Real Physics from “Unphysical” Simulations

Steven G. Johnson
MIT Applied Mathematics, MIT Physics

Simulations: Sources to Fields

Basic building block of most electromagnetic computations
= solver that can go from sources (e.g. electric currents **J**) to electromagnetic fields (e.g. electric field **E**)

Maxwell

$$\nabla\times\nabla\times\mathbf{E} + \varepsilon\ddot{\mathbf{E}} = -\dot{\mathbf{J}}$$ time domain

$$(\nabla\times\nabla\times - \omega^2\varepsilon)\mathbf{E} = i\omega\mathbf{J}$$ frequency (ω) domain

+ many variations … for example, the Equivalence Principle maps currents to/from incident waves, and maps volume unknowns (fields) to interface unknowns (surface integral equations, Mie, etc.).

- Computers: discretize (e.g. finite differences/elements) and solve as a large (sparse) matrix equation/ODE: $Mx = b$

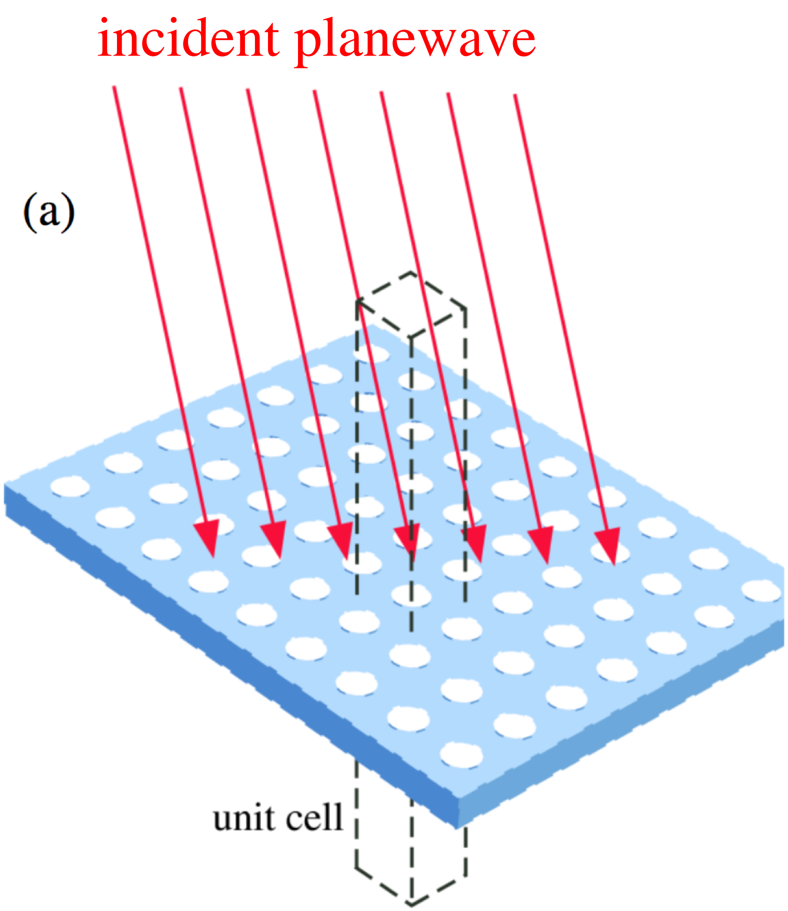
(One common exception: mode solvers …
find **J**=0 time-harmonic fields.

Actually closely related: will return to this later.)

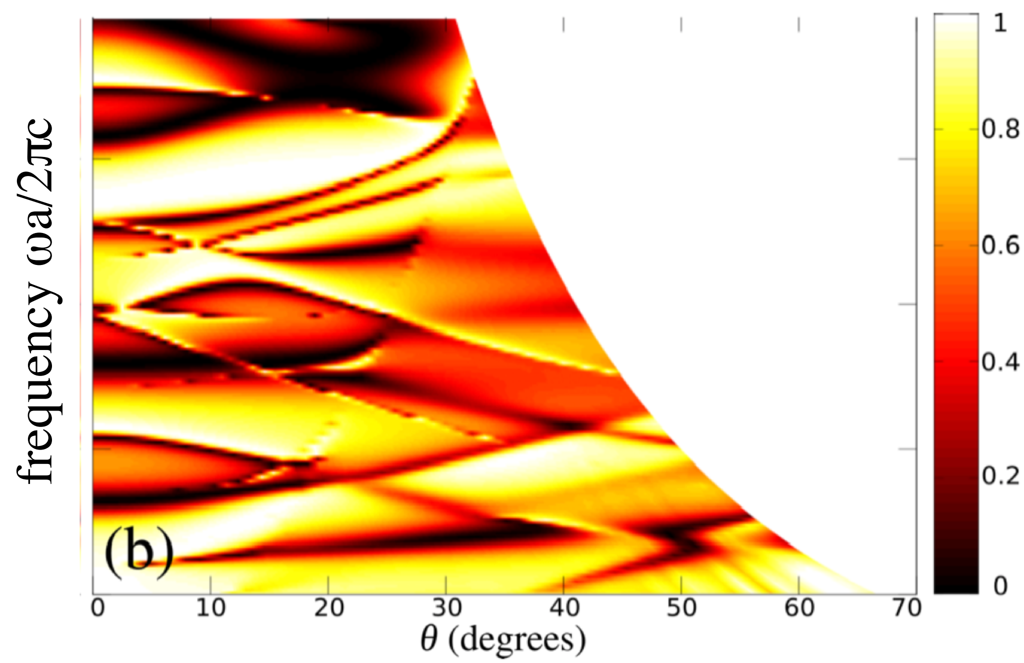
Numerical Experiments

a very common … and very useful! … way to use simulations:

mimic a laboratory experiment



typical example: reflection spectrum



an unoriginal observation, but perhaps still underutilized: Computers Can Do More

In a computer, simulation, you can measure the field amplitude and phase anywhere/everywhere, put sources anywhere …

and are not limited to physical materials, sources, or other parameters (e.g. ω).

Lots of ways to exploit this to gain understanding, save computation time, or extract information in ways that have no direct experimental analogue.

an old idea (1980s?), still underappreciated outside large-scale optimization community:

Adjoint Sensitivity Analysis

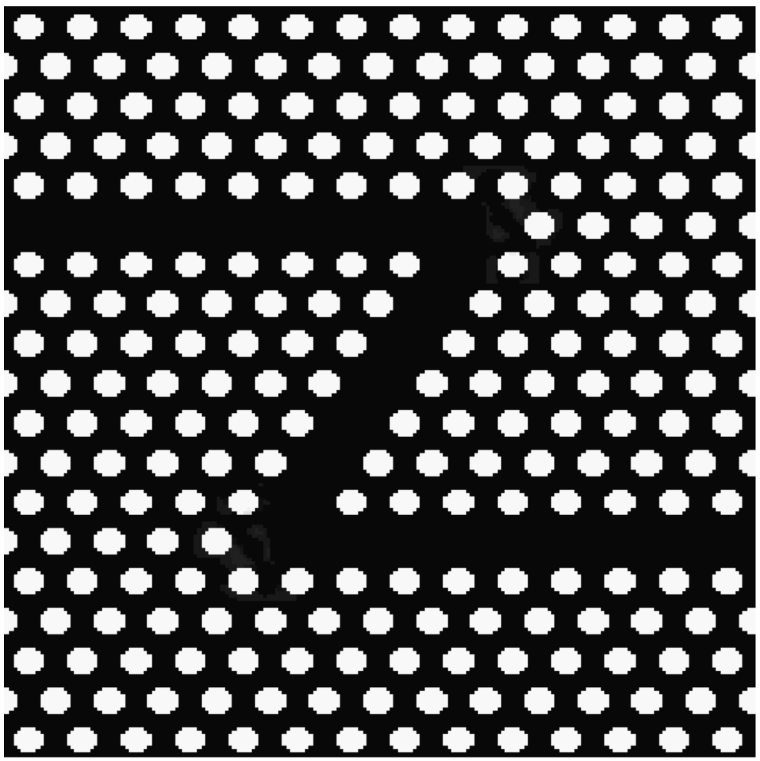
Suppose we are computing transmission T, and want to know the sensitivity $\partial T/\partial p$ to some parameter p.

Easy? Just use a finite-difference approx.: $\frac{\partial T}{\partial p} \approx \frac{T(p+\Delta p)-T(p)}{\Delta p}$.

- Problem: if you have N >> 1 parameters, need N+1 simulations.
  — Totally impractical for 3d simulations if N=1000?
  — But why would you need this?

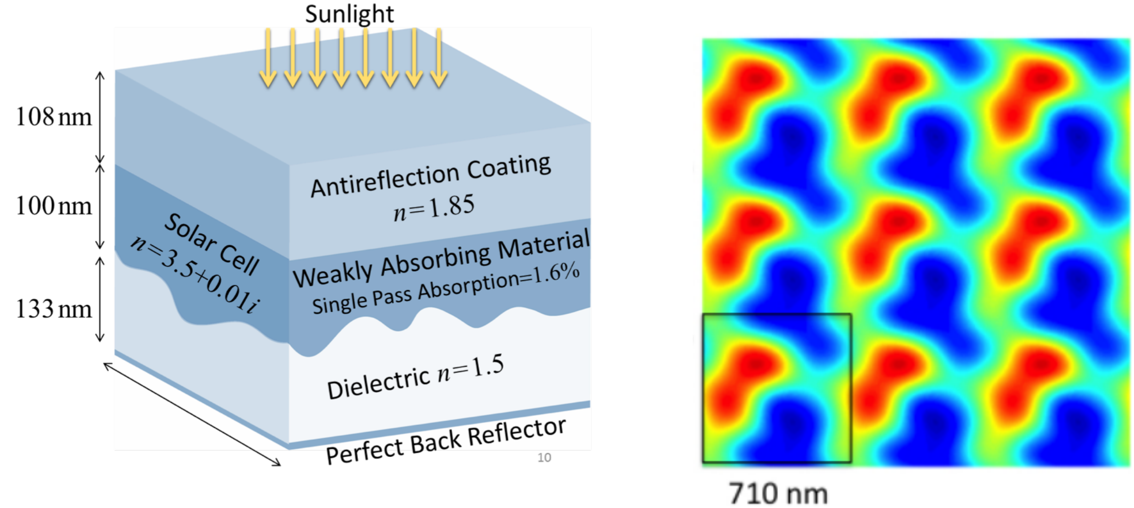
Large-scale optimization in photonics: "Every pixel" is a degree of freedom

bend optimization

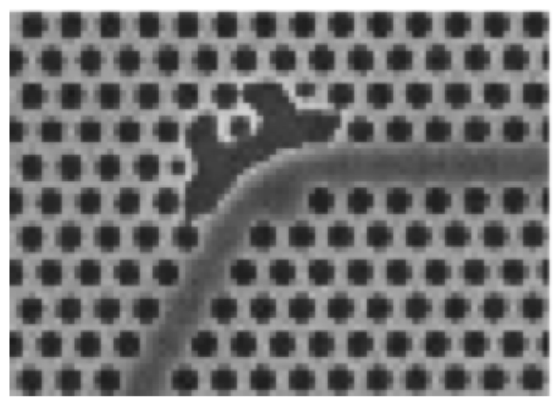


Sigmund et al.,
Opt. Express **12**, 1996 (2004)

solar-cell backreflector optimization

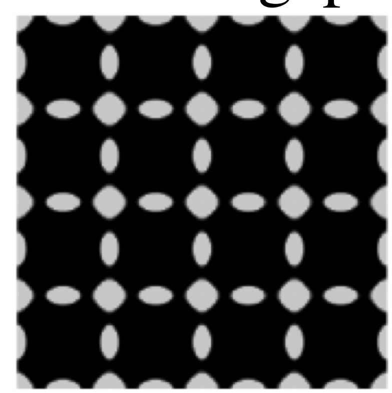


Ganapati et al. IEEE Jour. of Photovolt. **4**, 175 (2014)



