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

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

Lord Rayleigh
Development of Classical EM Computations

1. Analytical solutions

2. Semi-analytical solutions: series expansions

   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 inhomogeneous space
     (e.g. Fourier series, Chebyshev polynomials, …)
     & plug into PDE and solve for coefficients
Development of Classical EM Computations

1. **Analytical solutions**

   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, …

2. **Semi-analytical solutions & spectral methods**

   **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

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 $\sim e^{-i\omega t}$ ($J = 0$)
  - frequency-domain response: $E, H$ from $J(x)e^{-i\omega t}$
  - time-domain response: $E, H$ from $J(x, t)$
  - PDE or integral equation?

• What discretization?
  - finite differences (FD)
  - finite elements (FEM) / boundary elements (BEM)
  - spectral / Fourier
  - infinitely many unknowns
  - finitely many unknowns
  - …

• 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

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Understanding Photonic Devices

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 \( \sim e^{-i\omega t} \)

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

First task: get rid of this mess

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

\[
\nabla \times -\nabla \times \vec{H} = \omega^2 \vec{H}
\]

(eigen-operator) (Hermitian for lossless/real \( \varepsilon \! \)!) (eigen-value) (eigen-field)
Building Blocks: Periodic Media

homogeneous media

common thread: translational symmetry

discrete periodicity: photonic crystals

periodic in one direction
periodic in two directions
periodic in three directions
Periodic Hermitian Eigenproblems

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

\[ \mathbf{H}(\mathbf{x}, t) = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \mathbf{H}_{\mathbf{k}}(\mathbf{x}) \]

planewave
periodic “envelope”

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

Corollary 2: \( \mathbf{H}_{\mathbf{k}} \) given by finite unit cell, so \( \omega \) are discrete \( \omega_n(\mathbf{k}) \)
Electronic and Photonic Crystals

atoms in diamond structure

dielectric spheres, diamond lattice

Periodic Medium

Bloch waves:

Band Diagram

electron energy

wavevector

strongly interacting fermions

weakly-interacting bosons

… many design degrees of freedom

photon frequency

wavevector

Photonic Band Gap
Solving the Maxwell Eigenproblem

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

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

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

Finite cell \( \Rightarrow \) discrete eigenvalues \( \omega_n \)

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

\[ 1 \] Limit range of \( \mathbf{k} \): irreducible Brillouin zone

\[ 2 \] Limit degrees of freedom: expand \( \mathbf{H} \) in finite basis

\[ 3 \] Efficiently solve eigenproblem: iterative methods
Solving the Maxwell Eigenproblem: 1

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

   — Bloch’s theorem: solutions are periodic in $\mathbf{k}$

   first Brillouin zone

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

   irreducible Brillouin zone: reduced by symmetry

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

3. Efficiently solve eigenproblem: iterative methods
Solving the Maxwell Eigenproblem: 2a

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

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

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

finite matrix problem: \[ \mathbf{A}\mathbf{h} = \omega^2 \mathbf{B}\mathbf{h} \]

inner product: \[ \langle \mathbf{f} | \mathbf{g} \rangle = \int \mathbf{f}^* \cdot \mathbf{g} \]

Galerkin method:

\[
A_{ml} = \langle \mathbf{b}_m | \hat{\mathbf{A}} | \mathbf{b}_l \rangle \quad B_{ml} = \langle \mathbf{b}_m | \mathbf{b}_l \rangle
\]

3. Efficiently solve eigenproblem: iterative methods
Solving the Maxwell Eigenproblem: 2b

1. Limit range of \( k \): irreducible Brillouin zone

2. Limit degrees of freedom: expand \( H \) in finite basis
   — must satisfy constraint: \((\nabla + ik) \cdot H = 0\)

Planewave (FFT) basis

\[
H(x_t) = \sum_G H_G e^{iG \cdot x_t}
\]

constraint: \( H_G \cdot (G + k) = 0 \)

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

Finite-element basis

constraint, boundary conditions:

Nédélec elements


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

3. Efficiently solve eigenproblem: iterative methods

[ figure: Peyrilloux et al., J. Lightwave Tech. 21, 536 (2003) ]
Solving the Maxwell Eigenproblem: 3a

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

$$Ah = \omega^2 Bh$$

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

Faster way:
— start with initial guess eigenvector $h_0$
— iteratively improve
— $O(Np)$ storage, $\sim O(Np^2)$ 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 $\omega_0$ minimizes:

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

minimize by preconditioned conjugate-gradient (or…)
Band Diagram of 2d Model System
(radius 0.2a rods, ε=12)

irreducible Brillouin zone

\[ \vec{k} \]

\[ \omega (2\pi c/a) = a/\lambda \]

Photonic Band Gap

gap for \( n > \sim 1.75:1 \)
The Iteration Scheme is *Important* (minimizing function of $10^4$–$10^8$+ variables!)

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

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

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

— $d$ is $\nabla f$ + (stuff): *conjugate* to previous search dirs

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

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

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

— $d$ is (approximate $A^{-1}$) $[\nabla f + (\text{stuff})]$
The Iteration Scheme is *Important*
(minimizing function of ~40,000 variables)
The Boundary Conditions are Tricky

\[ \mathbf{E}_\parallel \text{ is continuous} \]

\[ \mathbf{E}_\perp \text{ is discontinuous} \]

\[ (\mathbf{D}_\perp = \varepsilon \mathbf{E}_\perp \text{ is continuous}) \]

Use a tensor \( \varepsilon \): 

\[
\begin{pmatrix}
\langle \varepsilon \rangle \\
\langle \varepsilon \rangle
\end{pmatrix}
\begin{pmatrix}
\mathbf{E}_\parallel \\
\mathbf{E}_\perp
\end{pmatrix}
\]

[ Meade et al. (1993) ]
The $\varepsilon$-averaging is **Important**

Correct averaging changes *order* of convergence from $\Delta x$ to $\Delta x^2$

Reason in a nutshell:

- Averaging = smoothing $\varepsilon$
- ...must pick smoothing with zero 1st-order perturbation

[Farjadmour et al. (2006)]
Closely related to anisotropic metamaterial, e.g. multilayer film in large-\(\lambda\) 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 \(E\):

\[ E_{\parallel} \text{ continuous } \Rightarrow \varepsilon_{\parallel} = \langle \varepsilon \rangle \]

\[ D_{\perp} = \varepsilon E_{\perp} \text{ continuous } \Rightarrow \varepsilon_{\perp} = \langle \varepsilon^{-1} \rangle^{-1} \]
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)
any state in the gap cannot couple to bulk crystal $\rightarrow$ localized
to be continued…

Further reading:


Bloch-mode eigensolver: [http://jdj.mit.edu/mpb](http://jdj.mit.edu/mpb)
Computational Nanophotonics: Cavities and Resonant Devices

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Resonance

an oscillating mode trapped for a long time in some volume (of light, sound, …)

frequency $\omega_0$

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

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

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

modal volume $V$

[ Notomi et al. (2005). ]

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


[ 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, …)

frequency $\omega_0$

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

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

energy in cavity $\sim e^{-\omega_0t/Q}$

modal volume $V$

$\sim$ volume where residue is large

near $\omega_0$, Green’s function is dominated by

collection of the pole $\sim$ a “resonant mode” profile

simple pole

at $\omega_0 - i/\tau$

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

response to a narrowband pulse

$\sim$ 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 $\omega$

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

$\Rightarrow$ electric “dyadic” Green’s function $G_{\omega}(x, y) = [E^{(1)} \ E^{(2)} \ E^{(3)}]$

... any electric current $J(x)e^{-i\omega t}$ then gives the “convolution” $E(x) = G_{\omega} \ast J = \int G_{\omega}(x, y)J(y)d^3y$

At eigenvalue/resonance frequency $\omega_0$ ($\nabla \times \mu^{-1} \nabla \times E_0 = \omega_0^2 \varepsilon E_0$), the operator $(\nabla \times \mu^{-1} \nabla \times -\omega_0^2 \varepsilon)$ becomes singular.

