## Solving the Maxwell Eigenproblem

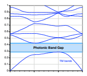
*Finite cell* → *discrete* eigenvalues $\omega_n$

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

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

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

where: $\mathbf{H}(x,y)\, e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$



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

## Solving the Maxwell Eigenproblem: 2a

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis ($N$)

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

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

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

$$\langle \mathbf{f}|\mathbf{g}\rangle = \int \mathbf{f}^* \cdot \mathbf{g} \qquad A_{m\ell} = \langle \mathbf{b}_m|\hat{A}|\mathbf{b}_\ell\rangle \qquad B_{m\ell} = \langle \mathbf{b}_m|\mathbf{b}_\ell\rangle$$

3. Efficiently solve eigenproblem: iterative methods

## Solving the Maxwell Eigenproblem: 2b

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis
   — must satisfy constraint: $(\nabla + i\mathbf{k}) \cdot \mathbf{H} = 0$

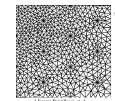
**Planewave (FFT) basis**

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

constraint: $\mathbf{H}_{\mathbf{G}} \cdot (\mathbf{G} + \mathbf{k}) = 0$

uniform "grid," periodic boundaries, simple code, $O(N \log N)$

**Finite-element basis**



[ figure: Peyrilloux *et al.*, *J. Lightwave Tech.* **21**, 536 (2003) ]

constraint, boundary conditions: Nédélec elements

[ Nédélec, *Numerische Math.* **35**, 315 (1980) ]

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

3. Efficiently solve eigenproblem: iterative methods

## Solving the Maxwell Eigenproblem: 3a

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

$$Ah = \omega^2 Bh$$

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

Faster way:
— start with *initial guess* eigenvector $h_0$
— *iteratively* improve
— $O(Np)$ storage, ~ $O(Np^2)$ time for p eigenvectors
(p smallest eigenvalues)

## Solving the Maxwell Eigenproblem: 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:

"variational theorem"

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

minimize by preconditioned conjugate-gradient (or…)

## 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

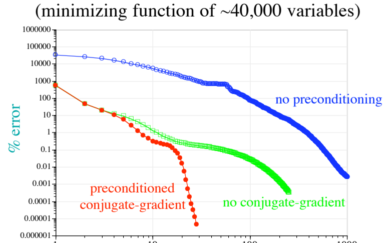
Conjugate-gradient: minimize $(h + \alpha\, d)$
— $d$ is $\nabla f$ + (stuff): *conjugate* to previous search dirs

Preconditioned steepest descent: minimize $(h + \alpha\, d)$
— $d$ = (approximate $A^{-1}$) $\nabla f$ ~ Newton's method

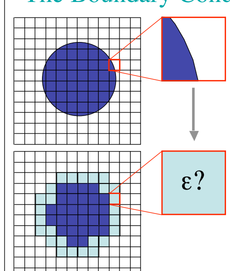
Preconditioned conjugate-gradient: minimize $(h + \alpha\, d)$
— $d$ is (approximate $A^{-1}$) [$\nabla f$ + (stuff)]

## The Iteration Scheme is *Important*

(minimizing function of ~40,000 variables)




## The Boundary Conditions are Tricky




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

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

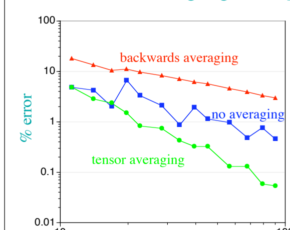
($\mathbf{D}_{\perp} = \varepsilon\mathbf{E}_{\perp}$ is continuous)

Any single scalar ε fails:
(mean **D**) ≠ (any ε) (mean **E**)

*Use a tensor* ε:

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

## The ε-averaging is *Important*




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

(similar effects in other E&M numerics & analyses)