Computational EM Overview

Steven G. Johnson
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

James Clerk Maxwell
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
  — …

• 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

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

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

First task: get rid of this mess

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

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

- eigen-operator
  (Hermitian for lossless/real \( \varepsilon \!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!}
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**:

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

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

**Corollary 2:** \( \bar{H}_{\bar{k}} \) 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

electro energy

wavevector

Electron Band Gap

Photon Band Gap

Strongly interacting fermions

Weakly-interacting bosons

… many design degrees of freedom
Solving the Maxwell Eigenproblem

Finite cell $\rightarrow$ discrete eigenvalues $\omega_n$

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

$$(\nabla + ik) \times \frac{1}{\varepsilon} (\nabla + ik) \times H_n = \frac{\omega_n^2}{c^2} H_n$$

constraint: $$(\nabla + ik) \cdot H_n = 0$$

where field = $H_n(x) e^{i(k \cdot x - \omega t)}$

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

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

   - Bloch’s theorem: solutions are periodic in \( \mathbf{k} \)

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

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

3. Efficiently solve eigenproblem: iterative methods

irreducible Brillouin zone: reduced by symmetry
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 ($N$)

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

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…)

variational / min–max theorem
Band Diagram of 2d Model System
(radius 0.2a rods, ε=12)

\[ \text{frequency } \Omega = \frac{a}{\lambda} \]

irreducible Brillouin zone

\[ \vec{k} \]

\[ \Gamma \quad X \quad M \quad \Gamma \]

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 $(h + \alpha d)$
— $d =$ (approximate $A^{-1}$) $\nabla f$  ~ Newton’s method

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

\[ E_{\parallel} \text{ is continuous} \]
\[ E_{\perp} \text{ is discontinuous} \]
\[ (D_{\perp} = \varepsilon E_{\perp} \text{ is continuous}) \]

Use a tensor \( \varepsilon \):

\[
\begin{pmatrix}
\langle \varepsilon \rangle \\
\langle \varepsilon \rangle \\
\langle \varepsilon^{-1} \rangle^{-1}
\end{pmatrix}
\begin{pmatrix}
E_{\parallel} \\
E_{\perp}
\end{pmatrix}
\]

[ 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 $\varepsilon$
- = 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-\(\lambda\) limit

\[ \mathbf{\varepsilon}_{ij}^{\text{eff}} = \frac{\langle D_i \rangle}{\langle E_j \rangle} = \frac{\langle \varepsilon E_i \rangle}{\langle E_j \rangle} = \frac{\langle D_i \rangle}{\langle \varepsilon^{-1} D_j \rangle} \]

Key to anisotropy is differing continuity conditions on \(\mathbf{E}\):

\( \mathbf{E}_\parallel\) continuous \(\Rightarrow\) \(\varepsilon_\parallel = \langle \varepsilon \rangle\)

\(\mathbf{D}_\perp = \varepsilon \mathbf{E}_\perp\) 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)
any state in the gap cannot couple to bulk crystal — 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

Steven G. Johnson
MIT Applied Mathematics
Resonance

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 \( Q = \frac{\omega_0 \tau}{2} \)

equality in cavity \( \sim e^{-\omega_0 t/Q} \)

modal volume \( V \)

\[ \omega_0 = 420 \text{ nm} \]

[ Notomi et al. (2005). ]

[ Schliesser et al., 
\textit{PRL} \textbf{97}, 243905 (2006) ]


[ C.-W. Wong, 
\textit{APL} \textbf{84}, 1242 (2004). ]
Resonance = Pole in Green’s Function

an oscillating mode trapped for a long time in some volume (of light, sound, …) lifetime \( \tau >> \frac{2\pi}{\omega_0} \)

frequency \( \omega_0 \)

quality factor \( Q = \frac{\omega_0 \tau}{2} \)

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

modal volume \( V \)