$G_{\omega}$ blows up = “pole” at $\omega_0^2$

Similarly, 6×6 Green’s function $\Gamma_{\omega}(x, y)$ gives

$$\begin{bmatrix} E \\ H \end{bmatrix} = \psi$$

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

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

- Best methods compute lowest-$\omega$ eigenvals, but $N^d$ supercells have $N^d$ modes below the cavity mode — expensive

- Best methods are for Hermitian operators, but losses requires non-Hermitian
Time-Domain Eigensolvers
(finite-difference time-domain = FDTD)

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

• Excite with broad-spectrum dipole (↑) source

Response is many sharp peaks, one peak per mode

complex $\omega_n$


decay rate in time gives loss

tricky signal processing

$\Delta \omega$
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.

\[
\nabla \times E = -\frac{\partial B}{\partial t} \quad \nabla \times H = \frac{\partial D}{\partial t} + J
\]

\[
D = \varepsilon E \quad B = \mu H
\]

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=ε⁻¹D

\[
\begin{align*}
E_x &= \frac{\Delta t}{\varepsilon \Delta y} \left( H_z^{j+0.5} - H_z^{j-0.5} \right) \\
E_y &= \frac{\Delta t}{\varepsilon \Delta x} \left( H_z^{i+0.5} - H_z^{i-0.5} \right)
\end{align*}
\]

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

\[
\begin{align*}
H_z &= \frac{\Delta t}{\mu} \left( \frac{E_x^{j+1} - E_x^j}{\Delta y} + \frac{E_y^i - E_y^{i+1}}{\Delta x} \right)
\end{align*}
\]

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 $\omega > 0$.

$$\text{fields } \sim f(y,z)e^{i(kx-\omega t)}$$  \hspace{1cm} (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

$$\tilde{x} = x + \frac{i\sigma}{\omega} x$$

unchanged (no reflection)

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 \( x \).

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

(allow \( x \)-dependent PML strength \( \sigma \))

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

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

nondispersive materials: \( k/\omega \sim \text{constant} \)

so decay rate independent of \( \omega \)
(at a given incidence angle)
PML Step 3: Effective materials

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

\[
\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E} + \mathbf{J},
\]

coordinate transformations are equivalent to transformed materials.

\[
\begin{align*}
\{\varepsilon, \mu\} &\rightarrow \frac{J\{\varepsilon, \mu\}J^T}{\det J} \\
\end{align*}
\]

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

\[
\frac{\partial x}{\partial \tilde{x}}
\]

\[
\begin{pmatrix}
\{\varepsilon, \mu\} &\rightarrow \{\varepsilon, \mu\} \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
(1 + i\sigma / \omega)^{-1} & 1 + i\sigma / \omega \\
1 + i\sigma / \omega & 1 + i\sigma / \omega
\end{pmatrix}
\]

for isotropic starting materials:

PML = effective anisotropic “absorbing” $\varepsilon$, $\mu$
Photonic-crystal PML?

FDTD (Meep) simulation:

\[ \varepsilon \text{ not even continuous in } x \text{ direction, much less analytic!} \]

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) ]


... & 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 $\varepsilon$ reflection doesn’t $\to 0$ as $\Delta x \to 0$

… similar to non-PML scalar $\sigma$

in uniform $\varepsilon=1$ medium, PML reflection $\to 0$ for exact wave equation
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 $\rightarrow 0$!

