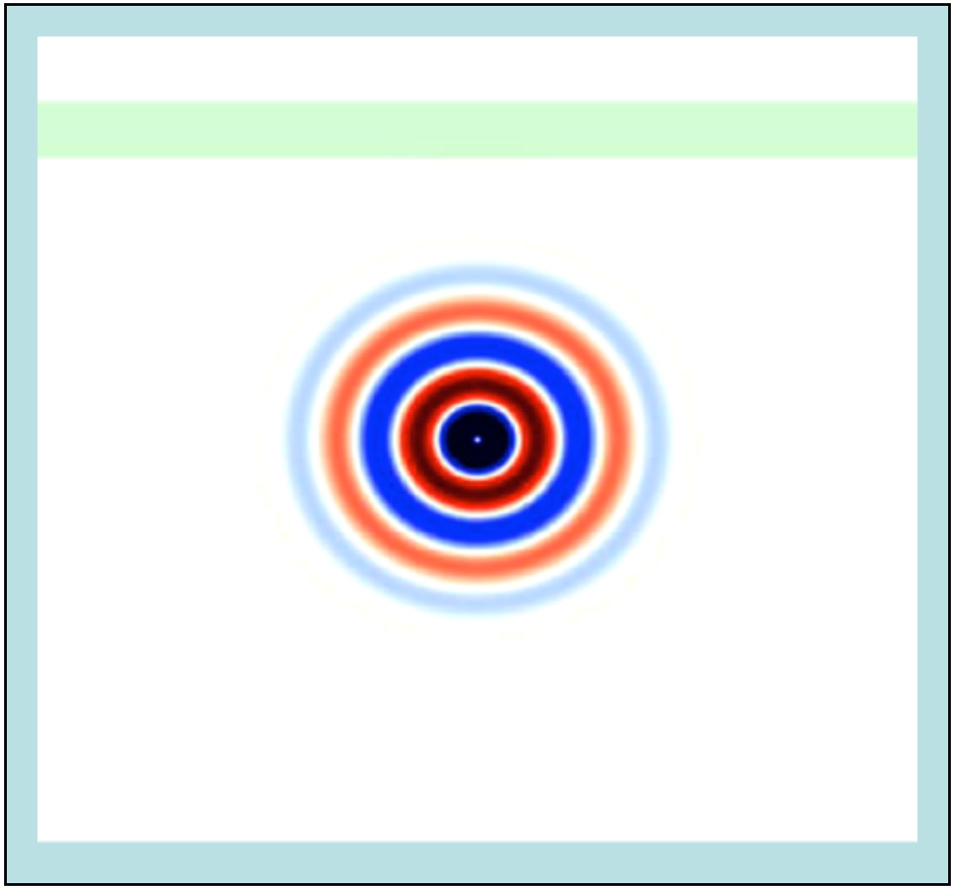
Works *remarkably well*.

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).

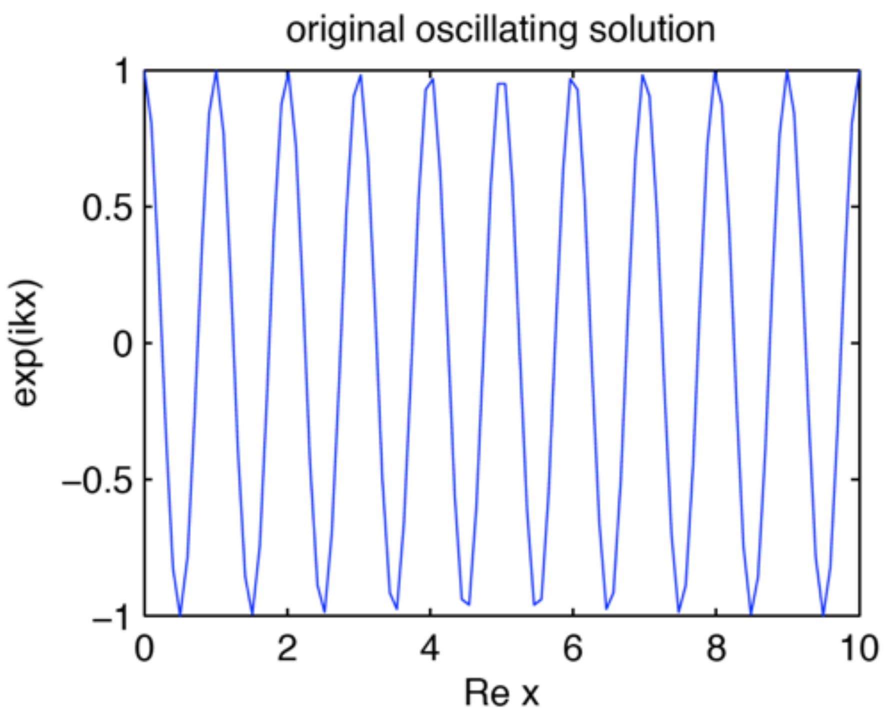
PML Starting point: propagating wave

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

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

$(usually, k > 0)$

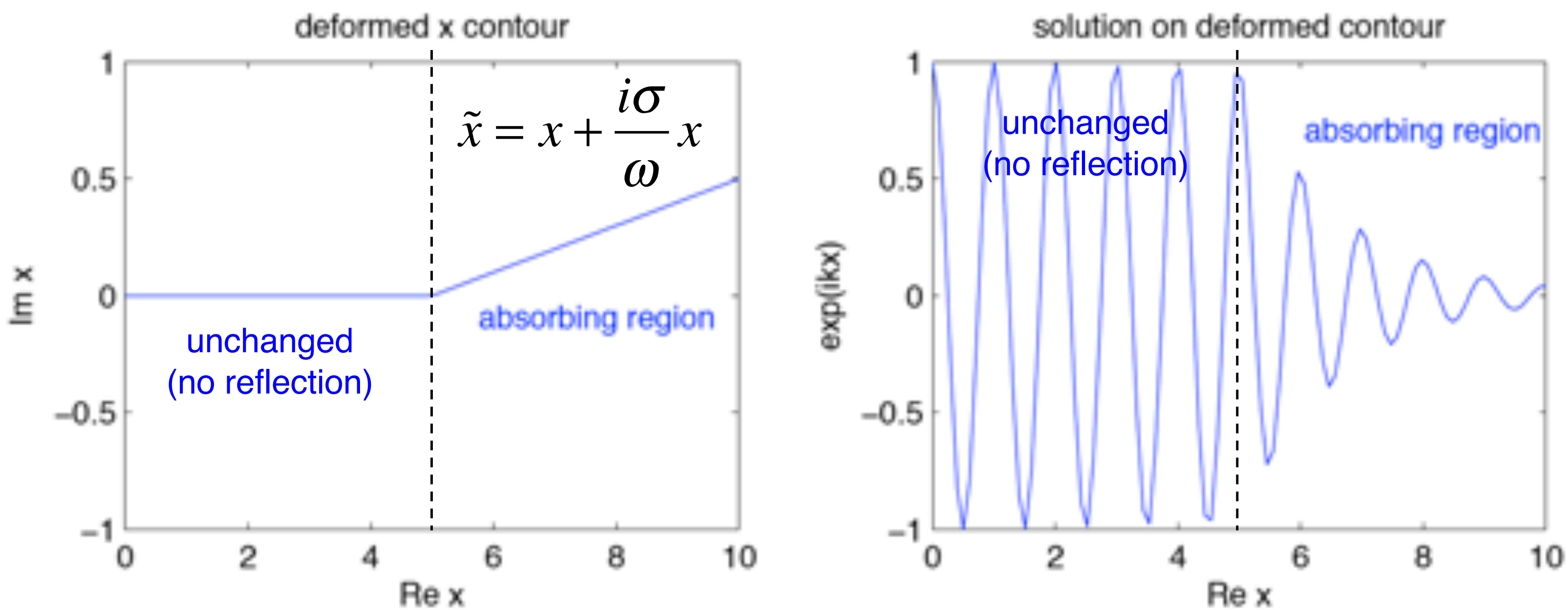
[rare "backward-wave" cases defeat PML (Loh, 2009)]



(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)

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

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

nondispersive materials: k/ω ~ 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:

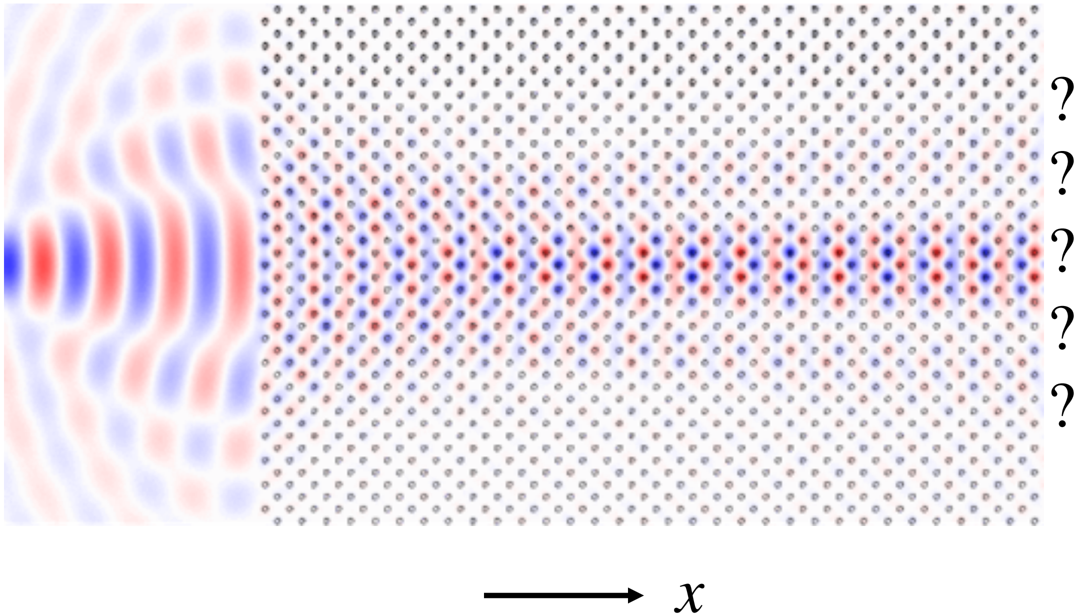
effective conductivity

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

PML = effective anisotropic "absorbing" ε, μ

Photonic-crystal PML?

FDTD (Meep) simulation:

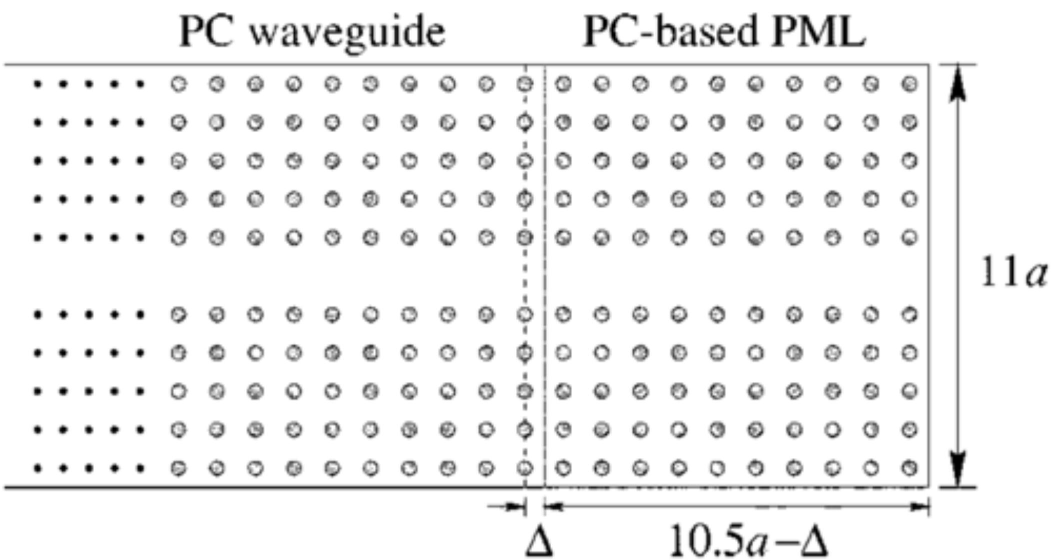


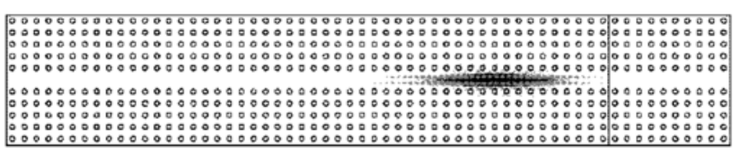
ε not even *continuous*
in x direction,
much less analytic!

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

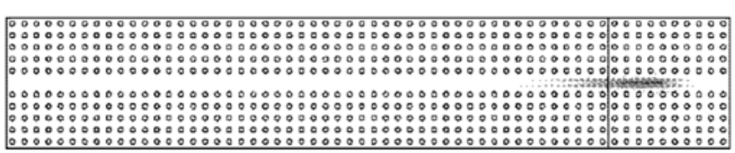
Photonic-crystal PMLs: Magic?

[Koshiba, Tsuji, & Sasaki (2001)]

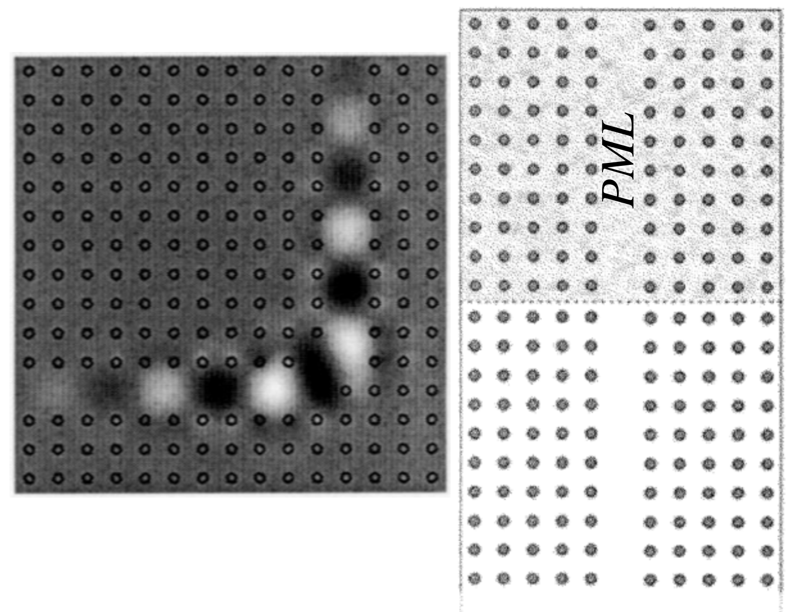




(b)



[Kosmidou *et al* (2003)]



… & several other authors …

Low reflections claimed

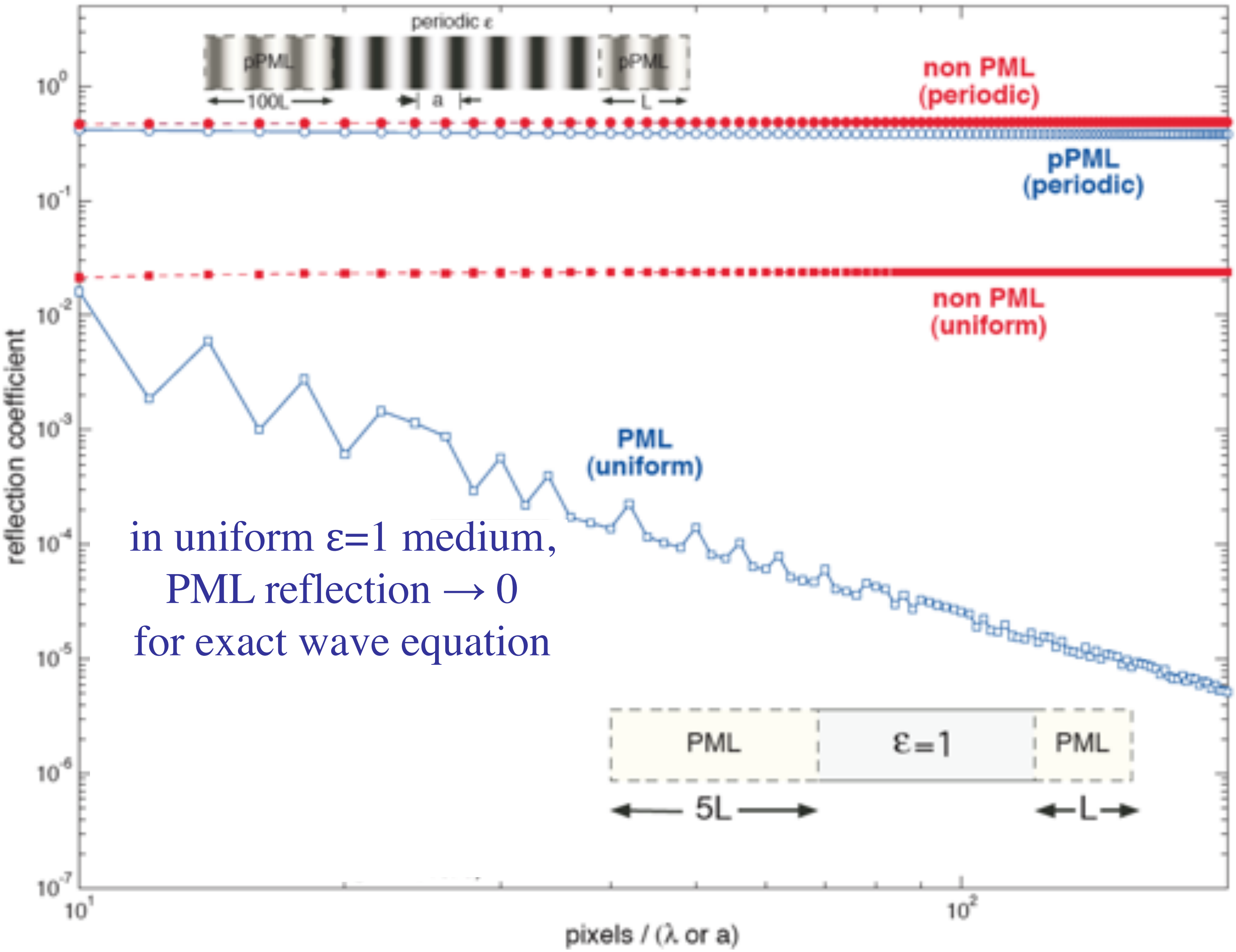
— is PML working?

Something suspicious:

very thick absorbers.

Failure of Photonic-crystal "pseudo-PML"

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



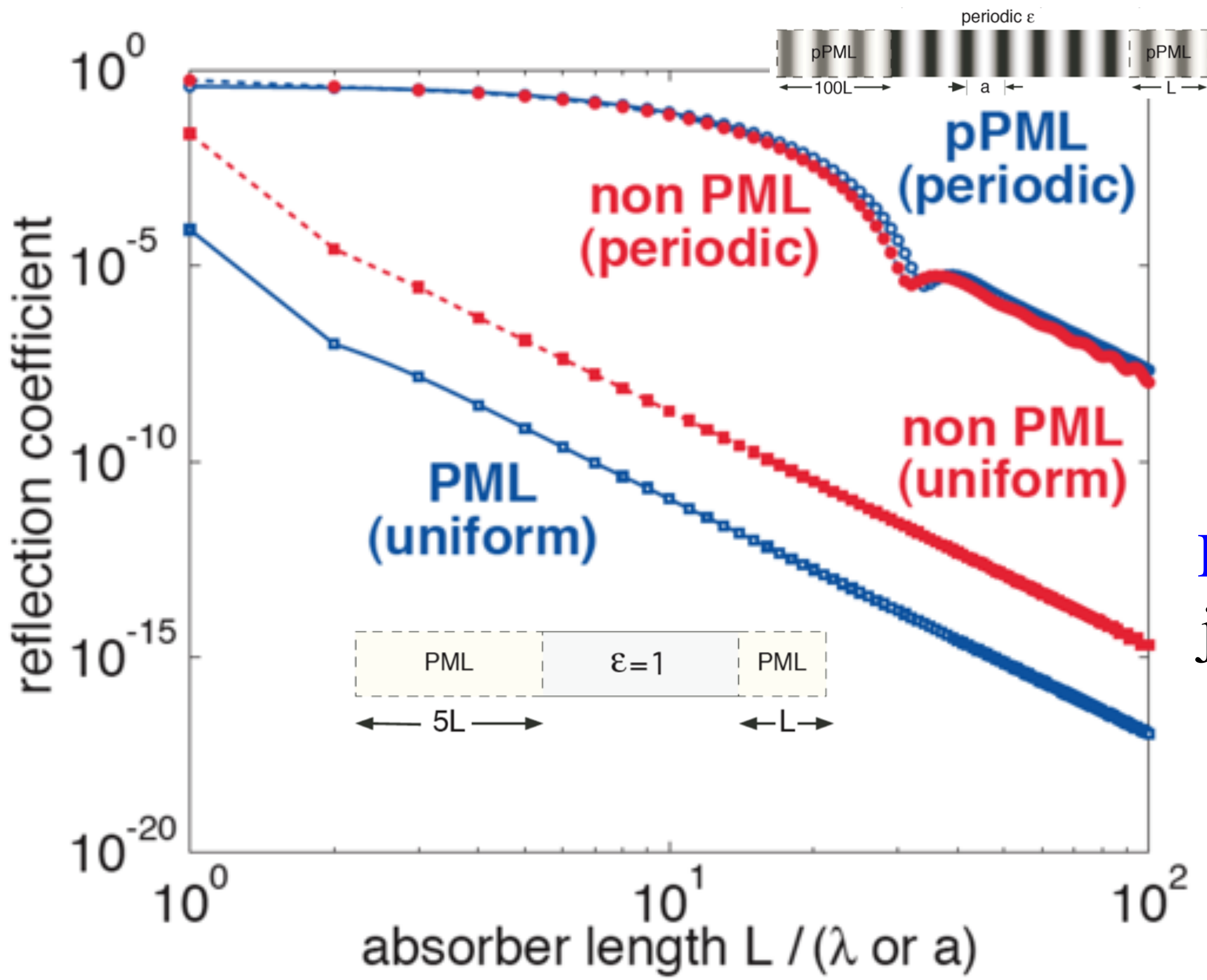
1d test case:

(pseudo-) PML in periodic ε reflection doesn't → 0 as $\Delta x \to 0$

… similar to non-PML scalar σ

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

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



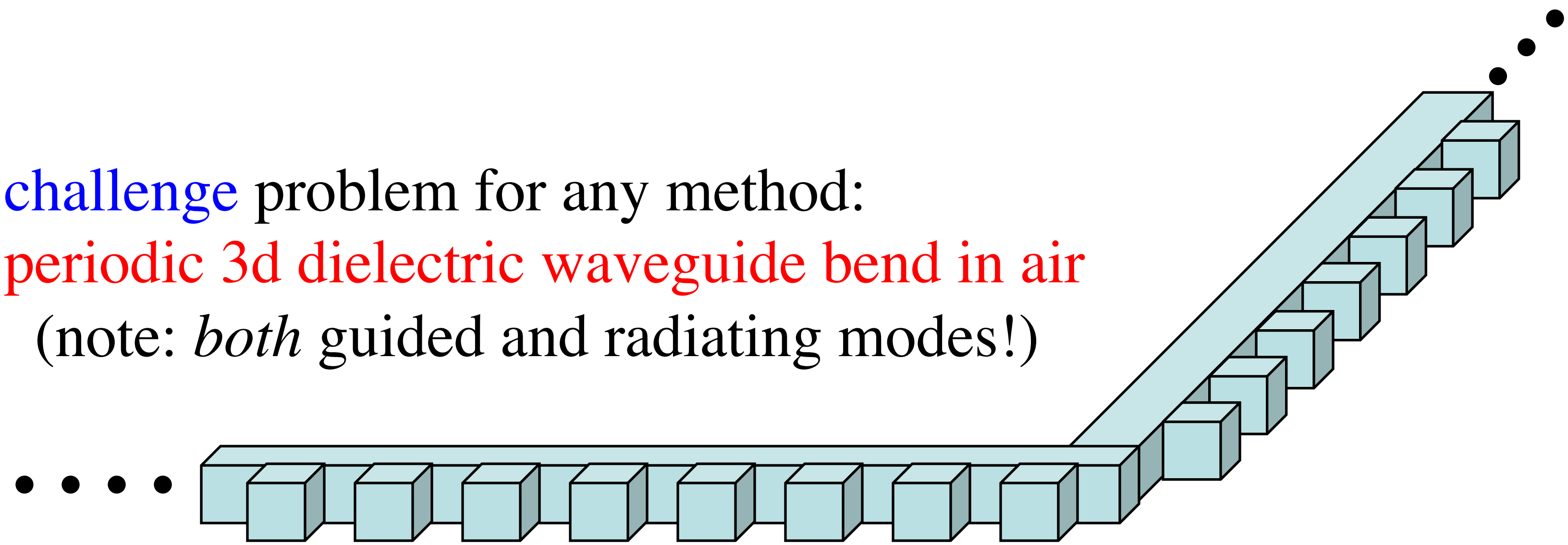
Any absorber, turned on gradually enough, will have reflections → 0!

PML (when it works) just helps coefficient.

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!)

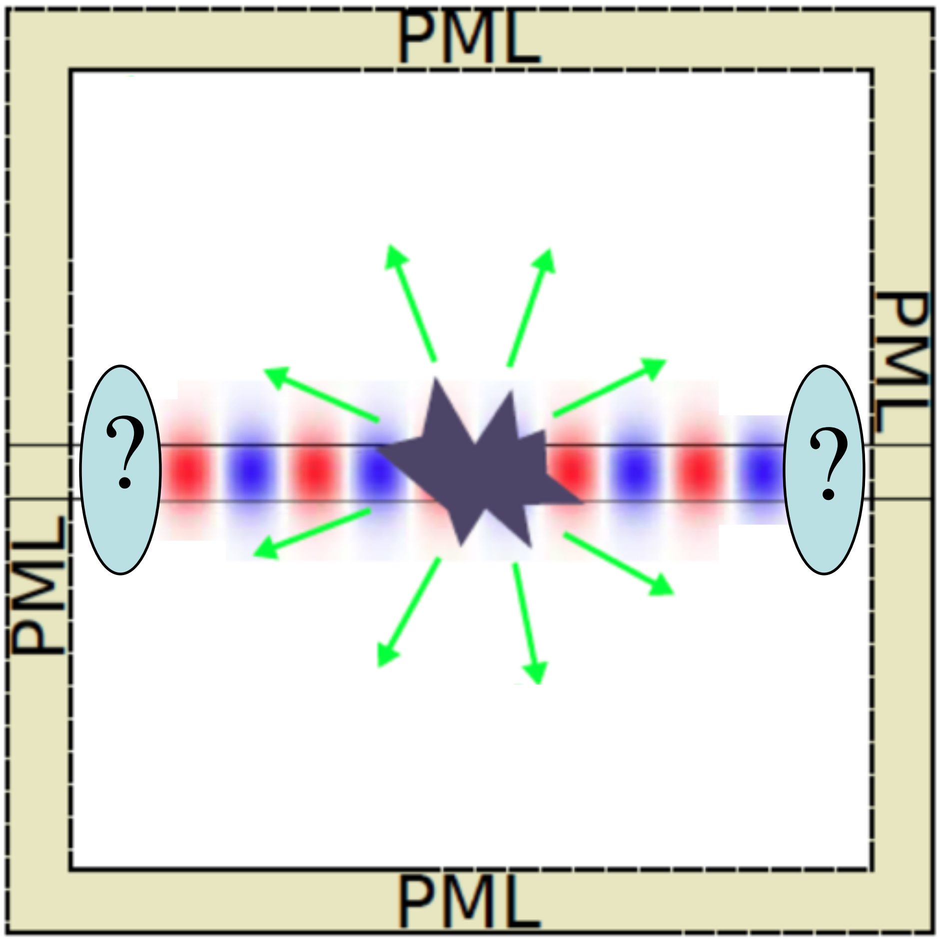


… DtN / Green's function / Bloch modes (incl. radiation!) expensive

Computational Nanophotonics: Sources & Integral Equations

Steven G. Johnson
MIT Applied Mathematics

How can we excite a desired incident wave?



