Fast Eigenvalue Solvers for Three Dimensional Maxwell's Equations

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Plan

- Maxwell's equations
  - Dielectric materials
  - Dispersive metallic materials
  - Complex media
- Explicit representations of matrices for Yee's scheme
  - Dispersive metallic materials
  - Numerical results
- Eigen-decompositions of discrete double-curl operator and SVD of discrete single-curl operator
- Null-space free methods
  - Dielectric materials
  - Complex media

Maxwell's Equations

Maxwell's Equations for electromagnetic waves

$$\nabla \times E = \imath\omega B, \qquad \nabla \times H = -\imath\omega D$$

$$\nabla \cdot (\varepsilon E) = 0, \qquad \nabla \cdot (\mu H) = 0$$

Dielectric materials

$$D = \varepsilon E, \qquad B = \mu H$$

Metamaterials

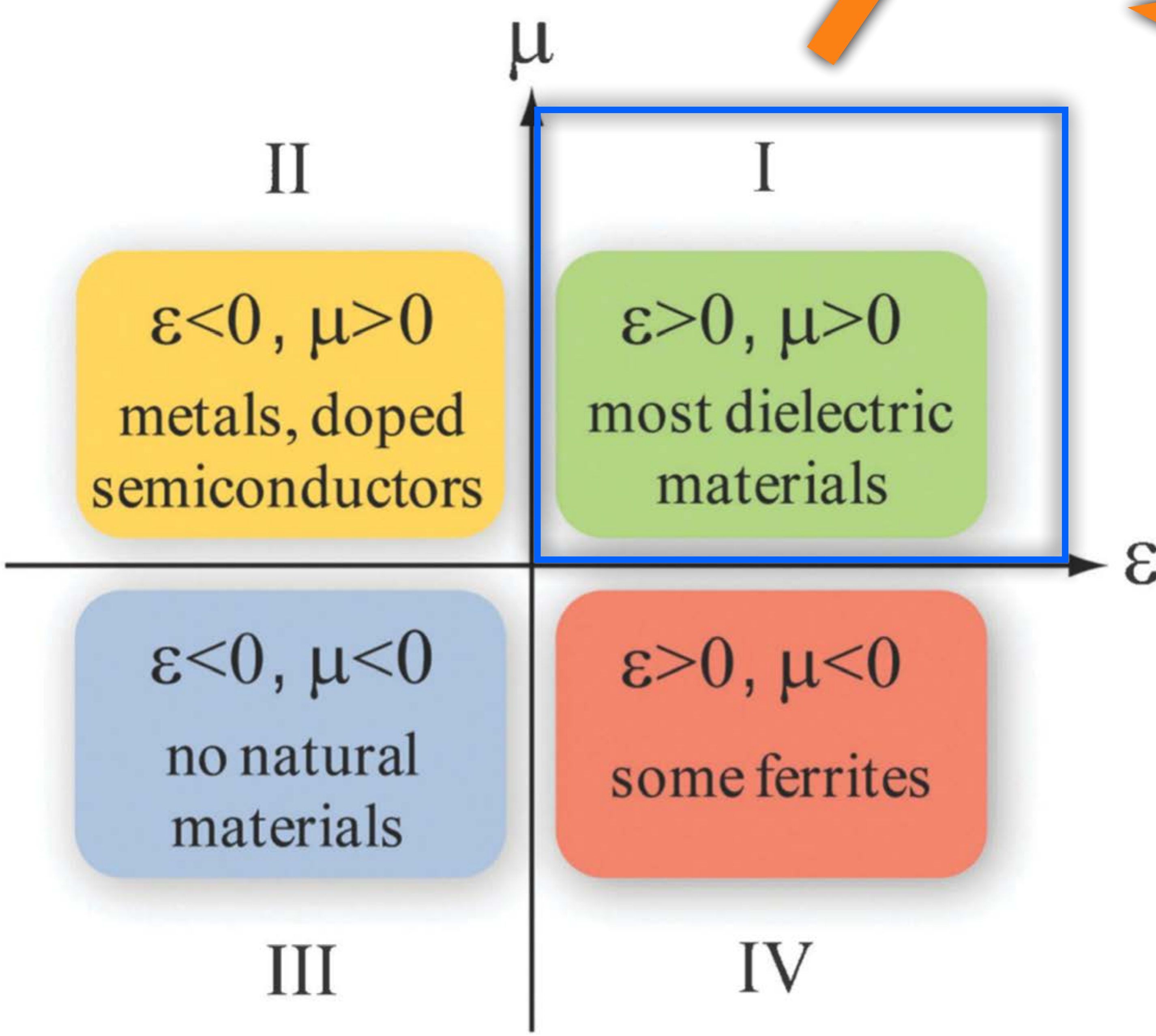
$$D = \varepsilon E + \xi H,$$

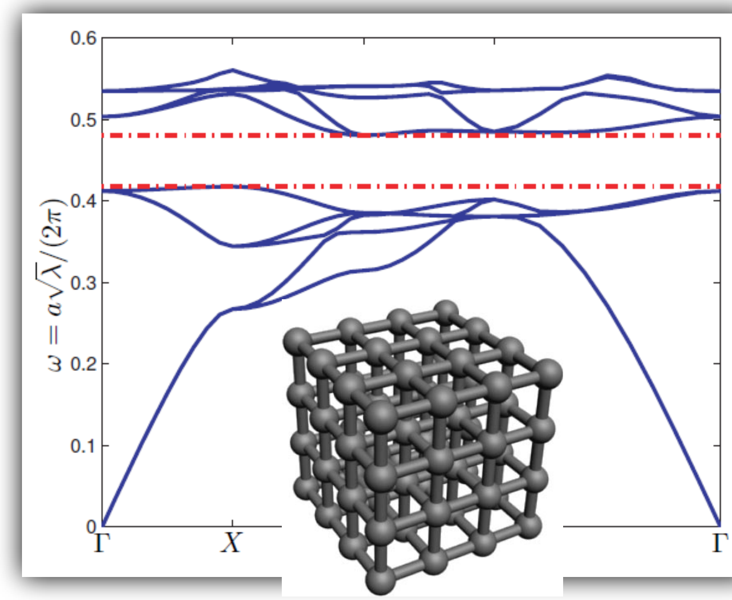
$$B = \mu H + \zeta E$$

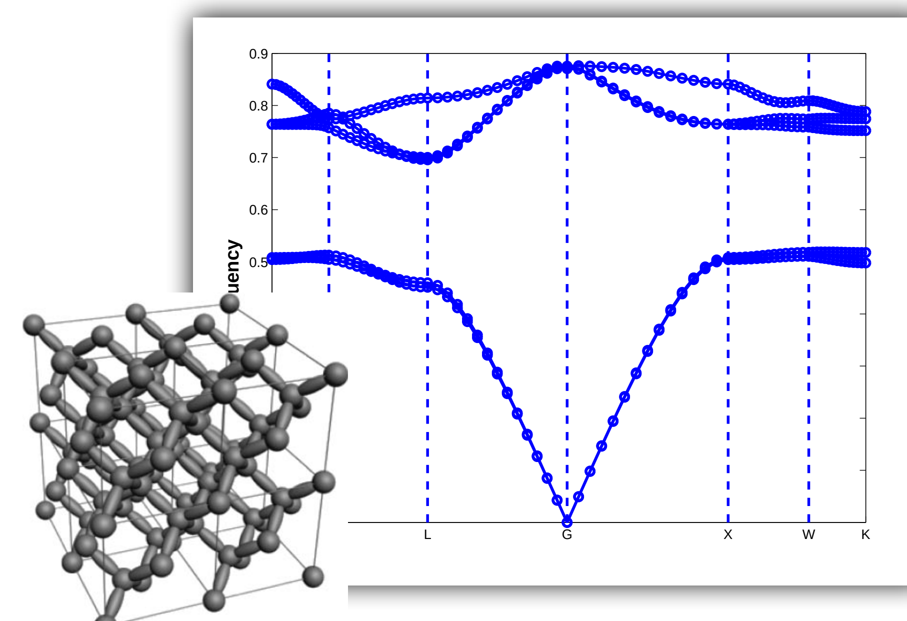
Dielectric materials (3D)

$$\boxed{\nabla \times \nabla \times E = \mu_0 \omega^2 \varepsilon(\mathbf{x}) E}$$

$$\varepsilon(\mathbf{x}) = \begin{cases} \varepsilon_1 & \text{in material 1} \\ \varepsilon_2 & \text{in material 2} \end{cases}$$



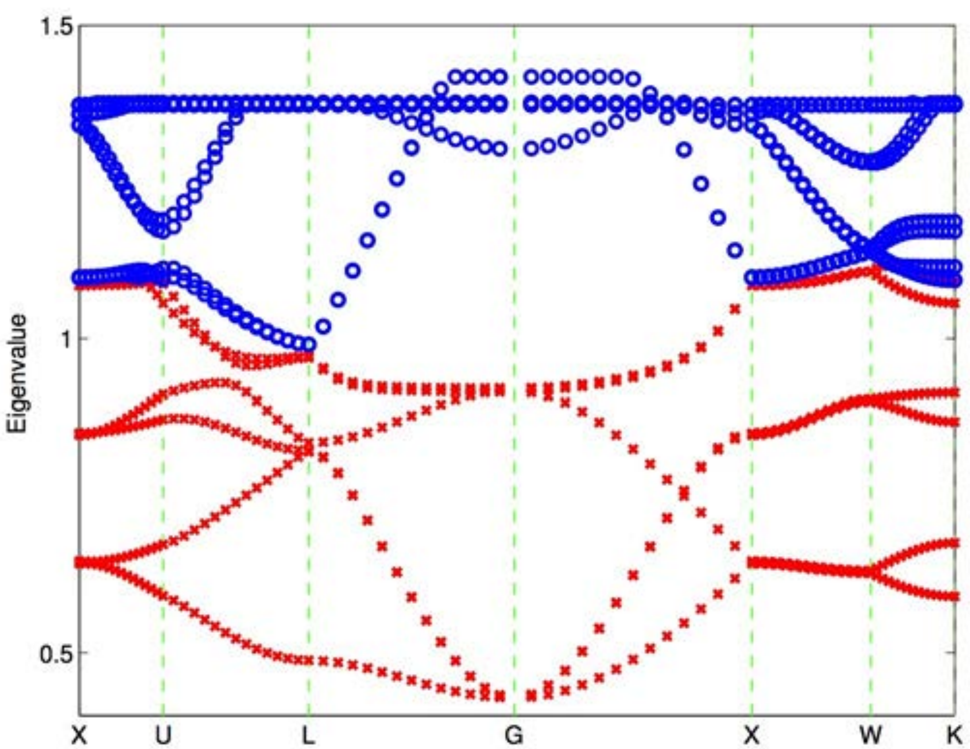


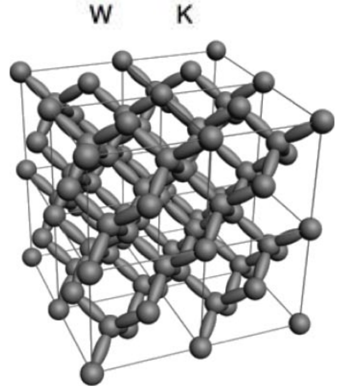


Dispersive metallic materials (3D)