~ volume where residue is large

near \( \omega_0 \), Green’s function is dominated by contribution of the pole ~ a “resonant mode” profile

simple pole at \( \omega_0 - i / \tau \)

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

decay rate in time gives loss


tricky signal processing
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:

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

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

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 \(E=ε^{-1}D\)

\[
E_x^j + = \frac{Δt}{ε Δy} \left( H_z^{j+0.5} - H_z^{j-0.5} \right)
\]
\[
E_y^i - = \frac{Δt}{ε Δx} \left( H_z^{i+0.5} - H_z^{i-0.5} \right)
\]

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

\[
H_z^{j+0.5} - ε^{-1} \frac{Δt}{μ} \left( \frac{E_x^{j+1} - E_x^j}{Δy} + \frac{E_y^i - E_y^{i+1}}{Δx} \right)
\]

CFL/Von Neumann stability: \(cΔt < 1 / \sqrt{Δx^{-2}+Δy^{-2}}\)
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 \textit{artificially truncate space} for a computer simulation.

In a wave equation, a hard-wall \textit{truncation} gives reflection artifacts.

An old goal: \textit{“absorbing boundary condition” (ABC)} that absorbs outgoing waves.

\textbf{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 $\omega > 0$.

$$\text{fields } \sim f(y, z)e^{i(kx-\omega t)} \quad \text{(usually, } k > 0)$$

(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

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

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 $s$)

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

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: $k/\omega \sim$ 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 (Ward & Pendry, 1996: “transformational optics”)

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

for isotropic starting materials:

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

$\times$ PML Jacobian

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

FDTD (Meep) simulation:

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

\( \varepsilon \) not even continuous in \( x \) direction, much less analytic!
Photonic-crystal PMLs: **Magic?**

<table>
<thead>
<tr>
<th>PC waveguide</th>
<th>PC-based PML</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Waveguide Diagram" /></td>
<td><img src="image2.png" alt="PML Diagram" /></td>
</tr>
</tbody>
</table>

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

\[ \text{[Oskooi et al, Optics Express 16, 11376 (2008)]} \]

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

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
\[ f^+ = \begin{pmatrix} E \\ H \end{pmatrix} \]
in ambient medium
(possibly inhomogeneous, e.g. waveguide or photonic crystal)

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 \( f^- \)
The *Principle of Equivalence* in classical EM

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

(close connection to Schur complement [Kuchment])

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

[ review article: arXiv:1301.5366 ]
starting point: solution in all space

incident fields $f^+$

medium $\chi$

$\Omega$

6-component fields:

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

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

$$\left( \begin{array}{cc} \nabla \times & \nabla \times \\ -\nabla \times & \nabla \times \end{array} \right) f^+ = -i\omega \chi f^+$$
constructing solution in $\Omega$

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

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

$$
= -i\omega \chi f + c
$$
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 $\hat{c}(x,\omega) \leftrightarrow c(x,t)$

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

– 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

example: 90° bend of single-mode dielectric waveguide

simple constant-amplitude line-current $J$

accumulate (discrete-time) Fourier transforms of fields:

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

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° bend of single-mode dielectric waveguide

\[
\text{waveguide width} / \lambda
\]
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
(required for incident planewave)

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

$\iff$ curved line
$\theta = \text{asec}(ck_x/\omega)$
in $(\omega, \theta)$ plot
Fun possibilities in FDTD:

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

- **Doppler shift** from moving oscillating dipole
  - $v = 0.3c$

- **Cerenkov radiation** from **moving point charge** in dielectric medium
  - $v = 1.05 \frac{c}{n}$ (0.35 pixels/$\Delta t$)
Cerenkov radiation

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

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

for any integer $m$

⇒ no minimum $v$

[ Smith–Purcell effect ]

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

[ Luo, Ibanescu, Johnson, & Joannopoulos (Science, 2002) ]
Surface-integral equations (SIEs) and boundary-element methods (BEMs)

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


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 \textit{integral equation} for surface unknowns only.
The Principle of Equivalence in classical EM