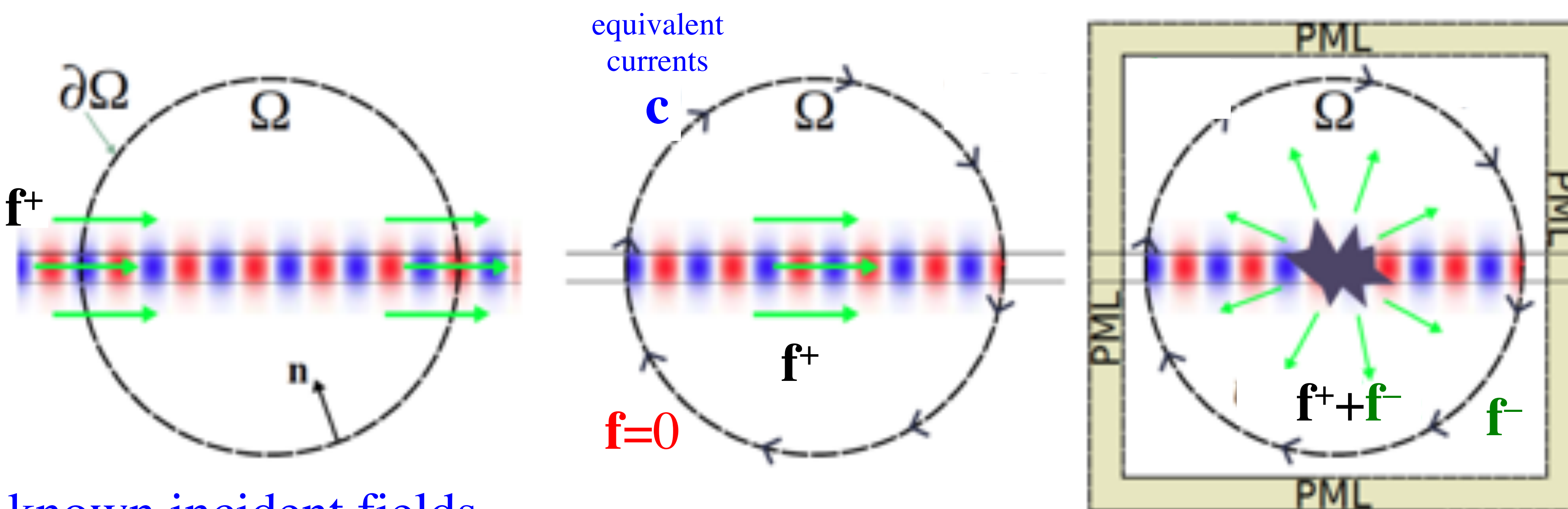
Want some current source to excite incident waveguide mode, planewave, etc…

— 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

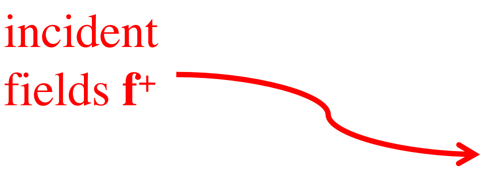
(or Stratton–Chu equivalence principle)
(formalizes Huygens' Principle)
(or total-field/scattered-field, TFSF)
(near-to-far-field transformation)

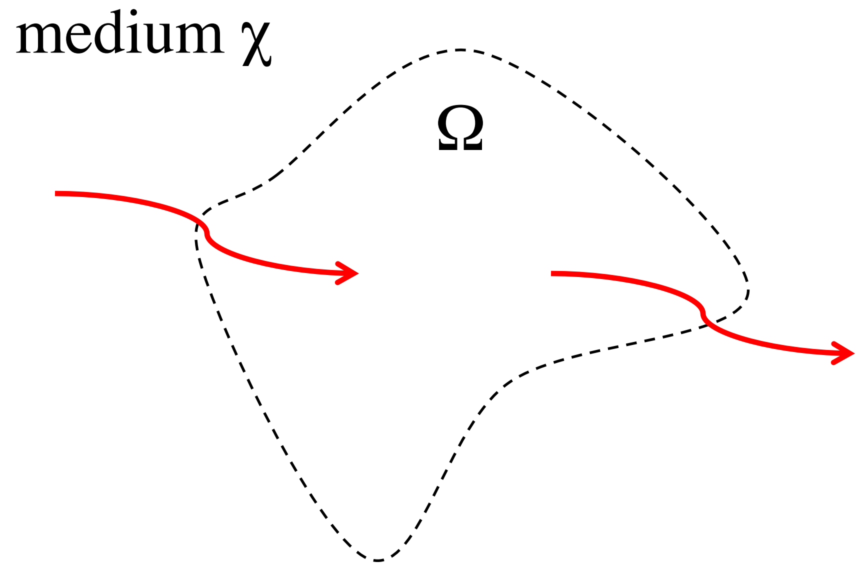
(close connection to Schur complement [Kuchment])

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

[review article: arXiv:1301.5366]

starting point: solution in all space





6-component fields:

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

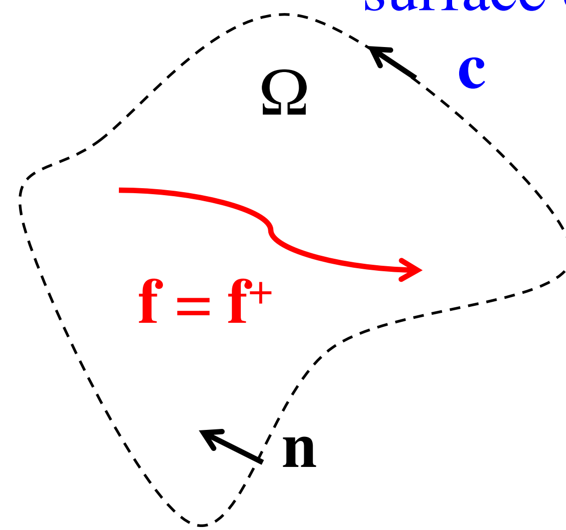
solve (source-free) Maxwell PDE (in frequency domain):

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

constructing solution in Ω

equivalent
"6"-component
surface currents

$\mathbf{f} = 0$



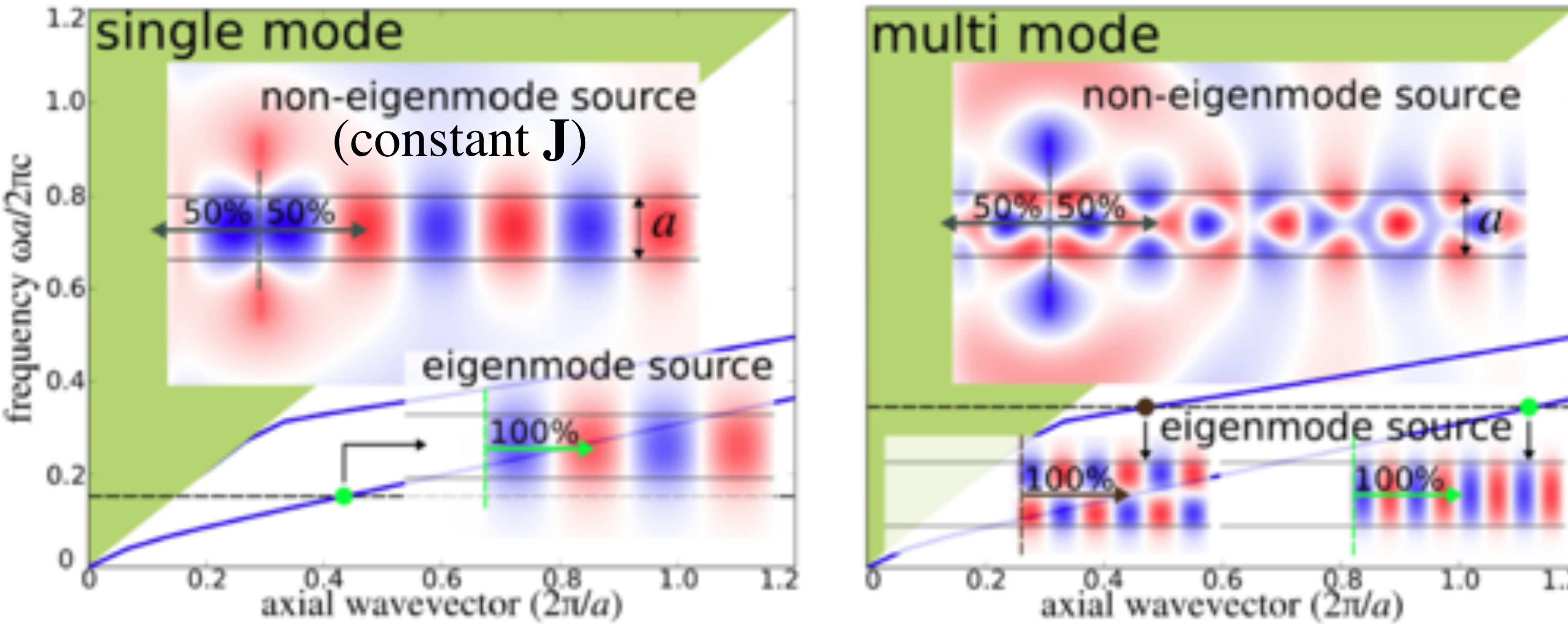
construct **c** so that **f** is a new solution:

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix}\mathbf{f} = -i\omega\chi\mathbf{f} + \delta(\partial\Omega)\begin{pmatrix} -n\times\mathbf{H}^{+} \\ n\times\mathbf{E}^{+} \end{pmatrix} \begin{matrix} \text{"electric" current} \\ \text{"magnetic" current} \end{matrix}$$

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

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

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

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

narrow-bandwidth

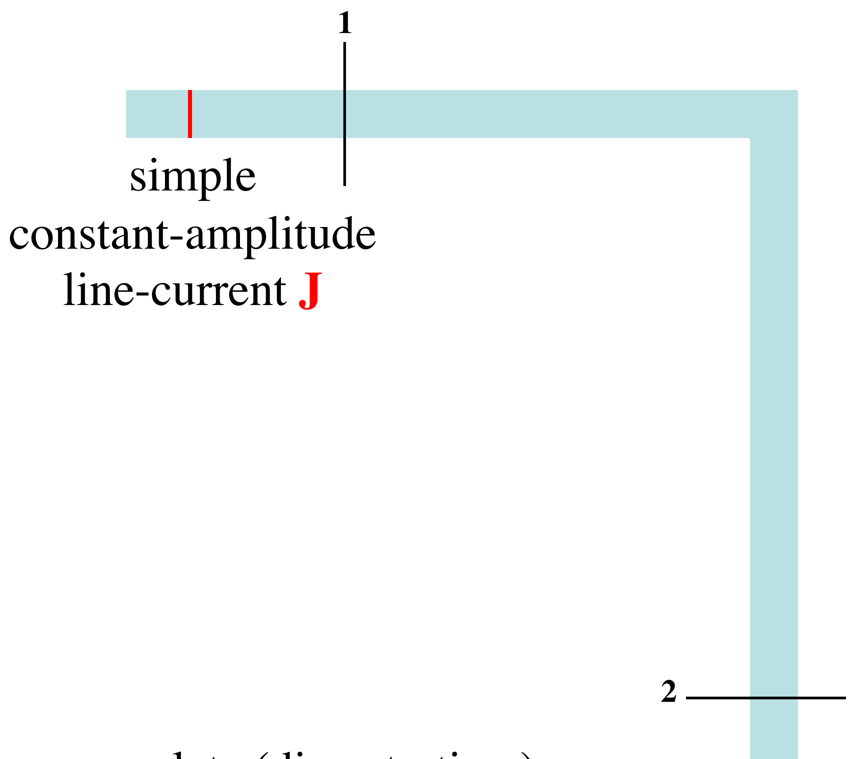
– convolutions expensive, can be approximated by finite-time (FIR/IIR) calculations using DSP techniques
– specialized methods are known for planewave sources

(have numerical dispersion!)

time domain only

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 $\hat{\mathbf{f}}^{1}_{\text{bend}} - \hat{\mathbf{f}}^{1}_{\text{straight}}$

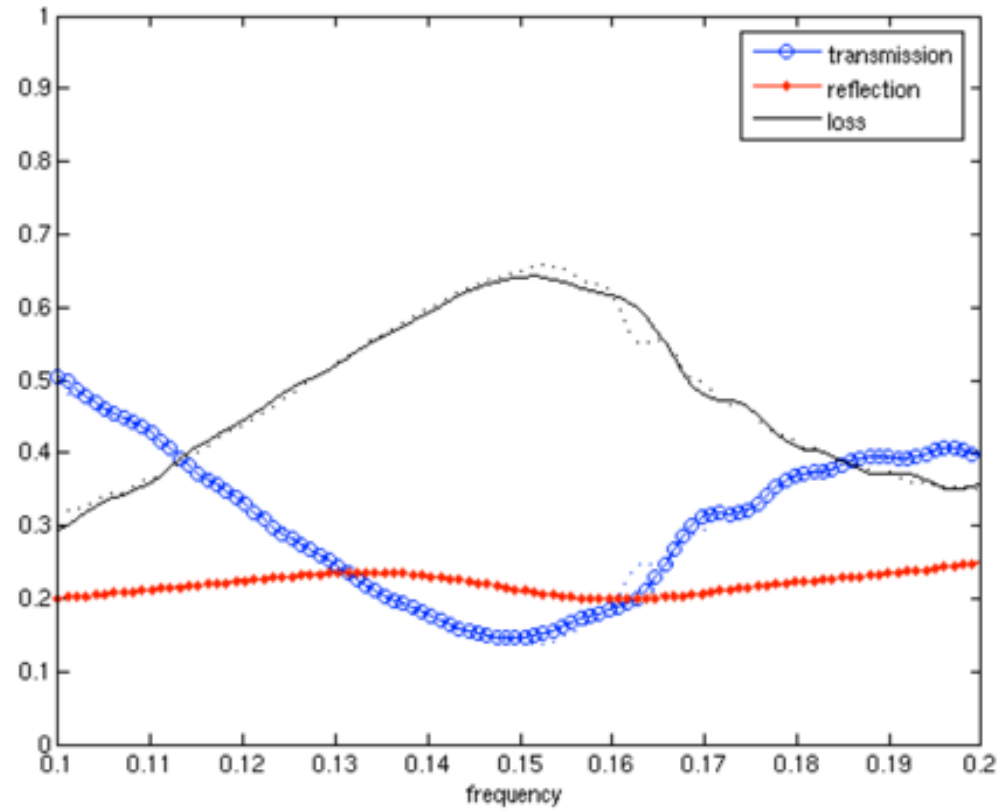
accumulate (discrete-time) Fourier transforms of fields:

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

at desired frequencies ω

Shortcut: Subtract two simulations

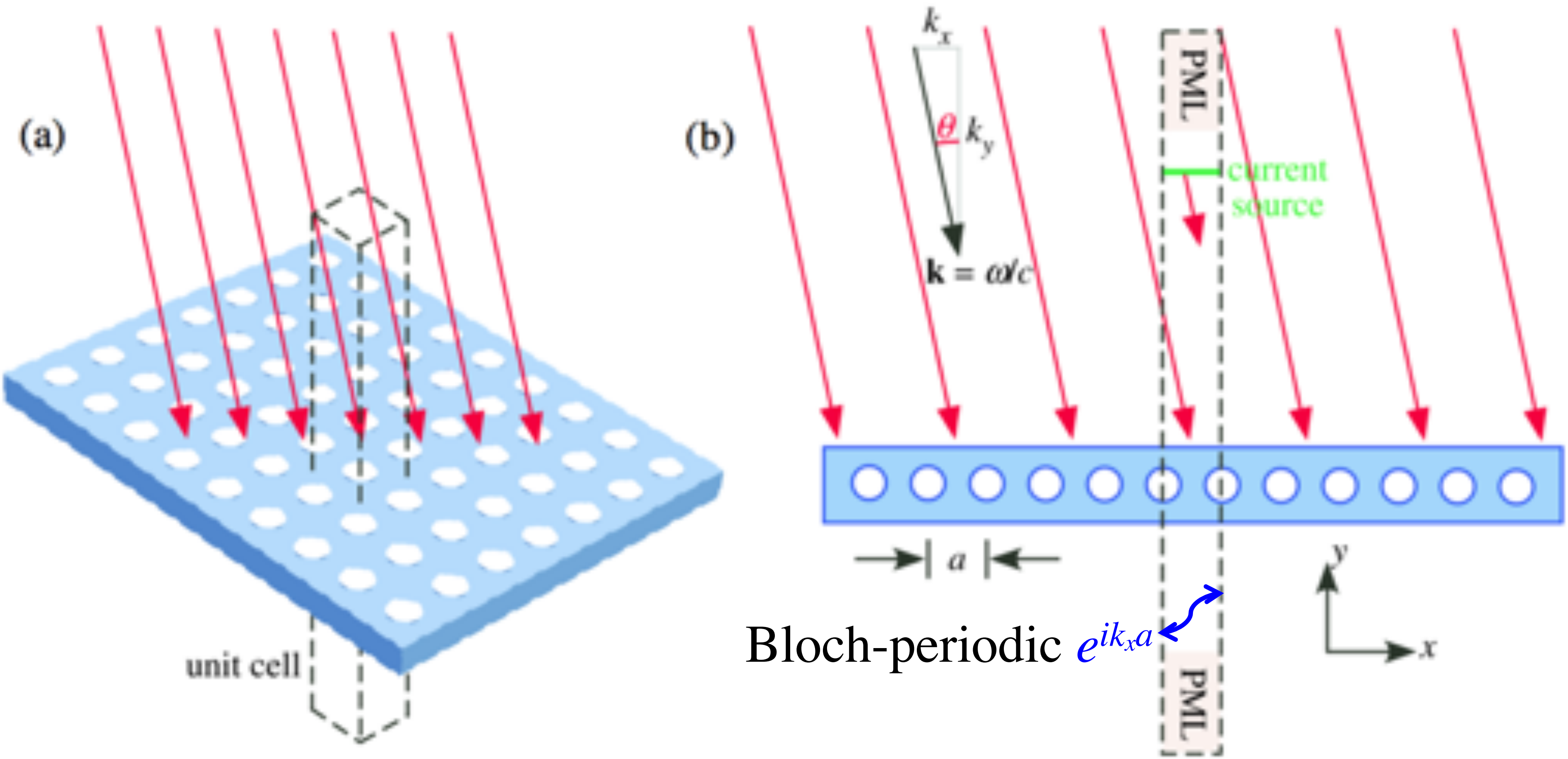
example: 90˚ bend of single-mode dielectric waveguide



(waveguide width) / λ

Shortcut: Planewave sources for periodic media

[review article: arXiv:1301.5366]

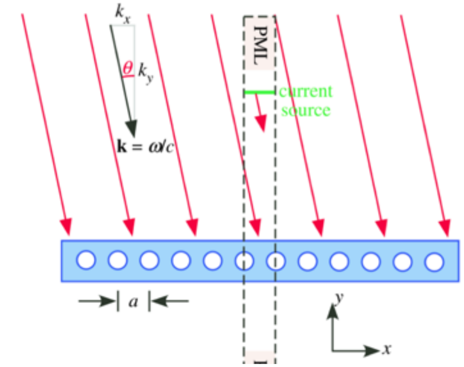


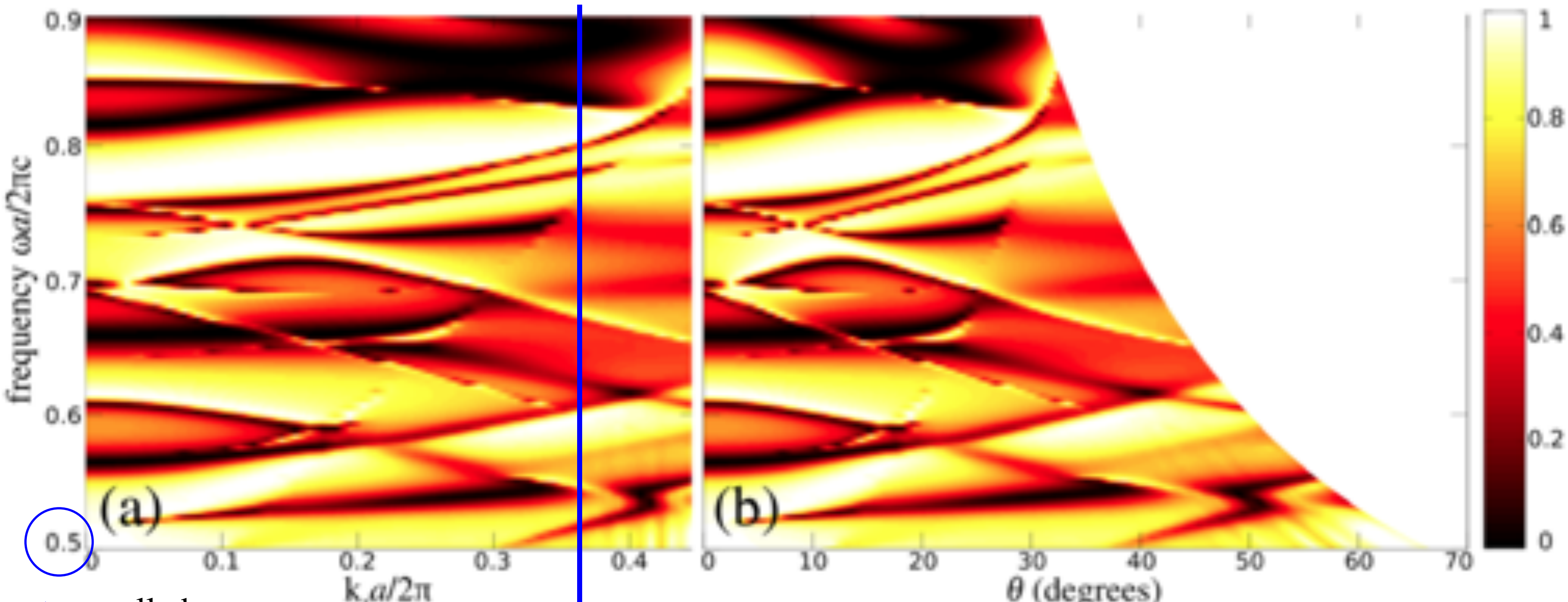
trick #1: incident & scattered fields are Bloch-periodic/quasiperiodic

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

Reflection spectra example for periodic media

(Fano resonance lineshapes)





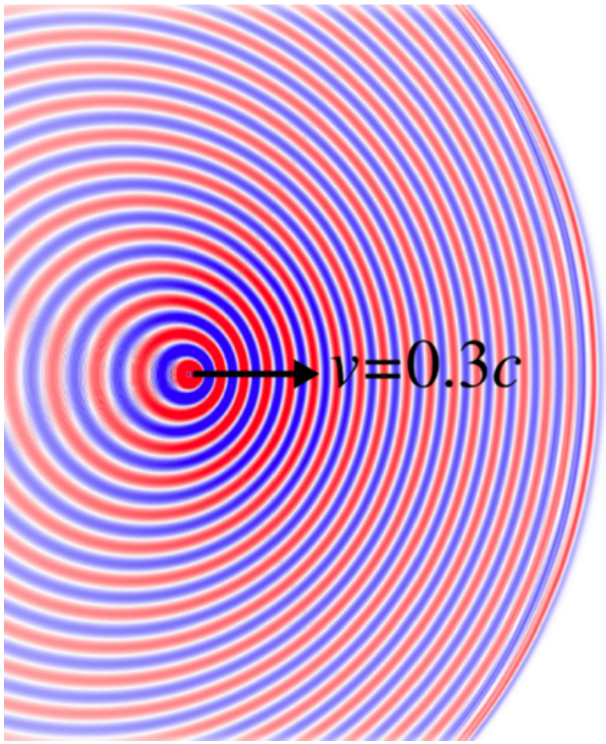
note: ω all above light line
(req. for incident planewave)

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

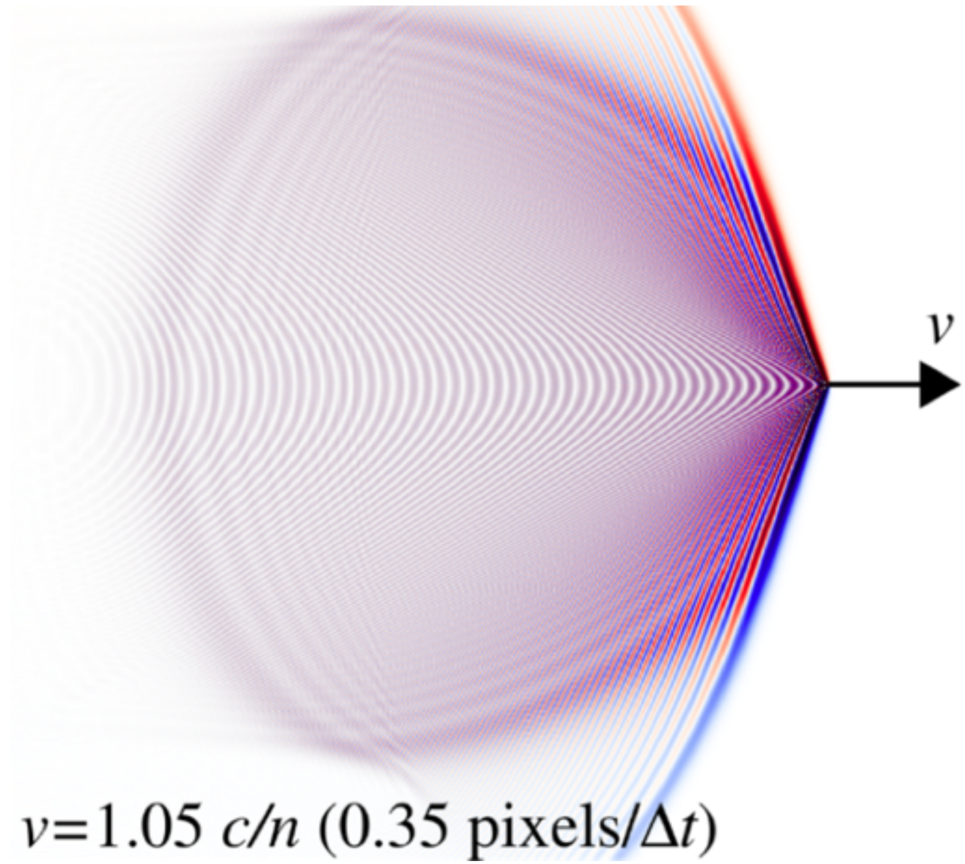
$\omega/c \sin(\theta) = k_x$
$\Leftrightarrow$ curved line
$\theta = \mathrm{asin}(ck_x/\omega)$
in (ω,θ) plot

Fun possibilities in FDTD:

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

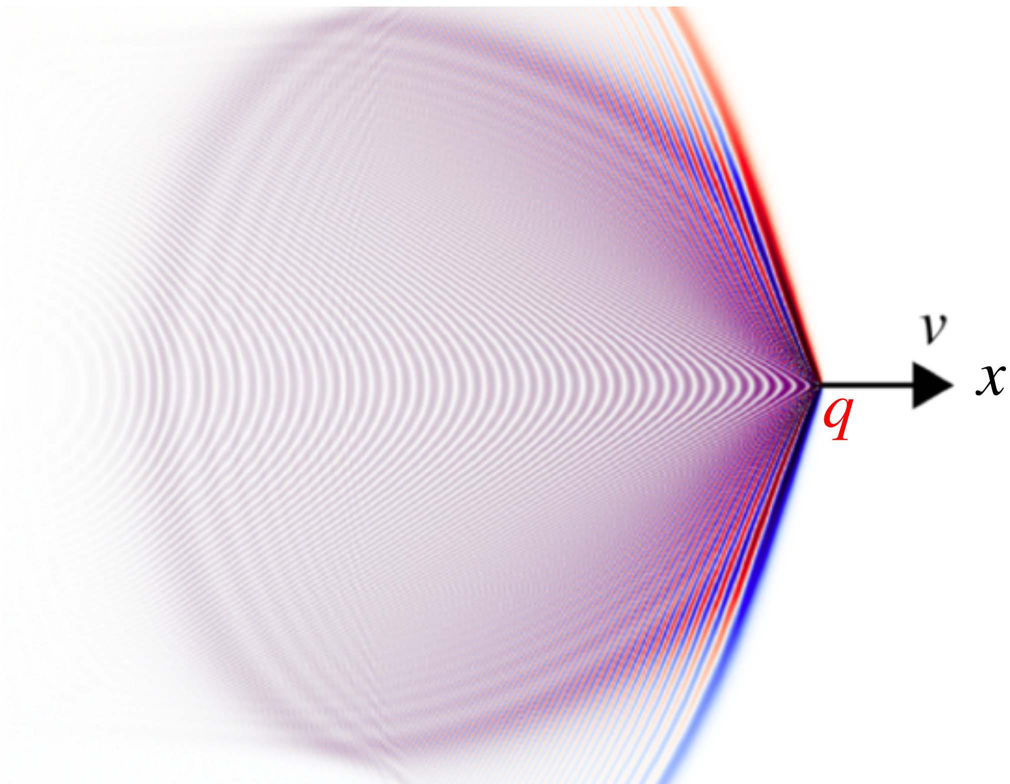


Doppler shift from moving oscillating dipole



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 $\omega(k)=kv$

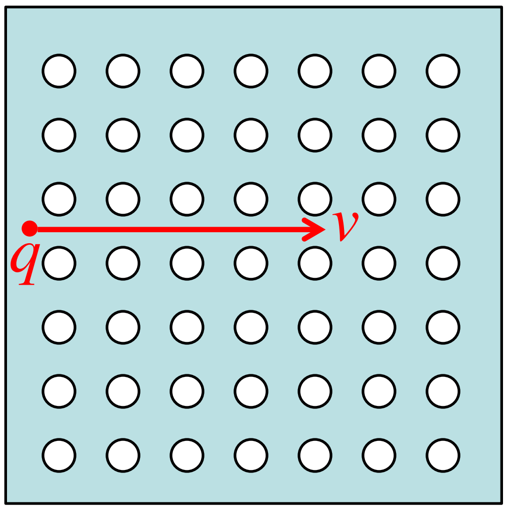
excites radiating mode $\omega(k_x,k_y)$