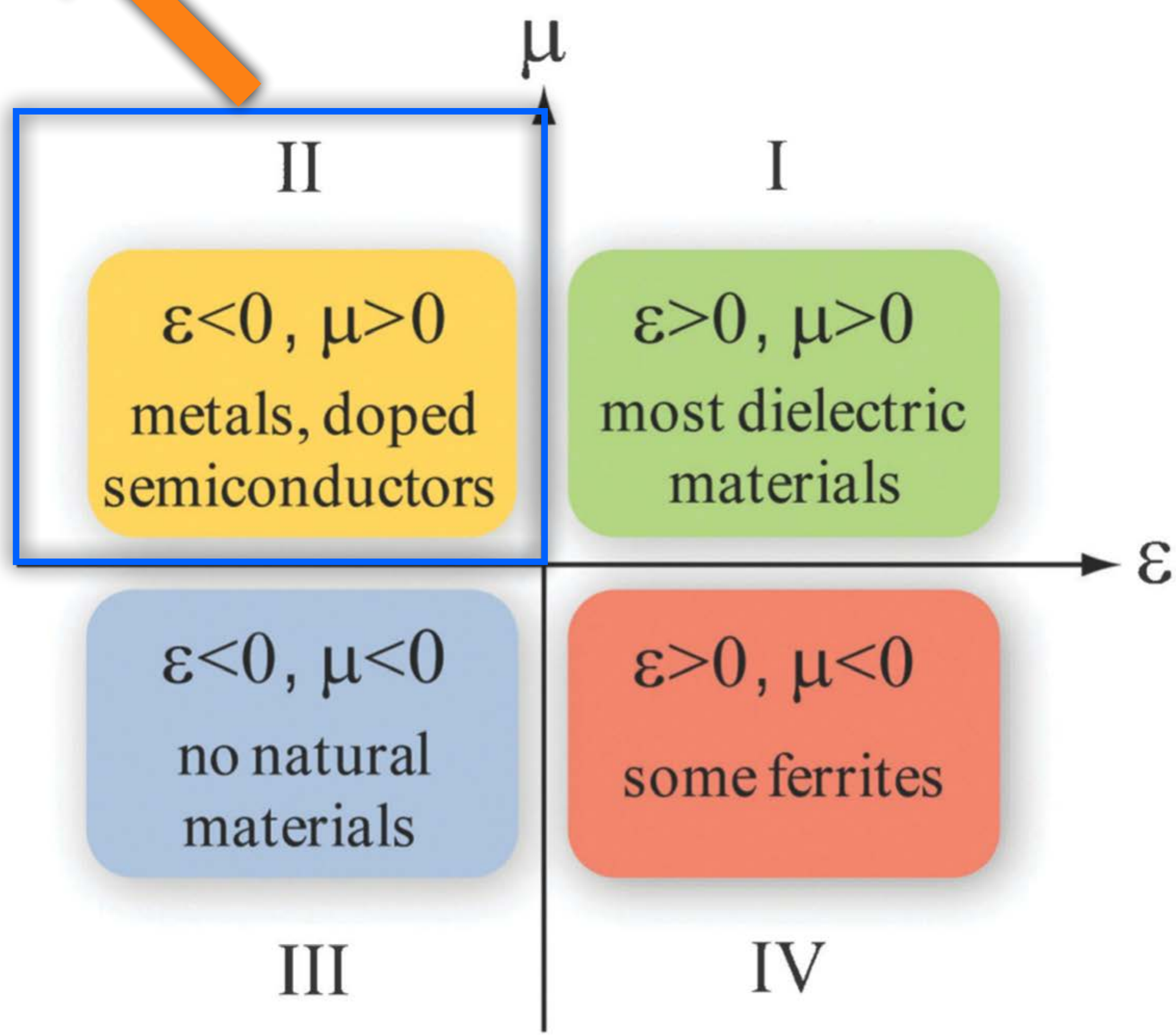
$$\boxed{\nabla \times \nabla \times E = \mu_0 \omega^2 \varepsilon(\mathbf{x}, \omega) E}$$

$$\varepsilon(\mathbf{x}, \omega) = \begin{cases} \varepsilon_1(\omega) & \text{in material 1} \\ \varepsilon_2 & \text{in material 2} \end{cases}$$