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

incident fields $f^{0+}$

6-component fields:

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

Maxwell PDE:

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

…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:

$$\left( \begin{array}{cc} \nabla \times & \nabla \times \\ -\nabla \times & \end{array} \right) f = -i\omega \chi^0 f + \delta(\text{surface}) \left( \begin{array}{c} -n \times H \\ n \times E \\ c \end{array} \right)$$

$= -i\omega \chi^0 f + c$
The Principle of Equivalence I

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

incident fields \( f^{0+} \)

same scattered fields \( f^{0-} \) of \( c \)

"equivalent" 6-component surface currents

medium 0

\[ f=0 \ (!!) \]

medium 0

convolution with 6x6 Green’s function \( \Gamma^0 \) of homogenous medium 0

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

\[ \text{medium 1} \]

\[ f = 0 \]

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

*opposite-sign 6-component surface currents*

convolution with

6x6 Green’s function \( \Gamma^1 \)

of *homogenous* medium 1

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

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

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

\( \mathbf{c} \) determined by continuity of tangential fields at 0/1 interface:

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

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

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

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

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

Galerkin method — require error \( \perp \) basis:

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

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

\[
c = \sum_n x_n b_n \quad \Rightarrow \quad N \text{ discrete unknowns } x_n
\]

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

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

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

\[ c^2 = \sum_n x_n^2 b_n^2 \]

\[ c^1 = \sum_n x_n^1 b_n^1 \]

⇒ linear equations \( Mx = s \)

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

… + straightforward generalizations to more objects, nested objects, etcetera
SIE basis choices

• Can use *any* basis for $\mathbf{c} = \text{any basis of surface functions}$
  … 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 $\mathbf{b}_n$ 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

**silver nanotip**

[ Johannes Feist, Harvard ]

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

**complex impedance** of passive structures

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

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

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

  — 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)

SCUFF-EM

[ http://homerreid.ath.cx/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.

http://homerreid.com/scuff-EM

* to be released by end of October-ish
SCUFF usage outline

The steps involved in solving any BEM scattering problem:

1. **Mesh object surfaces into triangles.**
   Not done by SCUFF-EM; high-quality free meshing packages exist (e.g. GMSH).

2. **Assemble the BEM matrix $M$ 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

<table>
<thead>
<tr>
<th>Regions</th>
<th>Surfaces</th>
<th>.scuffgeo File</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exterior</td>
<td>UpperSurface</td>
<td>REGION Exterior MATERIAL Vacuum</td>
</tr>
<tr>
<td>UpperVolume</td>
<td>EquatorialPlane</td>
<td>REGION UpperVolume MATERIAL Gold</td>
</tr>
<tr>
<td>LowerVolume</td>
<td>LowerSurface</td>
<td>REGION LowerVolume MATERIAL Silicon</td>
</tr>
</tbody>
</table>

```
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

<table>
<thead>
<tr>
<th>Unit cell mesh</th>
<th>First 25 lattice cells</th>
</tr>
</thead>
</table>

**.scuffgeo file**

```plaintext
LATTICE
    VECTOR 0.75 0
    VECTOR 0 0.75
ENDLATTICE

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

(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 $\Gamma^*c$) one can obtain any desired fields, but…

It is much more efficient to compute as much as possible directly from $c$ ($\sim n \times$ 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 $c$:
  — scattered/absorbed power, force, torque, …
• Net effects of quantum/thermal fluctuations in matter can be computed from norm/det/trace of $M$ or $M^{-1}$:
  — thermal radiation, Casimir (van der Waals) forces, …
Resonant modes (and eigenvalues)

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

\[
\text{det } M(\omega) = 0
\]

For passive (\( \Rightarrow \) 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
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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Topology optimization