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

= phase velocity in x direction

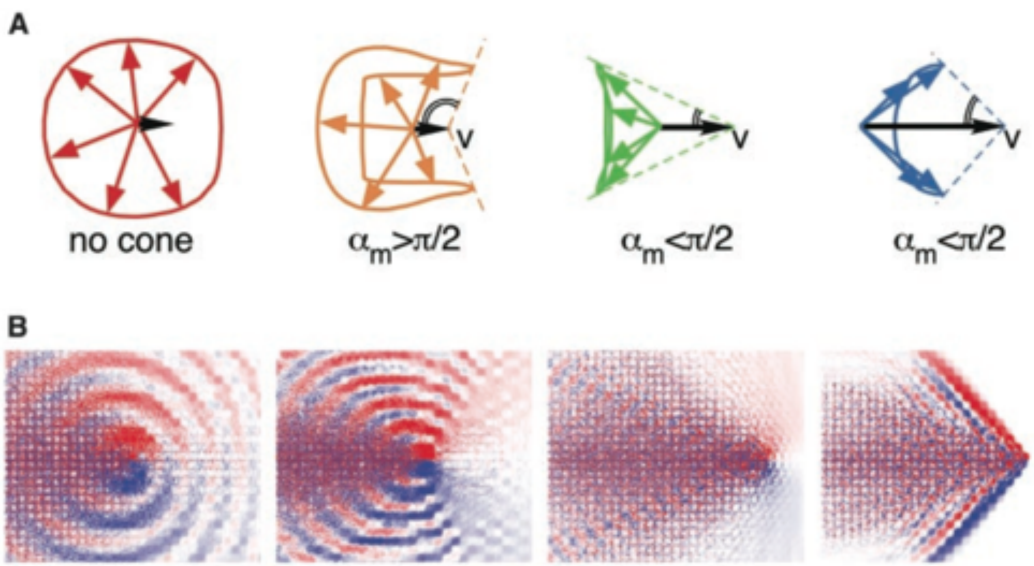
$\geq c/n$ in index-n medium

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

$\Rightarrow$ 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)

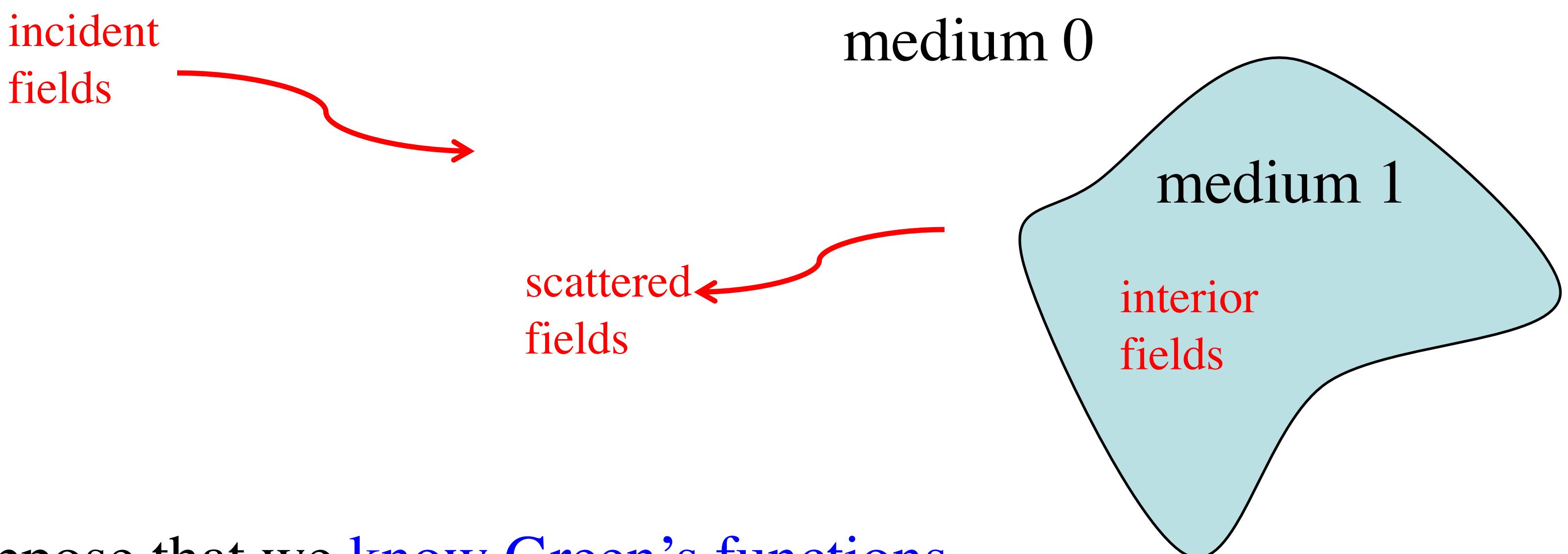
[see e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]

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

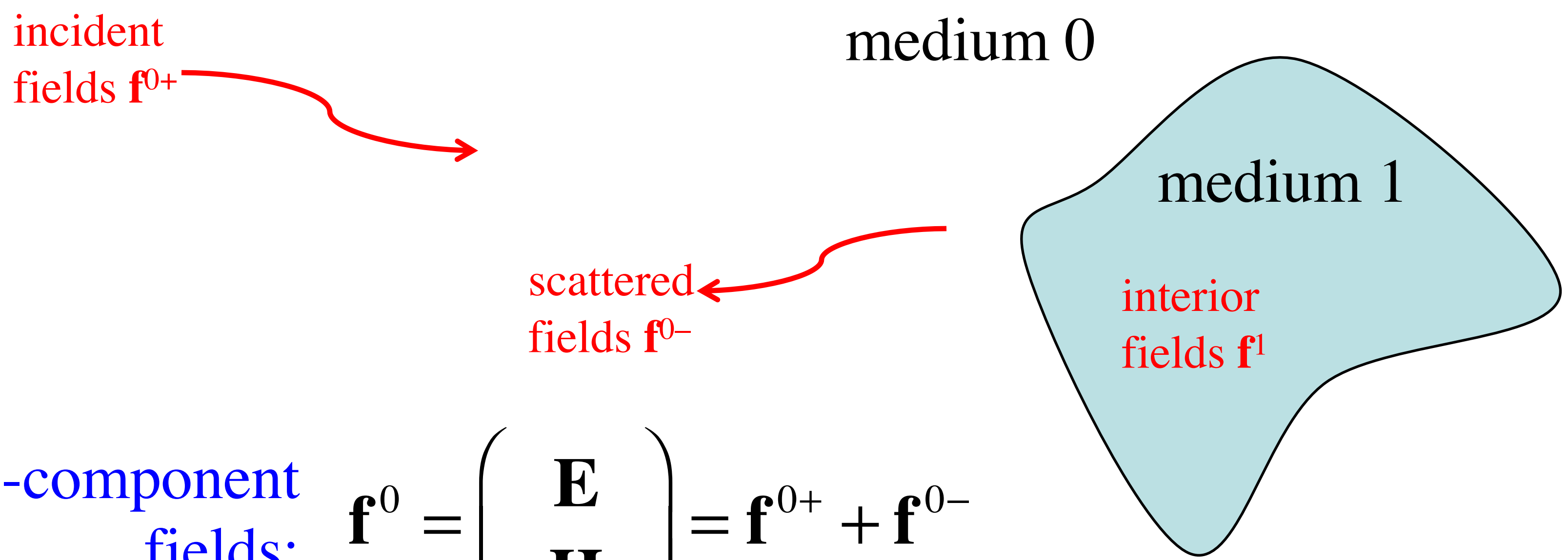
— known analytically for homogeneous media

— 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*]



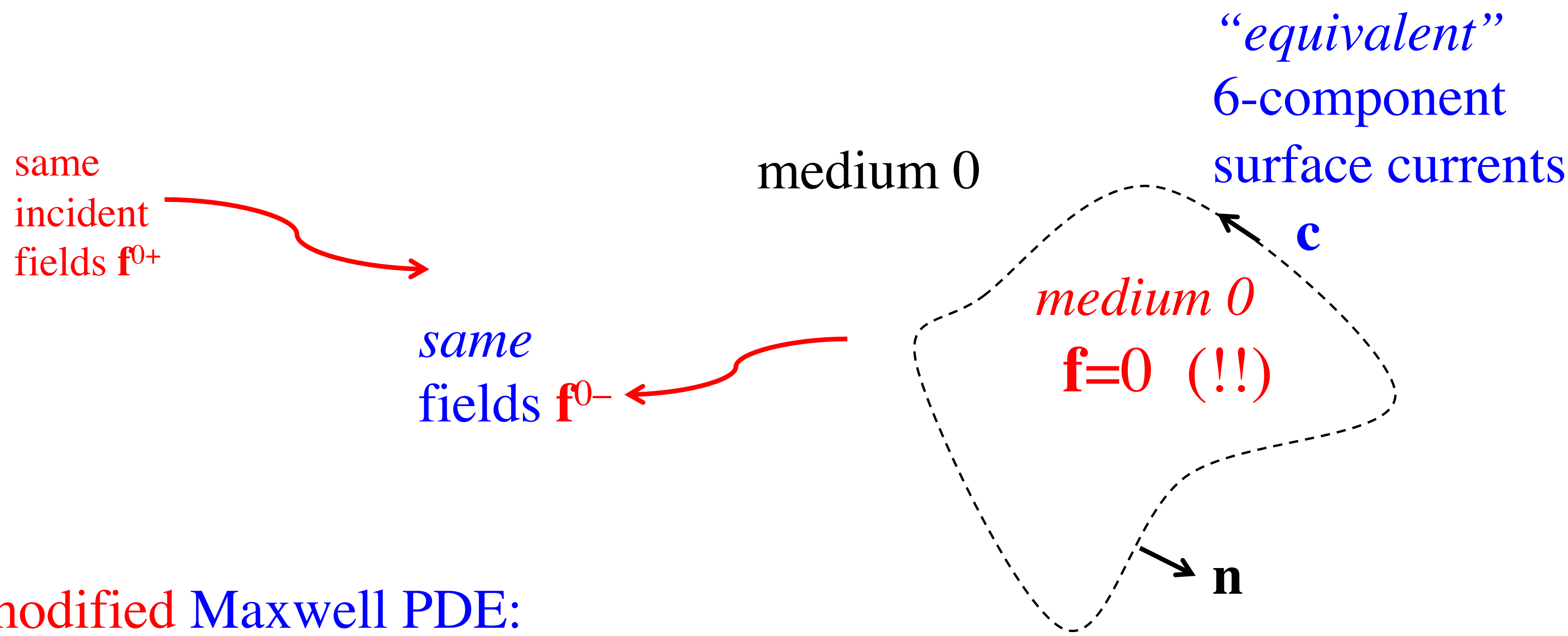
6-component fields: $$\mathbf{f}^0 = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathbf{f}^{0+} + \mathbf{f}^{0-}$$

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:

$$\begin{pmatrix} & \nabla\times \\ -\nabla\times & \end{pmatrix}\mathbf{f} = -i\omega\chi\mathbf{f} + \delta(\partial\Omega)\begin{pmatrix} -n\times\mathbf{H}^{0} \\ n\times\mathbf{E}^{0}\end{pmatrix} \begin{matrix} \text{“electric” current} \\ \text{“magnetic” current}\end{matrix}$$

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

The *Principle of Equivalence* I

"equivalent"
6-component
surface currents
c

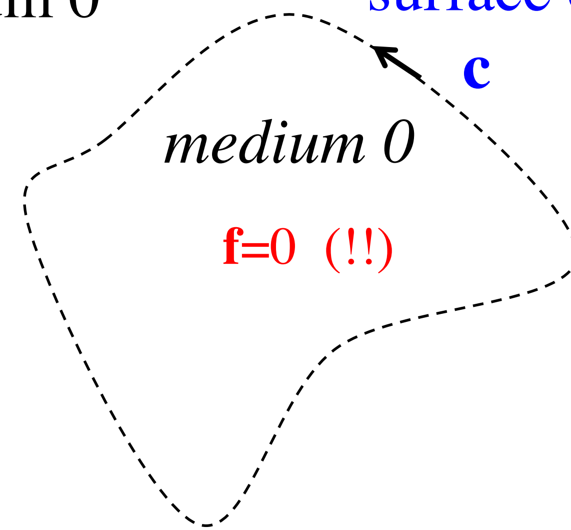
incident
fields $\mathbf{f}^{0+}$

medium 0

medium 0

$\mathbf{f}=0$ (!!)

same
~~scattered~~
fields $\mathbf{f}^{0-}$ of **c**



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

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

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

The *Principle of Equivalence* II

opposite-sign
6-component
surface currents

medium 1

$-\mathbf{c}$

$\mathbf{f}=0$

medium 1

$$\mathbf{f}^1 = -\underbrace{\Gamma^1 * \mathbf{c}}$$

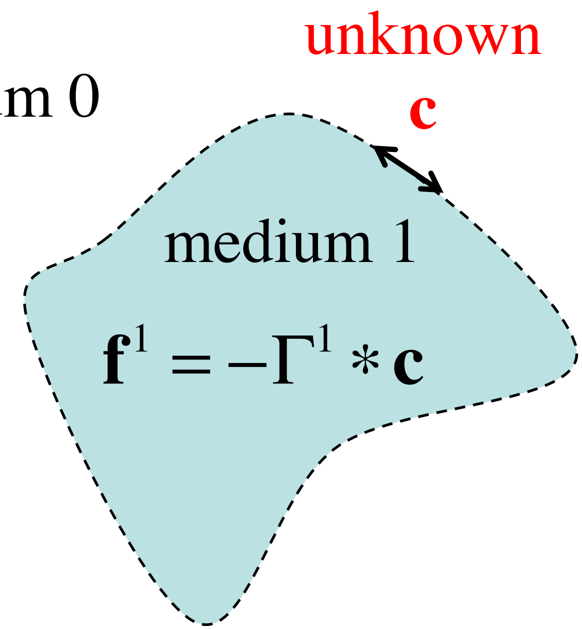
convolution with
6x6 Green's function Γ^1
of *homogenous* medium 1

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

Surface-Integral Equations (SIE)

medium 0

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



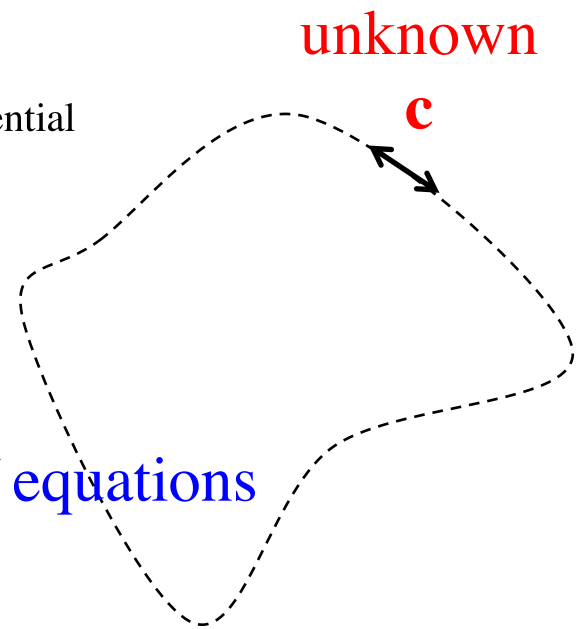
c determined by
continuity of tangential fields
at 0/1 interface:

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

[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→∞)
for surface-tangential vector fields

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

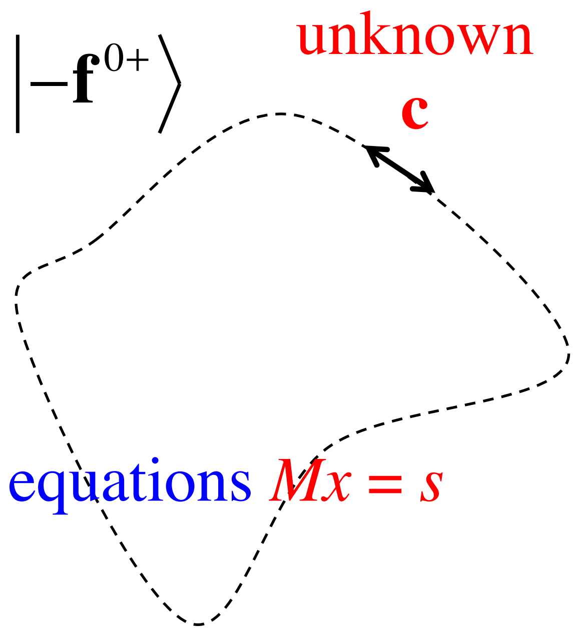
N discrete unknowns x_n ⇒ N equations

[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** $\mathbf{b}_\mathrm{n}$ (n=1,…,N→∞)
for surface-tangential vector fields

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

N discrete unknowns x_n

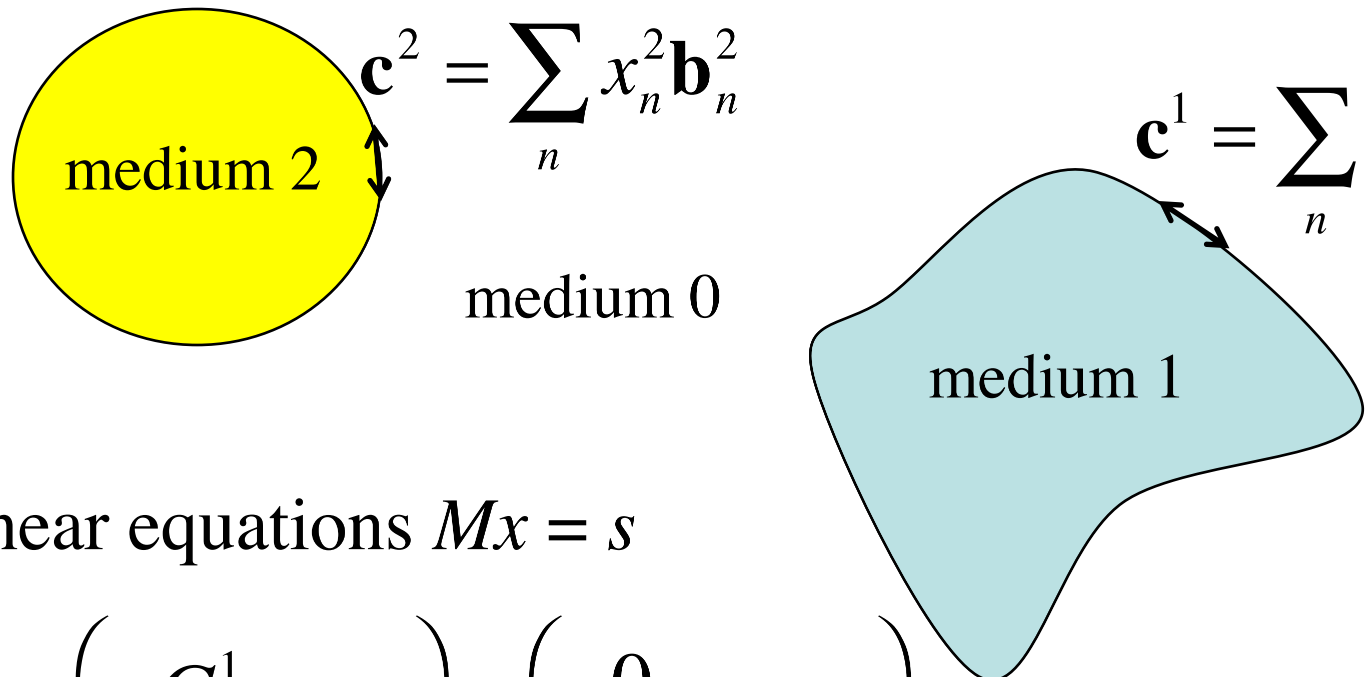
⇒ N equations $Mx = s$

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

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

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

Discretized SIE: Two Objects



$$\mathbf{c}^2 = \sum_n x_n^2 \mathbf{b}_n^2$$

$$\mathbf{c}^1 = \sum_n x_n^1 \mathbf{b}_n^1$$

$\Rightarrow$ linear equations $Mx = s$

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

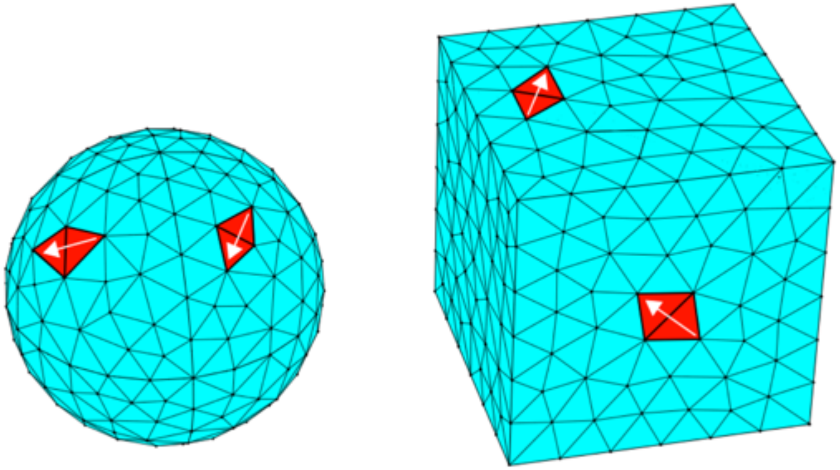
… + straightforward generalizations to more objects, nested objects, etcetera

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**



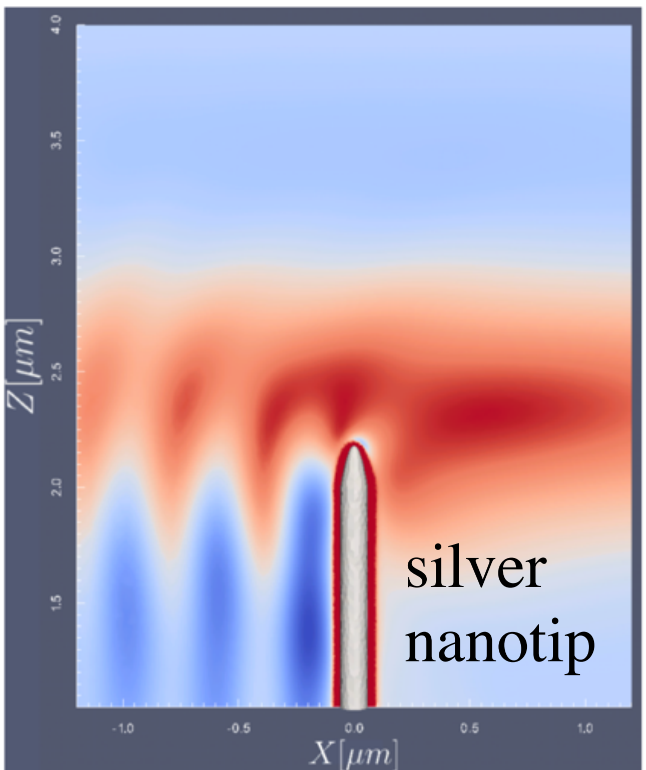
"RWG" basis (1982):

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

BEM strengths

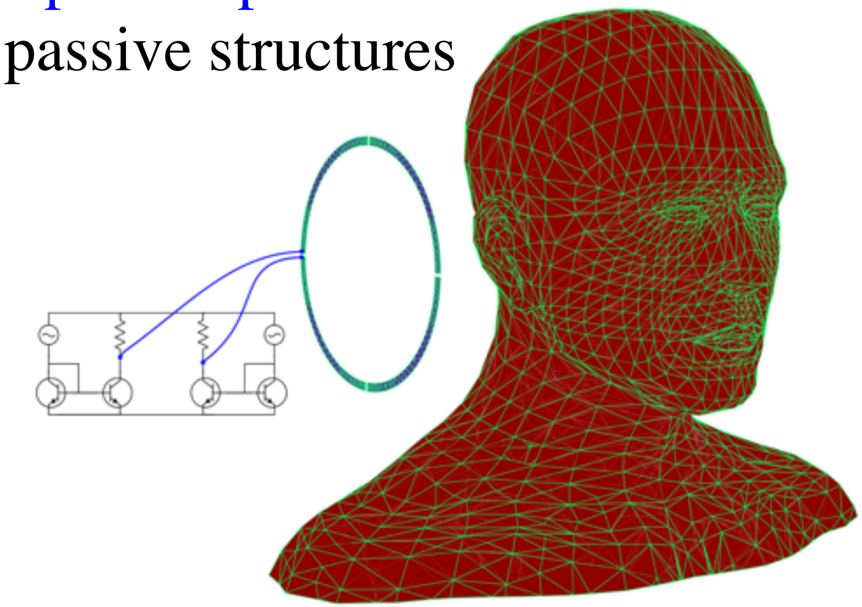
especially small surface areas in a large (many-λ) volume, e.g.:

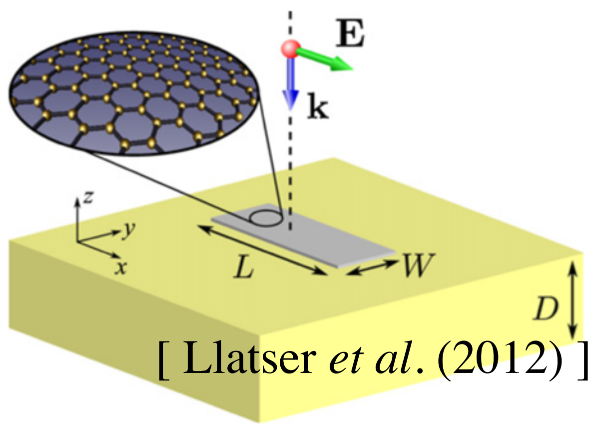
surface plasmons (metals):
extremely sub-λ fields



[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

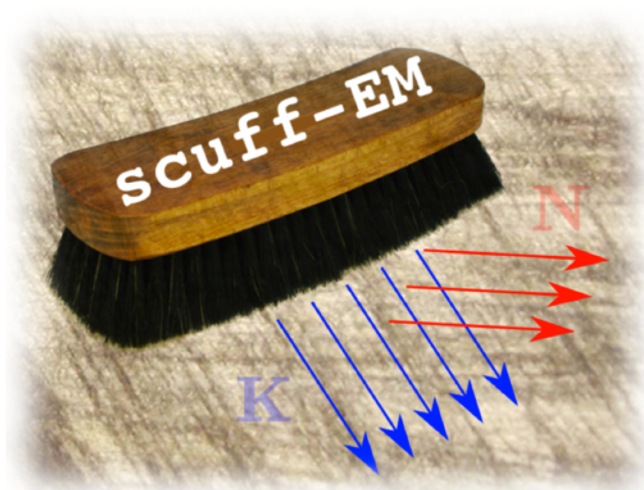
  — M is *not sparse*, but:
  often small enough for dense solvers ($\lesssim 10^4 \times 10^4$)
  + "fast solvers:" approximate sparse factorizations
  (fast multipole method, etc.)