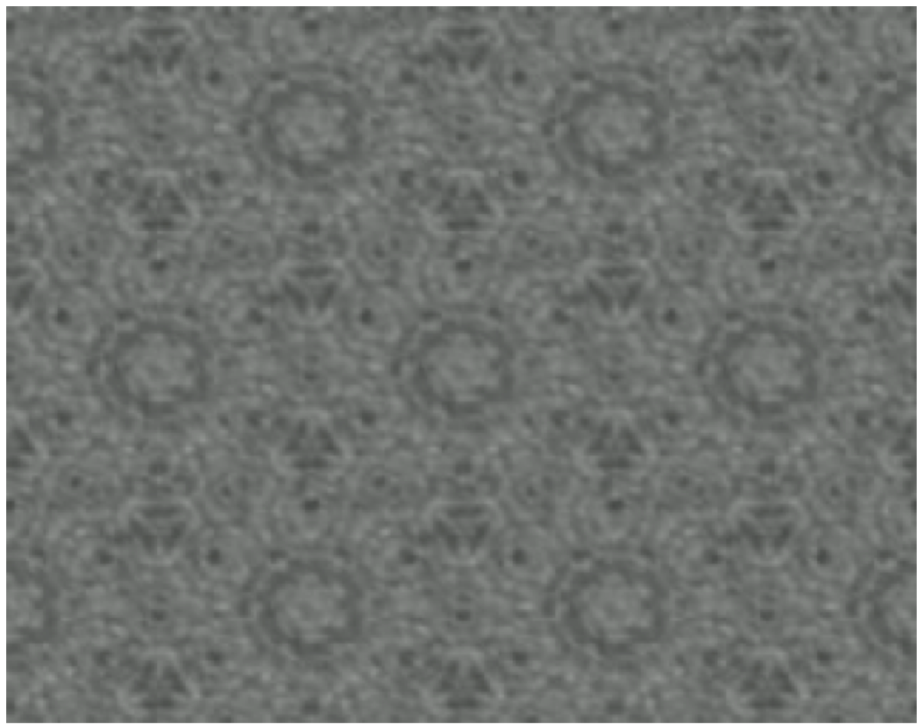
OE **12**, 5916 (2004)

2d band gaps



Dobson (1999)

Optimizing 1st complete (TE+TM) 2d gap from random starting guess



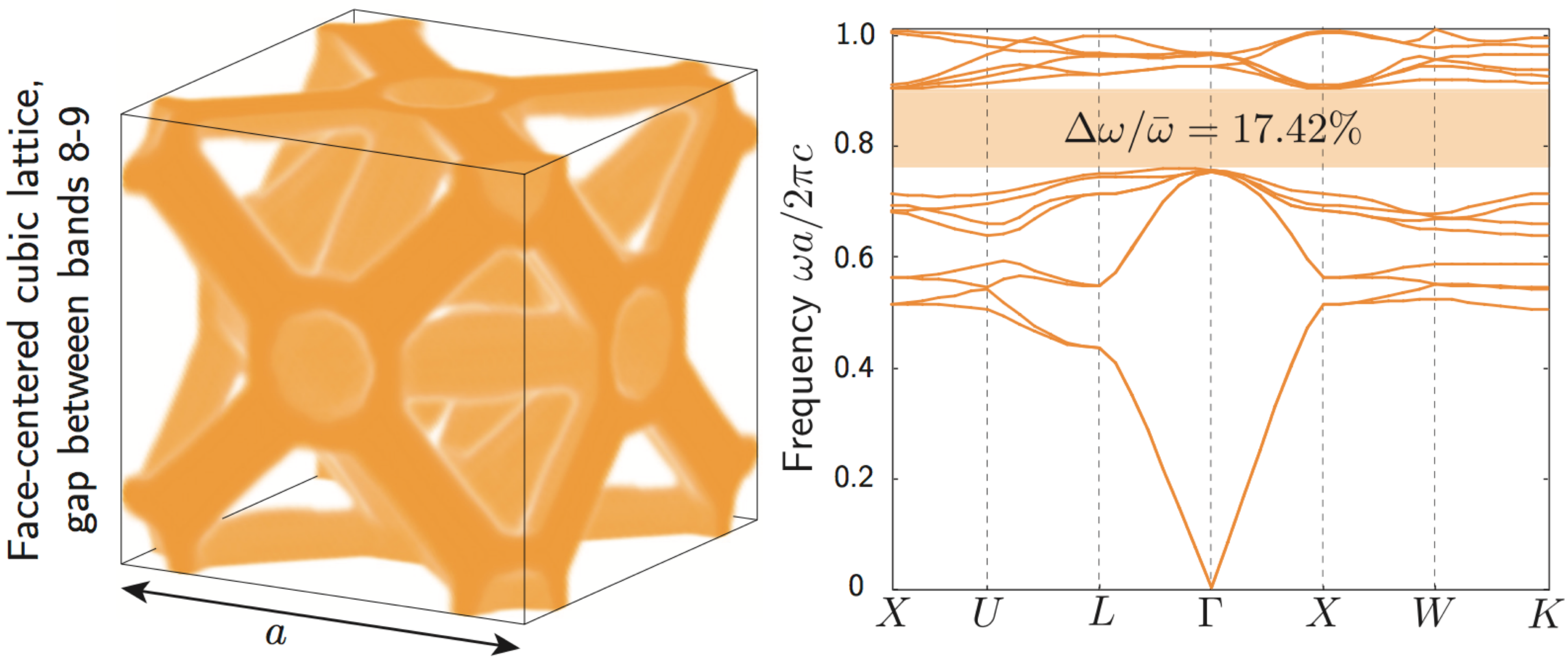
20.7% gap (ε = 12:1)

[Oskooi & Johnson, ScD thesis (2010)]

Even ~10^6 of degrees of freedom

[Men, Lee, Freund, Peraire, Johnson, *Opt. Express* (2014).]

3d bandgap optimization: Every "voxel" is degree of freedom



(e) FCC8 (no. 225)

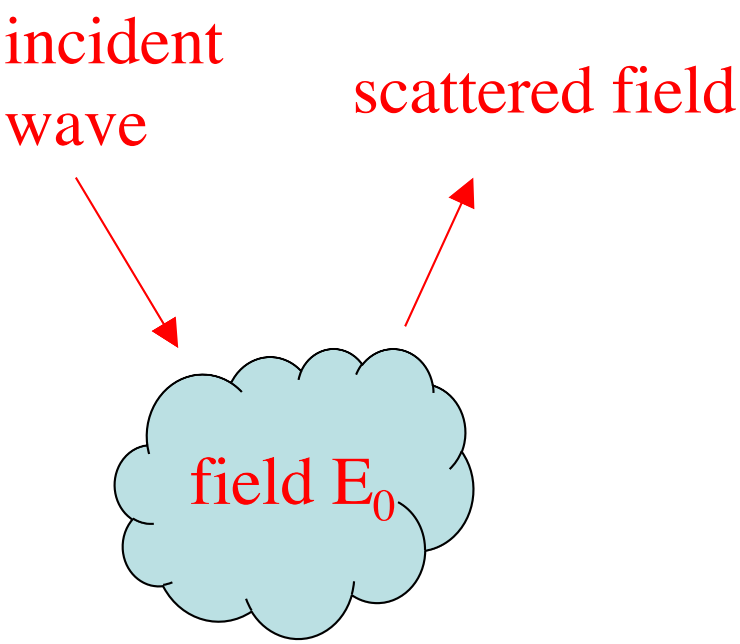
Impossible to explore/optimize a 10^6-dimensional parameter space without derivatives.

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

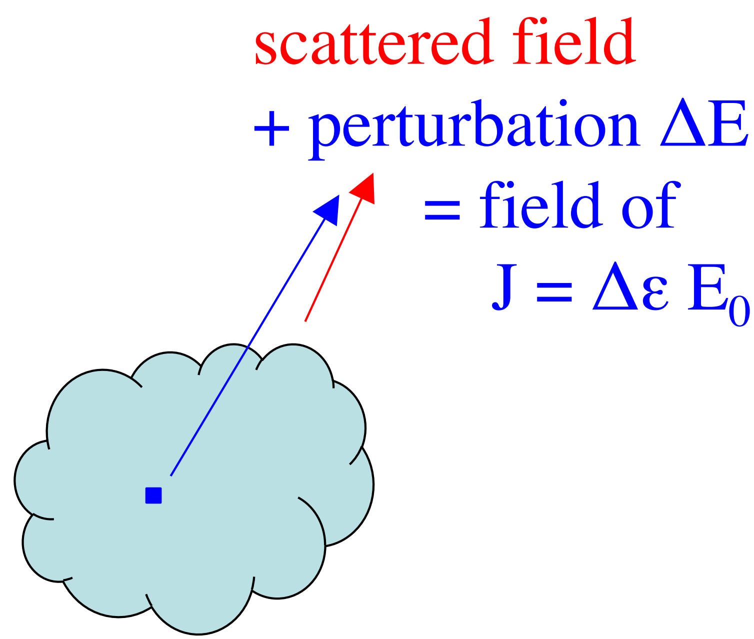
(Only local optimization with this many parameters, but can still find very good designs, sometimes with provable guarantees.)