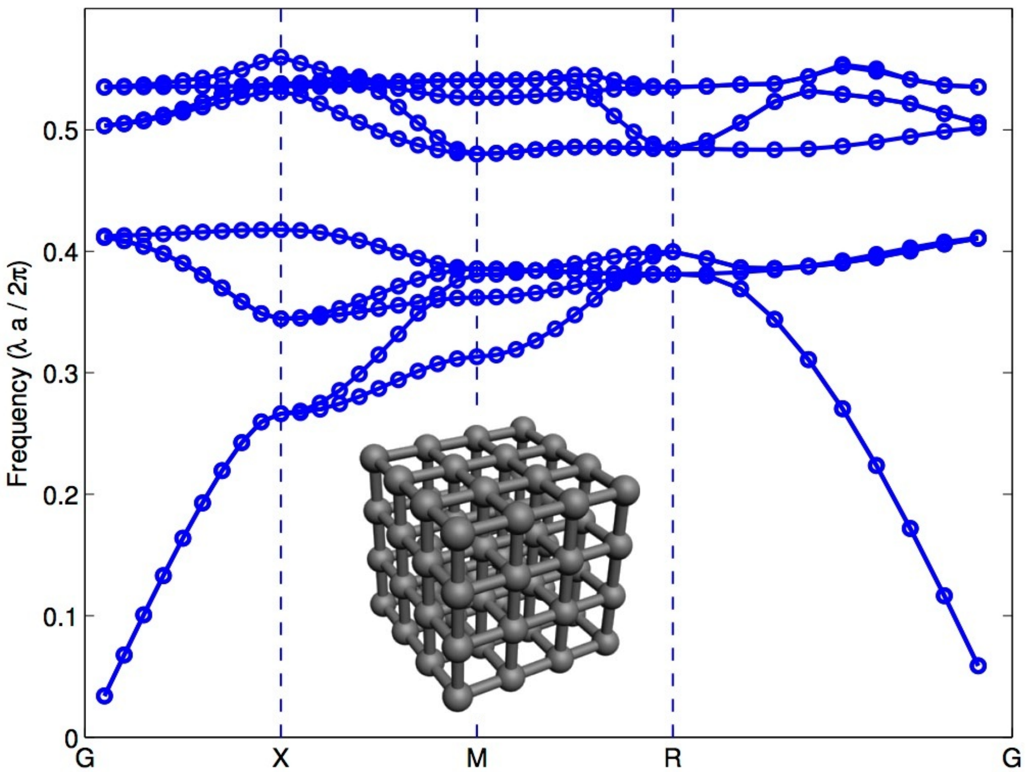


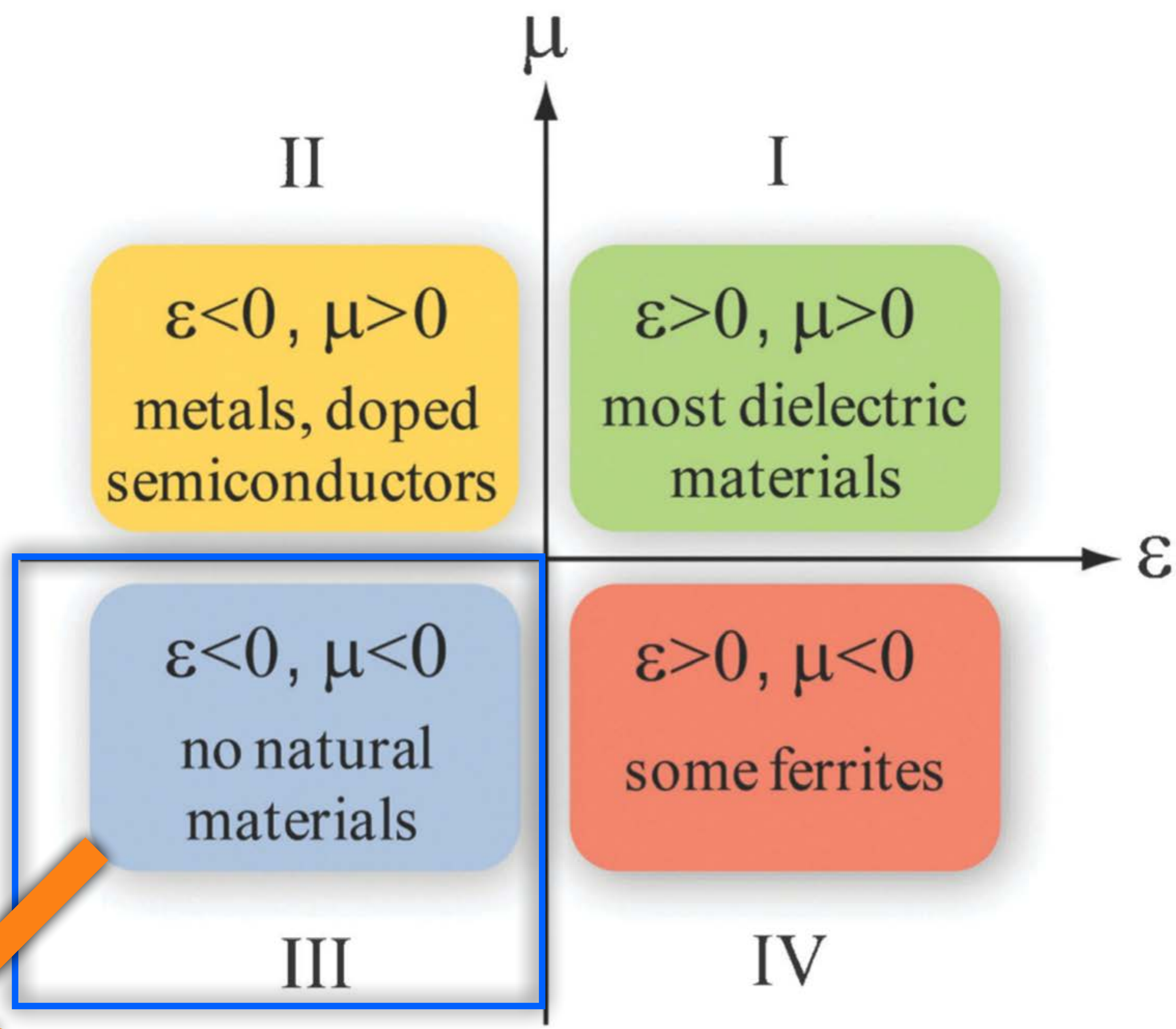


Face-Centered Cubic



Complex Media (3D)