  — 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

[https://github.com/HomerReid/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.

https://github.com/HomerReid/scuff-em

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.**

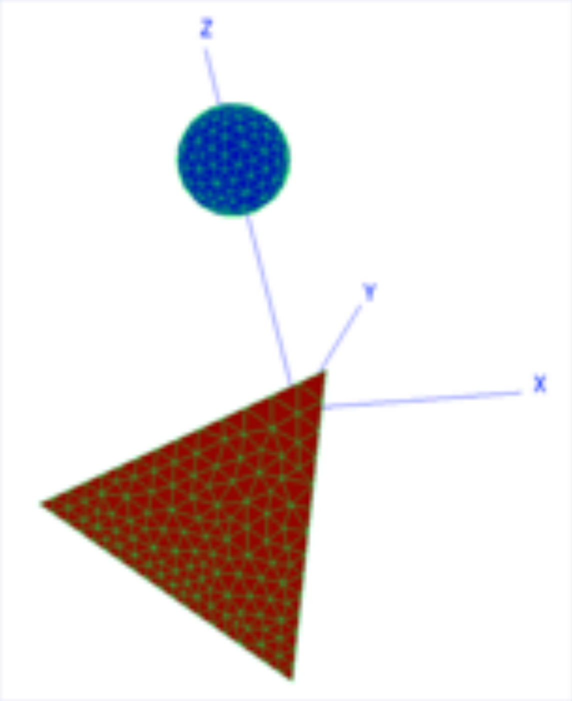
Innovations unique to SCUFF-EM:

- 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 SiO_2 tetrahedron:

The geometry:



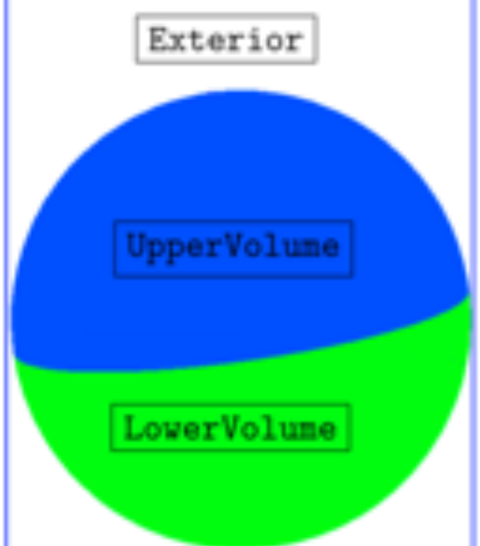
The .scuffgeo file:

```
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
```

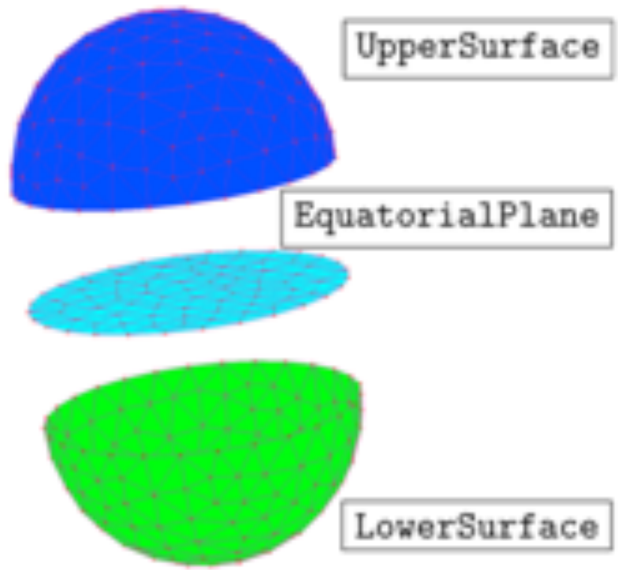
$\Longrightarrow$ Handle displacements and rotations without re-meshing.