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

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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)

\[ f^+ + f^- = 0 \]

equivalent currents

want to construct surface currents

\[ c = \begin{pmatrix} J \\ K \end{pmatrix} \]

giving same \( f^+ \) in \( \Omega \)

do simulations in finite domain + inhomogeneities / interactions

= scattered field \( f^- \)

known incident fields

\[ f^+ = \begin{pmatrix} E \\ H \end{pmatrix} \]

in ambient medium

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

[ review article: arXiv:1301.5366 ]
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: \[ f^+ = \begin{pmatrix} E \\ H \end{pmatrix} \]

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

\[
\begin{pmatrix}
\nabla \times \\
-\nabla \times 
\end{pmatrix} f^+ = -i\omega\chi f^+
\]
constructing solution in $\Omega$

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

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

"electric" current

"magnetic" current

$$= -i\omega \chi f + c$$
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 $\omega$, so injecting a pulse $p(t)$ requires a convolution with $\hat{c}(x,\omega)$

\[
\text{currents}(x,t) = p(t) * c(x,t) \approx p(t) \hat{c}(x,\omega)
\]

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

– specialized methods are known for planewave sources (have numerical dispersion!)
Shortcut: Subtract two simulations

equation: 90° bend of single-mode dielectric waveguide

simple constant-amplitude line-current $\mathbf{J}$

accumulate (discrete-time) Fourier transforms of fields:

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

at desired frequencies $\omega$

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

- incident: Poynting flux of $\hat{f}^2_{\text{straight}}$
- transmitted: flux of $\hat{f}^2_{\text{bend}}$
- reflected: flux of $\hat{f}^1_{\text{bend}} - \hat{f}^1_{\text{straight}}$
Shortcut: Subtract two simulations

example: $90^\circ$ bend of single-mode dielectric waveguide
Shortcut: Planewave sources for periodic media

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

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

[ review article: arXiv:1301.5366 ]
Reflection spectra example for periodic media

*(Fano resonance lineshapes)*

**note:** \( \omega \) all above light line
(req. for incident planewave)

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

\[
\frac{\omega}{c} \sin(\theta) = k_x
\]
\( \Leftrightarrow \) curved line

\( \theta = \text{asin}(ck_x/\omega) \)
in \((\omega, \theta)\) 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

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

\[ \Rightarrow \text{ current density} \]

\[ J_x = qv\delta(x - vt) \]

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

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

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 
\[ v = \frac{\omega(k_x,k_y)}{(k_x + 2\pi m/a)} \]
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* ]


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

same incident fields $f^{0+}$

same fields $f^{0-}$

modified Maxwell PDE:

$$
\begin{pmatrix}
  \nabla \times \\
  \nabla \times 
\end{pmatrix} f = -i \omega \chi f + \delta(\partial \Omega) \begin{pmatrix}
  -n \times H^0 \\
  n \times E^0
\end{pmatrix} = -i \omega \chi f + c
$$

“equivalent” 6-component surface currents

medium 0

$c$

$n$

medium 0

$f=0$ (!!)
The Principle of Equivalence I

incident fields $f^{0+}$

medium 0

same scattered fields $f^{0-}$ of $c$

medium 0

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

convolution with $6 \times 6$ Green’s function $\Gamma^0$ of homogenous medium 0

[e.g. Harrington, Time-Harmonic Electromagnetic Fields]
The Principle of Equivalence II

\[ f_1 = -\Gamma^1 \ast \mathbf{c} \]

opposite-sign 6-component surface currents

medium 1

\[ f = 0 \]

convolution with 6x6 Green's function \( \Gamma^1 \) of homogenous medium 1

[e.g. Harrington, *Time-Harmonic Electromagnetic Fields*]
Surface-Integral Equations (SIE)

\[ f^0 = f^{0+} + \Gamma^0 \ast c \]

\[ f^1 = -\Gamma^1 \ast c \]

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

\[ \left( \Gamma^0 + \Gamma^1 \right) \ast c \bigg|_{\text{tangential}} = -f^{0+} \bigg|_{\text{tangential}} \]

[ e.g. Harrington, *Time-Harmonic Electromagnetic Fields* ]
Discretizing the Maxwell SIE

\[(\Gamma^0 + \Gamma^1) \times c \bigg|_{\text{tangential}} = -f^{0+} \bigg|_{\text{tangential}}\]

pick some basis \(b_n\) \((n=1, \ldots, N \to \infty)\) for surface-tangential vector fields

\[c = \sum_n x_n b_n \quad \text{\(N\) discrete unknowns \(x_n\)} \implies N \text{ equations}\]