$$\begin{bmatrix} \nabla\times & 0 \\ 0 & \nabla\times \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \imath\omega \begin{bmatrix} \zeta & \mu \\ -\varepsilon & -\xi \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix}$$

Maxwell's Equations

Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method

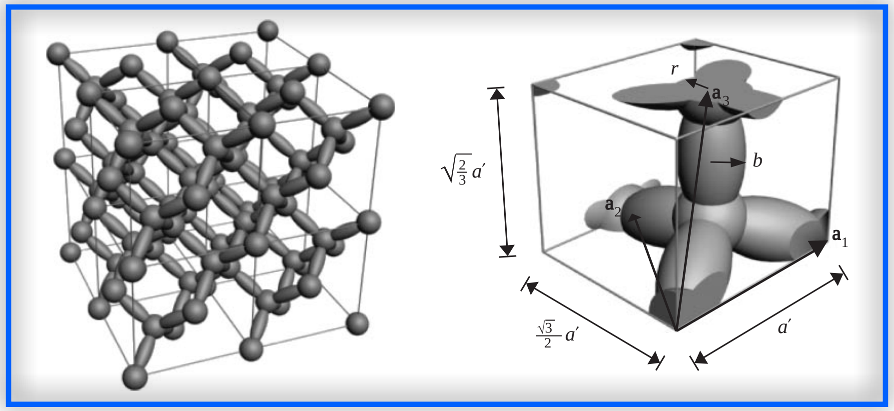
Explicit Representations of matrices for Yee's scheme

Bloch Theorem

- We are interested in finding E satisfying the quasi-periodic condition

$$E(\mathbf{x}+\mathbf{a}_\ell) = e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_\ell} E(\mathbf{x})$$

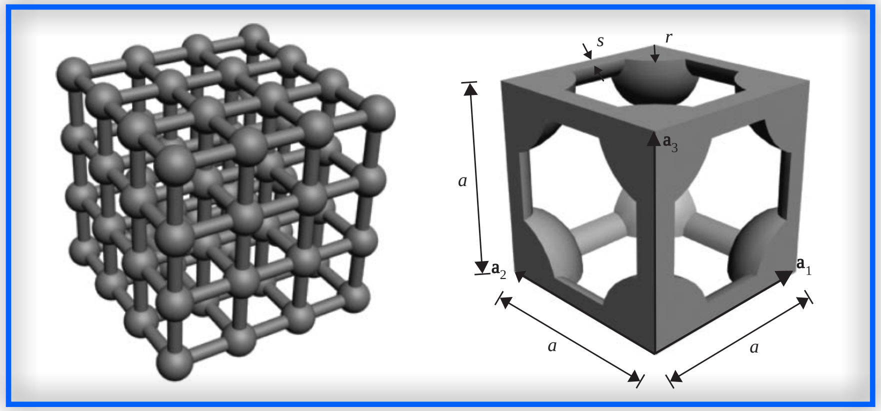
- Face-centered cubic (FCC)



$$\mathbf{a}_1 = \frac{a}{\sqrt{2}}[1,0,0]^\top, \ \mathbf{a}_2 = \frac{a}{\sqrt{2}}\left[\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right]^\top$$

$$\mathbf{a}_3 = \frac{a}{\sqrt{2}}\left[\frac{1}{2}, \frac{1}{2\sqrt{3}}, \sqrt{\frac{2}{3}}\right]^\top$$

- Simple cubic (SC)



$$\mathbf{a}_1 = a\begin{bmatrix}1 & 0 & 0\end{bmatrix}, \quad \mathbf{a}_2 = a\begin{bmatrix}0 & 1 & 0\end{bmatrix},$$
$$\mathbf{a}_3 = a\begin{bmatrix}0 & 0 & 1\end{bmatrix}$$

Figures taken from Chern, Chang, Chang, Hwang, 2004

Discrete Double-Curl Operator

- Curl operator

$$\nabla \times E = \begin{bmatrix} \frac{\partial E_3}{\partial y} - \frac{\partial E_2}{\partial z} \\ \frac{\partial E_1}{\partial z} - \frac{\partial E_3}{\partial x} \\ \frac{\partial E_2}{\partial x} - \frac{\partial E_1}{\partial y} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

- Central face points (finite diff. Yee's scheme)

$$C = \begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{bmatrix} \in \mathbb{C}^{3n \times 3n}$$

$$\boxed{C_1 = I_{n_2 n_3} \otimes K_1 \in \mathbb{C}^{n \times n}, \ C_2 = I_{n_3} \otimes K_2 \in \mathbb{C}^{n \times n}, \ C_3 = K_3 \in \mathbb{C}^{n \times n}}$$