Geometries in SCUFF

Regions



Surfaces



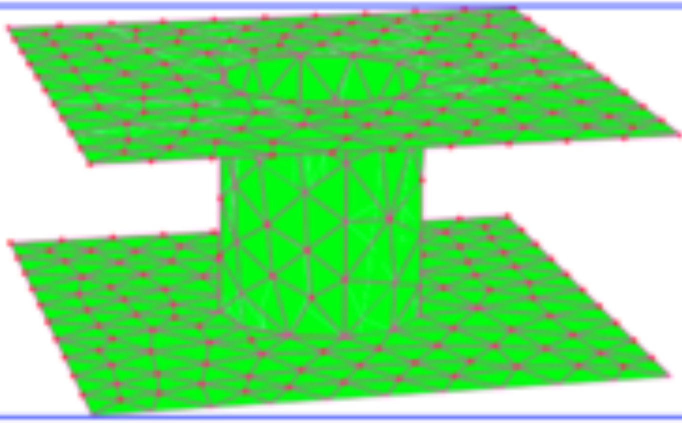
.scuffgeo File

```
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

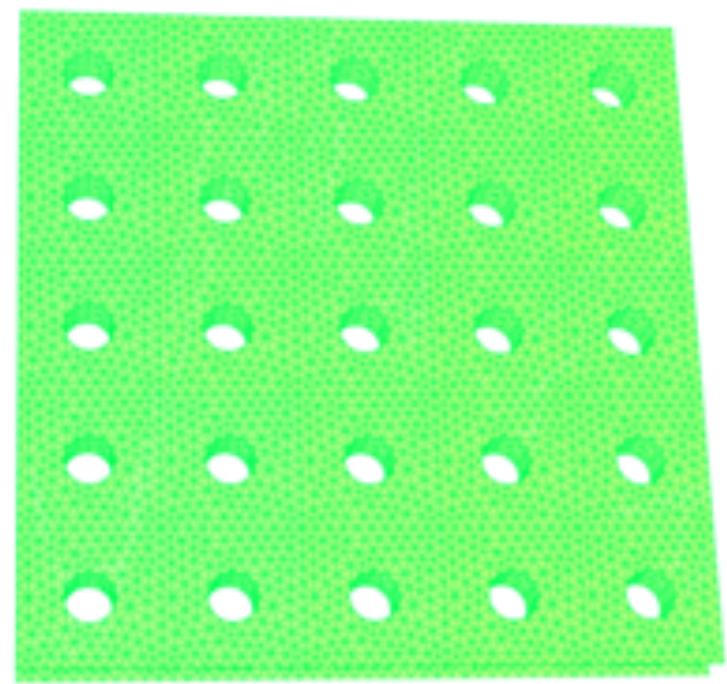
Unit cell mesh



`.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** ($\sim \mathbf{n} \times$ 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, …

https://arxiv.org/abs/1307.2966

- 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 ($\Rightarrow$causal) systems, solutions can only occur for $\operatorname{Im} \omega \leq 0$.

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

to be continued…

Further reading:

Free FDTD software: http://jdj.mit.edu/meep
Free BEM software:
http://homerreid.ath.cx/scuff-EM/

Review on wave sources:
arXiv:1301.5366 [in Taflove, Oskooi, & Johnson, eds., *Advances in FDTD Comput. EM* (2013)]

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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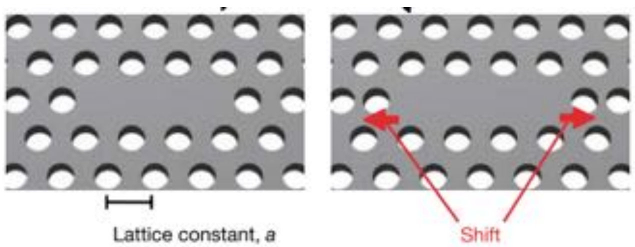
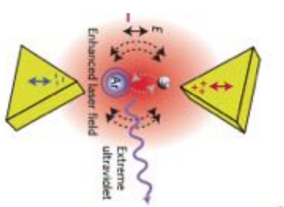
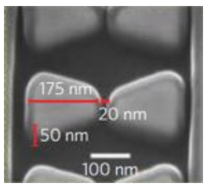
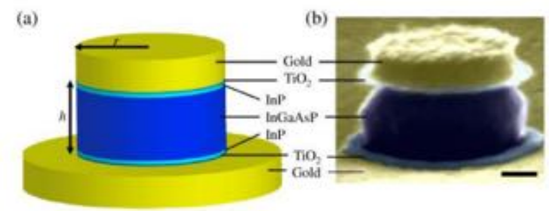
Optical design = optimization

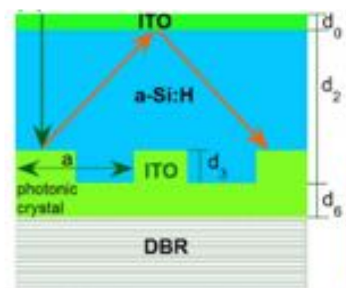
traditional approach: intuition + “tweaking” few parameters





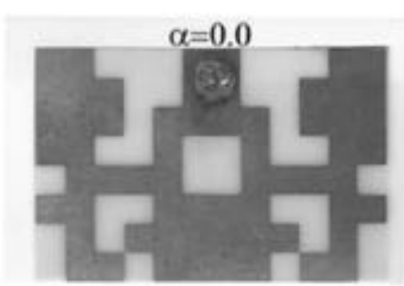


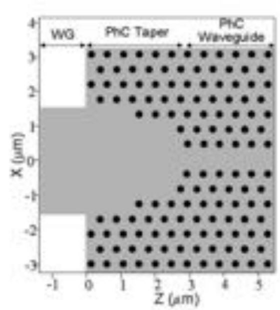




[Noda et. al. 2003]
[Brongersma et. al. 2010]
[Yu et. al. 2010]
[Zhou et. al. 2010]

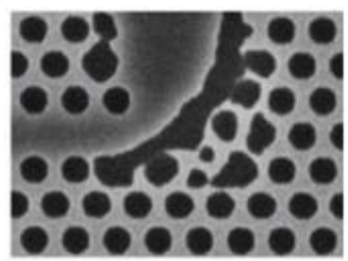
“black-box” optimization
(typically << 100 params)

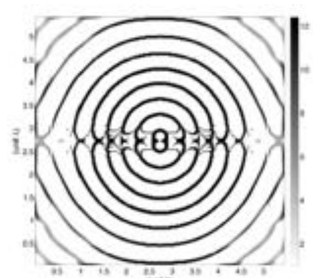




[Villegas et. al. 2004] [Hakansson et. al. 2005]

gradient-based (“adjoint”)
optimization (>10^5 params, 3D)



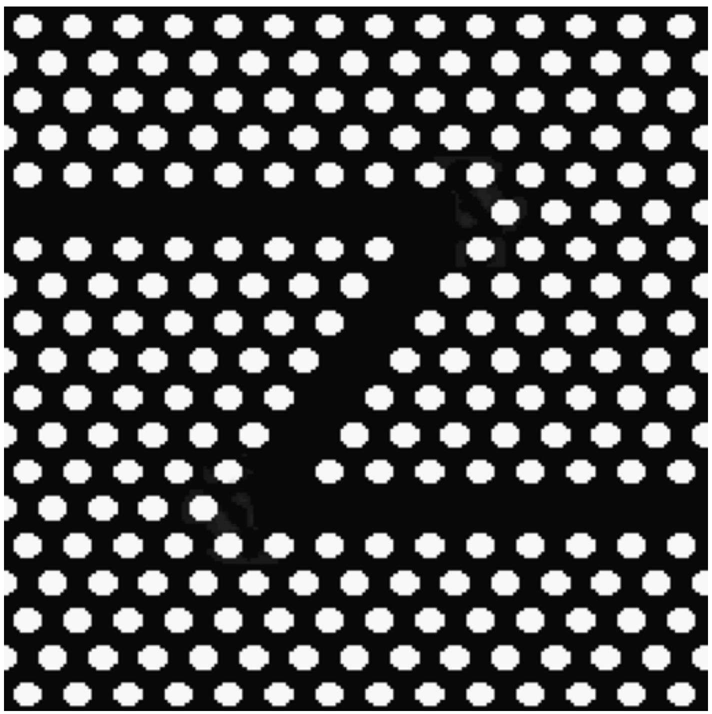


[Sigmund et. al. *Las. Phot. Rev.* 5, 308 (2011)]

[X. Liang & SG Johnson *Opt. Exp.* 21, 30812 (2013)]

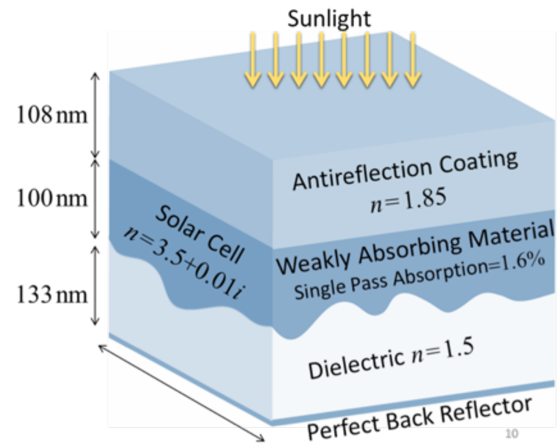
Large-scale optimization in photonics: "Every pixel" is a degree of freedom

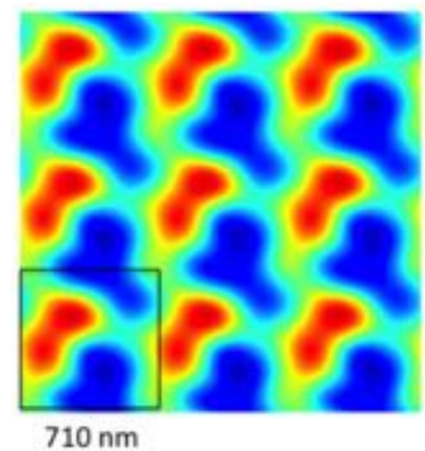
bend optimization



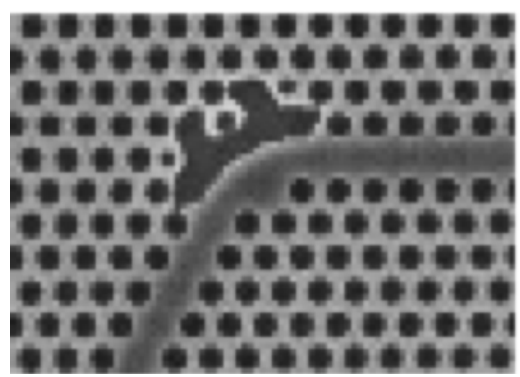
Sigmund et al.,
Opt. Express **12**, 1996 (2004)

solar-cell backreflector optimization



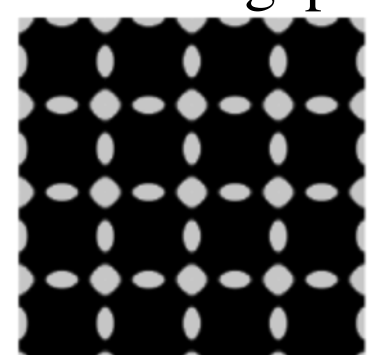


Ganapati et al. IEEE Jour. of Photovolt. **4**, 175 (2014)



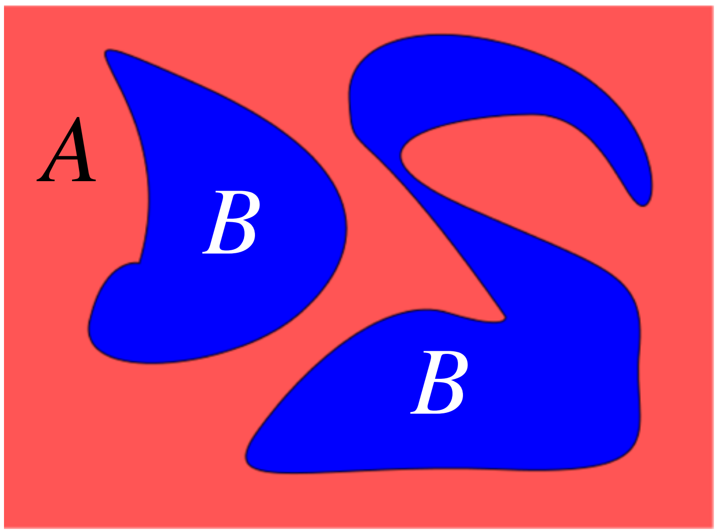
OE **12**, 5916 (2004)

2d band gaps



Dobson (1999)

Topology optimization



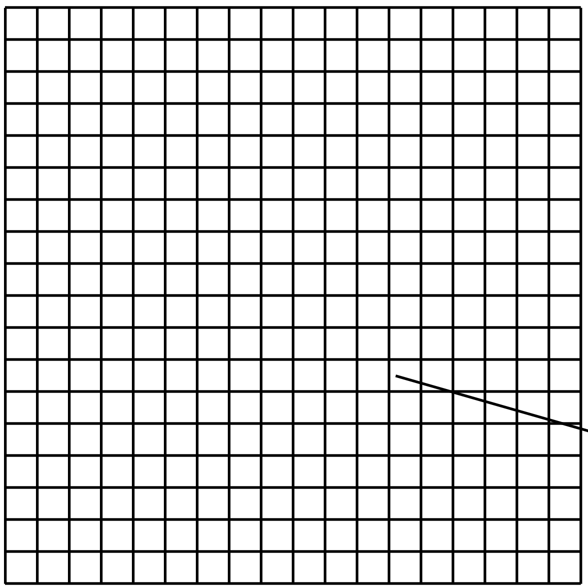
Given two (or more) materials *A* and *B*, determine what arrangement — including what topology — optimizes some objective/constraints.

Electromagnetism:
Materials (mostly) described by permittivity (dielectric constant) ε
(susceptibility χ=ε–1)

Discretizing Topology Optimization

for computer, need finite-dimensional, differentiable parameters

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* …

"Density-based topology optim."
Continuous relaxation: material varies in [A,B] at each pixel

(+ filtering methods to constrain minimum feature sizes and "binary-ize" result)

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

Outline

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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

photonics: mostly local optima in non-convex problems

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.

Leads to "density based" topology optimization, many methods to impose feature-size constraints etc.

Derivatives are essential

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

subject to m constraints

$$f_i(x) \leq 0$$

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

For n ≥ 1000's of parameters, impractical unless you have

$$\nabla_x f_i(x)$$

$$i = 0, 1, 2, \ldots, m$$

computed "analytically" (not by finite differences).

minimize an objective function f_0 with respect to n design parameters x

(also called *decision parameters*, *optimization variables*, etc.)

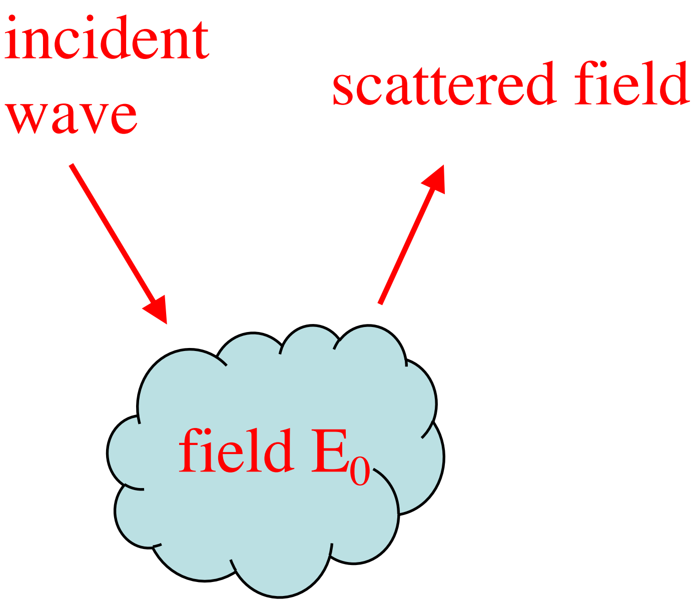
Impossible to explore/optimize a 10^6-dimensional parameter space without derivatives.

(Gradient tells you which direction to go for improvement.)

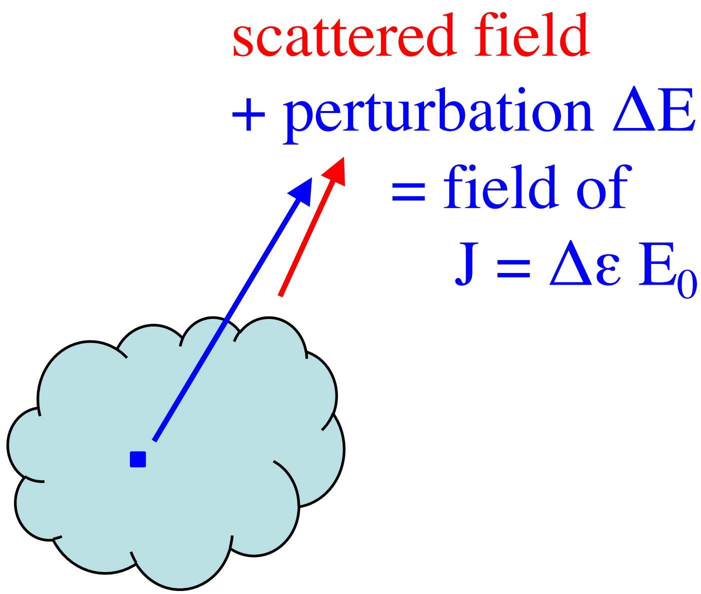
(Only local optimization with this many parameters, but can still find very good designs, sometimes with provable guarantees.)

Amazing fact of adjoint methods: all 10^6 derivatives with two simulations

physical intuition: Born approximation + reciprocity



"forward" solve

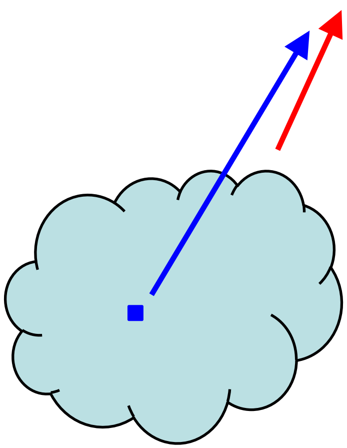


perturbed pixel $\Delta\varepsilon$,
expensive: repeat for each pixel?

Amazing fact of adjoint methods: all 10^6 derivatives with two simulations

physical intuition: Born approximation + reciprocity

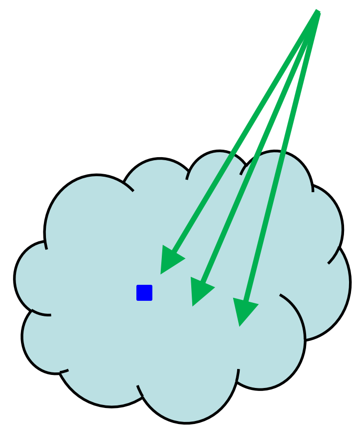
scattered field
+ perturbation ΔE
= field of
$J = \Delta\varepsilon\, E_0$



perturbed pixel $\Delta\varepsilon$,
repeat for each pixel?

=
(reciprocity)

source at scattered
measurement point



solve **one adjoint problem**
*… get fields at **all** perturbed pixels*

Adjoint methods, in math

cost of ∇f ~ one extra f(x) evaluation

[google "adjoint method" for reviews]

toy example: maximizing transmitted power from a source

Maxwell's equations discretized as:

$$\underbrace{M(x)}_{\substack{\text{Maxwell matrix} \\ \text{(parameters x)}}}\overset{\text{EM fields}}{e} = \overset{\text{source}}{s}$$