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

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

• Not uncommon for optimum to yield $A$ or $B$ almost everywhere
• Possible to add “penalty” to objective for intermediate values
Discretizing Topology Optimization

for computer, need finite-dimensional parameter space

some computational grid

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

…or…

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

e.g. in electromagnetism, let $\varepsilon$ at each pixel vary in $[A,B]$. 
Dobson et al. (Texas A&M)

TM gap, bands 3 & 4

TM bands 6 & 7


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

(square lattices only)

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

optimize TM localization in supercell


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


bend optimization


OE 12, 5916 (2004)

T-junctions
*JOSA B* 22, 1191 (2005)

low-index (scalar approx.)
dispersion-compensating fibers
*JOSA B* 25, 88 (2008)
Dispersion optimization
Sigmund, Jensen, Pederson et al. [www.topopt.dtu.dk]

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

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

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

...also band gaps for 2d (scalar) phononic crystals...
Kao, Osher, and Yablonovitch
2d TM and TE square-lattice gaps via level sets


TM gap,
bands 6 & 7

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

TE gap,
bands 5 & 6
Frei et al. (UIUC)

2d TM “directional” emission
via level-set method

via topology optimization
APL 86, 111114 (2005)

optimizing 3d $Q$
(level-set + MMA)
Other Topology Optimizers

2d TM bend

“2d” (really 1d) TE filter

2d TM gap ($\Delta w$) bands 3 & 4
He et al.,
Optimization with many discrete degrees of freedom

2d TM “bender”
moving cylinders around
(steepest-descent)

2d TM “lens” design

genetic algorithms: moving cylinders around
Outline

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A general optimization problem

\[
\begin{align*}
\text{minimize } & f_0(x) \\
\text{subject to } & f_i(x) \leq 0, \quad i = 1, 2, \ldots, m
\end{align*}
\]

\(x\) 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
\(f_i(x) = h(x)\) and \(f_{i+1}(x) = -h(x)\)
(although, in practical algorithms, equality constraints
typically require special handling)
Important considerations

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

- For general nonlinear functions, most algorithms only guarantee a local optimum
  - that is, a feasible \( x_0 \) such that \( f_0(x_0) \leq f_0(x) \) for all feasible \( x \)
    within some neighborhood \( \|x-x_0\| < R \) (for some small \( R \))
- A much harder problem is to find a global optimum: the minimum of \( f_0 \) for all feasible \( x \)
  - exponentially increasing difficulty with increasing \( n \), practically impossible to guarantee that you have found global minimum without knowing some special property of \( f_0 \)
  - many available algorithms, problem-dependent efficiencies
    - not just genetic algorithms or simulated annealing (which are popular, easy to implement, and thought-provoking, but usually very slow!)
    - for example, non-random systematic search algorithms (e.g. DIRECT), partially randomized searches (e.g. CRS2), repeated local searches from different starting points ("multistart" algorithms, e.g. MLSL), …
**Convex Optimization**

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

*All* the functions $f_i \ (i=0\ldots m)$ are *convex*:

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

For a convex problem (convex objective & constraints) *any* local optimum *must* be a global optimum

$\Rightarrow$ efficient, robust solution methods available
Important Convex Problems

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

all of these have very efficient, specialized solution methods
Non-convex local optimization: a typical generic outline

[ many, many variations in details !!! ]

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

2. Optimize the model problem $\Rightarrow$ new $x$
   — use a trust region to prevent large steps

3. Evaluate new $x$:
   — if “acceptable,” go to 1
   — if bad step (or bad model), update trust region / model and go to 2
Important special constraints

• Simplest case is the *unconstrained* optimization problem: \( m = 0 \)
  – e.g., line-search methods like steepest-descent, nonlinear conjugate gradients, Newton methods …

• Next-simplest are *box constraints* (also called *bound constraints*): \( x_k^{\text{min}} \leq x_k \leq x_k^{\text{max}} \)
  – easily incorporated into line-search methods and many other algorithms
  – many algorithms/software only handle box constraints

• ...