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

physical intuition: Born approximation + reciprocity



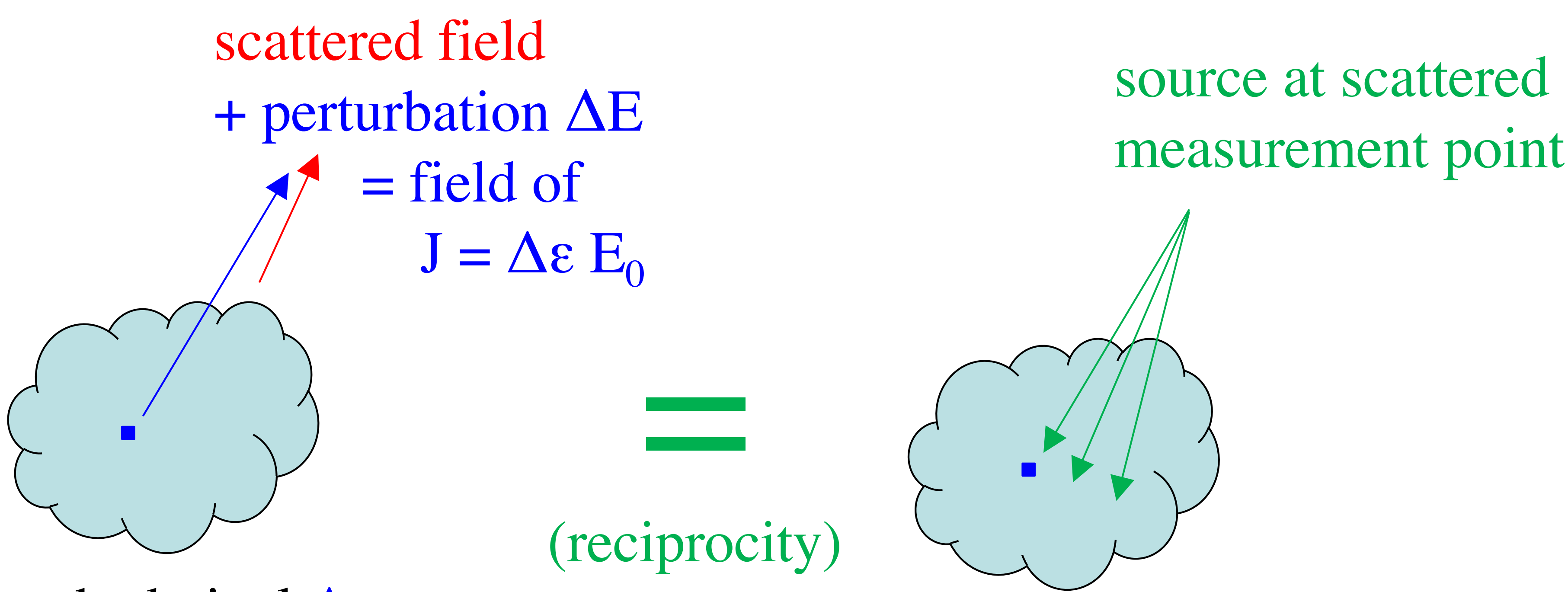
"forward" solve



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



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

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:

[real variables, e = real/imag parts]

$$M(x)e = s$$

EM fields

source

Maxwell matrix (parameters x)

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")

Even “weirder” sources: Complex ω

Example problem: Maximal-scattering/absorption nanoparticles

motivation:
smoke grenades

particle:
given χ,
not shape

incident light,
wavelength λ,
intensity I_0

vol
V

scattered light,
power P_{scat}

extinction cross-section $\sigma_{ext} = (P_{abs} + P_{scat}) / I_0$

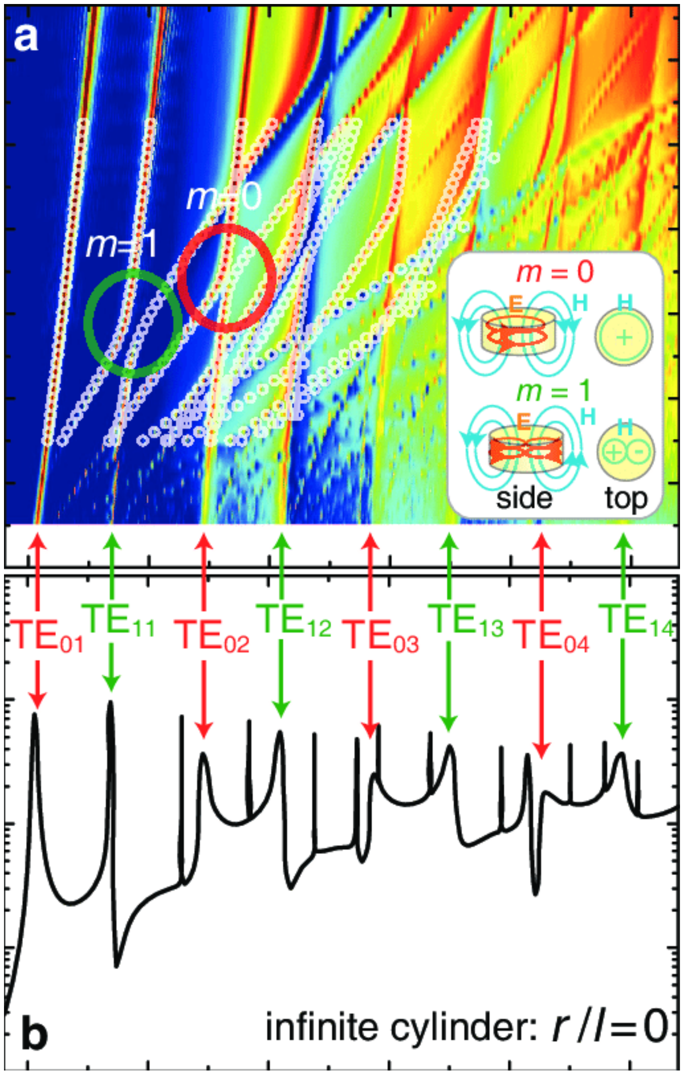
Key question: What is the best σ_{ext} / volume?

… averaged incident angles & polarizations

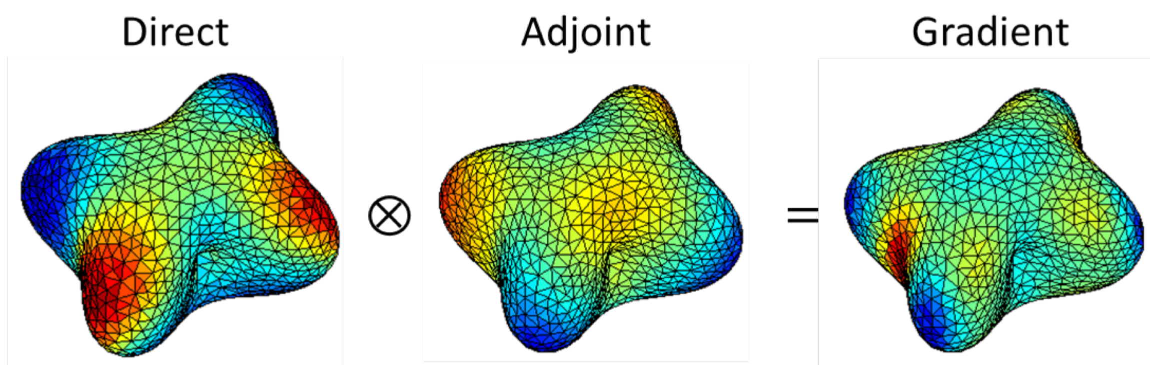
(averaged over some bandwidth)

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

Bandwidth = Many solves ☹



Rybin et. al (2017): arXiv:1706.02099



Very efficient surface-integral equation (BEM) solver for angle-average cross-section σ and its gradient at a single frequency.

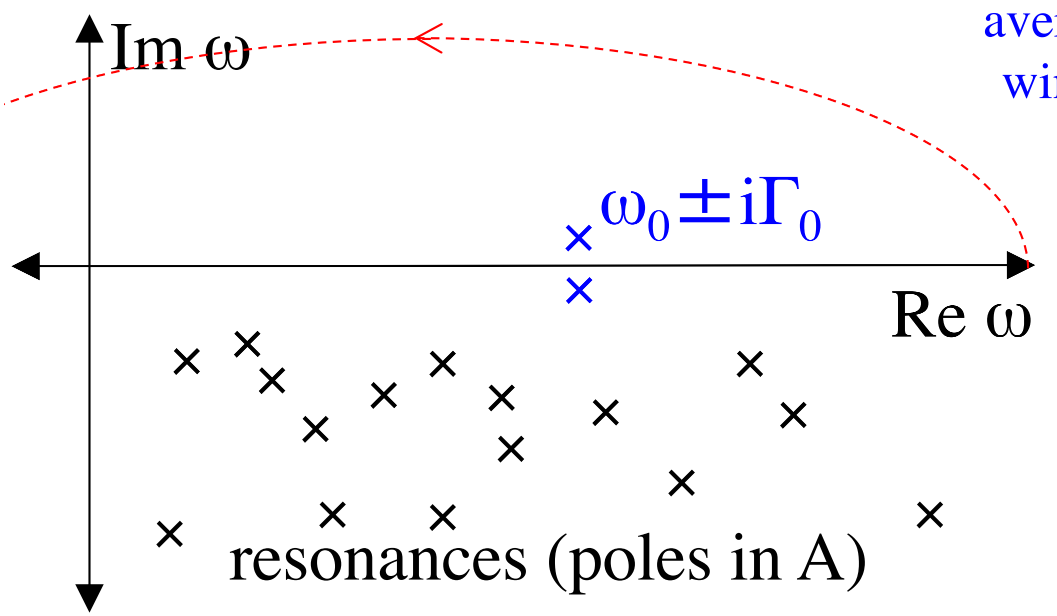
But integrating over visible spectrum (many resonance spikes) requires solving many frequencies.

Optical theorem + Passivity

- Optical theorem: σ_{ext} = Im (forward scattering amplitude A)
- Passivity/causality: A(ω) analytic for Im ω > 0

$$\text{average } \sigma_{ext} = \mathrm{Im}\int_{-\infty}^{\infty} A(\omega)\,\underbrace{\frac{\Gamma_0/\pi}{(\omega-\omega_0)^2+\Gamma_0^2}}_{\text{averaging window}}\,d\omega = \mathrm{Im}[2A(\omega_0+i\Gamma_0)]$$

via contour integration



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

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

(numerical results eventually pointed the way to general analytical bounds on σ/V and other quantities, given only material and not the shape)

[Owen Miller et. al. *Phys. Rev. Lett.* **112**, *123903* (2014)]
[Owen Miller et. al. *Optics Express* **24**, *3329* (2016)]
[+ subsequent papers]

Prof. Owen Miller
Yale

Solvers “like” complex ω!

In frequency domain, Im $\omega > 0$
moves away from resonances =
better conditioning

Is there an analogous approach/advantage
in time-domain?

(In time domain, Fourier-transform response to a broadband pulse to get many ω, but requires long simulation to capture long-lived resonances.)