[real variables, e = real/imag parts]

Quadratic objective: $f(x) = e^T Q e$

[Q assumed symmetric]

$$\frac{\partial f}{\partial x_i} = 2e^T Q \frac{\partial e}{\partial x_i} = -2e^T Q M^{-1} \frac{\partial M}{\partial x_i} e = 2a^T \frac{\partial M}{\partial x_i} e$$

adjoint problem: $M^T a = Qe$ = one extra solve with transposed (adjoint) M

(Don't let the reciprocity intuition fool you.)

There is a general prescription that is independent of the physics — even for nonreciprocal, nonlinear, and time-varying problems.

(google "adjoint method notes")

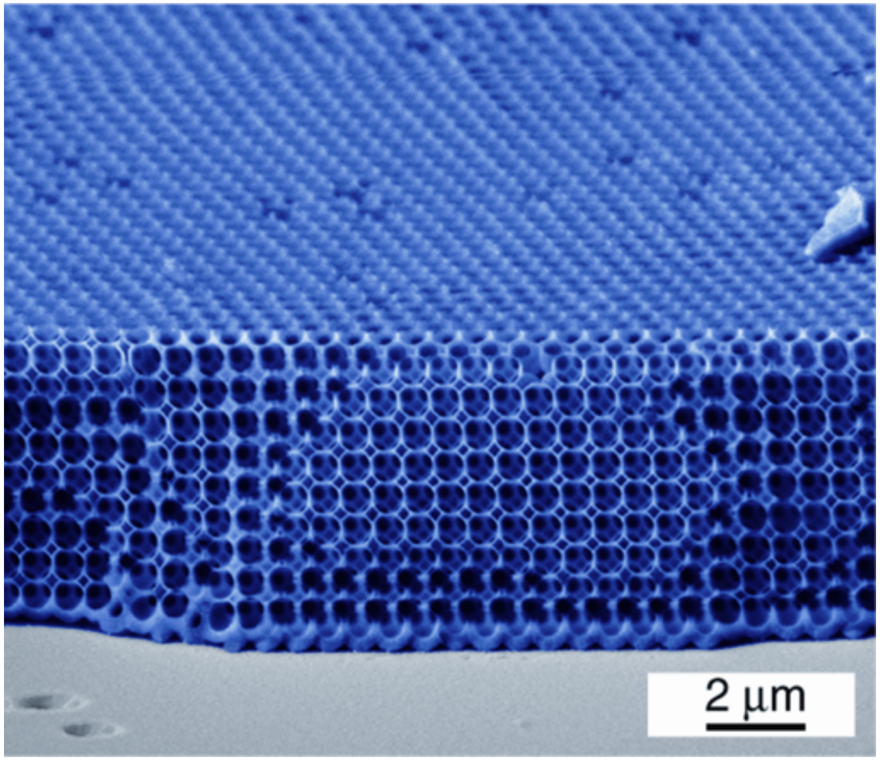
(also known as "reverse mode" differentiation or, in machine learning, as "backpropagation")

Sometimes, non-obvious transformations are required to make the problem differentiable.

Designing photonic band gaps

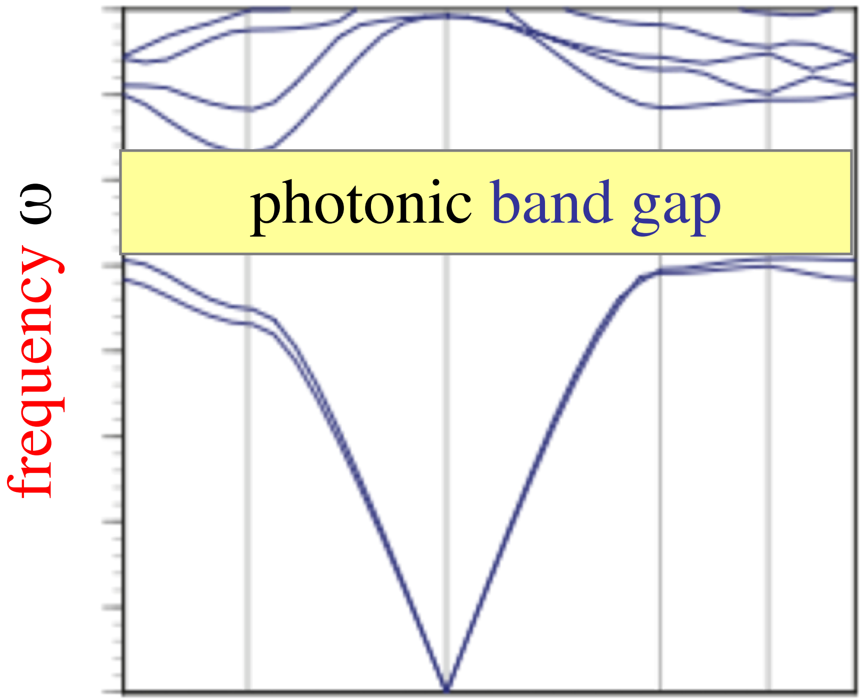
periodic structures ("photonic crystals") have

Bloch-wave "quasiperiodic" solutions = periodic(x) × $e^{ikx-i\omega t}$



[Y. A. Vlasov *et al.*, *Nature* **414**, 289 (2001).]

band diagram (dispersion relation)



wavevector k

In the gap, crystal is "optical insulator" that can trap light.

Maximizing photonic band gap over all periodic structures?

we want:

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

frequently not differentiable

an equivalent problem ("epigraph" transformation for "minimax" problems):

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

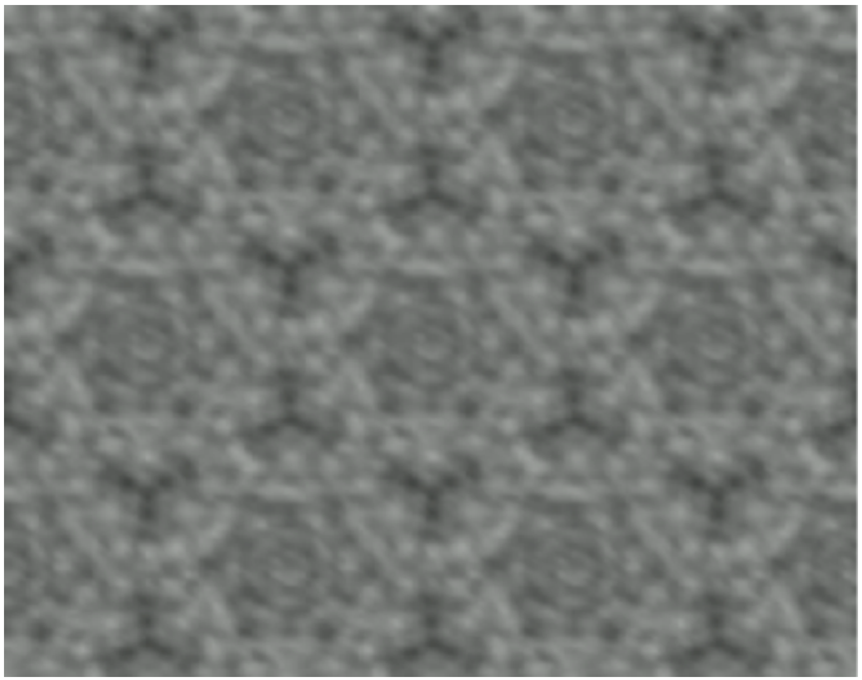
subject to:

…with (mostly?) differentiable nonlinear constraints:

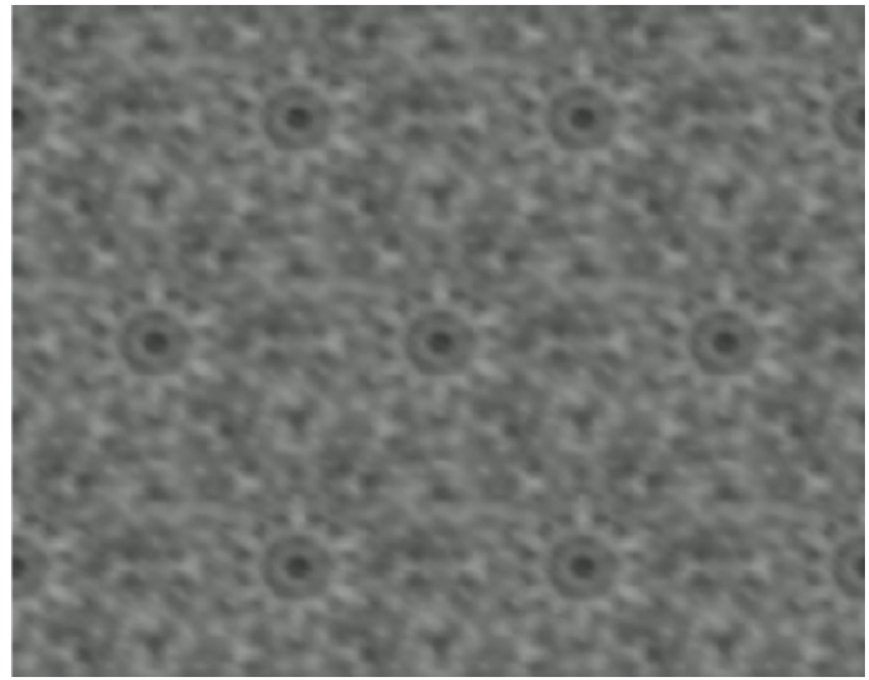
$$f_1 \geq \omega_n(\mathbf{k}) \qquad \text{for } \mathbf{k}\in\mathcal{K}$$
$$f_2 \leq \omega_{n+1}(\mathbf{k})$$

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)

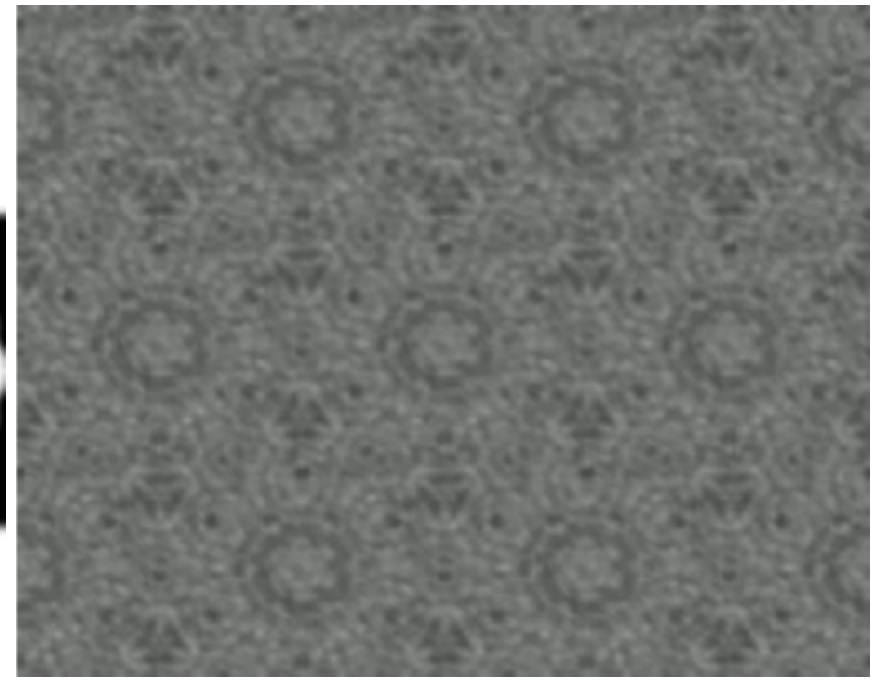


51.4% TE gap (ε = 12:1)

30 iterations of optimizer

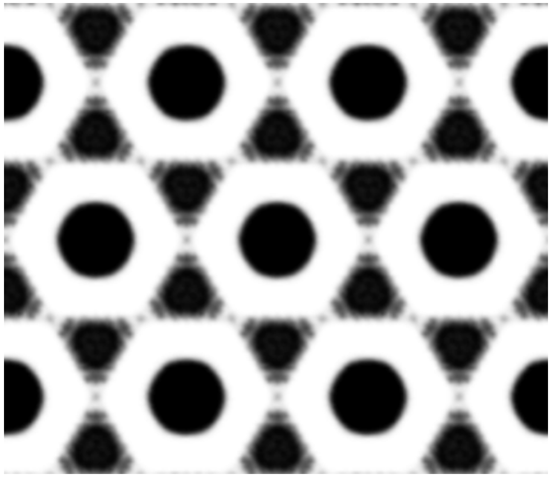
Optimizing 1st complete (TE+TM) 2d gap

21.1% gap (ε = 12:1)



20.7% gap (ε = 12:1)

+ some local minima



–0.5% gap

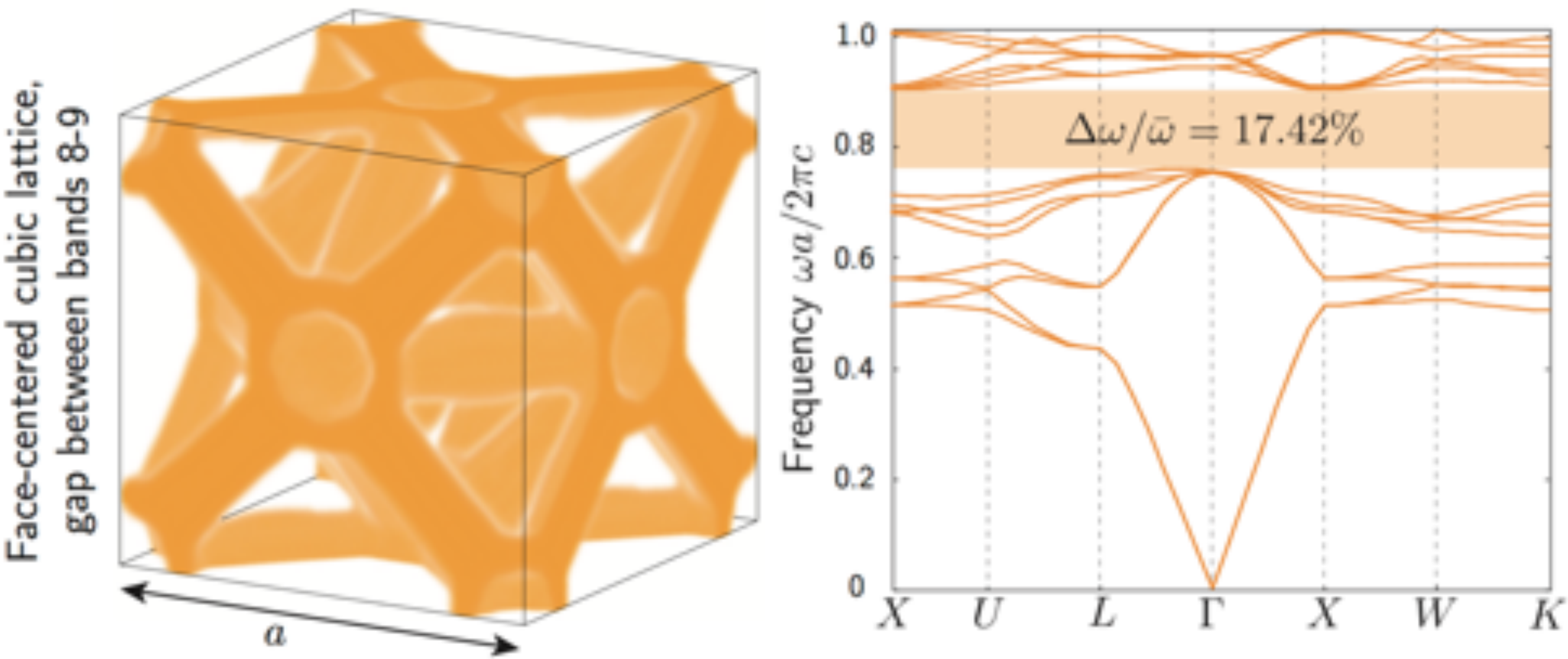
–2% gap

–10% gap

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

3d gap optimization

[given symmetry group + which bands]

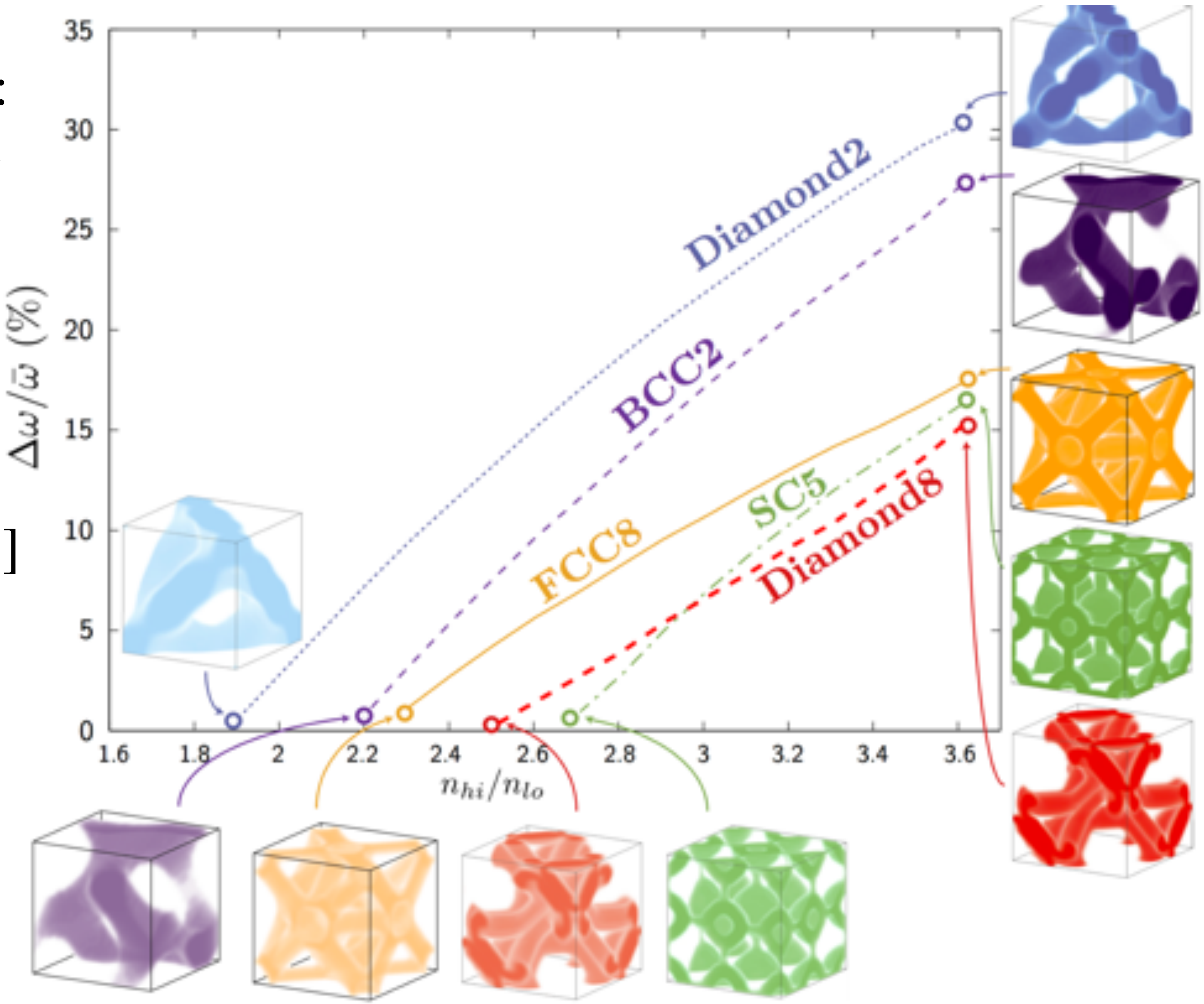


(e) FCC8 (no. 225)

~ 100x100x100 = 10^6 degrees of freedom (ε in every "voxel")

Gap vs Index Contrast

"negative" result: seems to indicate diamond lattice of holes [previously discovered "by hand": Ho *et al*. (1990)] is best, and has gap for $\Delta n \geq 1.9{:}1$



Key questions occur *before* choosing optimization algorithm:

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

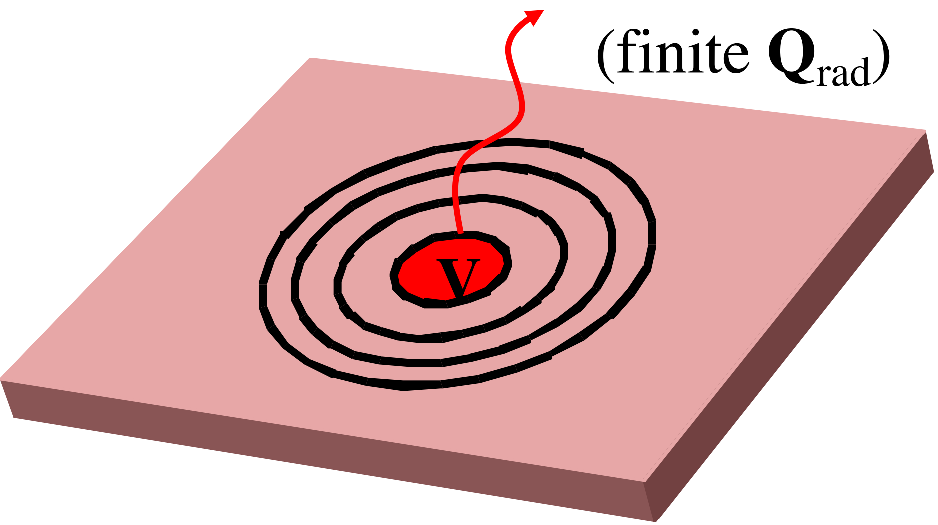
- Which objective function & constraints?
  — many choices for a given design goal,

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

Outline

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

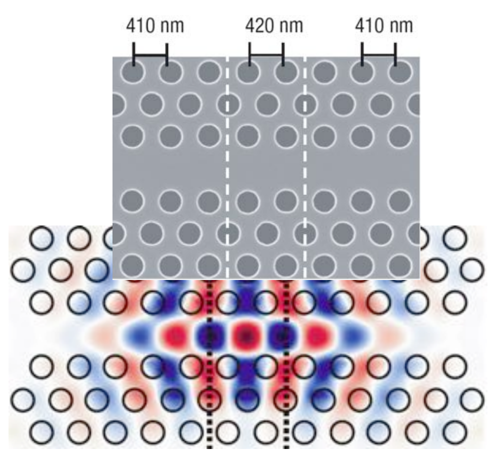
3d Microcavity Design Problem



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

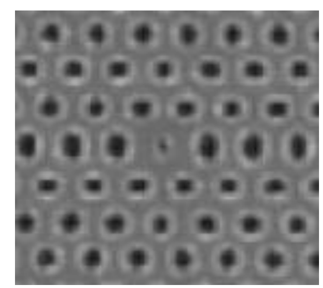
Many *ad hoc* designs,
trading off Q_{rad} and V…

ring resonators

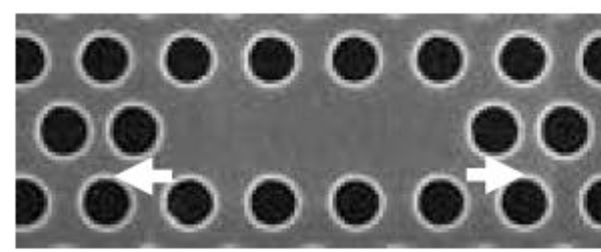


[Song, (2005)]

[Loncar, 2002]

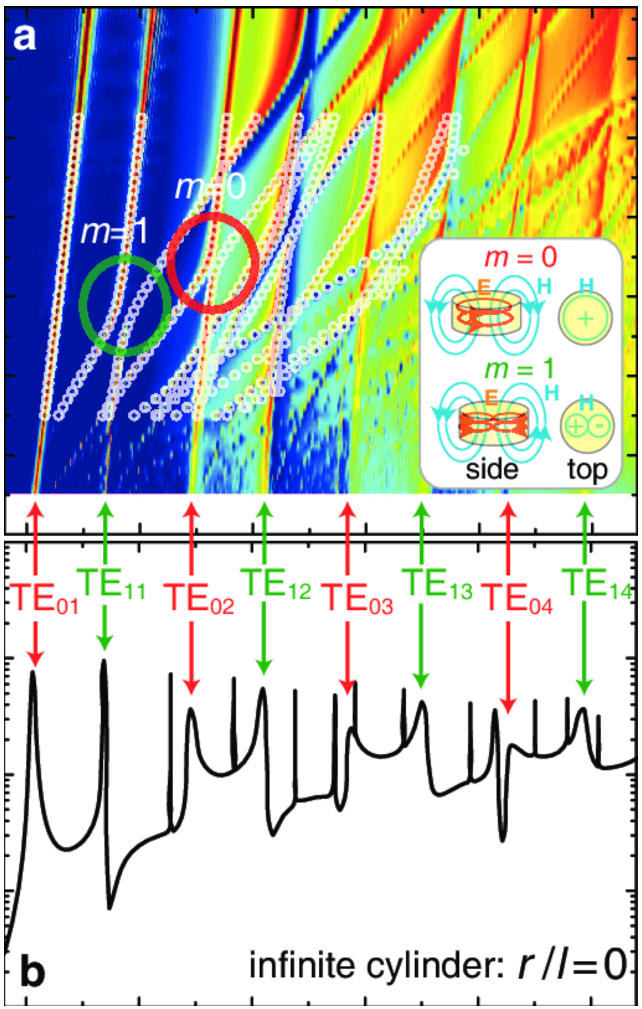


(“defects” in periodic structures)

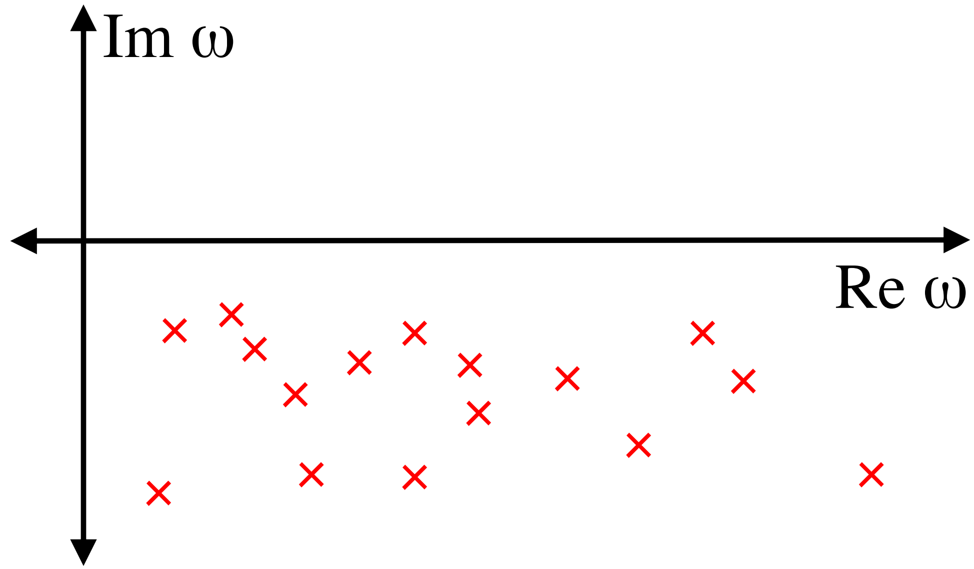


[Akahane, 2003]

Resonances = complex ω ~ frequency - *i* loss



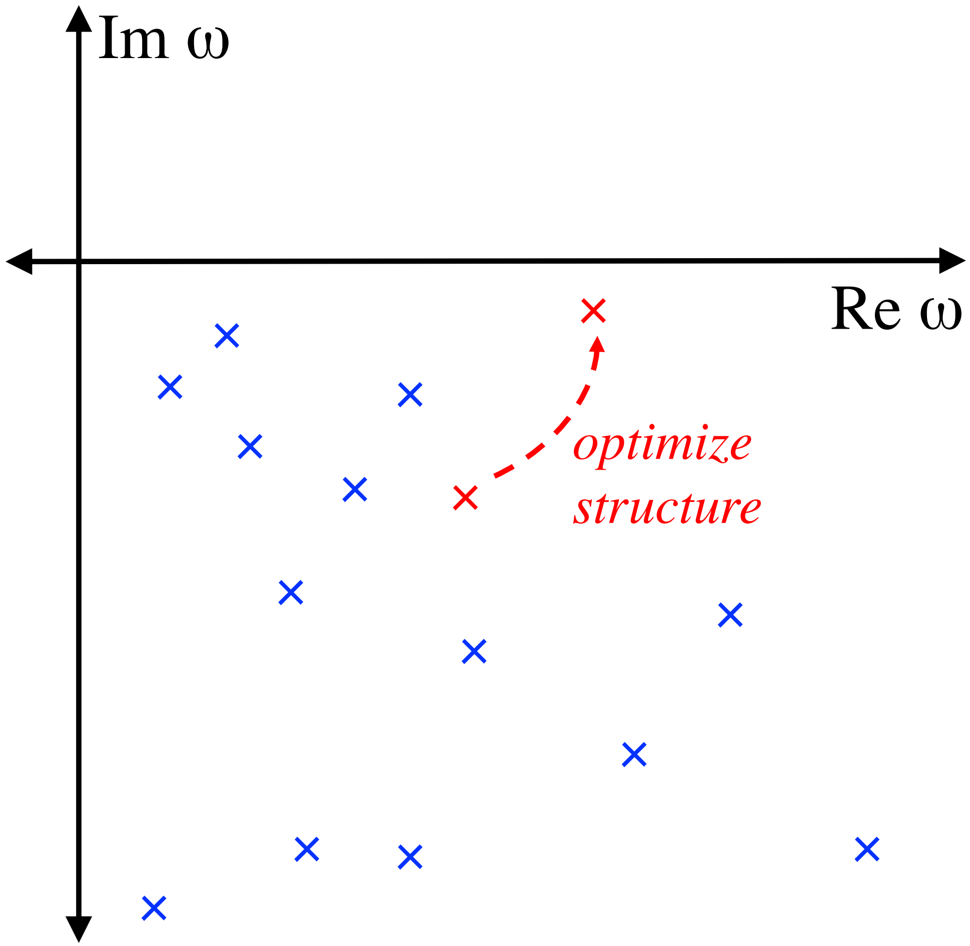
Rybin et. al (2017): arXiv:1706.02099



resonances = poles in scattering
= poles in Green's function
= singular Maxwell operator M(ω)

$$\underbrace{(\nabla\times\nabla\times-\omega^2\varepsilon)}_{\text{M(ω) singular at resonance ω}}\mathbf{E} = \mathrm{i}\omega\mathbf{J} = \mathbf{0}$$

Optimize resonances?



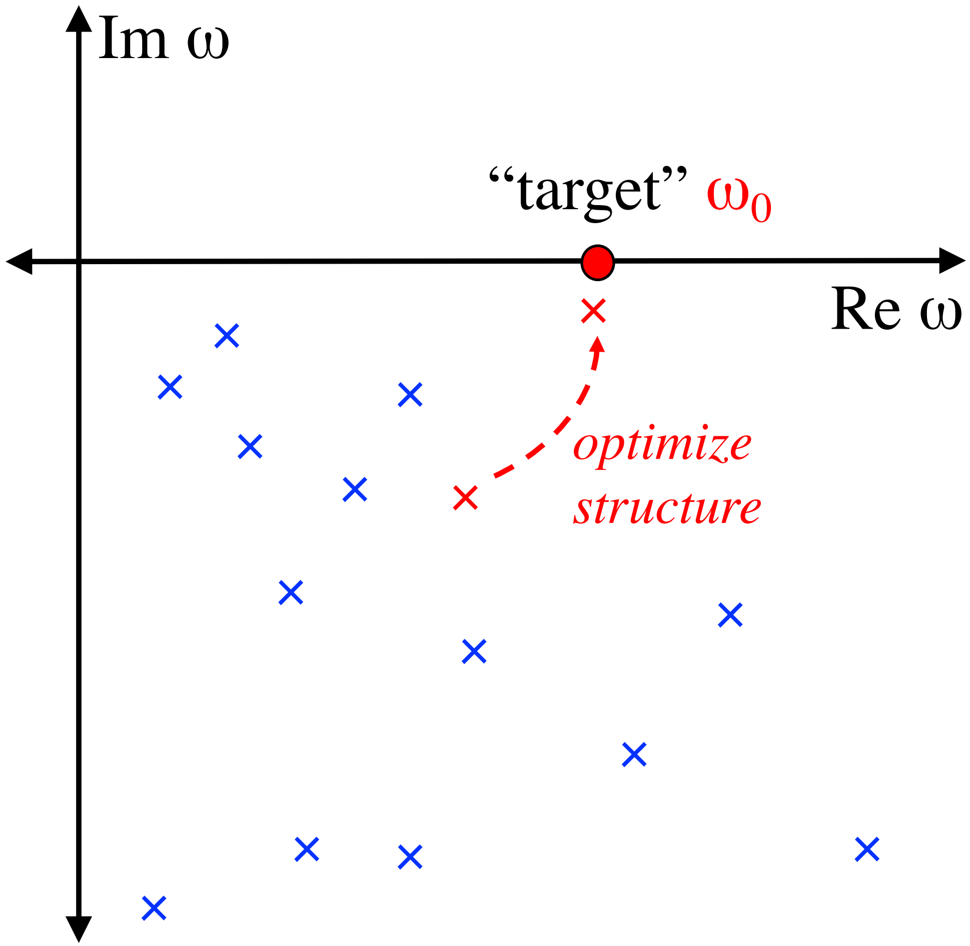
Challenges:

Which eigenvalue?

Interior eigenvalue of big non-Hermitian…

Tracking eigenvalue (no discontin. jumps!)

Optimize resolvent instead



maximize

$\mathrm{Re}\,\psi^{*}M(\omega_0)^{-1}\psi$

$= \mathrm{Re}\,f(\omega)$

instead for some ψ

… many key physical quantities in this form!

= total power expended by a source or incident wave ψ

[X. Liang & S. G. Johnson, *Optics Express* (2013).]

Back to cavity optimization…

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

[review: arXiv:1301.5366]

= approximation for LDOS (local density of states)
= power expended by dipole source Re $\psi^* M(\omega_0)^{-1}\psi$ for ψ = dipole

Naively, should we maximize Q/V or LDOS?

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

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

Real design problem: maximize LDOS
averaged over desired bandwidth $\omega_0 \pm \Gamma_0$

[Liang & Johnson (2013)]

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

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

Why a "density of states"

[review: arXiv:1301.5366]

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

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

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

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

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

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

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

loss → 0: a localized measure of spectral density