• Linear equality constraints \( Ax = b \)
  – for example, can be explicitly eliminated from the problem by writing \( x = Ny + x \), where \( x \) is a solution to \( Ax = b \) and \( N \) is a basis for the nullspace of \( A \)
Derivatives of $f_i$

• Most-efficient algorithms typically require user to supply the gradients $\nabla_x f_i$ of objective/constraints
  – you should *always* compute these analytically
    • rather than use finite-difference approximations, better to just use a derivative-free optimization algorithm
    • in principle, one can always compute $\nabla_x f_i$ with about the same cost as $f_i$, using adjoint methods
  – gradient-based methods can find (local) optima of problems with millions of design parameters

• Derivative-free methods: only require $f_i$ values
  – easier to use, can work with complicated “black-box” functions where computing gradients is inconvenient
  – *may* be only possibility for nondifferentiable problems
  – need $> n$ function evaluations, bad for large $n$
Removable non-differentiability

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

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

equivalent to *minimax* problem:

\[
\min \left( \max_{x \in \mathbb{R}^n} \{ f_0(x), -f_0(x) \} \right)
\]

...still nondifferentiable...

...equivalent to *constrained* problem with a “temporary” variable \( t \):

\[
\min_{x \in \mathbb{R}^n, t \in \mathbb{R}} t \quad \text{subject to:} \quad t \geq f_0(x) \quad (f_1(x) = f_0(x) - t) \\
\quad \quad \quad \quad \text{subject to:} \quad t \geq -f_0(x) \quad (f_2(x) = -f_0(x) - t)
\]
Example: Chebyshev linear fitting

find the fit that minimizes the maximum error:

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

… nondifferentiable minimax problem

equivalent to a linear programming problem (LP):

\[
\begin{align*}
\min \ t & \\
\text{subject to } 2N \text{ constraints:} & \\
& x_1 a_i + x_2 - b_i - t \leq 0 \\
& b_i - x_1 a_i - x_2 - t \leq 0
\end{align*}
\]
Gap Optimization via nonlinear constraints

we want:

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

not differentiable at accidental degeneracies

an equivalent problem:

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

subject to:

$$f_1 \geq \omega_n(k)$$
$$f_2 \leq \omega_{n+1}(k)$$

...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 ($e = 12:1$)  
51.4% TE gap ($e = 12:1$)

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

21.1% gap (e = 12:1)

20.7% gap (e = 12:1)
+ some local minima

−0.5% gap

−2% gap

−10% gap

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

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

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

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

density of each pixel varies continuously from 0 (air) to max

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

optimized structure, deformed under load

Some Sources of Software

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

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

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

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

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

• Some more detailed photonics examples.
Key questions occur *before* choosing optimization algorithm:

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

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

  … can make an *enormous difference* in the computational *feasibility*
  & the *robustness* of the result.
Today: Three Examples

• Optimizing photonics without solving Maxwell’s equations
  — transformational inverse design

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

• Optimizing eigenvalues without eigensolvers
  — microcavity design and the
    frequency-averaged local density of states
Today: Three Examples

• Optimizing photonics without solving Maxwell’s equations
  — transformational inverse design

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

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

[ X. Liang et al., manuscript in preparation ]
3d Microcavity Design Problem

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 $V$…

ring resonators

[ Loncar, 2002 ]

[ Song, (2005) ]

[ Akahane, 2003 ]

(defects" in periodic structures)
Topology optimization? Mostly 2d…

[ Kao and Santosa, 2008 ]

in-plane $Q$, no $V$

Vuckovic (2011): $\sim \min V$

2d heuristic for the radiation loss

Can we formulate a \textit{practical} approach to solve the \textit{full} problem, computing the \textit{true} 3d radiation loss?

Goals: understand ultimate limits on cavity performance, & eventually push cavity design into new regimes
Not just maximizing $Q$ or $Q/V$!

Typical figure of merit is “Purcell factor” $Q/V$  
($\sim$ enhancement of light-matter coupling)

Naively, should we maximize $Q/V$?