Complex ω in the Time Domain?

E field is solution of: $(\nabla\times\nabla\times-\omega^2\varepsilon)\mathbf{E} = i\omega\mathbf{J}$

ω and ε only appear together!

complex contour deformation

⇒ change from ω to $\omega\, f(\omega)$ is equivalent (same E) to changing material to $f(\omega)^2\, \varepsilon(\omega\, f(\omega), x)$ (+ Jacobian factor in frequency integrals)

Can get all the advantages of complex frequency but for **real frequency/time** with **transformed materials**

[Alternatively, use $f(\omega)\, \varepsilon(\omega\, f(\omega), x)$ and $f(\omega)\, \mu(\omega\, f(\omega), x)$ to get same E and H]

Complex ω in the Time Domain

A. P. McCauley et al., "Casimir forces in the time domain: Applications," *Physical Review A*, vol. 81, p. 012119, January 2010.

One possible ω contour that leads to passive, causal materials

$$\omega \rightarrow \xi\sqrt{1+\frac{i\sigma}{\xi}} \quad \Leftrightarrow \quad \left(1+\frac{i\sigma}{\xi}\right)\varepsilon$$

= conductive medium

time domain: real-frequency response in conductive medium

$$\left.\begin{aligned} \frac{\partial \mu \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E} \\ \frac{\partial \varepsilon \mathbf{E}}{\partial t} &= \nabla \times \mathbf{H} - \sigma\varepsilon\mathbf{E} - \mathbf{J} \end{aligned}\right\}$$

off-the-shelf FDTD software already supports conductive media … damping = short simulation!

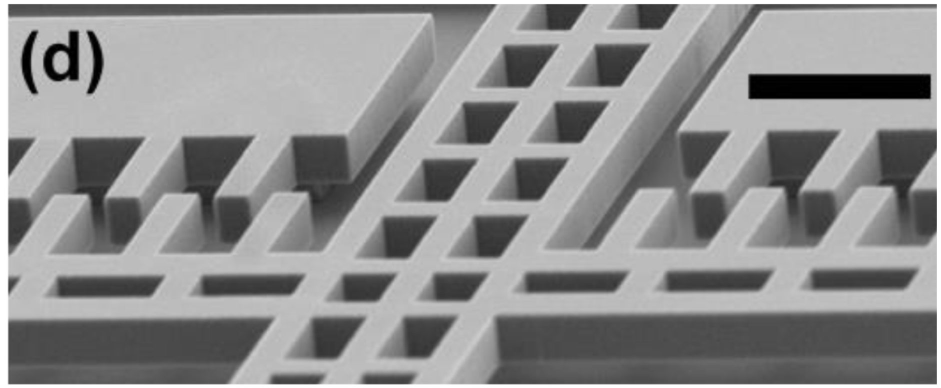
[Rodriguez, McCauley *et al*. *PNAS* **106** 6883 (2010)]

Complex ω = ω average: Lots of uses

3d optimization of microcavities
(frequency-averaged LDOS = Purcell factor)

[Liang & Johnson (2013)]

Modeling Casimir/van der Waals force

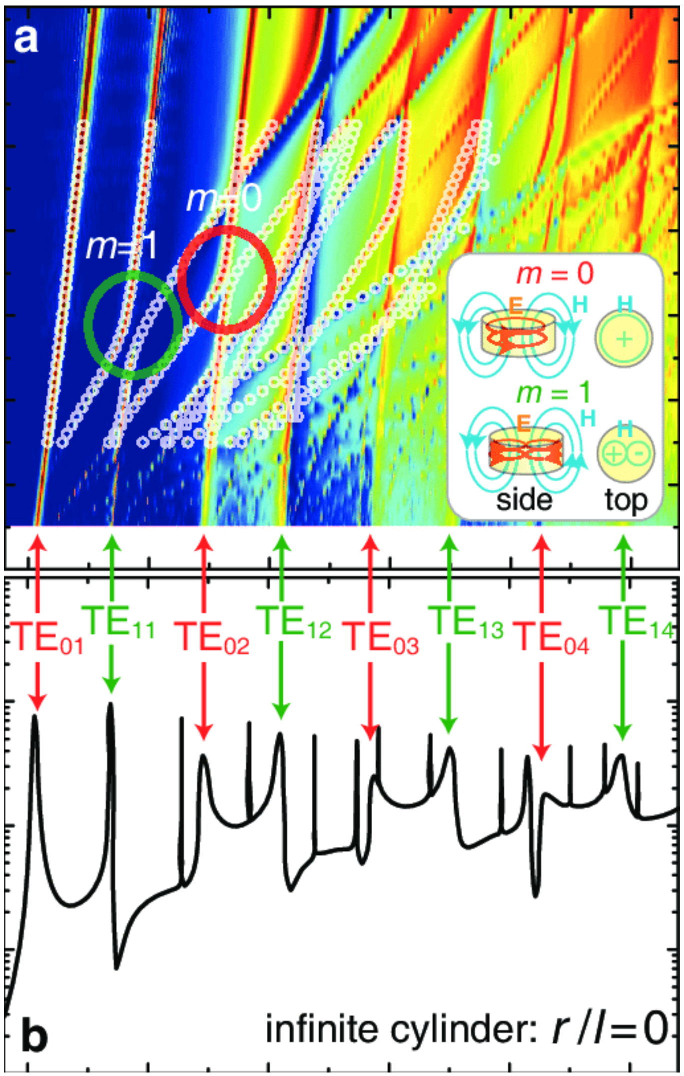


integrating fluctuations over all ω
= much nicer integral over Im ω

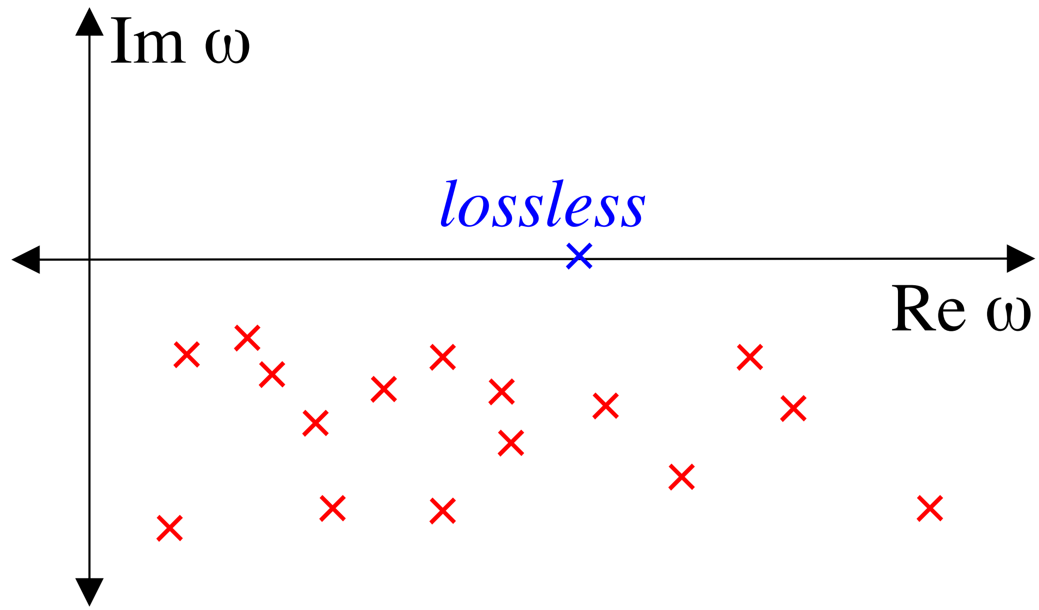
[Rodriguez et al., *Nature Photonics* (2011)]

- General derivation of Wheeler–Chu limits via contour integration
  [Sohl, Gustafsson, Kristensson (2007)]
- Proof that cloaking bandwidth scales ~ 1/diameter [Hashemi (2010)]
- Upper bounds on ω-averaged light-matter interactions [Miller (2018)]

Familiar complex ω: Resonances



Rybin et. al (2017): arXiv:1706.02099

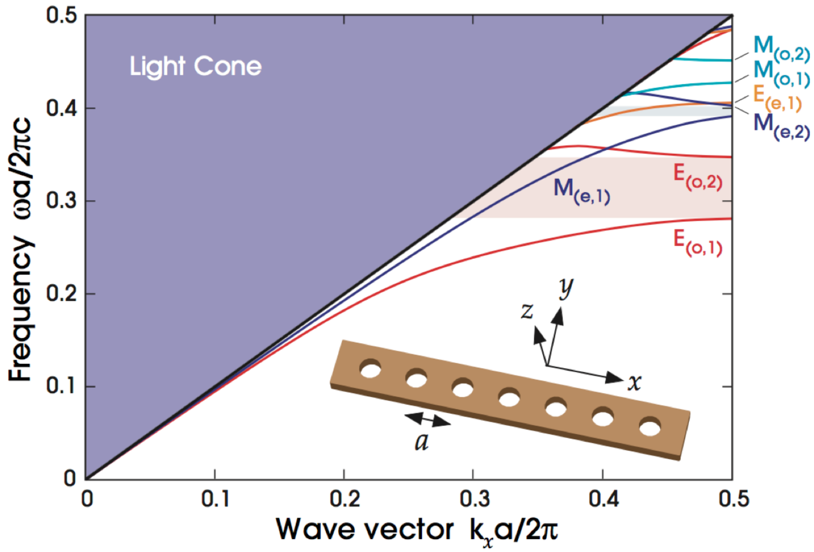


resonances = poles in scattering
= poles in Green's function
= singular Maxwell operator M(ω)