Finite Diff. Assoc. with Quasi-Periodic Cond.

$$\boxed{E(\mathbf{x}+\mathbf{a}_\ell) = e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_\ell} E(\mathbf{x})}$$

$$K_1 = \frac{1}{\delta_x}\begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \\ e^{\imath 2\pi \mathbf{k}\cdot\boxed{\mathbf{a}_1}} & & & -1 \end{bmatrix} \in \mathbb{C}^{n_1\times n_1},$$

$$K_2 = \frac{1}{\delta_y}\begin{bmatrix} -I_{n_1} & I_{n_1} & & \\ & \ddots & \ddots & \\ & & -I_{n_1} & I_{n_1} \\ e^{\imath 2\pi \mathbf{k}\cdot\boxed{\mathbf{a}_2}}\boxed{J_2} & & & -I_{n_1} \end{bmatrix} \in \mathbb{C}^{(n_1 n_2)\times(n_1 n_2)},$$

$$K_3 = \frac{1}{\delta_z}\begin{bmatrix} -I_{n_1 n_2} & I_{n_1 n_2} & & \\ & \ddots & \ddots & \\ & & -I_{n_1 n_2} & I_{n_1 n_2} \\ e^{\imath 2\pi \mathbf{k}\cdot\boxed{\mathbf{a}_3}}\boxed{J_3} & & & -I_{n_1 n_2} \end{bmatrix} \in \mathbb{C}^{n\times n},$$

Finite Diff. Assoc. with Quasi-Periodic Cond.

- SC lattice

$$J_2 = I_{n_1} \quad \text{and} \quad J_3 = I_{n_1 n_2}$$

- FCC lattice

$$\boxed{J_2} = \begin{bmatrix} 0 & e^{-\imath 2\pi \mathbf{k}\cdot \boxed{\mathbf{a}_1}} I_{n_1/2} \\ I_{n_1/2} & 0 \end{bmatrix} \in \mathbb{C}^{n_1 \times n_1}, \quad \text{and}$$

$$\boxed{J_3} = \begin{bmatrix} 0 & e^{-\imath 2\pi \mathbf{k}\cdot \boxed{\mathbf{a}_2}} I_{\frac{1}{3}n_2} \otimes I_{n_1} \\ I_{\frac{2}{3}n_2} \otimes \boxed{J_2} & 0 \end{bmatrix} \in \mathbb{C}^{(n_1 n_2)\times(n_1 n_2)}.$$

Eigen-decomp. of C_1, C_2, C_3 for SC lattice

Define unitary matrix T as

$$
\begin{aligned}
T &= \frac{1}{\sqrt{n}}\left((D_{\mathbf{a}_3,n_3}U_{n_3}) \otimes (D_{\mathbf{a}_2,n_2}U_{n_2}) \otimes (D_{\mathbf{a}_1,n_1}U_{n_1})\right) \\
&= \frac{1}{\sqrt{n}}\left(D_{\mathbf{a}_3,n_3} \otimes D_{\mathbf{a}_2,n_2} \otimes D_{\mathbf{a}_1,n_1}\right)\boxed{\left(U_{n_3} \otimes U_{n_2} \otimes U_{n_1}\right)}
\end{aligned}
$$

with

$$
U_m = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ e^{\theta_{m,1}} & e^{\theta_{m,2}} & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ e^{(m-1)\theta_{m,1}} & e^{(m-1)\theta_{m,2}} & \cdots & 1 \end{bmatrix} \in \mathbb{C}^{m\times m}.
$$

Then it holds that

$$
\begin{aligned}
C_1 T &= \delta_x^{-1} T\left(I_{n_3} \otimes I_{n_2} \otimes \Lambda_{\mathbf{a}_1,n_1}\right) \equiv T\Lambda_1, \\
C_2 T &= \delta_y^{-1} T\left(I_{n_3} \otimes \Lambda_{\mathbf{a}_2,n_2} \otimes I_{n_1}\right) \equiv T\Lambda_2, \\
C_3 T &= \delta_z^{-1} T\left(\Lambda_{\mathbf{a}_3,n_3} \otimes I_{n_2} \otimes I_{n_1}\right) \equiv T\Lambda_3.
\end{aligned}
$$

Eigen-decomp. of C_1, C_2, C_3 for FCC lattice

Define unitary matrix T as

$$T = \frac{1}{\sqrt{n}} \begin{bmatrix} T_1 & T_2 & \cdots & T_{n_1} \end{bmatrix} \in \mathbb{C}^{n \times n},$$

$$T_i = \begin{bmatrix} T_{i,1} & T_{i,2} & \cdots & T_{i,n_2} \end{bmatrix} \in \mathbb{C}^{n \times (n_2 n_3)},$$

$$T_{i,j} = (D_{\mathbf{z},i+j} \boxed{U_{n_3}}) \otimes (\mathbf{y}_{i,j} \otimes \mathbf{x}_i),$$

$$\mathbf{x}_i = D_{\mathbf{x}} \boxed{\begin{bmatrix} 1 & e^{\theta_{\mathbf{x},i}} & \cdots & e^{(n_1-1)\theta_{\mathbf{x},i}} \end{bmatrix}^\top},$$

$$\mathbf{y}_{i,j} = D_{\mathbf{y},i} \boxed{\begin{bmatrix} 1 & e^{\theta_{\mathbf{y},j}} & \cdots & e^{(n_2-1)\theta_{\mathbf{y},j}} \end{bmatrix}^\top}.$$