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

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

Complex target ω_0 = Frequency average

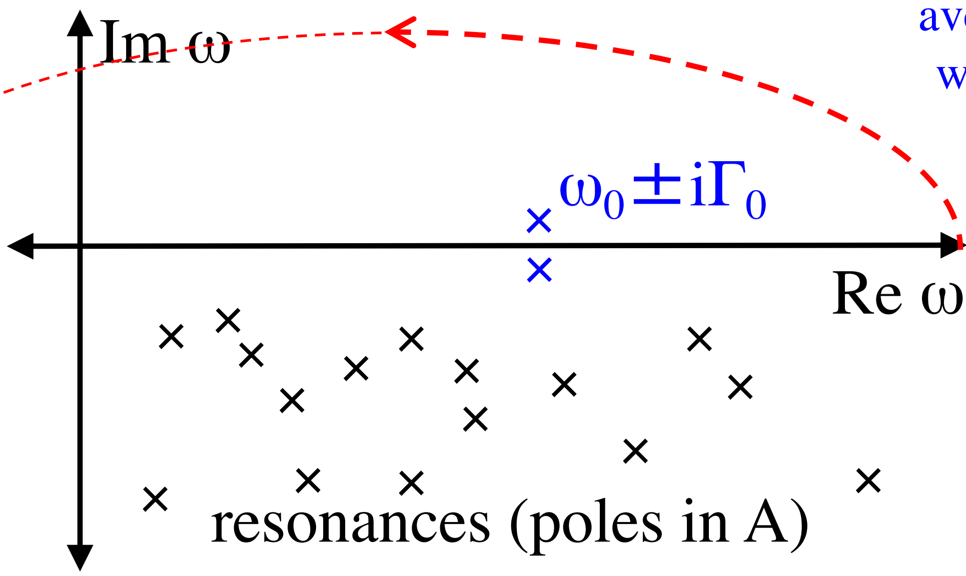
- Passivity/causality: $M(\omega)^{-1}$ analytic for $\text{Im}\,\omega > 0$

$$f(\omega) = \psi^* M(\omega_0)^{-1} \psi$$

$$\text{average} = \text{Re} \int_{-\infty}^{\infty} f(\omega) \frac{\Gamma_0/\pi}{(\omega-\omega_0)^2+\Gamma_0^2}\, d\omega = \text{Re}[2f(\omega_0 + i\Gamma_0)]$$

averaging window

via contour integration



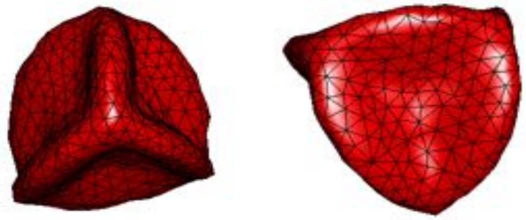
Get entire ω average with a single "unphysical" complex-ω solve!

[X. Liang & S. G. Johnson, *Optics Express* (2013).]

[Owen Miller et. al. *Phys. Rev. Lett. 112, 123903* (2014)]

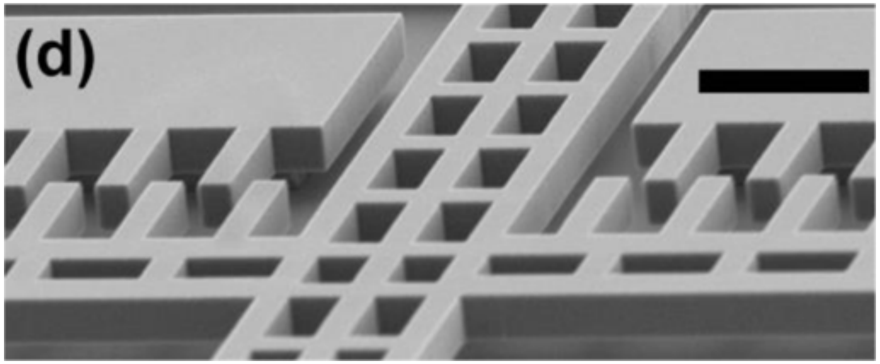
Complex ω = ω average: Lots of uses

3d optimization of absorbing particles (frequency-averaged absorbed+scattered power)



[Owen Miller et. al. (2014)]

Modeling Casimir/van der Waals force

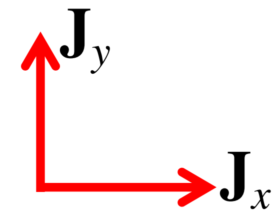


integrating fluctuations over all ω = much nicer integral over Im ω

[Rodriguez et al., *Nature Photonics* (2011)]

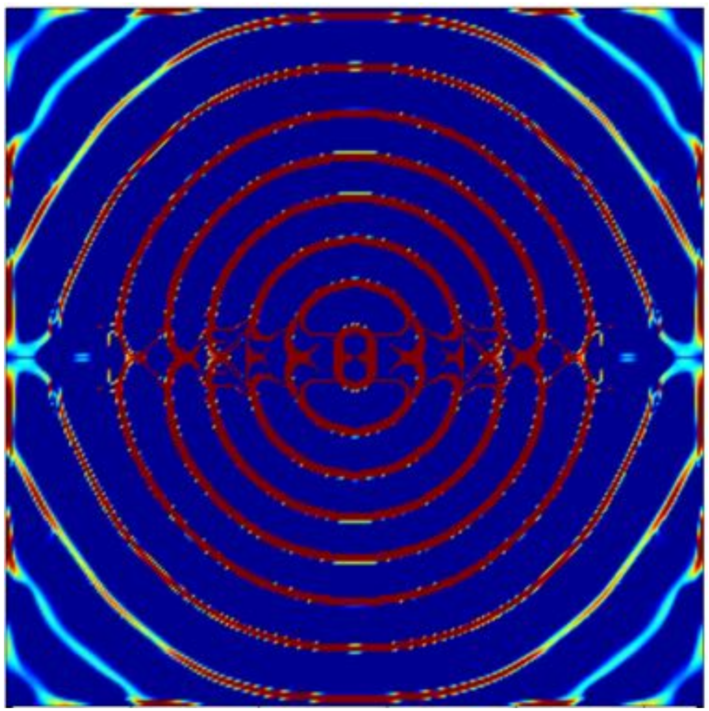
- General derivation of Wheeler–Chu limits via contour integration [Sohl, Gustafsson, Kristensson (2007)]
- Extension of "Miller" bounds to finite bandwidth [Shim (2019)]
- Proof that cloaking bandwidth scales ~ 1/diameter [Hashemi (2010)]

in-plane **J**

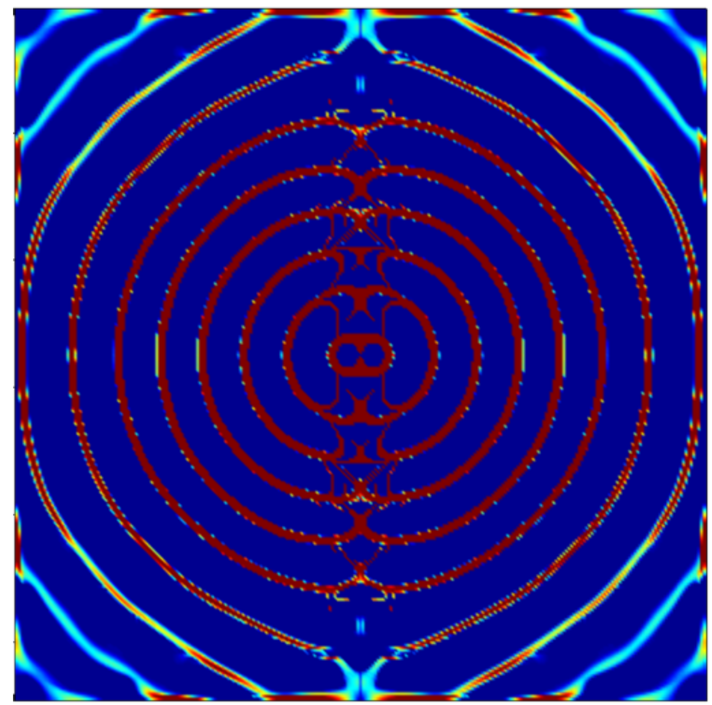


Maximizing LDOS for random in-plane J

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



4 out of 10

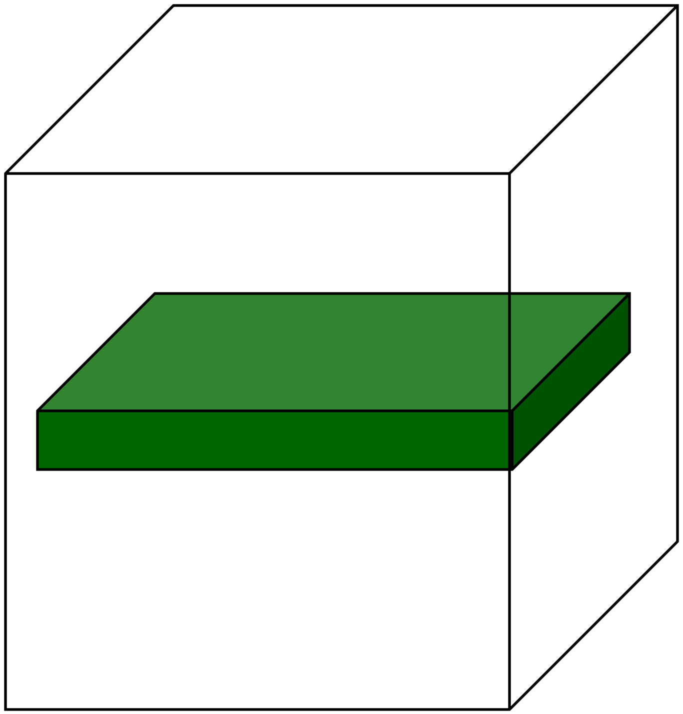


6 out of 10

Spontaneous symmetry breaking! "Picks" one polarization randomly

3d results: Photonic-crystal slab

[X. Liang & S. G. Johnson, *Optics Express* (2013).]



Optimize with Q_0=10^4

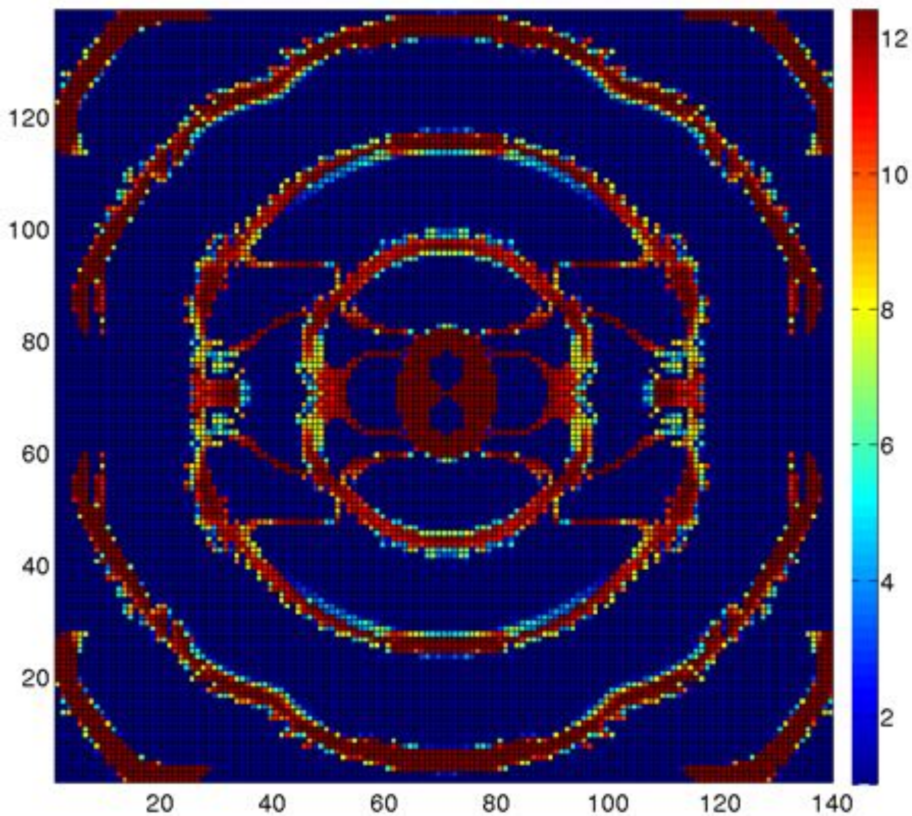
i.e. prefer $Q \geq 10^4$ but
after that mainly
minimize V

Next: 2d pattern in 3d slab

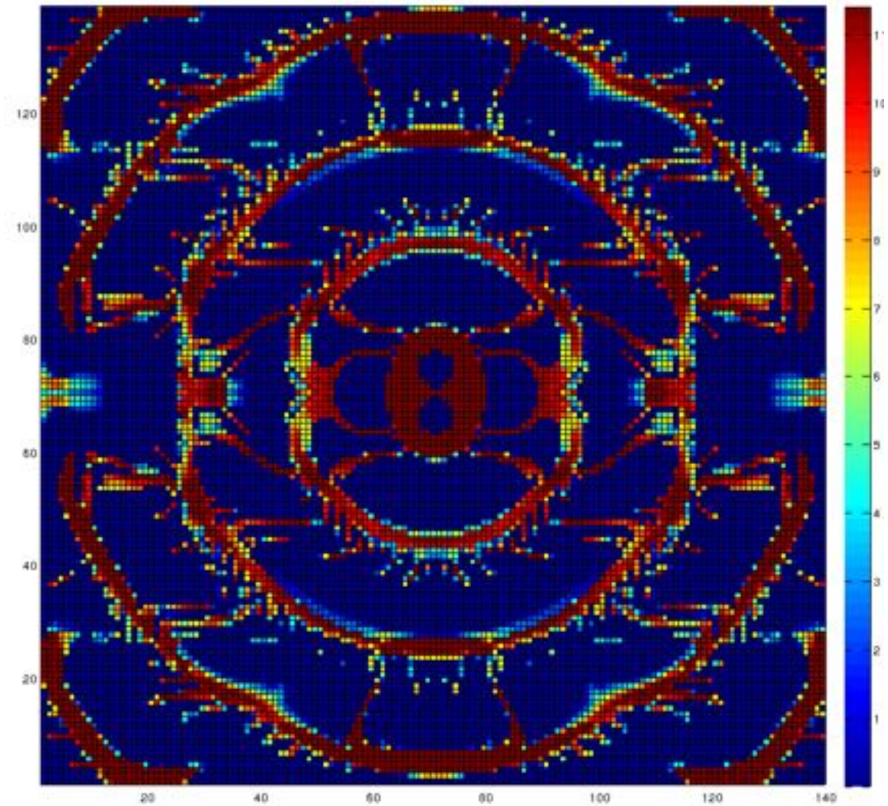
(including radiation loss via
PML absorbing boundaries)

3d Slab Results

[X. Liang & S. G. Johnson (2013).]



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…

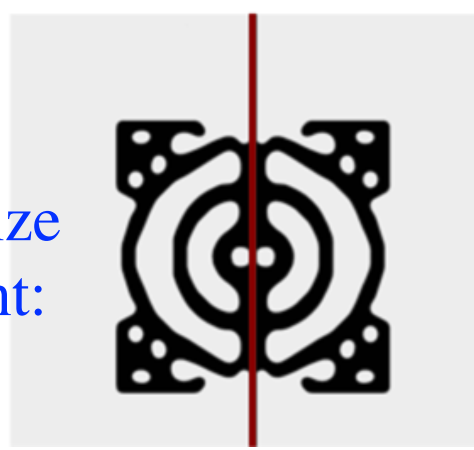
Manufacturability: Feature-size constraints

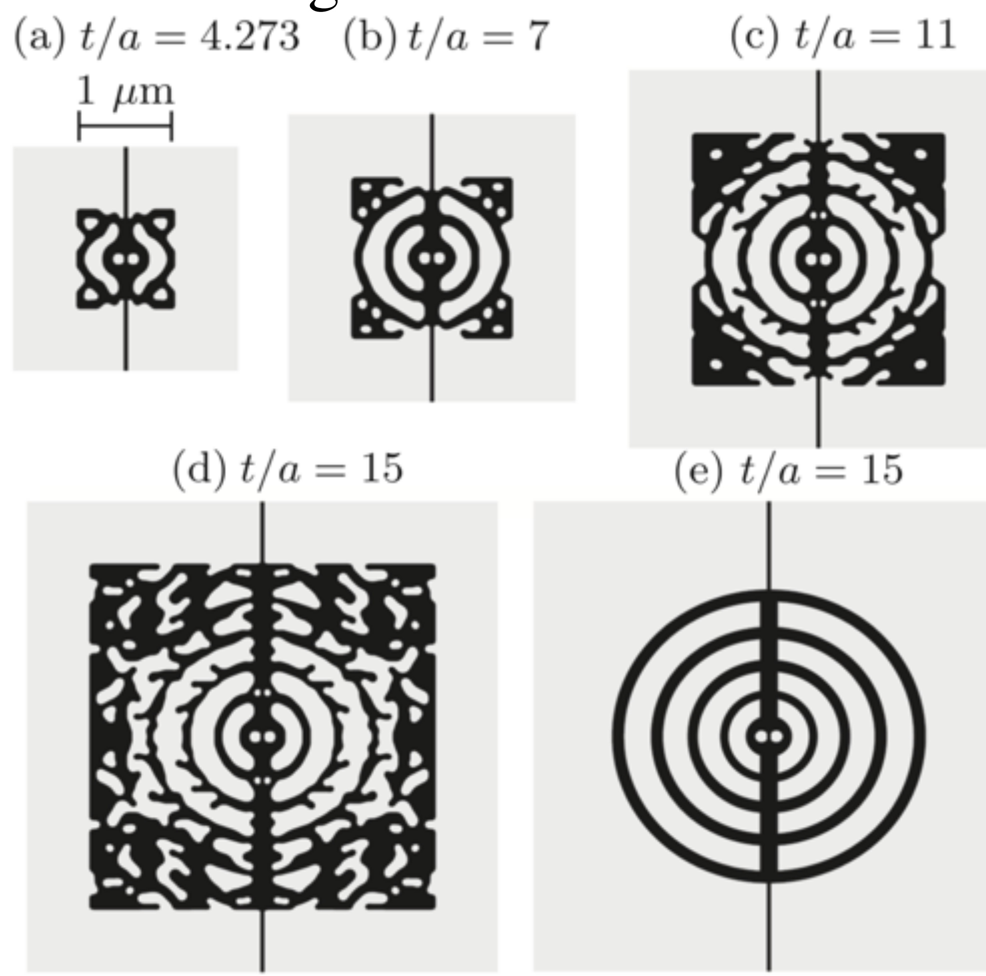
[Wang, Christiansen, Yu, Mørk, and Sigmund, *Appl. Phys. Lett.* **113**, 241101 (2018)]

Various techniques to impose a minimum feature size, connectivity, and other manufacturing constraints in TO.

no constraint:

feature-size constraint:

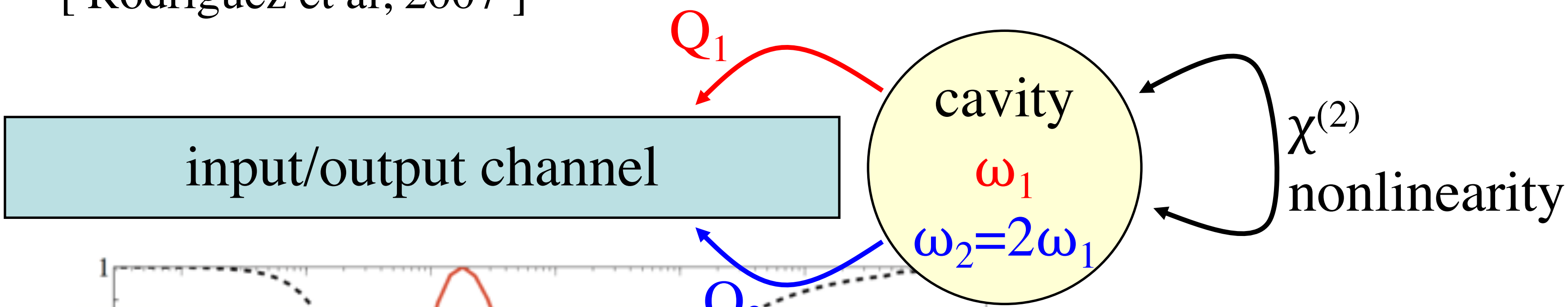


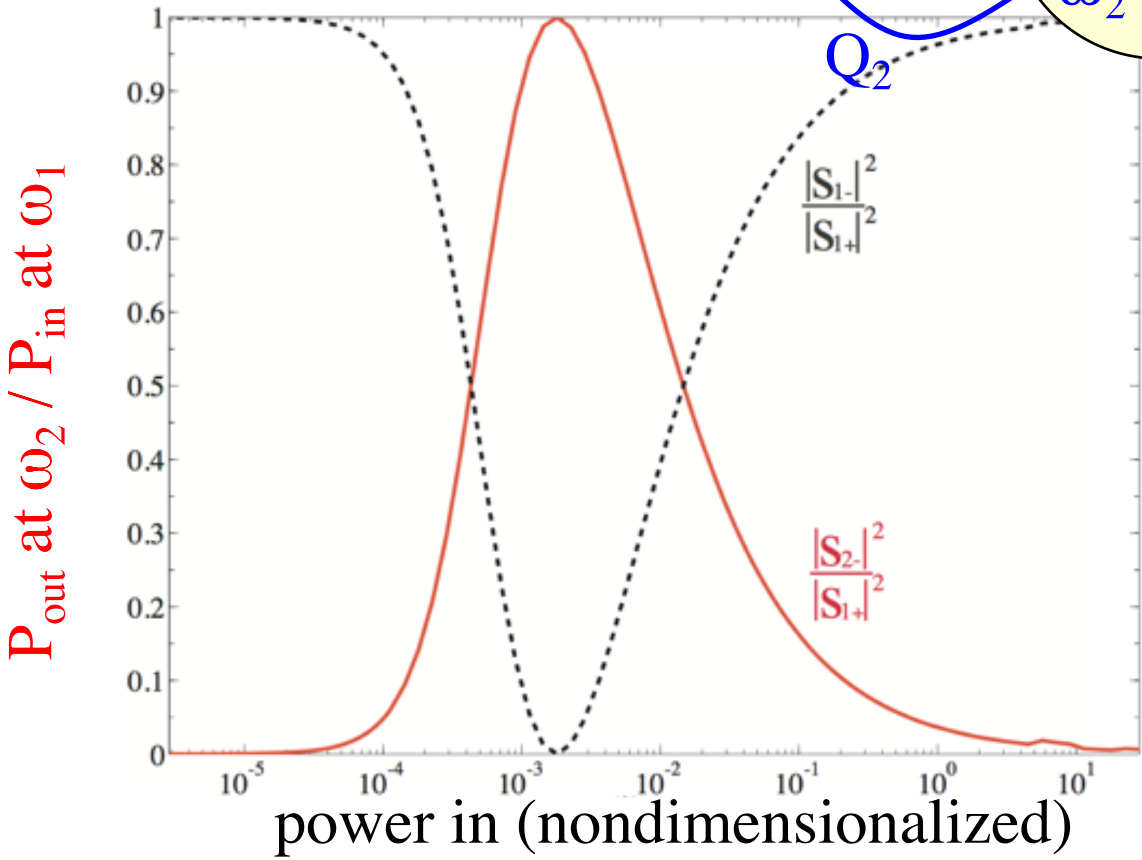


various size cavities

Intra-cavity 2nd-harmonic generation

[Rodriguez et al, 2007]



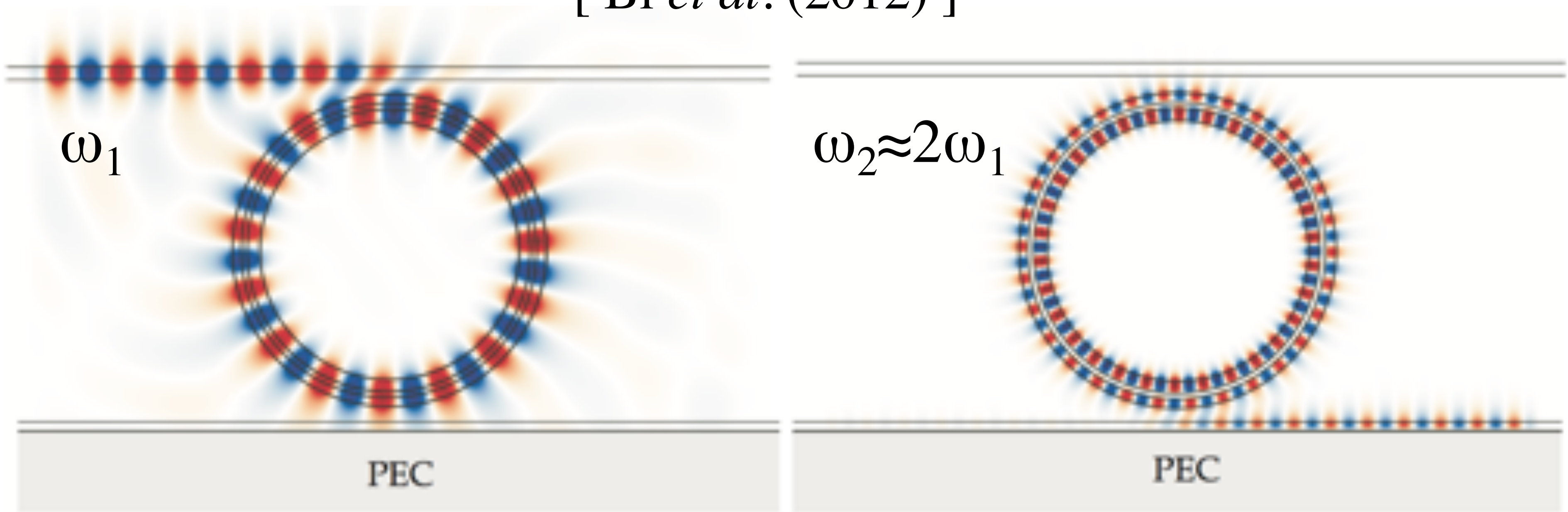


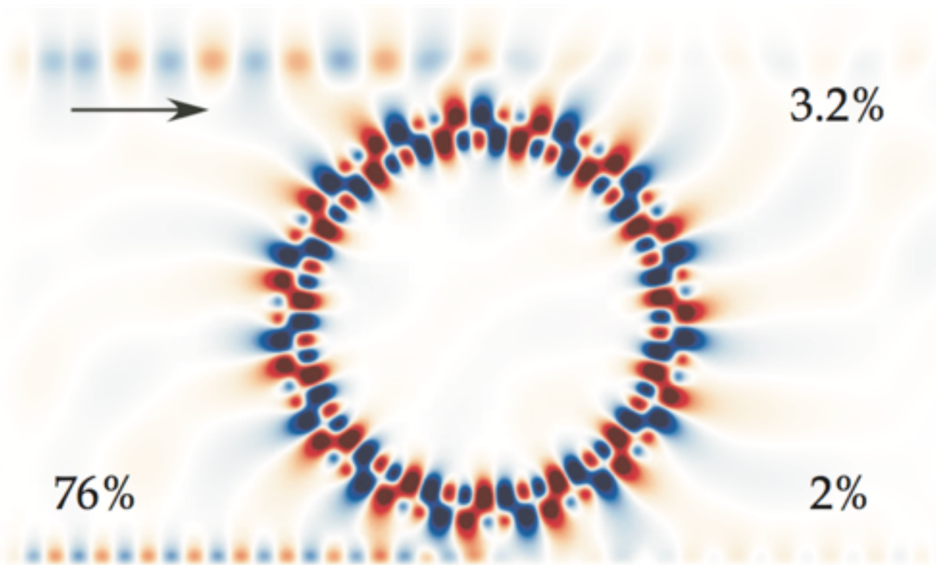
theory: 100% conversion at critical input power

… tricky part is designing cavity with simultaneous, spatially overlapping resonances at ω_1 & ω_2

Hand-design SHG cavity

[Bi *et al*. (2012)]





~80–90% efficiency (2d & 3d)
for AlGaAs, 30mW power, at teleco
wavelengths with 0.1% bandwidth

…

months of hand-tuning to find
compatible resonance modes

SHG by "LDOS" optimization

[Lin, Liang, Lončar, Johnson, and Rodriguez, *Optica*, vol. 3, pp. 233–238 (2016).]

key idea:

source J_1 at ω_1
$\Longrightarrow E_1$
$\Longrightarrow J_2 \sim \chi^{(2)} E_1{}^2$
$\Longrightarrow E_2$
$\Longrightarrow$ power at ω_2

Maximizing SHG
= maximizing
composition of
two scattering problems.

$$\max_{\bar{\varepsilon}_\alpha} \langle f(\bar{\varepsilon}_\alpha; \omega_1) \rangle = -\mathrm{Re}\left[\left\langle \int \mathbf{J}_2^* \cdot \mathbf{E}_2 \mathrm{d}\mathbf{r} \right\rangle\right],$$

$$\mathcal{M}_1 \mathbf{E}_1 = i\omega_1 \mathbf{J}_1,$$

$$\mathcal{M}_2 \mathbf{E}_2 = i\omega_2 \mathbf{J}_2, \omega_2 = 2\omega_1$$

where

$$\mathbf{J}_1 = \delta(\mathbf{r}_\alpha - \mathbf{r}_0)\hat{\mathbf{e}}_j, \qquad j \in \{x, y, z\}$$

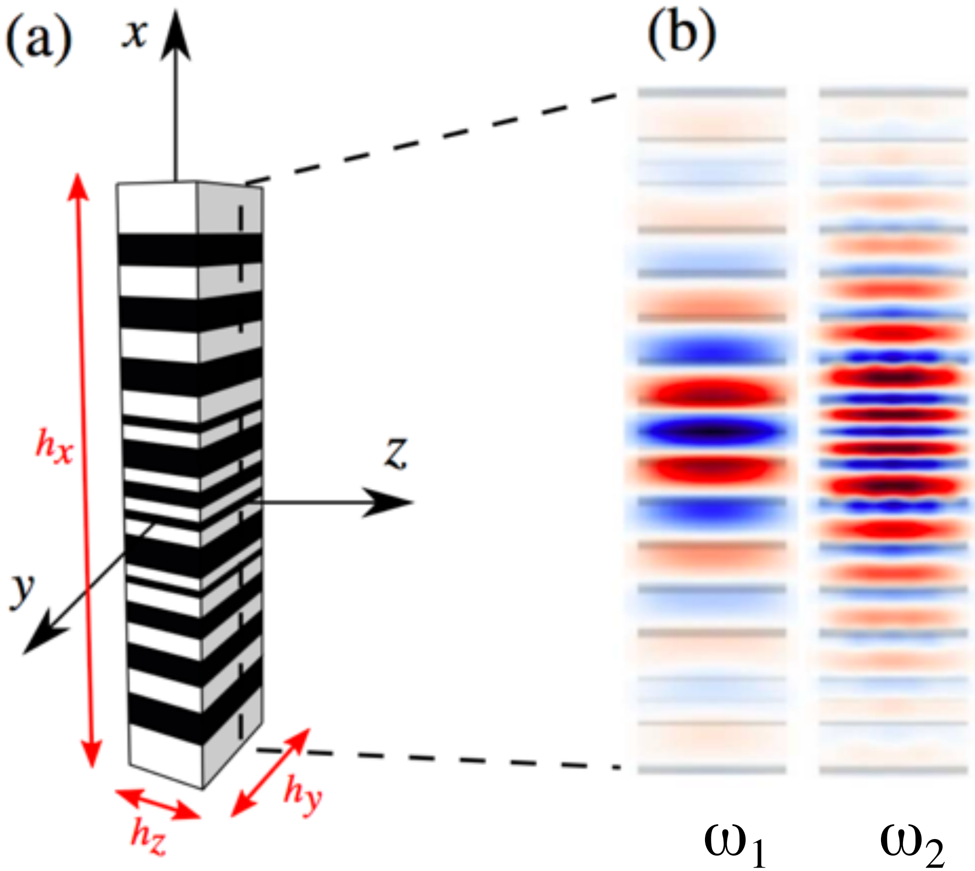
$$\mathbf{J}_2 = \bar{\varepsilon}(\mathbf{r}_\alpha) E_{1j}^2 \hat{\mathbf{e}}_j,$$

$$\mathcal{M}_l = \nabla \times \frac{1}{\mu} \nabla \times -\varepsilon_l(\mathbf{r}_\alpha)\omega_l^2, \qquad l = 1, 2$$

$$\varepsilon_l(\mathbf{r}_\alpha) = \varepsilon_m + \bar{\varepsilon}_\alpha(\varepsilon_{dl} - \varepsilon_m), \qquad \bar{\varepsilon}_\alpha \in [0, 1],$$

SHG by "LDOS" optimization

[Lin, Liang, Lončar, Johnson, and Rodriguez, *Optica*, vol. 3, pp. 233–238 (2016).]

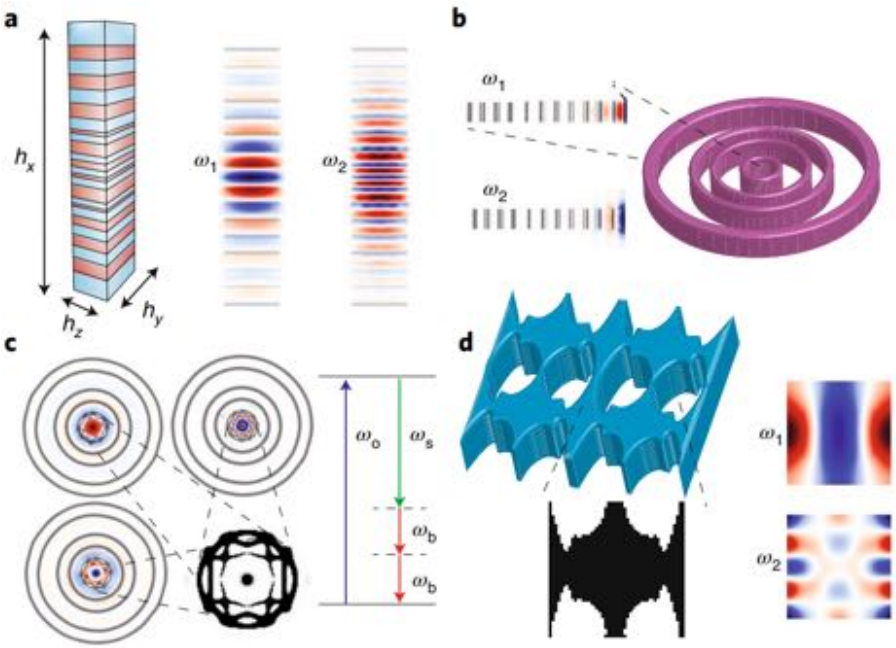


gave factor of 10 increase in mode-overlap figure of merit vs. best hand design

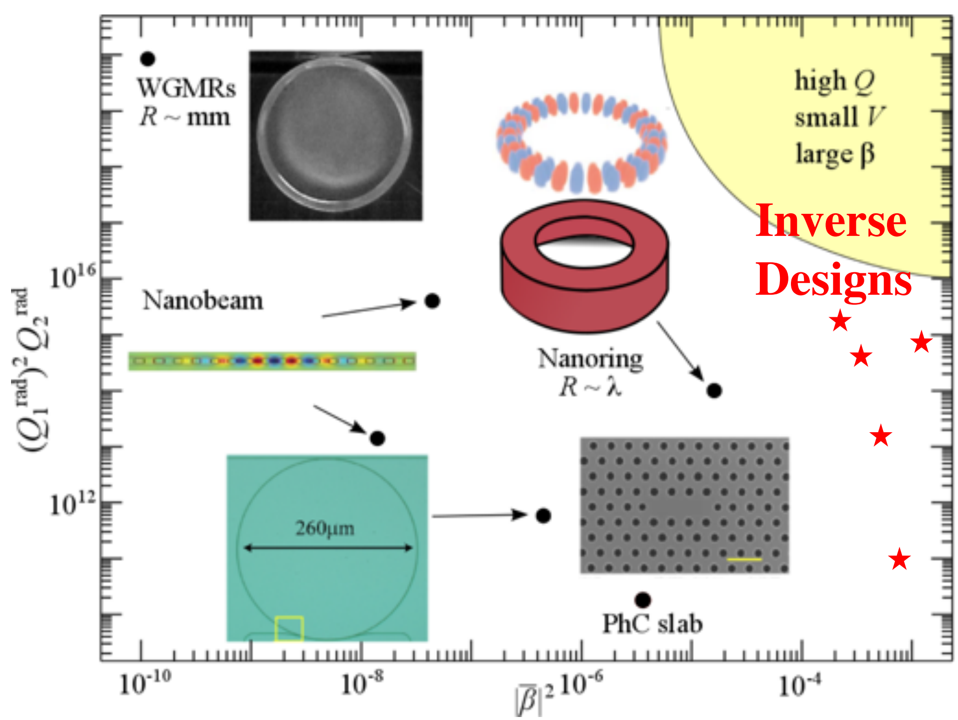
optimized VCSEL-like multilayer-film
(~hundreds of degrees of freedom)

Topology optimization for nonlinear frequency conversion

(figs courtesy Z. Lin)



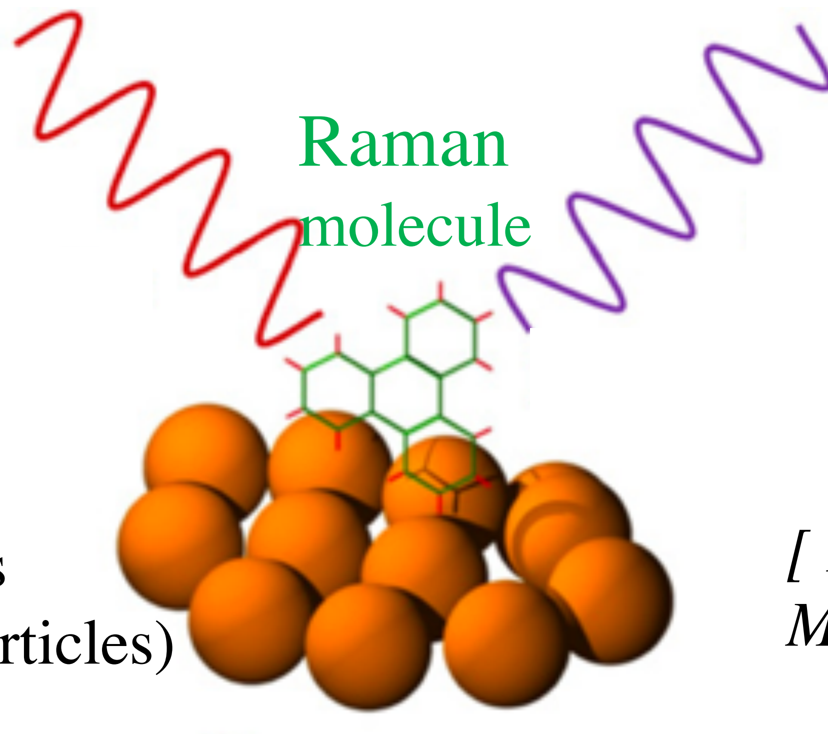
extension to 3d



[Lin *et al*, Optica Vol. 3, 233 (2016)]

Surface-enhanced Raman Scattering

[R. Christiansen, arXiv:1911.05002 (2019)]

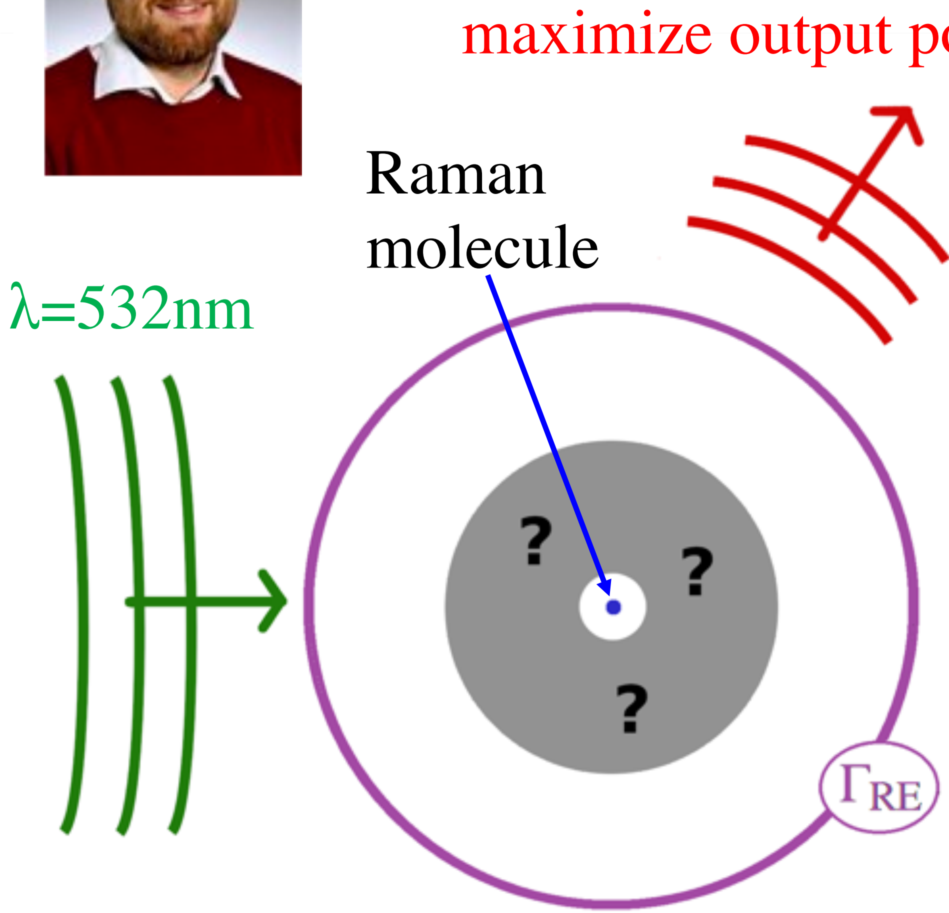


[Image:
M. K. Oo, UMich]

enhance Raman both by focusing incident wave and by enhancing emission (Purcell effect) … what structure is best?

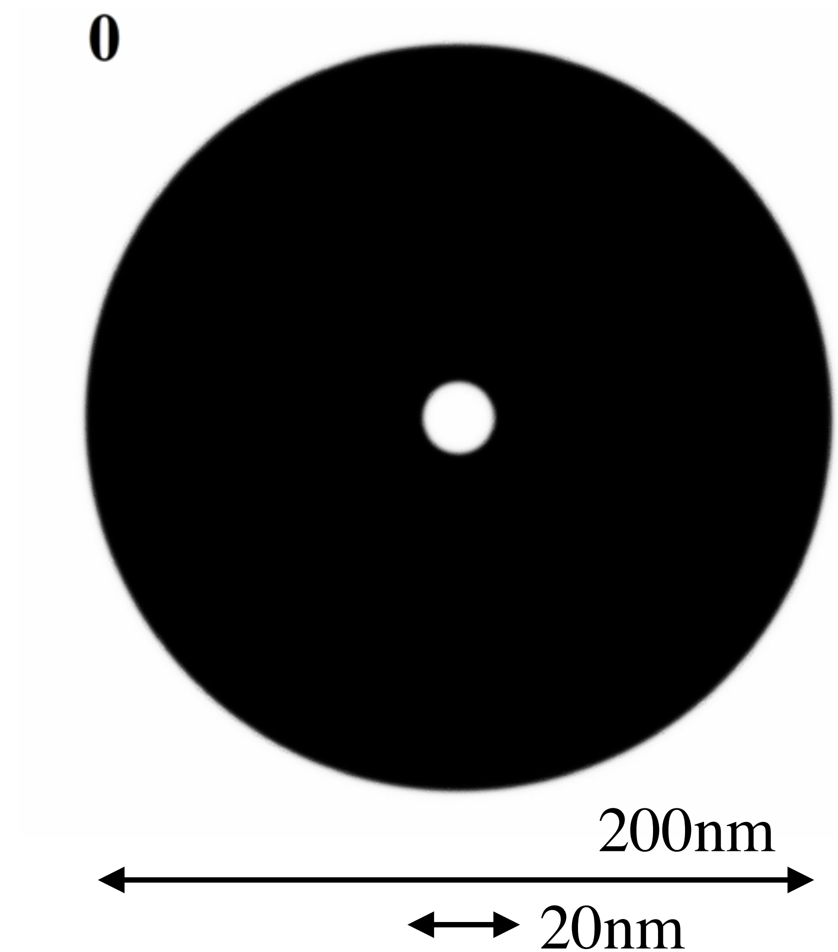
Optimization for Raman Scattering

[R. Christiansen, arXiv:1811.12936 (2019)]