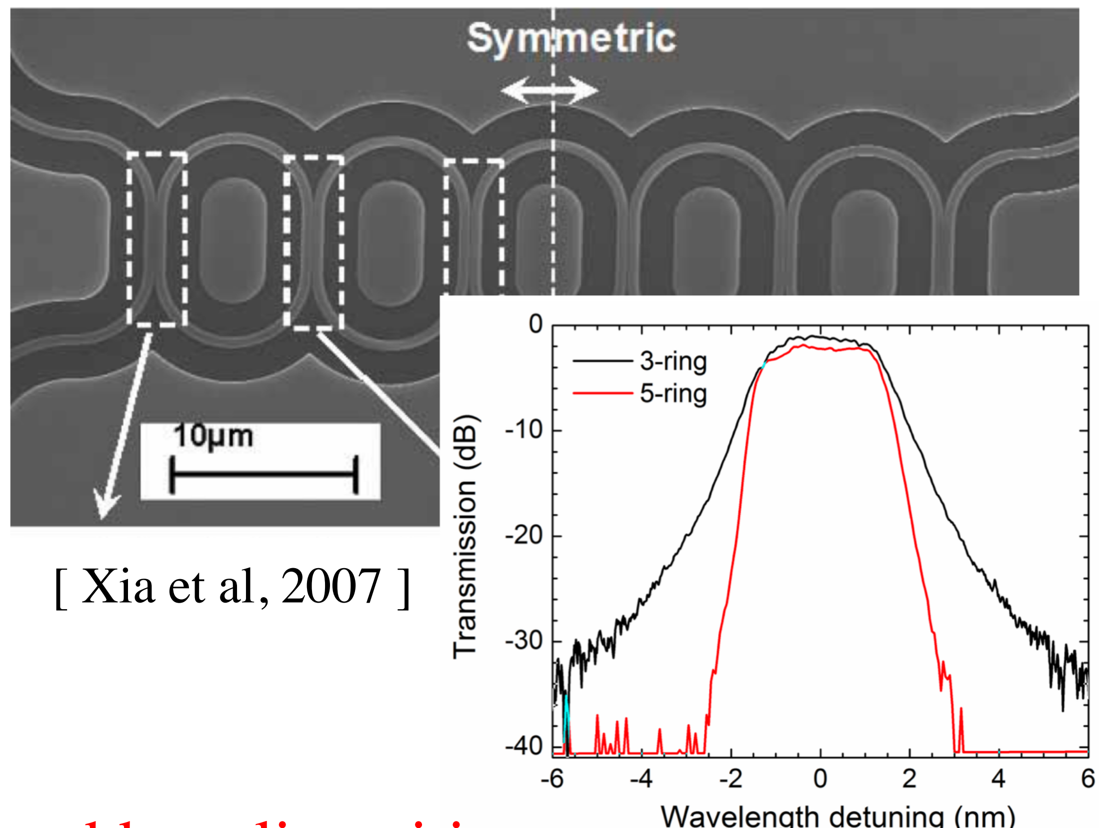
$$\underbrace{(\nabla\times\nabla\times-\omega^2\varepsilon)}_{\text{M(ω) singular at resonance ω}}\mathbf{E} = i\omega\mathbf{J} = \mathbf{0}$$

Review: Why find resonant modes?

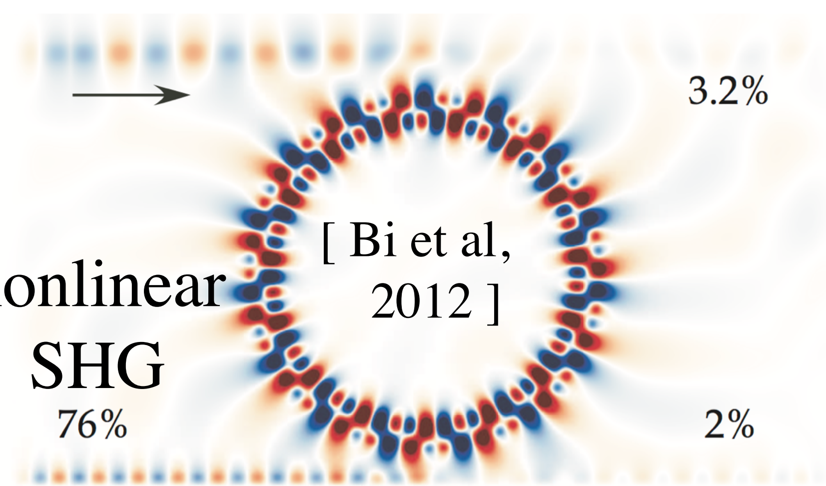
dispersion relations
= “map” of solutions



Given individual resonances + coupling,
can analyze/design arbitrary cascade:



[Xia et al, 2007]



nonlinear
SHG
76%

& add nonlinearities
and other “weak” effects analytically
that are very hard to simulate directly

Resonances = Complex-ω Solves!

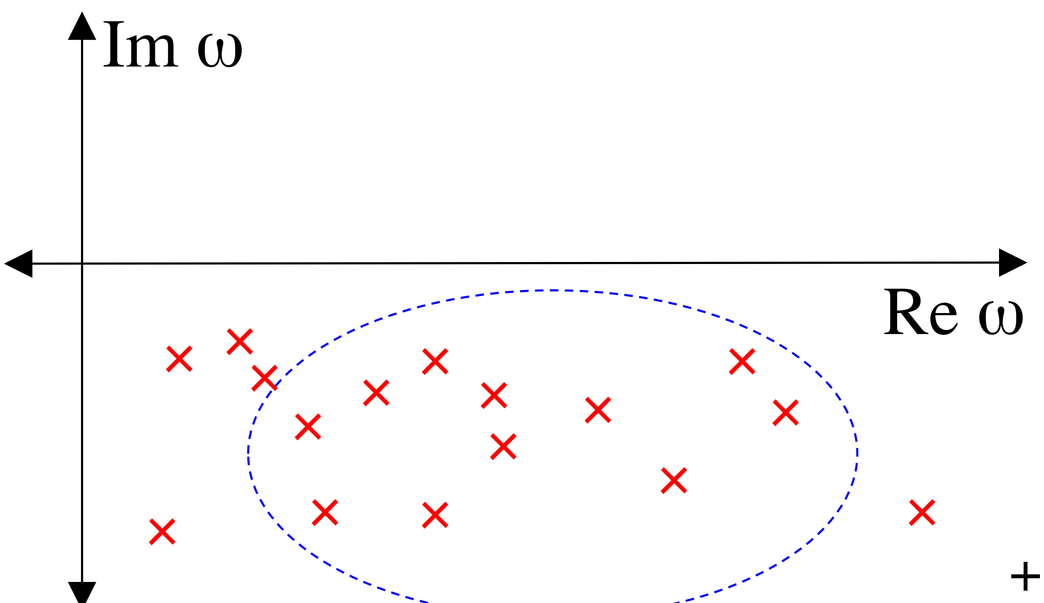
ω where M(ω) is singular = eigenproblem

(nonlinear if dispersive ε)

basic "shift-and-invert"/Newton technique given a rough guess for ω:

multiply a "random" vector by $M(\omega)^{-1}$, update ω, & repeat

(+ fancier algorithms, e.g. Arnoldi)



more recent technique:

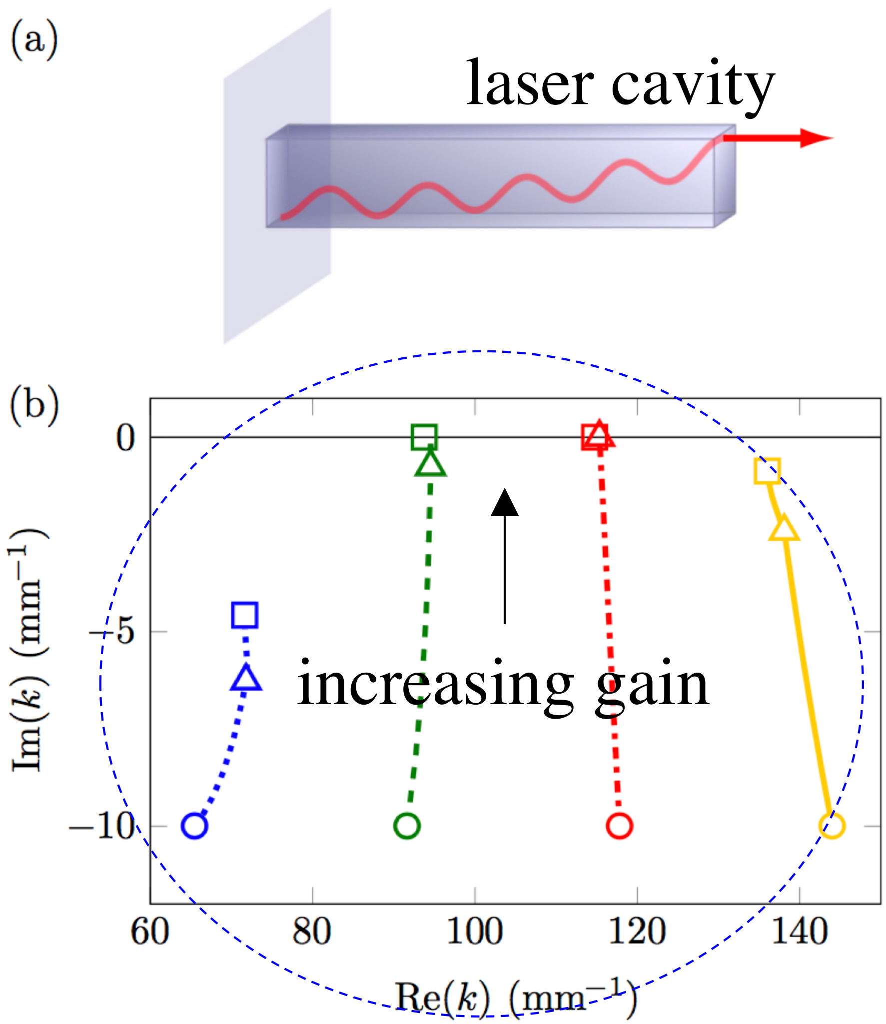
$$\oint M(\omega)^{-1}(\text{randoms})\,d\omega$$

… gives all resonances inside the contour!

[Beyn (2012)]

+ precursors in scattering-matrix methods
[e.g. Anemogiannis & Glytsis (1992)]

Resonances = Complex-ω Solves!



[Esterhazy, Liu et al. (2014)]

$$\oint M(\omega)^{-1}(\text{randoms})\,d\omega$$

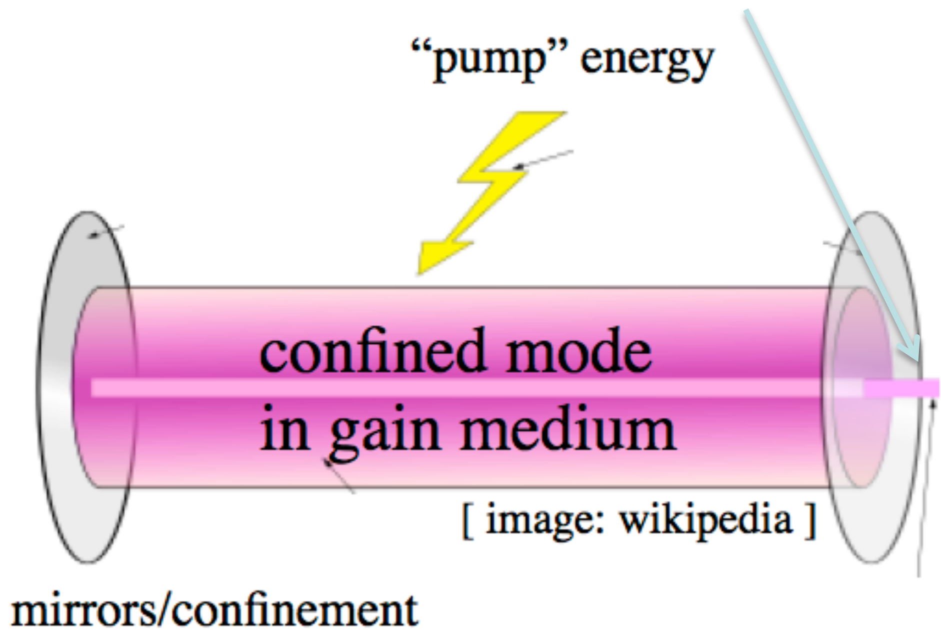
… gives all resonances inside the contour!
[Beyn (2012)]

We used this to track laser resonances as they approached threshold … & above threshold, a Newton solver solves nonlinear "SALT" equations of steady-state lasing. No time evolution!