[ e.g. Harrington, *Time-Harmonic Electromagnetic Fields* ]
Discretizing the Maxwell SIE

Galerkin method — require error \perp basis:

\[ \left\langle b_m \left| \left( \Gamma^0 + \Gamma^1 \right) \ast \left( \sum_n x_n b_n \right) \right\rangle = \left\langle b_m \right| -f^{0+} \right\rangle \]

pick some basis \( b_n \) (\( n=1, \ldots, N \rightarrow \infty \)) for surface-tangential vector fields

\( c = \sum_n x_n b_n \)  
\( N \) discrete unknowns \( x_n \)  
\( \Rightarrow N \) equations \( Mx = s \)

\[ M_{mn} = \left\langle b_m \left| \left( \Gamma^0 + \Gamma^1 \right) \ast b_n \right\rangle = G_{mn}^0 + G_{mn}^1 \]

\[ s_m = \left\langle b_m \right| -f^{0+} \right\rangle \]

[ e.g. Harrington, *Time-Harmonic Electromagnetic Fields* ]
Discretized SIE: Two Objects

\[
c^2 = \sum_n x^2_n b^2_n
\]

\[
c^1 = \sum_n x^1_n b^1_n
\]

\[M = G^0 + \begin{pmatrix} G^1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \end{pmatrix}
\]

\[\Rightarrow \text{linear equations } Mx = s\]

\[\cdots + \text{straightforward generalizations to more objects, nested objects, etcetera}\]
SIE basis choices

- Can use *any* basis for $c = \text{any basis of surface functions}$
  … 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 $b_n$ defined on *pairs of adjacent triangles* via degree-1 polynomials
BEM strengths
especially small surface areas in a large (many-\(\lambda\)) volume, e.g.:

**surface plasmons** (metals): extremely sub-\(\lambda\) fields

**complex impedance**
of passive structures

silver nanotip

[ Johannes Feist, Harvard ]

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

[ Llatser et al. (2012) ]
The bad news of BEM

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

- BEM system matrix $M_{mn} = \langle b_m | (\Gamma^0 + \Gamma^1) * b_n \rangle = G^0_{mn} + G^1_{mn}$

  - *singular integrals* for overlapping $b_m, b_n$
    …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 $\Gamma$
    (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)

[https://github.com/HomerReid/scuff-em]
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
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 \( M \) and RHS vector \( v \).**
   
   SCUFF-EM does this.

3. **Solve the linear system \( Mk = v \) for the surface currents \( k \).**
   
   SCUFF-EM uses LAPACK for this.

4. **Post-process to compute scattered fields \( \{E, H\}^{\text{scat}} \) from \( k \).**
   
   SCUFF-EM does this.

Innovations unique to SCUFF-EM:

- Bypass step 4: Compute scattered/absorbed power, force, and torque directly from \( k \)
- Bypass steps 3 and 4: Compute Casimir forces and heat transfer directly from \( M \)
Geometries in SCUFF

A gold sphere and a displaced and rotated SiO2 tetrahedron:

The geometry:

The .scuffgeo file:

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

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

⇒ Handle displacements and rotations without re-meshing.
Geometries in SCUFF

(discretization of SIE at junctions of 3+ materials is a bit tricky)
Periodic geometries in SCUFF

(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 $\mathbf{c}$, 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 $\mathbf{c}$ ($\sim \mathbf{n} \times$ surface fields). Examples:

- **Scattering matrices** (e.g. spherical-harmonic waves in $\rightarrow$ out): obtain directly from multipole moments of “currents”
- Any **bilinear function** of the surface fields can be computed directly from bilinear functions of $\mathbf{c}$:
  - 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 $\omega$ where this system is singular, i.e. the nonlinear eigenproblem

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

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

- 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](http://jdj.mit.edu/meep)

Free BEM software:


Review on wave sources:

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.
Outline

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• Some more detailed photonics examples.
Optical design = optimization

traditional approach: intuition + “tweaking” few parameters

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

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

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

[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


Solar-cell backreflector optimization

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

2d band gaps

OE 12, 5916 (2004)