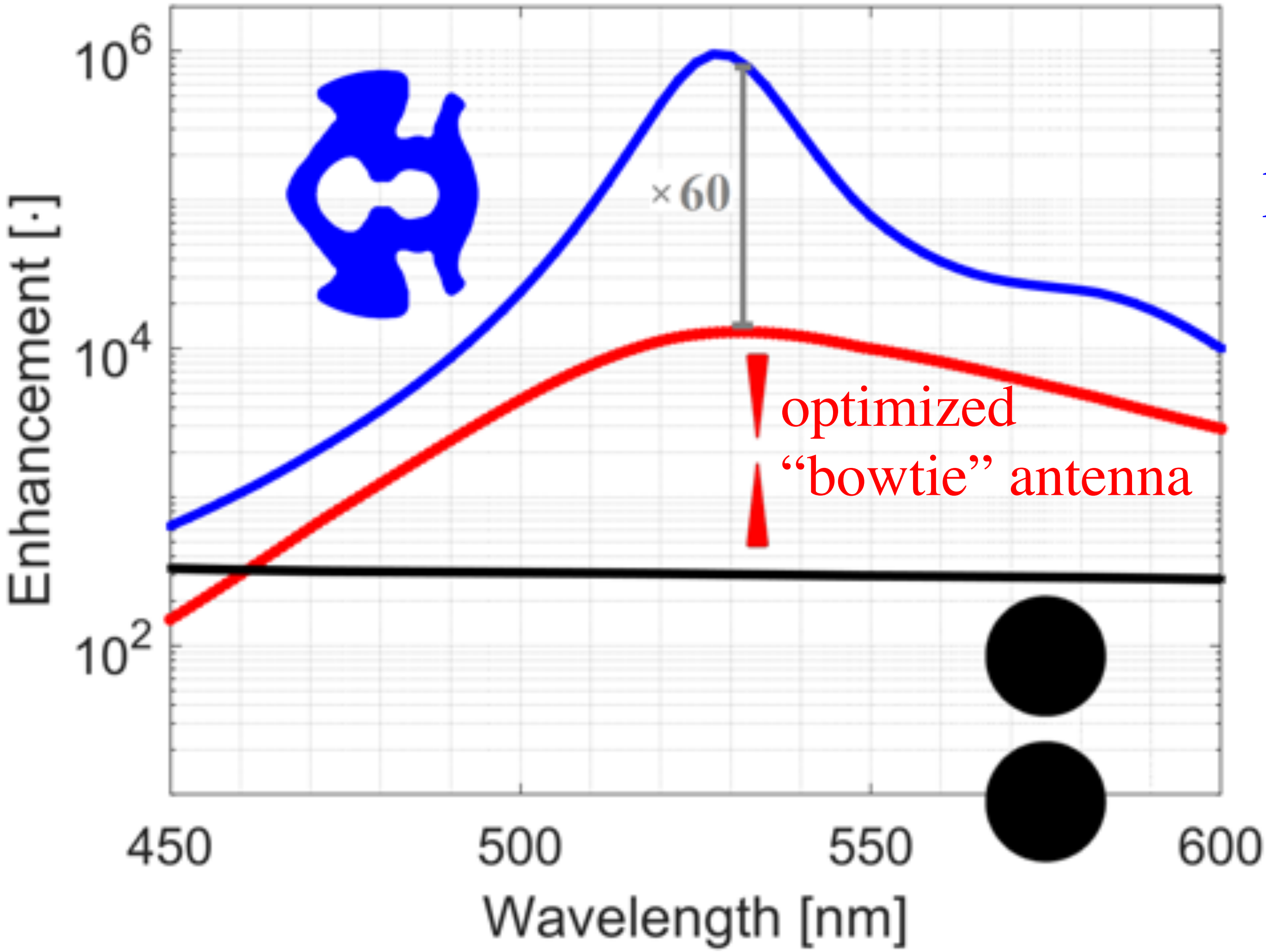
every "pixel" in ??? Region
is a design degree of freedom

Ag nanoparticle
optimization steps:



60 × better than typical resonators

[R. Christiansen, arXiv:1811.12936 (2019)]

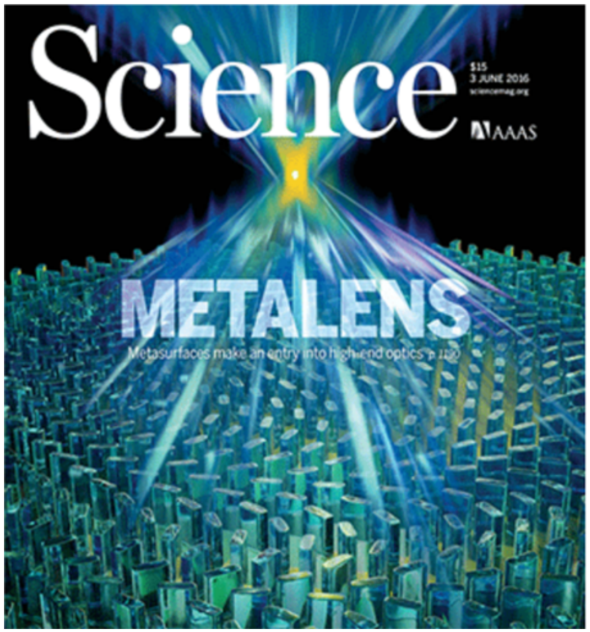


Very promising 2d results!

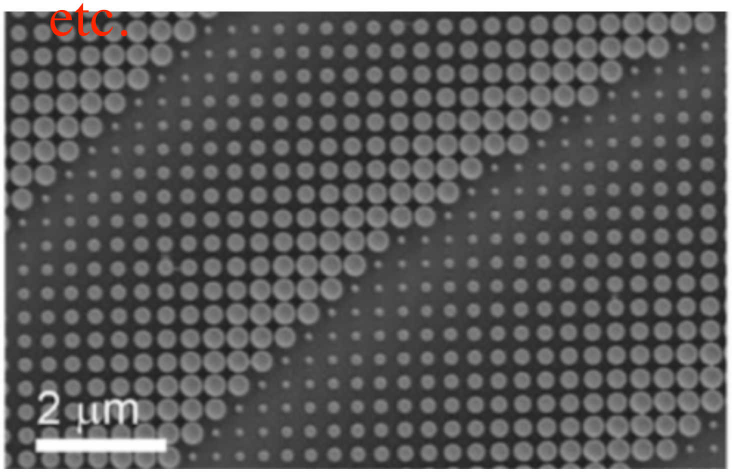
… 3d optimization currently running

“Metasurface” optical devices:

Large-area (often 100–1000λ) nanopatterned surfaces designed to reflect/transmit desired waves — e.g. flat-lens focusing, beamforming, etc.



(M.Khorasaninejad, W. T. Chen, R. C. Devlin, J.Oh, A. Y. Zhu ,F. Capasso, *Science*, June 3 2016)

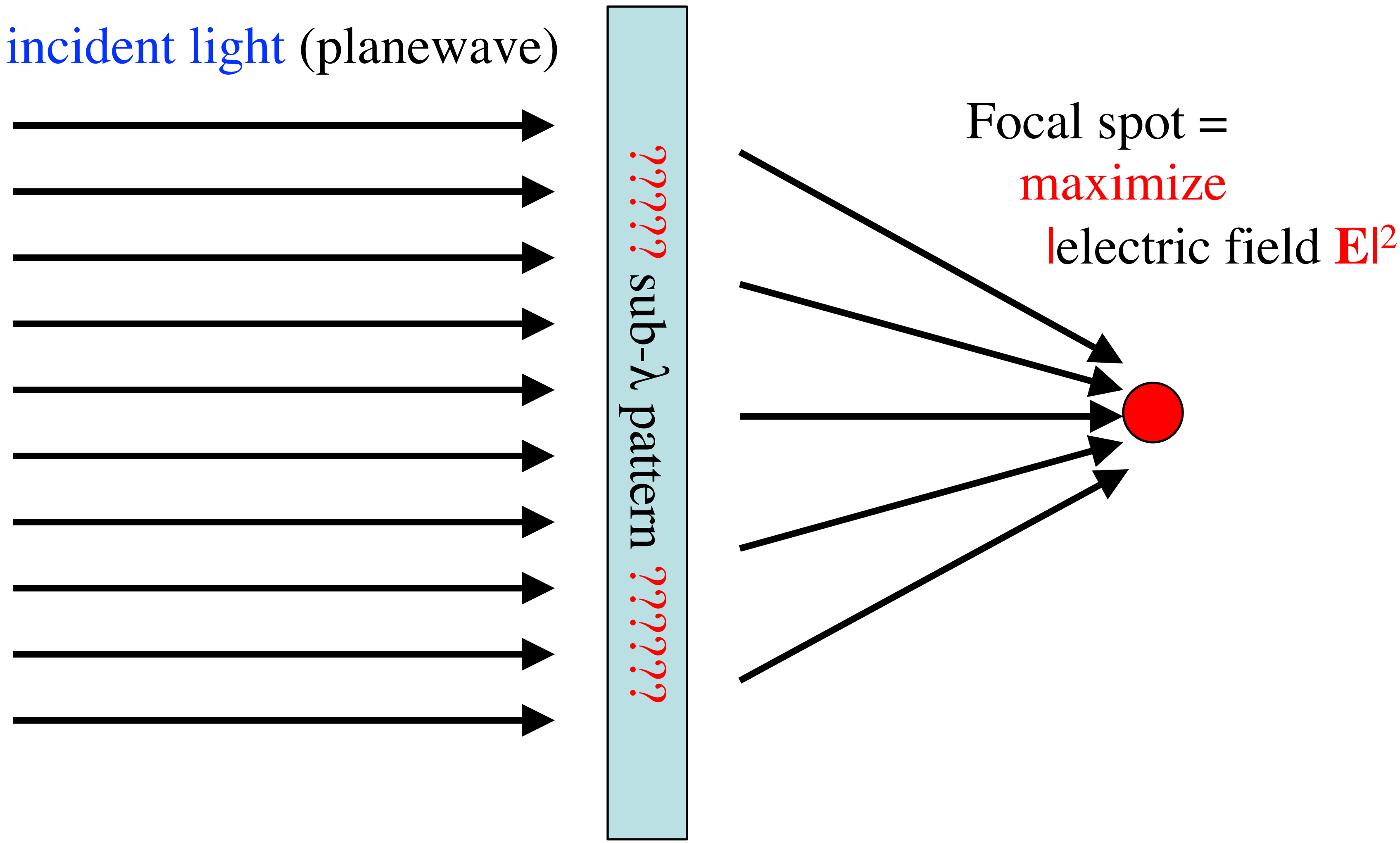


M. Khorasaninejad et al.,. IEEE J. Sel. Top. Quantum Electron. 23, 4700216 (2017)

Capasso group (Harva

“Meta:” << λ pattern acts like effective surface “impedance”. (Not really necessary.)

A typical "metalens" problem



Complication: focus multiple incident λ and/or angles simultaneously?

Why is it a hard problem?

- complex aperiodic pattern
- High material contrast
- Rapidly varying (λ), big

Capasso group (Harvard)

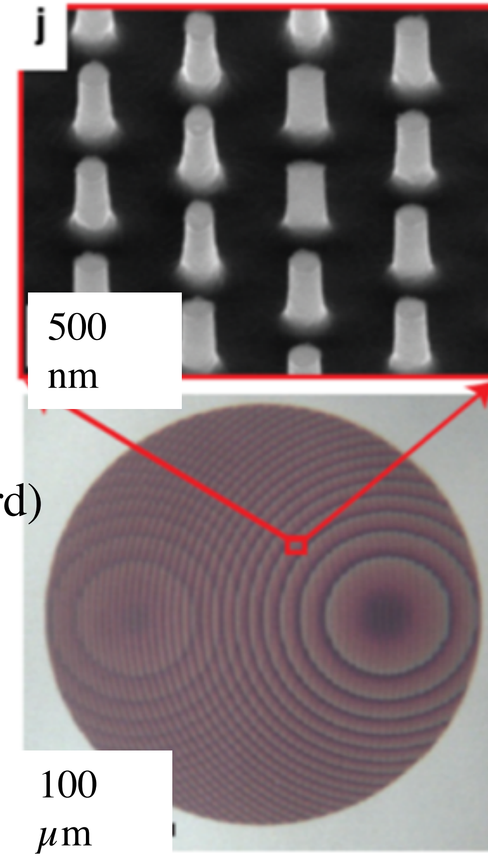
Very hard forward problem

Even if design is *given*, simulating it requires a super computer for *one* brute-force simulation

Inverse problem intractable?

We are not given the design!

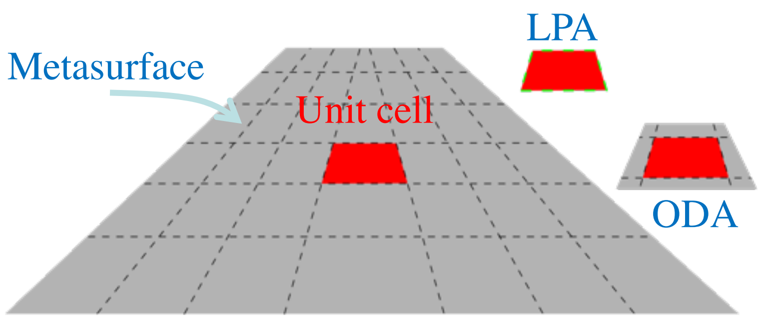
Ex: maximize I^2 at focal spot →
search 10^6 parameters for best focus



[Arbabi, A. et al. *Nat. Nanotechnol.* **10**, 937–943 (2015)]

Large-scale metasurface optimization by domain decomposition

[Pestourie et al. (2018); Lin et al. (2019)]



- Subdivide surface into small ($\lesssim 10\lambda$) cells, solve in parallel using either LPA or (better) overlapping non-periodic domains (ODA)
- "Stitch" together using *near-to-farfield transformation* to get fields anywhere.
- Optimize cells (*together*) for any desired objective.

many possible objective functions, (including broad-band/multi-ω)

focal-spot intensity:

$$f = \left| \int \mathbf{G_0}(\mathbf{r}, \mathbf{r}') \mathbf{J}_{\text{equiv}}(\mathbf{r}') d\mathbf{r}' \right|^2,$$

$$\mathbf{J}_{\text{equiv}} \sim \mathbf{E}_{||}$$

wavefront matching:

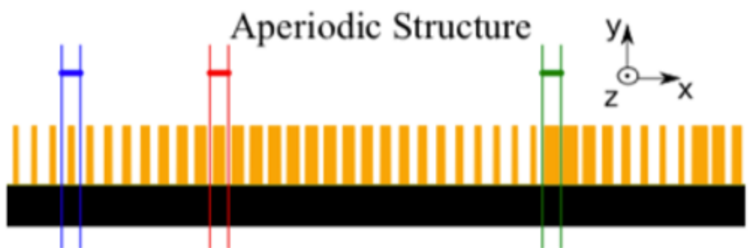
$$f = \int |\mathbf{E} - \mathbf{E_0}|^2 \, d\mathbf{r}$$

Important Notes:

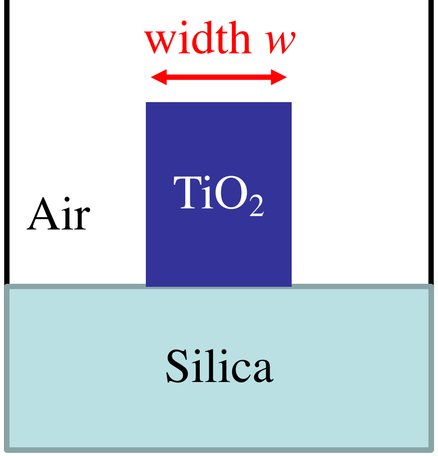
- *You cannot optimize each cell individually. All the DOFs (>10⁶) over the entire surface must be considered and updated together.*
- *No need to restrict oneself to sub-λ domains; domain >> λ tend to work better.*

Few parameters per cell: *library* approach

[R. Pestourie, et al., *Optics Express* (2018).]

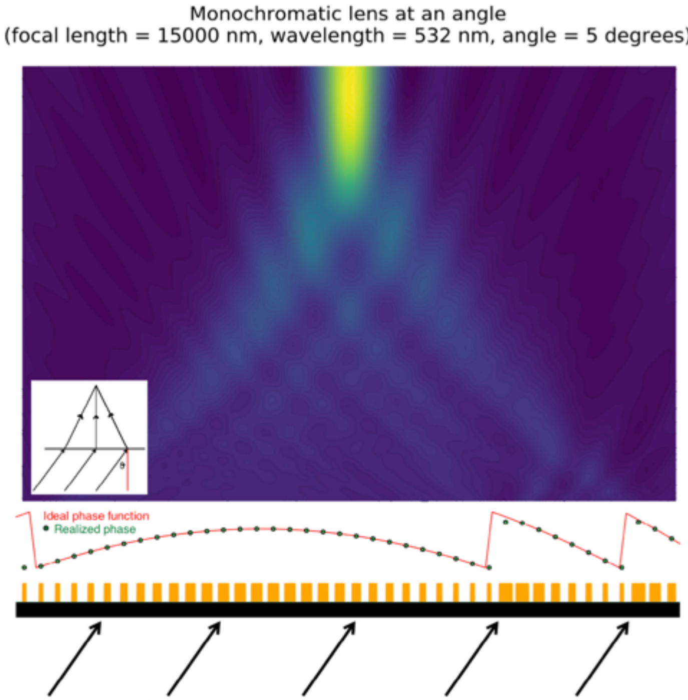


if each cell has only
a few parameters…



just precompute diffraction
coefficients vs. parameters (in LPA)

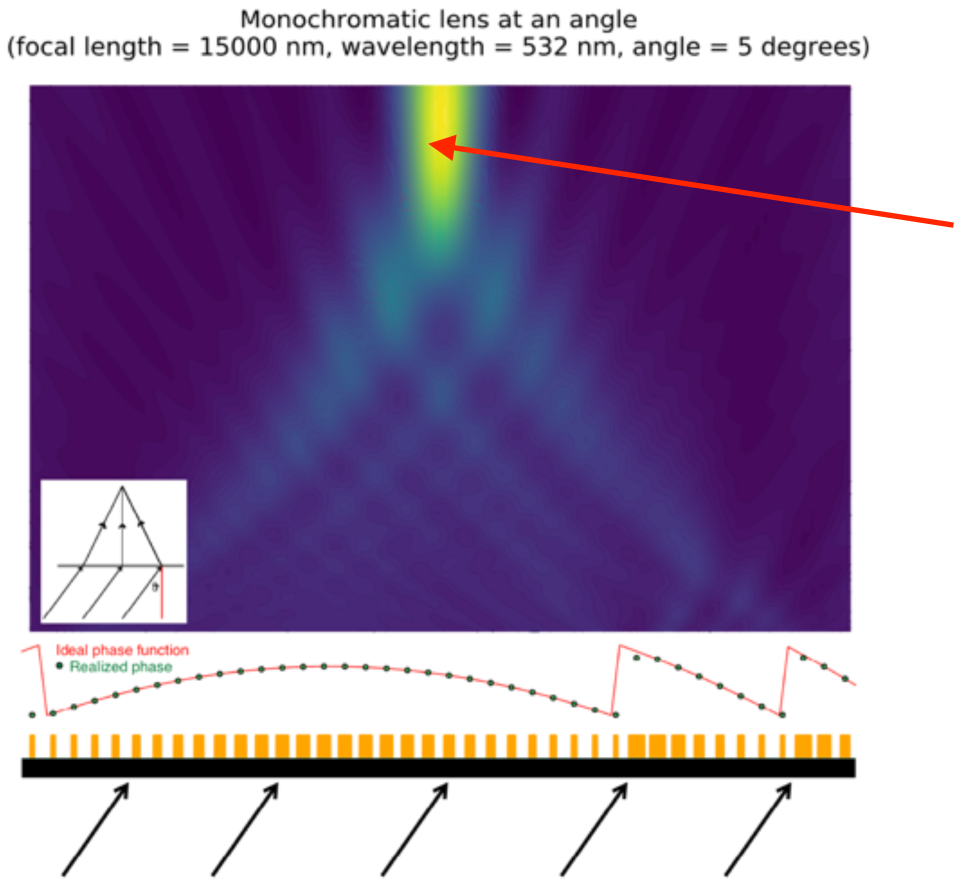
optimized metalens



few minutes
on a laptop!

just interpolate from this "library"
during optimization
over 1000s of parameters

A small metalens optimization problem



Maximize the 0th-order transmitted $|E|^2$ at a focal point as a function of pillar widths in every cell (here, 40 pillars).

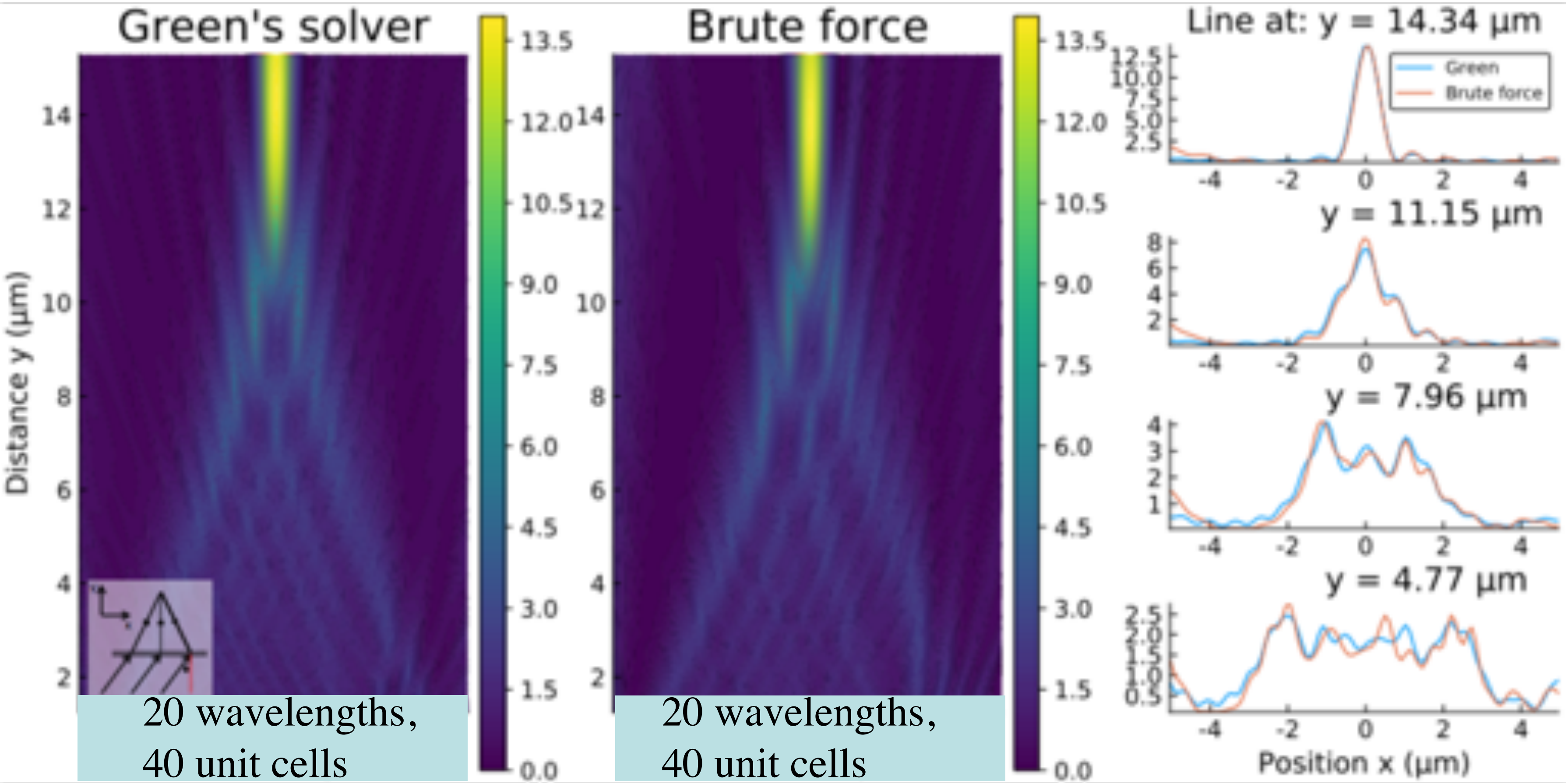
"Boring" off-the shelf nonlinear optimization algorithm: CCSA algorithm [Svanberg (2001)]

[R. Pestourie, et al., *Optics Express* (2018).]

Brute-force (FDFD) validation

180,000x faster

(0^{th}-order)



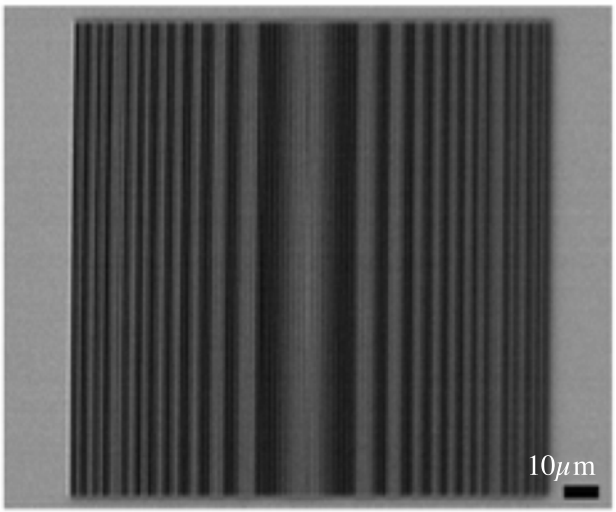
Seconds on a laptop

[R. Pestourie, et al., *Optics Express* (2018).]

Optimization + experiment: extended depth-of-focus metalens

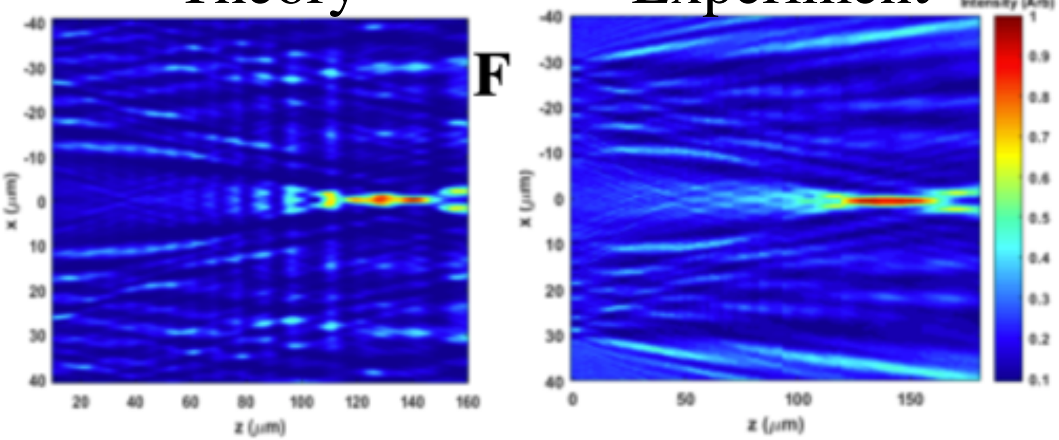
[collaboration with A. Majumdar, UW (2019)]

e-beam cylindrical lens



(SiN on fused silica)

Theory Experiment



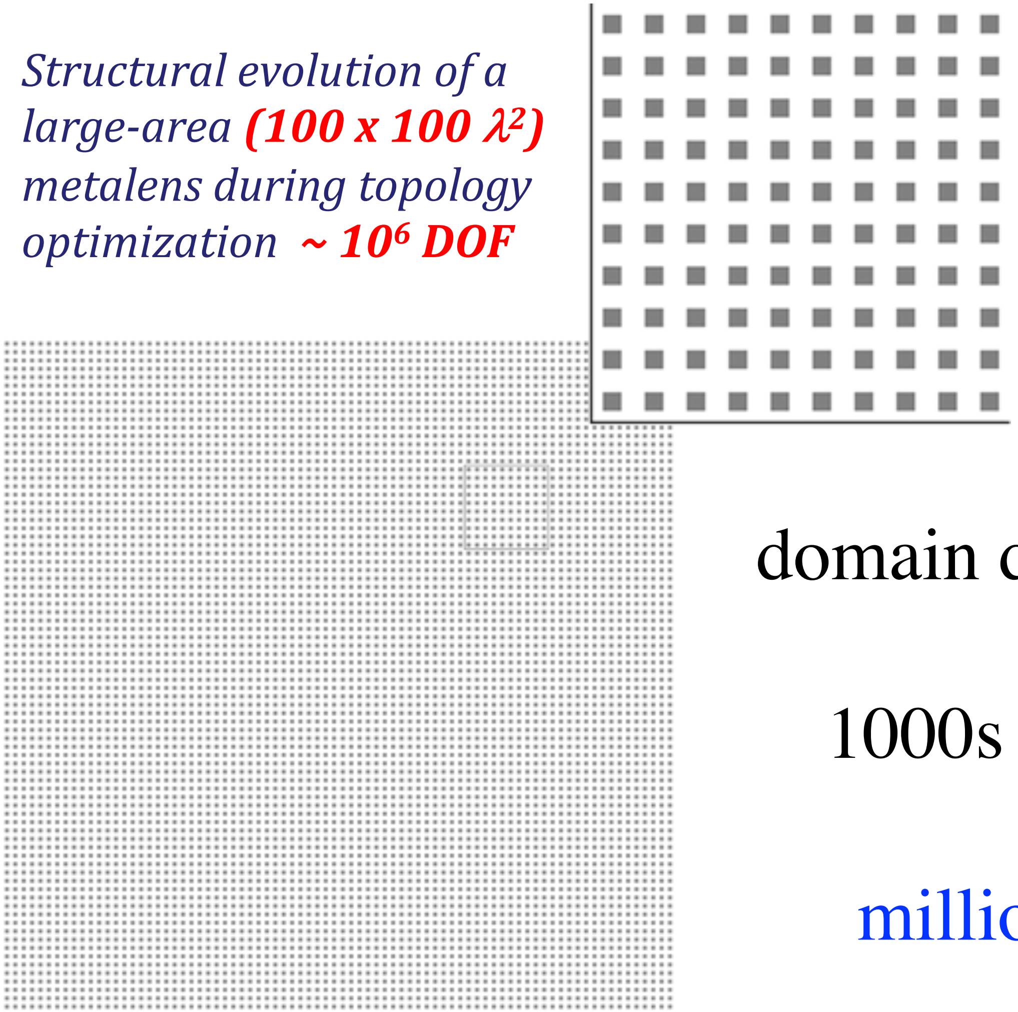
(λ = 633nm)

44μm depth of focus, focal length 133μm

Topology Optimization for Metasurfaces

[Lin et al. (2019)]

Structural evolution of a large-area ***(100 x 100 λ^2)*** *metalens during topology optimization* ***~ 10^6 DOF***



Every "pixel" is
a degree of freedom
… possibly in multiple layers!

domain decomposition (LPA / ODA)

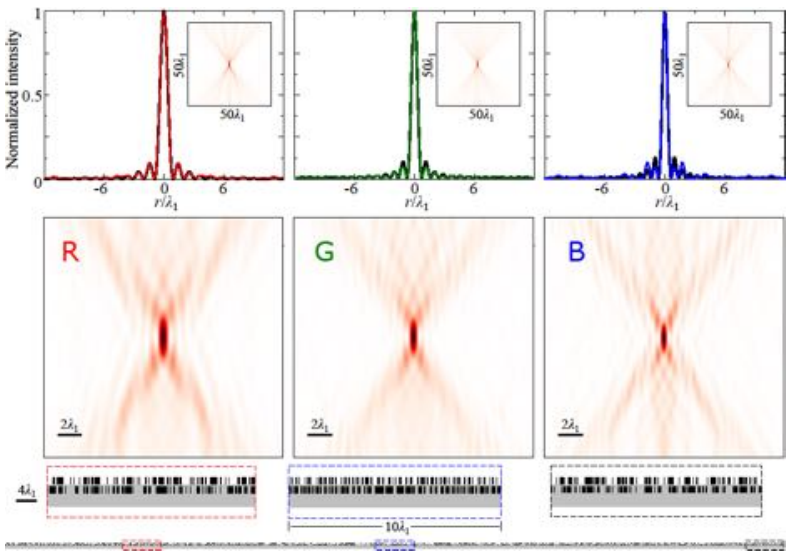
+

1000s of parameters per domain

=

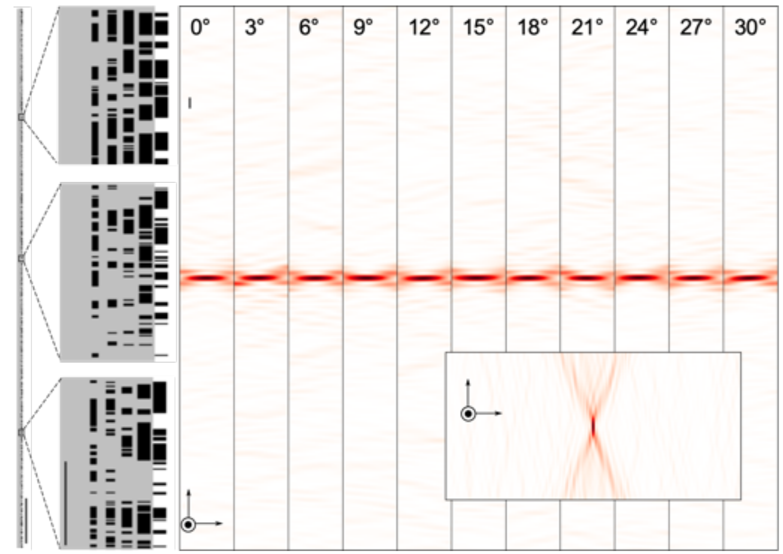
millions of parameters in total

Difficult metasurface designs



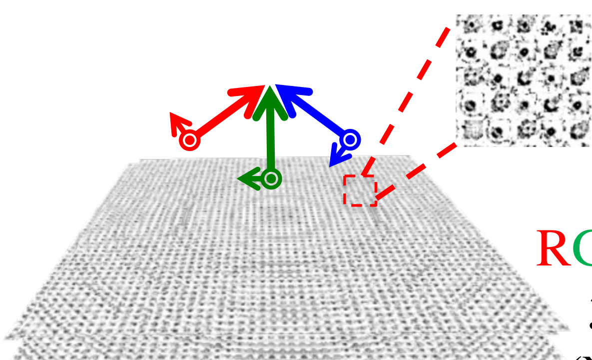
RGB 2-layer lens

(NA = 0.71, 200λ diameter, 50% efficiency)



Concentrator:

multiple angles, same focus



RGB 2-layer

3d lens

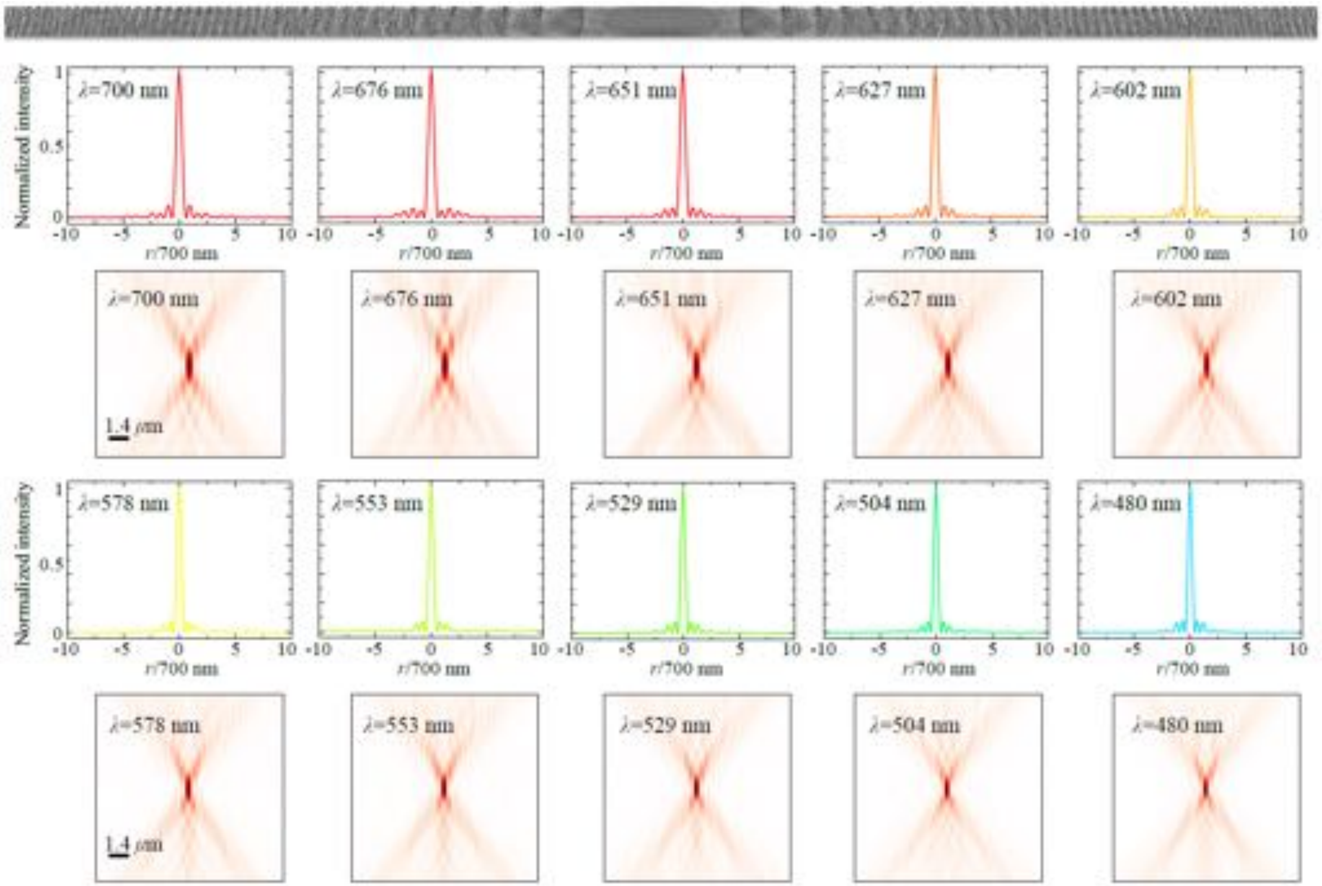
(NA = 0.44)

now fully achromatic lens…

Achromatic (480–700nm) metalens

[Lin et al (2019)]

Topology-optimization thrives in a large design space …



15 layers of 140 nm thickTiO_2

NA = 0.71

Lens size: 200 λs

Average focusing efficiency > 50%

Proof-of-concept 2D design:

large size

+ high NA

+ broadband

+ by far, the best efficiency

Note: Full FDTD validation of the entire lens.

Optimization is not just throwing parameters at a computer.

To get a tractable problem, domain-specific expertise goes into how you formulate the objective & parameters. Many physical similar choices that have very different mathematical properties!

Many design problems remain to be attacked, & several recent bounds far from attained.