Lasers

- a laser is a resonant cavity…
- with a gain medium…
- pumped by external power source

population inversion → stimulated emission



1d laser:
light bouncing
between 2 mirrors

Maxwell–Bloch equations:
simplest accurate spatio-temporal lasing model

- fully time-dependent, multiple unknown fields, nonlinear (Haken, Lamb, 1963): Maxwell + Lorentzian polarization resonance + 2-level atom population inversion

$$-\nabla \times \nabla \times (\mathbf{E}^+) - \varepsilon_c \ddot{\mathbf{E}}^+ = \frac{1}{\varepsilon_0} \ddot{\mathbf{P}}^+$$

Polarization induces inversion

Inversion drives polarization

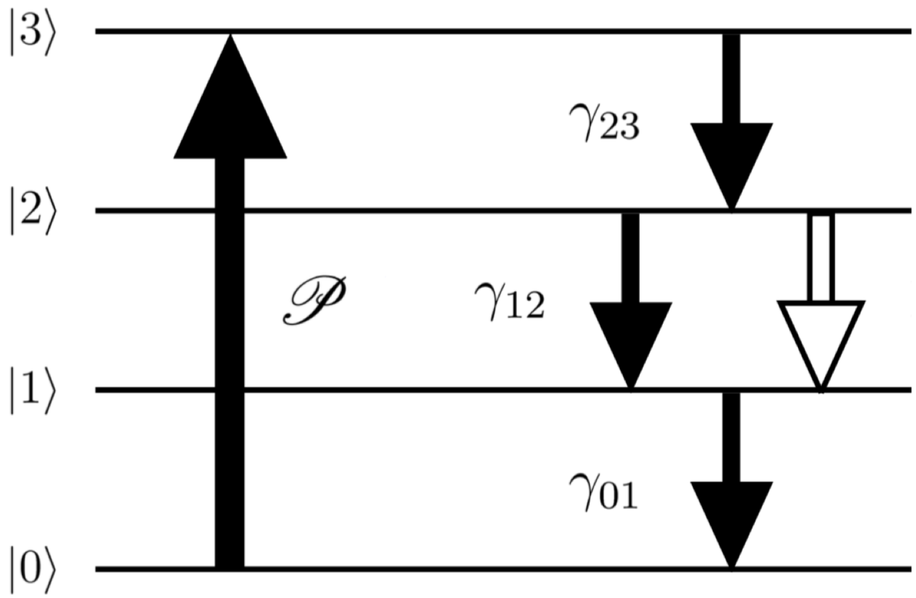
$$\dot{\mathbf{P}}^+ = (-i\omega_a - \gamma_\perp)\mathbf{P}^+ + \frac{1}{i\hbar}\mathbf{E}^+ D$$

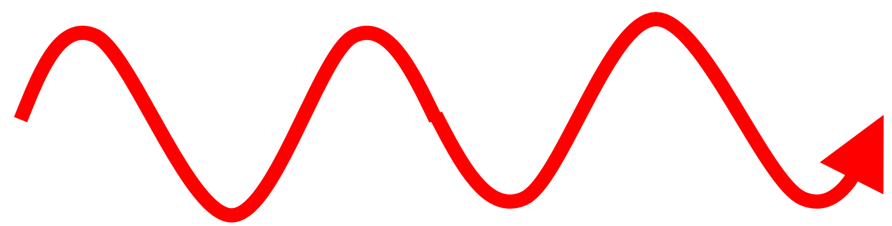
population inversion:

$$\dot{D} = \gamma_\parallel (D_0 - D) - \frac{2}{i\hbar}[\mathbf{E}^+ \cdot (\mathbf{P}^+)^* - \mathbf{P}^+ \cdot (\mathbf{E}^+)^*]$$

Conventional approach to study of laser

Time-domain **solution to Maxwell–Bloch**





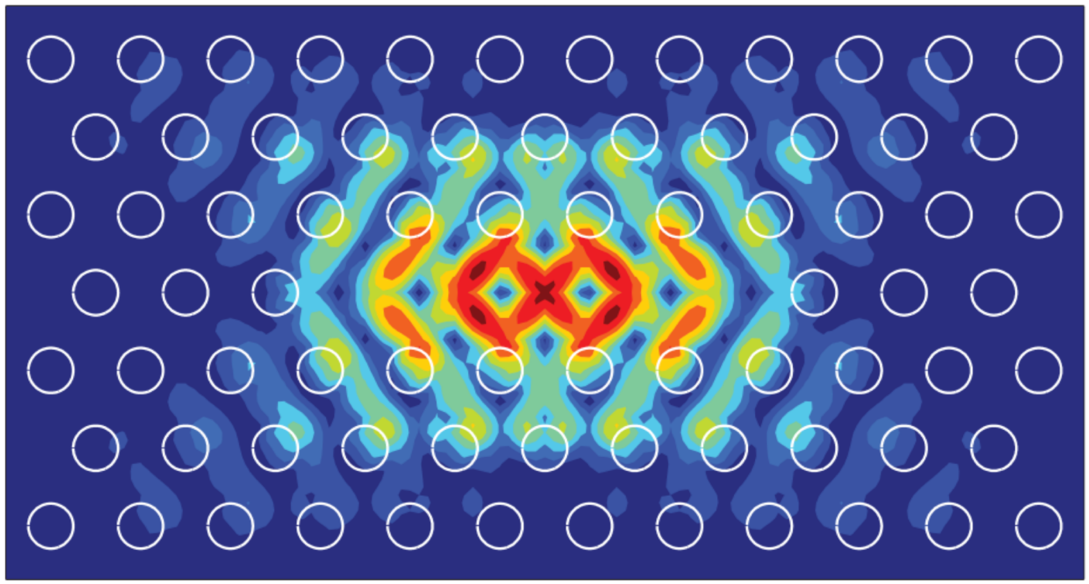
rate eq.
(population inversion) + Maxwell's eqs.

Challenge: $\gamma \ll \omega$

⇒ Takes too many time steps!
(Days of CPU time for 3D)

Brute-force Maxwell-Bloch solves

E.g., QD PC cavity laser



W. Carter et al., *PRA* (2017)

eventually reach steady state (SS). For example, each of our 2D $L15$ lasing simulations (shown below) takes roughly 20 hours to run, when 16 computational cores are used with 1024 Mb of memory each. This increased run time is roughly 400 times the

If a steady-state lasing solution exists, we'd rather solve for it directly *without* time-evolving

[Tureci, Stone, 2006]

$$\dot{D} = \gamma_{\|}(D_0 - D) - \frac{2}{i\hbar}[\mathbf{E}^+ \cdot (\mathbf{P}^+)^* - \mathbf{P}^+ \cdot (\mathbf{E}^+)^*]$$

key assumption:

$\gamma_{\perp}, \Delta\omega >> \gamma_{\|}$

valid for < 100μm microlasers

- "rotating-wave approximation"

  fast oscillations average out to zero

  … all oscillations are fast compared to $\gamma_{\|}$

… leads to: $\dot{D} \approx 0$

stationary-inversion approximation (SIE)

before

$$-\nabla\times\nabla\times(\mathbf{E}^+)-\varepsilon_c\ddot{\mathbf{E}}^+=\frac{1}{\varepsilon_0}\ddot{\mathbf{P}}^+$$

$$\dot{\mathbf{P}}^+=(-i\omega_a-\gamma_\perp)\mathbf{P}^++\frac{g^2}{i\hbar}\mathbf{E}^+D$$

$$\dot{D}=\gamma_{||}(D_0-D)-\frac{2}{i\hbar}[\mathbf{E}^+\cdot(\mathbf{P}^+)^*-\mathbf{P}^+\cdot(\mathbf{E}^+)^*]$$

after:

Steady-State Ab-Initio Lasing Theory,

"SALT"

[Tureci, Stone, 2006]

$$\boxed{\begin{gathered}\nabla\times\nabla\times\mathbf{E}_m=\omega_m^2\varepsilon_m\mathbf{E}_m\\ \varepsilon_m(\mathbf{x})=\varepsilon_c(\mathbf{x})+\frac{\gamma_\perp}{\omega_m-\omega_a+i\gamma_\perp}\left[\frac{D_0(\mathbf{x})}{1+\sum\left|\frac{\gamma_\perp}{\omega_\nu-\omega_a+i\gamma_\perp}\mathbf{E}_\nu\right|^2}\right]\end{gathered}}$$

Still nontrivial to solve:
equation is nonlinear in both

eigenvalue ω_m ← easier

eigenvector $\mathbf{E}_m$ ← harder

New numerical solvers:

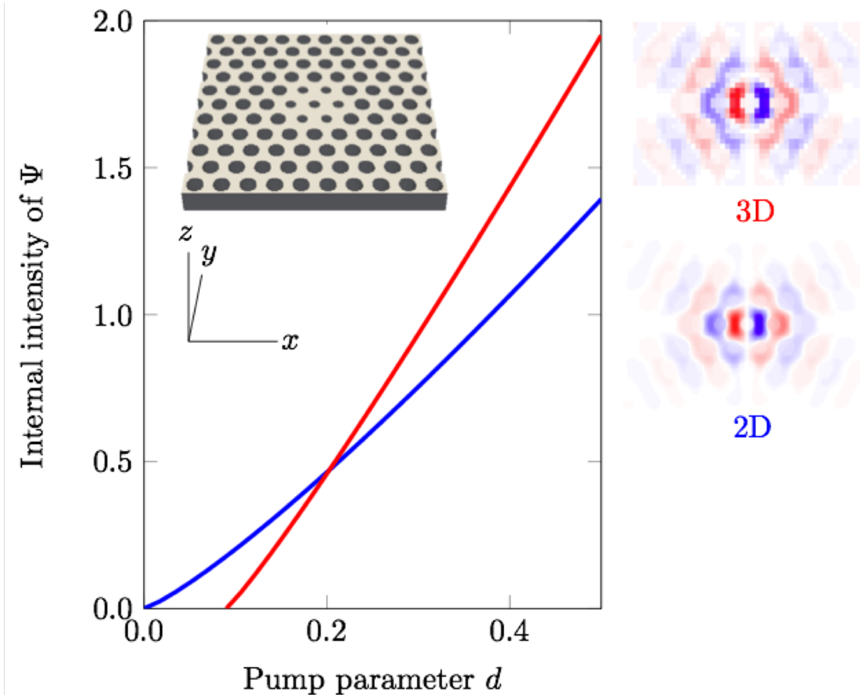
High-dimensional Newton from threshold modes