Dobson (1999)
Topography 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) $\varepsilon$ (susceptibility $\chi = \varepsilon - 1$)
Discretizing Topology Optimization
for computer, need finite-dimensional, differentiable parameters

some computational grid

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

… or …

“Density-based topology optim.”
Continuous relaxation: material varies in \([A,B]\) at each pixel

e.g. in electromagnetism, let \( \varepsilon \) at each pixel vary in \([A,B]\).
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A general optimization problem

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

subject to \( m \) constraints
\[ f_i(x) \leq 0 \quad i = 1, 2, \ldots, m \]

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)

\( x \) is a feasible point if it satisfies all the constraints

feasible region = set of all feasible \( x \)
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
\[
f_i(x) \leq 0 \quad i = 1, 2, \ldots, m
\]

For \(n \geq 1000\)’s of parameters, impractical unless you have
\[
\nabla_x f_i(x) \quad i = 0, 1, 2, \ldots, m
\]
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

incident wave \[
\text{field } E_0
\]

scattered field

"forward" solve

scattered field + perturbation $\Delta E$

= field of $J = \Delta \varepsilon E_0$

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 $\Delta E$ = field of $J = \Delta \varepsilon E_0$

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

(source at scattered measurement point) solve one adjoint problem … get fields at all perturbed pixels
Adjoint methods, in math

cost of $\nabla f \sim$ 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 ]

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 = Q e = $ 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−iωt}

In the gap, crystal is "optical insulator" that can trap light.
Maximizing photonic band gap over all periodic structures?

we want: 

\[
\max_{\varepsilon} \left( 2 \left[ \min_k \omega_{n+1}(k) \right] - \left[ \max_k \omega_n(k) \right] \right) - \left[ \min_k \omega_{n+1}(k) \right] + \left[ \max_k \omega_n(k) \right]
\]

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:

\[
f_1 \geq \omega_n(k) \quad \text{for } k \in \mathcal{K}
\]

\[
f_2 \leq \omega_{n+1}(k)
\]

...with

(mostly?) differentiable nonlinear constraints:
Optimizing 1st TM and TE gaps for a triangular lattice with 6-fold symmetry (between bands 1 & 2)

48.3% TM gap ($\varepsilon = 12:1$)  
51.4% TE gap ($\varepsilon = 12:1$)

30 iterations of optimizer
Optimizing 1st complete (TE+TM) 2d gap

21.1% gap ($\varepsilon = 12:1$)

20.7% gap ($\varepsilon = 12:1$)
+ 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 ]

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

(e) FCC8 (no. 225)
“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.
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3d Microcavity Design Problem

Want some 2d pattern that will **confine light in 3d** with **maximal lifetime** ("$Q_{\text{rad}}$") and **minimal modal volume** ("$V$")

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

[ Song, (2005) ]
[ Loncar, 2002 ]
[ Akahane, 2003 ]

("defects" in periodic structures)
Resonances = complex $\omega \sim$ frequency - $i$ loss


resonances = poles in scattering
= poles in Green’s function
= singular Maxwell operator $M(\omega)$

$$\nabla \times \nabla \times -\omega^2 \varepsilon \)E = i\omega J = 0$$

$M(\omega)$ singular at resonance $\omega$
Optimize resonances?

Challenges:

Which eigenvalue?

Interior eigenvalue of big non-Hermitian...

Tracking eigenvalue (no discontin. jumps!)
Optimize resolvent instead

maximize
$\text{Re} \psi^* M(\omega_0)^{-1} \psi$

instead for some $\psi$

$= \text{Re} f(\omega)$

... many key physical quantities in this form!

$= \text{total power expended by a source or incident wave } \psi$

[ 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)

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

Naively, should we maximize \( Q/V \) or LDOS?