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

Real design problem:

- maximize $Q$  
such that $V \leq V_0$  

or

- minimize $V$  
such that $Q \geq Q_0$

set by bandwidth, loss tolerance,  
& fabrication capabilities
Transforming the problem...

A series of nonobvious transformations makes the problem much easier.

- Minimize modal volume $V$
  - Subject to $Q \geq Q_0$

- Maximize mean LDOS (local density of states)
  - (= power of dipole)
  - Over bandwidth $\omega_0/Q_0$

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

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

Turn difficult eigenproblem into easier scattering problem:
- $Q/V$ is really just LDOS

Complex analysis:
- Contour integration
- + causality

Technical issue:
- Avoid optimizing along “narrow ridge”
- (avoid ill-conditioned Hessian)
**LDOS: Local Density of States**

[ review: arXiv:1301.5366 ]

Maxwell eigenproblem:

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

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

Maxwell vector-Helmholtz:

\[
\mathbf{E} = i\omega (\Theta - \omega^2)^{-1} \varepsilon^{-1} \mathbf{J}
\]

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

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

**special case of a dipole source: LDOS**

\[
\mathbf{J}(x) = e_\ell \delta(x - x_0) \quad \text{LDOS}_\ell(x_0, \omega) = \frac{4}{\pi} \varepsilon(x_0) P_\ell(x_0, \omega)
\]
Why a “density of states”

[ review: arXiv:1301.5366 ]

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

\[
\frac{1}{\varepsilon} \nabla \times \frac{1}{\mu} \nabla \times E \triangleq \Theta E = \omega^2 E \\
\langle E, E' \rangle = \int E \cdot \varepsilon E'
\]

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

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

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

\[
\text{DOS}(\omega) = \sum \delta (\omega - \omega^{(n)})
\]

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

\[
P = -\frac{1}{2} \text{Re} \langle E, \varepsilon^{-1} J \rangle
\]

\[
\varepsilon^{-1} J = \sum_n E^{(n)} \langle E^{(n)}, \varepsilon^{-1} J \rangle
\]
Minimize $1/\text{LDOS}$ at $\omega_0(1+i/2Q_0)$

...Let every pixel be a degree of freedom ($\varepsilon$ in $[1,12]$)
~ $10^5$ degrees of freedom

...Solve with (mostly) standard methods:
- FDFD solver (sparse-direct + GMRES)
- adjoint sensitivity analysis
- quasi-Newton optimization (L-BFGS)

Now, a few results...
2d test case: Out-of-plane $J$, starting from vacuum initial guess

finds “Bragg onion” structure

(No $Q$ vs. $V$ tradeoff)
2d test case: Out-of-plane J, starting from PhC initial guess

starting guess has PhC resonant mode already, but optimization converts back to Bragg onion
2d test case: **In-plane J (breaks symmetry)**, starting from vacuum initial guess
Maximizing LDOS for random in-plane $J$

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

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

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

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

and others…

after deleting “hairs”:
\[ Q \approx 10,000 \]
(without re-optimizing)
Today: Three Examples

• Optimizing photonics without solving Maxwell’s equations
  — transformational inverse design

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

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

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

a “nominal” optimization problem: minimize \( \text{objective}(p) \)
Robustness of optimized designs

a “nominal” optimization problem:  
\[
\begin{align*}
\text{minimize} & \quad \text{objective}(p,0) \\
\text{design parameters} & \quad p
\end{align*}
\]

**Problem:** real objective is inexact, due to uncertainties in modeling, fabrication, materials, etcetera

… is a function \( \text{objective}(p,u) \) of \( p \) and unknown/uncertain parameters \( u \in U \)

**Problem:** optimization sometimes finds solutions that are “delicate” and destroyed by uncertainty

… i.e. \( \text{objective}(p, \text{actual } u) >> \text{objective}(p,0) \)