[Esterhazy et al., PRA (2014)]

SALT: lasing steady state
= "ordinary" EM eigenproblem

$$\nabla \times \nabla \times \mathbf{E}_m = \omega_m^2 \varepsilon_m \mathbf{E}_m$$

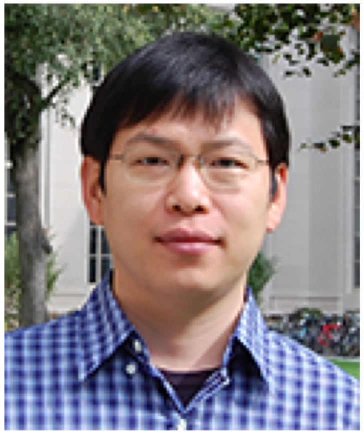
with nonlinear permittivity ε



$$\varepsilon_m = \varepsilon_c(\mathbf{x}) + \frac{\gamma_0}{\omega_m - \omega_0 + i\gamma_0} \frac{D_0(\mathbf{x}, d)}{1 + \sum_n \left| a_n \frac{\gamma_0}{\omega_n - \omega_0 + i\gamma_0} \mathbf{E}_n \right|^2}$$

(Lorentzian gain spectrum, mode amplitudes a_n)

full 3d nonlinear PDE solvers



SALT via off-the-shelf solvers

[Wonseok Shin et al, manuscript in preparation (2018)]

Problem: Newton's method requires you to rip your existing optimized Maxwell solver to shreds and re-assemble it into the SALT Jacobian matrix

… $|E|^2$ terms mean you need to write in terms of real matrices of real/imaginary parts

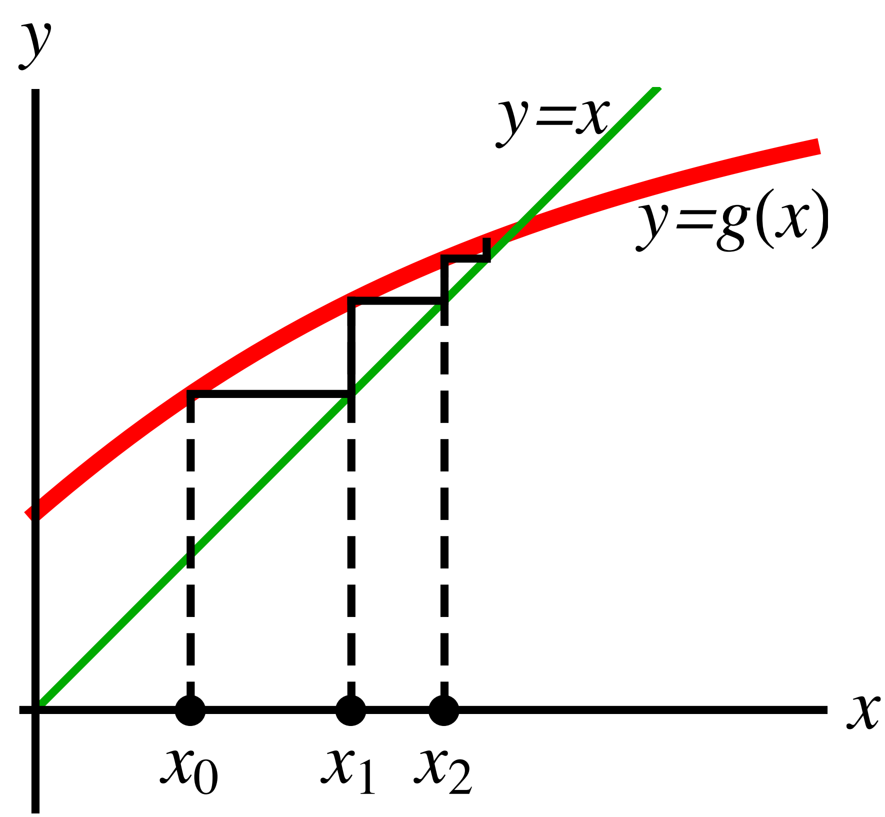
… we don't want to re-invent wheel on optimized code, preconditioners etc.

SALT solver with *existing* Maxwell solver

Key ingredient: *fixed-point iteration*

$$f(x) = 0 \implies g(x) \equiv f(x) + x = x \quad \text{(fixed-point eq.)}$$

$$x_{n+1} = g(x_n)$$



no Jacobian Required!

Anderson acceleration for fixed point

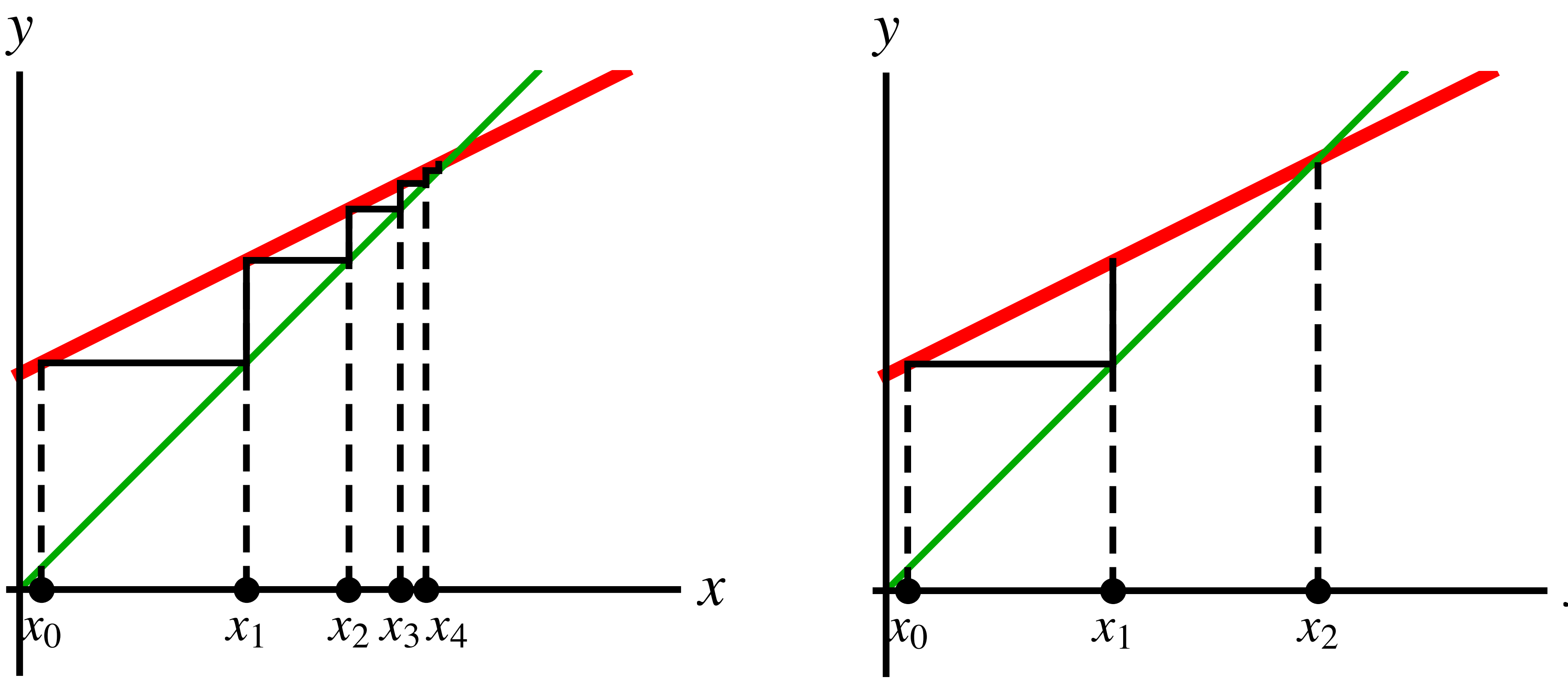
[Anderson (1965); Walker and Ni (2011): equivalence to GMRES]

Fixed-point

$$x_{n+1} = g(x_n)$$

Anderson

$$x_{n+1} = w_1\, g(x_n) + \cdots + w_k\, g(x_{n-k+1})$$



For calculating 1 lasing mode in 2D:

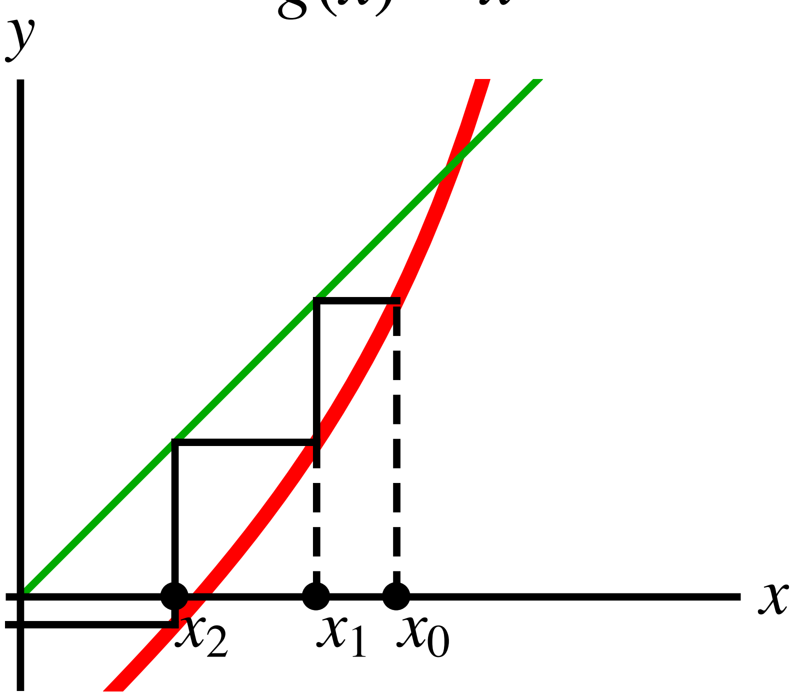
n **∼100**

n **≈ 2–3**

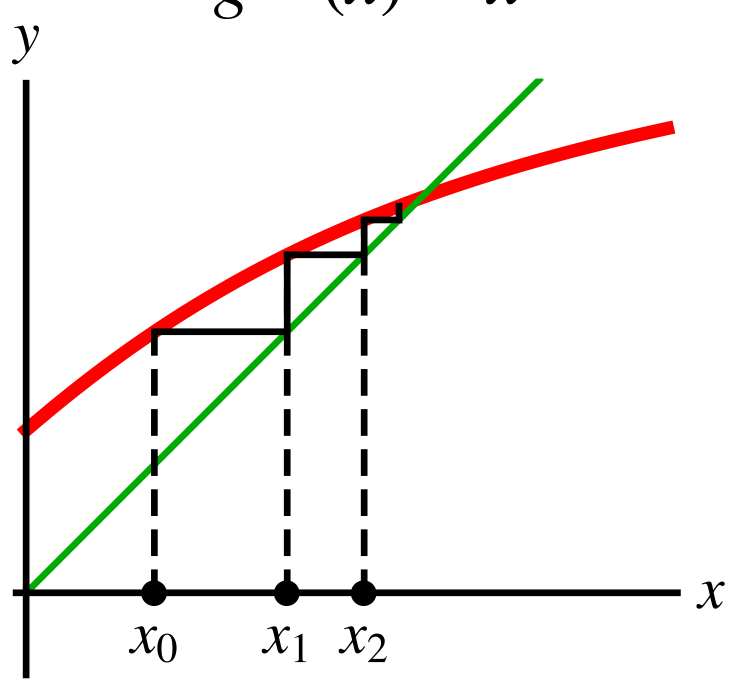
Infinitely many fixed-point formulations!