Then it holds that

$$C_1 T = T \left(\Lambda_{n_1} \otimes I_{n_2 n_3} \right) \equiv T \Lambda_1,$$

$$C_2 T = T \left(\left(\oplus_{i=1}^{n_1} \Lambda_{i,n_2} \right) \otimes I_{n_3} \right) \equiv T \Lambda_2,$$

$$C_3 T = T \left(\oplus_{i=1}^{n_1} \oplus_{j=1}^{n_2} \Lambda_{i,j,n_3} \right) \equiv T \Lambda_3.$$

Explicit Represent. of matrices

Dispersive metallic materials

Eigen-decomposition of double-curl and SVD of single-curl

Numerical results

$$C_1 T = T\Lambda_1, \quad C_2 T = T\Lambda_2, \quad C_3 T = T\Lambda_3$$

Null-space free method

Dispersive metallic materials (3D)

- Maxwell's Equation

$$\nabla \times \nabla \times E = \omega^2 \varepsilon(r,\omega) E$$

- Lossless Drude model

$$\varepsilon(r,\omega) = \begin{cases} 1 - \frac{\omega_p^2}{\omega^2} & \text{in material 1} \\ 1 & \text{in material 2} \end{cases}$$

- Resulting eigenvalue problem

$$\left(A + \omega_p^2 B_d\right) x = \omega^2 x \equiv \lambda x$$

where B_d is a diagonal matrix and

$$A = C^* C$$

Dispersive metallic materials (3D)

- Lossy Drude model (or Drude-Lorentz model)

$$\boxed{\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \imath\Gamma_p\omega}}$$

$$\boxed{\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + \imath\Gamma_p\omega} + \sum_{j=1}^{2}\Omega_j A_j\left(\frac{e^{\imath\phi_j}}{\Omega_j - \omega - \imath\Gamma_j} + \frac{e^{-\imath\phi_j}}{\Omega_j + \omega + \imath\Gamma_j}\right)}$$

- Resulting nonlinear eigenvalue problem

$$\left(A - \omega^2 B_n - \omega^2\varepsilon(\omega)B_d\right)x = 0 \qquad B_n + B_d = I$$

- Multiplying the common denominator, it results

$$C(\lambda)x \equiv \left(\lambda^3 I + \lambda^2 A_2 + \lambda A_1 + A_0\right)x = 0$$

where

$$\boxed{P(\omega)x = \left(\omega^7 A_7 + \omega^2 A_6 + \cdots + \omega A_1 + A_0\right)x = 0}$$

$$A_2 = \imath\Gamma_p I, \quad A_1 = -\omega_p^2 B_d - A, \quad A_0 = -\imath\Gamma_p A$$

FFT-based preconditioner

$$\left(A+\omega_p^2 B_d\right)x=\omega^2 x\equiv\lambda x$$

- Solve the linear system

$$\left(A+\omega_p^2 B_d-\sigma I\right)\mathbf{z}=\mathbf{b}$$

- Consider the preconditioned

$$\boxed{M=(A-\tau I),}$$

where τ is the average of the diagonal entries of $\sigma I-\omega_p^2 B_d$

$$\left(\lambda^3 I+\lambda^2 A_2+\lambda A_1+A_0\right)x=0$$

$$\left(\omega^7 A_7+\omega^2 A_6+\cdots+\omega A_1+A_0\right)x=0$$

$$\boxed{(A+D)\,\mathbf{z}=\mathbf{b}}$$

Solving $(A - \tau I)\mathbf{y} = \mathbf{d}$

$$\boxed{(A - \tau I)\mathbf{y} = \mathbf{d}}$$

$$G = \begin{bmatrix} C_1^\top & C_2^\top & C_3^\top \end{bmatrix}^\top \qquad A = I_3 \otimes (G^* G) - GG^*$$

$$\boxed{\{I_3 \otimes (G^* G) - \tau I\}\, \mathbf{y} = \mathbf{d} + GG^* \mathbf{y}}$$

$$C = \begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{bmatrix} \qquad CG = 0 \qquad GG^* \mathbf{y} = -\tau^{-1} GG^* \mathbf{d}$$

$$\boxed{\{I_3 \otimes (G^* G) - \tau I\}\, \mathbf{y} = \mathbf{d} - \tau^{-1} GG^* \mathbf{d}}$$

Solving $(A - \tau I)\mathbf{y} = \mathbf{d}$

$$\boxed{\{I_3 \otimes (G^* G) - \tau I\}\, \mathbf{y} = \mathbf{d} - \tau^{-1} G G^* \mathbf{d}}$$

$$G = \begin{bmatrix} C_1^\top & C_2^\top & C_3^\top \end{bmatrix}^\top$$

$$\Lambda_q = \Lambda_1^* \Lambda_1 + \Lambda_2^* \Lambda_2 + \Lambda_3^* \Lambda_3$$

$$C_1 T = T \Lambda_1, \quad C_2 T = T \Lambda_2, \quad C_3 T = T \Lambda_3$$

$$\begin{aligned} &(I_3 \otimes \Lambda_q - \tau I)\, \tilde{\mathbf{y}} \\ &= \left(I - \tau^{-1} \begin{bmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{bmatrix} \begin{bmatrix} \Lambda_1^* & \Lambda_2^* & \Lambda_3^* \end{bmatrix} \right) \boxed{(I_3 \otimes T)^* \mathbf{d},} \qquad \mathbf{y} = \boxed{(I_3 \otimes T)\, \tilde{\mathbf{y}}.} \end{aligned}$$