😊 Trivial design problem: maximum \( Q/V = \infty \)
\[ \text{[ for lossless materials,} \]
\[ \text{e.g. perfect ring resonator of } \infty \text{ radius] } \]

Real design problem: maximize LDOS
\[ \text{averaged over desired bandwidth } \omega_0 \pm \Gamma_0 \]
\[ \text{[ Liang & Johnson (2013)]} \]
LDOS: Local Density of States

[ review: arXiv:1301.5366 ]

Maxwell eigenproblem:

\[
\frac{1}{\varepsilon} \nabla \times \frac{1}{\mu} \nabla \times E \equiv \Theta E = \omega^2 E
\]

\[
\langle E, E' \rangle = \int E^* \cdot \varepsilon E'
\]

Power radiated by a current \( \mathbf{J} \) (Poynting’s theorem)

\[
P = -\frac{1}{2} \text{Re} \int E^* \cdot \mathbf{J} \, d^3x = -\frac{1}{2} \text{Re} \langle E, \varepsilon^{-1} \mathbf{J} \rangle
\]

special case of a dipole source: LDOS

\[
\mathbf{J}(x) = e_\ell \delta(x - x_0)
\]

\[
\text{LDOS}_\ell(x_0, \omega) = \frac{4}{\pi} \varepsilon(x_0) P_\ell(x_0, \omega)
\]
Why a “density of states”

[ review: arXiv:1301.5366 ]

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

\[ \langle E, E' \rangle = \int E \cdot \varepsilon E' \]

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

loss \( \rightarrow 0 \): a localized measure of spectral density

\[ LDOS_\ell(x, \omega) = \sum_n \delta(\omega - \omega^{(n)}) \varepsilon(x) |E^{(n)}_\ell(x)|^2 \]

\[ \text{DOS}(\omega) = \sum_n \delta(\omega - \omega^{(n)}) \]
Complex target $\omega_0 = \text{Frequency average}$

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

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

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

via contour integration

Get entire $\omega$ average with a single “unphysical” complex-$\omega$ solve!

Complex $\omega = \omega$ 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 $\omega$

= much nicer integral over $\text{Im}\ \omega$

[ 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 $\sim 1/diameter$ [ Hashemi (2010) ]
Maximizing LDOS for random in-plane $\mathbf{J}$

$$= \max [\text{LDOS}(\omega, J_x) + \text{LDOS}(\omega, J_y)]/2$$

Spontaneous symmetry breaking! “Picks” one polarization randomly
3d results: Photonic-crystal slab


Optimize with $Q_0=10^4$

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

Next: 2d pattern in 3d slab

(including radiation loss via PML absorbing boundaries)
3d Slab Results
[X. Liang & S. G. Johnson (2013).]

after deleting “hairs”:
\[ Q \sim 10,000 \]
(without re-optimizing)

\[ Q \sim 30,000, \ V \sim 0.06(\lambda/n)^3 \]

vs. hand-optimized:
\[ Q \sim 100,000, \ V \sim 0.7(\lambda/n)^3 \]
\[ Q \sim 300,000, \ V \sim 0.2(\lambda/n)^3 \]

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

(a) $t/a = 4.273$  (b) $t/a = 7$  (c) $t/a = 11$

(d) $t/a = 15$  (e) $t/a = 15$
Intra-cavity 2$^{\text{nd}}$-harmonic generation

[ Rodriguez et al, 2007 ]

\[ \chi^{(2)} \]

nonlinearity

\[ \omega_1, \omega_2 = 2\omega_1 \]

cavity

input/output channel

theory: 100% conversion at critical input power

\[ P_{\text{out}} / P_{\text{in}} \text{ at } \omega_1 \]

… tricky part is designing cavity with simultaneous, spatially overlapping resonances at $\omega_1$ & $\omega_2$
Hand-design SHG cavity

[ Bi et al. (2012) ]

\[ \omega_1 \approx 2 \omega_1 \]

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

... months of hand-tuning to find compatible resonance modes
key idea:

source $J_1$ at $\omega_1$

$\Rightarrow E_1$

$\Rightarrow J_2 \sim \chi^{(2)} E_1^2$

$\Rightarrow E_2$

$\Rightarrow$ power at $\omega_2$

Maximizing SHG

= maximizing composition of two scattering problems.