$$f(x) = 0 \implies g(x) \equiv f(x) + x = x$$
$$\implies x = g^{-1}(x)$$

$g(x) = x$



$g^{-1}(x) = x$



1. We re-formulated SALT in converging fixed-point form.
2. Inversion performed by any Maxwell solver!

E-field iteration (a bit technical…)

notation:
E = ψ

$$f(\psi,\omega,a) = \left[-\nabla\times\nabla\times \quad +\omega^2\left(\varepsilon_c + \gamma(\omega)\ \frac{D_0}{1+a^2\ |\psi|^2}\right)\right]\psi$$

$$= A(\psi,\omega,a)\ \psi$$

$$0 = f + \Delta f$$

$$= f + \cancel{(\partial_\psi f)\ \Delta\psi} + (\partial_\omega f)\ \Delta\omega + (\partial_a f)\ \Delta a$$

$$= f + \boxed{\Delta_\psi f} + (\partial_\omega f)\ \Delta\omega + (\partial_a f)\ \Delta a$$

Apply "implicit Newton step" : $\Delta_\psi f = A(\psi)\ \Delta\psi + \psi\ B(\psi,\Delta\psi)$

$$= f + [A(\psi)\ \Delta\psi + B(\psi,\Delta\psi)\ \psi] + (\partial_\omega f)\ \Delta\omega + (\partial_a f)\ \Delta a$$

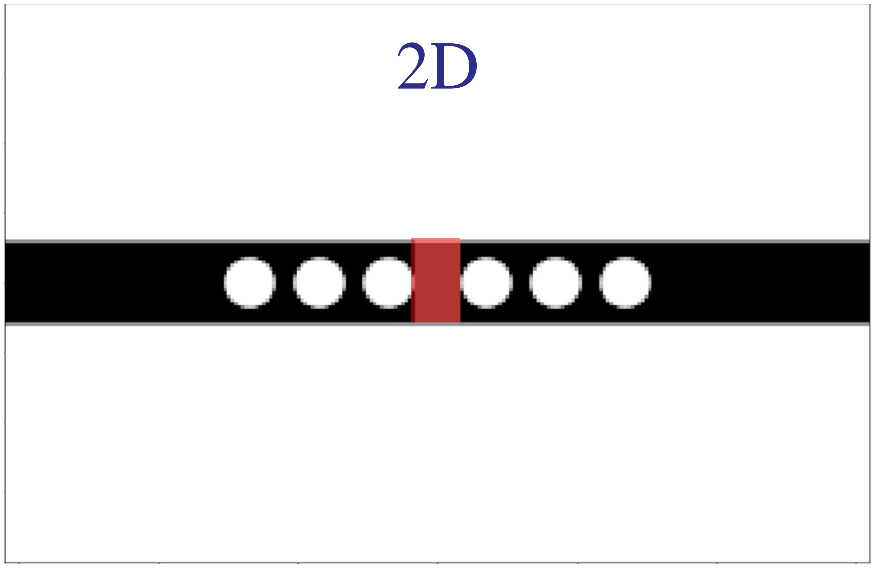
Want to find $\Delta\psi$, $\Delta\omega$, Δa satisfying this equation (to use them to move ψ, ω, a).

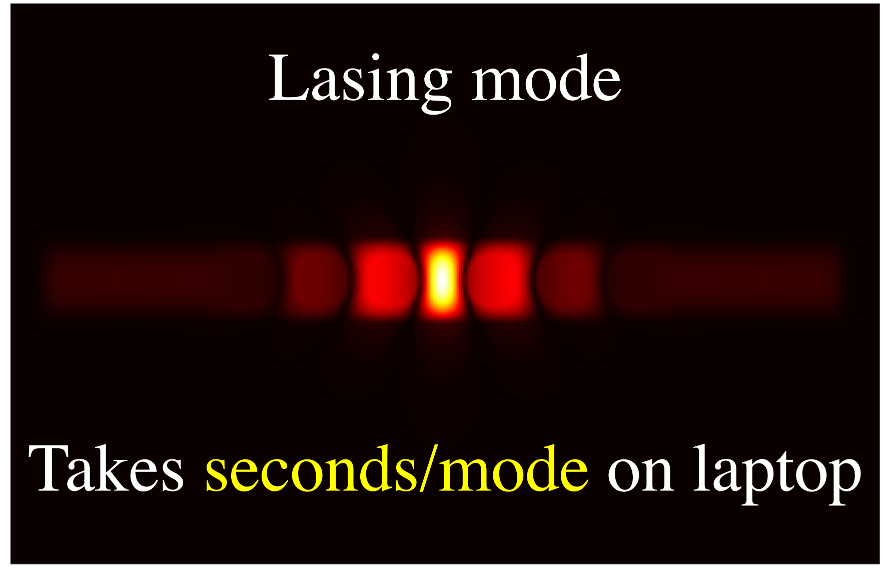
$\Rightarrow$ Solve eq. for $\Delta\psi$ using fixed-point iteration:

$$\Delta\psi = -\boxed{A(\psi)}^{-1}\ [f + B(\psi,\Delta\psi)\ \psi + (\partial_\omega f)\ \Delta\omega + (\partial_a f)\ \Delta a]$$

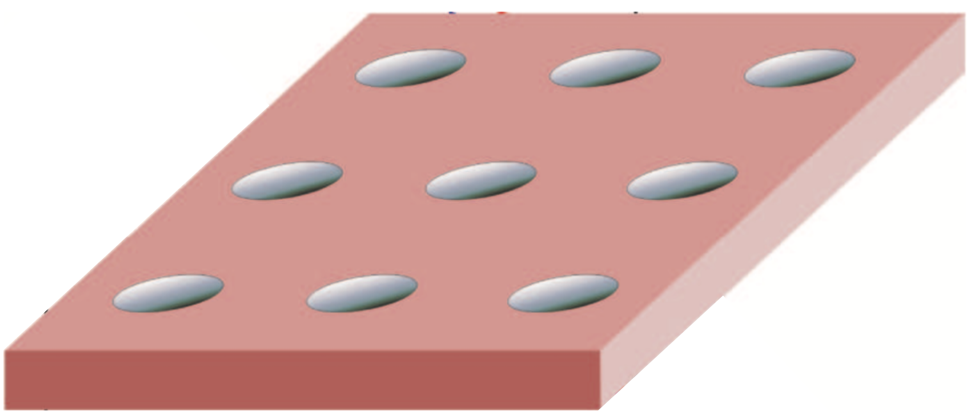
Maxwell operator → Any Maxwell solver can be used!
(FEM, BEM, spectral method, …)

Example Results

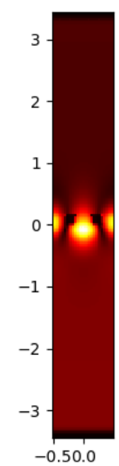




3D



Lasing mode



Takes mins/mode on laptop

Many, many other "weird" ways to use existing Maxwell solvers…

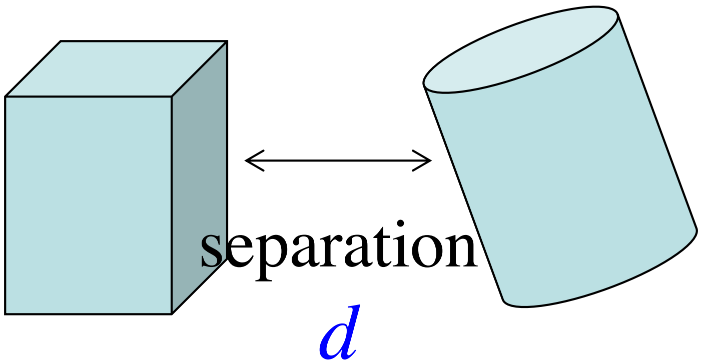
Sometimes they don't even involve solving Mx=b

discretized
Maxwell matrix
(FD, FEM, BEM…)

EM
fields

current
sources

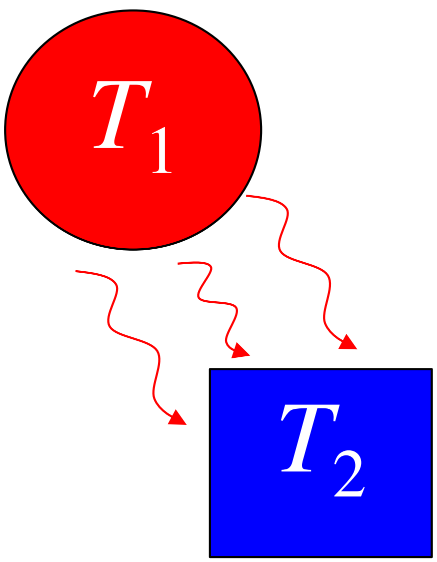
Casimir forces and heat transfer w/"standard" ω-domain matrix M



force in d direction =

$$-\frac{\hbar}{2\pi}\int_0^\infty \mathrm{tr}\left[M^{-1}\frac{\partial M}{\partial d}\right]d\omega$$

[BEM matrix M: Reid et al. (2011, 2014)
FDFD matrix M: Milton (2008)]



flux(ω) =

$$\|\mathrm{M}^{-1}\|_W \cdot (\text{planck spectrum})$$

[Rodriguez, Reid, SGJ (2012)]

… several linear-algebra algorithms to compute such matrix functions using ~few solves

finis

The interesting parts of computational science are not just coding or refinements to discretization schemes & solvers, but also include analytical transformations to turn intractable problems tractable, or extract new info from old code.