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

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

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

[ Povinelli, Johnson, Joannopoulos (2005) ]
[ Mutapcic, Boyd, Farjadpour, Johnson, Avniel (2009) ]
[ Oskooi et al., Optics Express 20, 21558 (2012). ]

going from uniform waveguide to periodic waveguide

\[ s(z) \]

\[ s = 0 \]

\[ s = 1 \]

\[ s(z) \]

\[ s = 0 \]

\[ s = 1 \]

\[ z = 0 \]

\[ z = L \]

\[ \text{design} \]

\[ \text{…100s of parameters…} \]

\[ \text{parameter } s = 0 \]

\[ \text{parameter } s = 1 \]

(e.g. \( s \sim \) flange width, hole radius, block width, …)

nominal problem:

Find \( s(z) \) minimizing loss...
A nominal optimum

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

any tiny manufacturing defect will kill this cancellation

(stretching design taper — a simple perturbation)
The solution: **Robust optimization**
(worst-case minimax)

- Minimize worst-case reflection:

\[
\min_{s} \max_{u} R(s, u)
\]

(manufacturing variation)

- Robust design still works when random disorder introduced:

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

[ Mutapcic, Boyd, Farjadvour, Johnson, Avniel (2009) ]
A more realistic, slow-light structure
[ Oskooi et al., Optics Express 20, 21558 (2012). ]

Slow-light waveguide for TE (in-plane polarization), tapers contain no narrow gaps, corresponds to contiguous, low-aspect ratio structure in 3d.

... Operate close to band edge, group velocity c/34.

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

Nominal optimum is worthless: reflections > 10%.

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

• Optimizing photonics without solving Maxwell’s equations
  — transformational inverse design

  [ Liu et al., manuscript in preparation. ]

• Ensuring manufacturability of narrow-band devices
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• Optimizing eigenvalues without eigensolvers
  — microcavity design and the
  frequency-averaged local density of states
Gradient-index Multimode Optics

Lipson group @ Cornell

can make smoothly varying “gradient-index” structures by grayscale lithography
(variable-thickness waveguide = gradient effective index)

Transformation optics: design materials that mathematically mimic coordinate transformations
Transformational Optics


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

= material transformations

\[
\varepsilon' = \varepsilon \frac{JJ^T}{\det J} \quad \mu' = \mu \frac{JJ^T}{\det J}
\]

\((J = \text{Jacobian matrix})\)

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

- transforms all modes same way, preserving relative phase \( \rightarrow \) multimode optics

**Cons:** most transformations give difficult-to-achieve \( \varepsilon, \mu \):

- anisotropy; \( \mu \neq \mu_0 \),

... “round” to isotropic index

\[
n \approx \sqrt{\varepsilon \mu / \varepsilon_0 \mu_0}
\]

- \( n \) may be too big / small
Transformational Inverse Design

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

... so optimization can rapidly search many transformations to find the “best” manufacturable design

want small radius $R$

“mode squeezer”

effective index

minimize waist ‘L’

multimode bend
Technical outline

For a given radius $R$, minimize the maximum anisotropy, subject to index constraints, over “all” transformations $x'(x)$:

$$\min_{x'(x)} \left[ \max_x \text{anisotropy}(x) \right] = \min_{x'(x), t} \min t$$

subject to: $1.6 \leq n(x) \leq 3.2$ \quad $t \geq \text{anisotropy}(x) = \text{“Distortion”} - 1$

at all $x$ \quad $-1 + \text{tr} J^T J / 2 \det J \geq 0$

($J = \text{Jacobian}$)

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

\~ 100 parameters

\~ 30,000 constraints

(100\times100 x grid)

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

[ use COBYLA derivative-free sequential LP algorithm of Powell (1994) ]
An optimized multimode bend

optimized index profile

FEM simulation

[ arXiv:1304.1553 ]
Experimental (Si/SiO$_2$) Realization

measured 14dB reduction in loss (conversion) of the fundamental mode ($\lambda=1.55\mu m$) vs. circular bend