\[
\max_{\tilde{\varepsilon}_a} \langle f(\tilde{\varepsilon}_a; \omega_1) \rangle = -\text{Re} \left[ \left\langle \int J_2^* \cdot E_2 \, dr \right\rangle \right],
\]

where

\[
M_1 E_1 = i\omega_1 J_1,
\]

\[
M_2 E_2 = i\omega_2 J_2, \quad \omega_2 = 2\omega_1
\]

\[
J_1 = \delta(\mathbf{r}_\alpha - \mathbf{r}_0)\hat{e}_j, \quad j \in \{x, y, z\}
\]

\[
J_2 = \tilde{\varepsilon}(\mathbf{r}_\alpha)E_{1j}^2\hat{e}_j,
\]

\[
M_l = \nabla \times \frac{1}{\mu} \nabla \times -\varepsilon_l(\mathbf{r}_\alpha)\omega_l^2, \quad l = 1, 2
\]

\[
\varepsilon_l(\mathbf{r}_\alpha) = \varepsilon_m + \tilde{\varepsilon}_\alpha(\varepsilon_{dl} - \varepsilon_m), \quad \tilde{\varepsilon}_\alpha \in [0, 1],
\]
SHG by “LDOS” optimization

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

gave factor of 10 increase in mode-overlap figure of merit vs. best hand design
Topology optimization for nonlinear frequency conversion

(figs courtesy Z. Lin)

extension to 3d

Surface-enhanced Raman Scattering


incident “pump” at $\omega$
emitted at $\omega - \Delta \omega$

resonant structures (metal particles)

[ 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


maximize output power

Raman molecule

every “pixel” in ??? Region is a design degree of freedom

Ag nanoparticle optimization steps:

$\lambda=532\text{nm}$

$200\text{nm}$

$20\text{nm}$
60 \times \text{better than typical resonators}


Very promising 2d results!

... 3d optimization currently running

optimized "bowtie" antenna
“Metasurface” optical devices:

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


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

incident light (planewave)

Focal spot = maximize $|\text{electric field } E|^2$

Complication: focus multiple incident $\lambda$ and/or angles simultaneously?
Why is it a hard problem?

- complex aperiodic pattern
- High material contrast
- Rapidly varying ($\lambda$), big

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 $l^2$ at focal spot → search $10^6$ parameters for best focus

Large-scale metasurface optimization by domain decomposition

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

- Subdivide surface into small ($\leq 10\lambda$) 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-$\omega$)

focal-spot intensity:
\[ f = \left| \int G_0(\mathbf{r}, \mathbf{r}') J_{\text{equiv}}(\mathbf{r}') d\mathbf{r}' \right|^2, \]
\[ J_{\text{equiv}} \sim E_\parallel \]

wavefront matching:
\[ f = \int |E - E_0|^2 d\mathbf{r} \]

Important Notes:
- You cannot optimize each cell individually. All the DOFs ($>10^6$) over the entire surface must be considered and updated together.
- No need to restrict oneself to sub-$\lambda$ domains; domain $>> \lambda$ tend to work better.
Few parameters per cell: *library* approach

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

- **Silica**
- **TiO₂**
- **Air**

if each cell has only a few parameters…

just precompute diffraction coefficients vs. parameters (in LPA)

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

optimized metalens

Monochromatic lens at an angle
(focal length = 15000 nm, wavelength = 532 nm, angle = 5 degrees)

few minutes on a laptop!
A small metalens optimization problem

Maximize the 0\textsuperscript{th}-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

(0th-order)

[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

44µm depth of focus, focal length 133µm
Topology Optimization for Metasurfaces
[ Lin et al. (2019) ]

Structural evolution of a large-area \((100 \times 100 \lambda^2)\) metalens during topology optimization \(\sim 10^6\) 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

Topography-optimization thrives in a large design space …

15 layers of
140 nm thick TiO$_2$
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.