This beautiful idea is proposed by Wei-Cheng Wang

T*p and Tq for SC lattice

$$T = \frac{1}{\sqrt{n}}((D_{\mathbf{a}_3,n_3}U_{n_3}) \otimes (D_{\mathbf{a}_2,n_2}U_{n_2}) \otimes (D_{\mathbf{a}_1,n_1}U_{n_1}))$$
$$= \frac{1}{\sqrt{n}}(D_{\mathbf{a}_3,n_3} \otimes D_{\mathbf{a}_2,n_2} \otimes D_{\mathbf{a}_1,n_1})\boxed{(U_{n_3} \otimes U_{n_2} \otimes U_{n_1})}$$

with

$$U_m = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ e^{\theta_{m,1}} & e^{\theta_{m,2}} & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ e^{(m-1)\theta_{m,1}} & e^{(m-1)\theta_{m,2}} & \cdots & 1 \end{bmatrix}, \quad \theta_{m,j} = \frac{\imath 2\pi j}{m}.$$

- $(U_{n_3} \otimes U_{n_2} \otimes U_{n_1})^* \mathbf{p}$ → 3D forward FFT
- $(U_{n_3} \otimes U_{n_2} \otimes U_{n_1}) \mathbf{q}$ → 3D backward FFT

Compute T*p for FCC lattice

Algorithm 4 Forward FFT-based matrix-vector product $T^*\mathbf{p}$ [15].

Input: Any vector $\mathbf{p} = \begin{bmatrix} \mathbf{p}_1^\top & \cdots & \mathbf{p}_{n_3}^\top \end{bmatrix}^\top \in \mathbb{C}^n$ with $\mathbf{p}_k = \begin{bmatrix} \mathbf{p}_{1,k}^\top & \cdots & \mathbf{p}_{n_2,k}^\top \end{bmatrix}^\top$ and $\mathbf{p}_{j,k} \in \mathbb{C}^{n_1}$ for $j = 1, \ldots, n_2$, $k = 1, \ldots, n_3$.

Output: The vector $\mathbf{f} \equiv T^*\mathbf{p}$.

```
for k = 1, ..., n_3 do
    Compute P_x(:, :, k) = [p_{1,k} ... p_{n_2,k}]^* E_x U_x.
end for
for i = 1, ..., n_1 do
    Compute P_y = [P_x(:, i, 1)  P_x(:, i, 2)  ...  P_x(:, i, n_3)]^T E_{y,i} U_y.
    Compute P_z = U_z^* [E_{z,i+1}^* P_y(:, 1)  E_{z,i+2}^* P_y(:, 2)  ...  E_{z,i+n_2}^* P_y(:, n_2)]
    Set f((i-1) n_2 n_3 + 1 : i n_2 n_3) = 1/sqrt(n_1 n_2 n_3) vec(P_z).
end for
```

$$\text{2: Compute } P_{\mathbf{x}}(:,:,k) = \boxed{\begin{bmatrix} \mathbf{p}_{1,k} & \cdots & \mathbf{p}_{n_2,k} \end{bmatrix}^* E_{\mathbf{x}} U_{\mathbf{x}}}.$$

$$\text{5: Compute } P_{\mathbf{y}} = \boxed{\begin{bmatrix} P_{\mathbf{x}}(:,i,1) & P_{\mathbf{x}}(:,i,2) & \cdots & P_{\mathbf{x}}(:,i,n_3) \end{bmatrix}^\top E_{\mathbf{y},i} U_{\mathbf{y}}}.$$

$$\text{6: Compute } P_{\mathbf{z}} = \boxed{U_{\mathbf{z}}^* \begin{bmatrix} E_{\mathbf{z},i+1}^* P_{\mathbf{y}}(:,1) & E_{\mathbf{z},i+2}^* P_{\mathbf{y}}(:,2) & \cdots & E_{\mathbf{z},i+n_2}^* P_{\mathbf{y}}(:,n_2) \end{bmatrix}}$$

$$\text{7: Set } \mathbf{f}((i-1)n_2 n_3 + 1 : i n_2 n_3) = \frac{1}{\sqrt{n_1 n_2 n_3}} \operatorname{vec}(P_{\mathbf{z}}).$$

1D forward FFT

Compute Tq for FCC lattice

Algorithm 5 Backward FFT-based matrix-vector product $T\mathbf{q}$ [15].

Input: Any vector $\mathbf{q} = \begin{bmatrix} \mathbf{q}_1^\top & \cdots & \mathbf{q}_{n_1}^\top \end{bmatrix}^\top \in \mathbb{C}^n$ with $\mathbf{q}_i = \begin{bmatrix} \mathbf{q}_{i,1}^\top & \cdots & \mathbf{q}_{i,n_2}^\top \end{bmatrix}^\top$ and $\mathbf{q}_{i,j} \in \mathbb{C}^{n_3}$ for $i = 1, \ldots, n_1, j = 1, \ldots, n_2$.

Output: The vector $\mathbf{g} \equiv T\mathbf{q}$.

for $i = 1, \ldots, n_1$ **do**
- Compute $Q_{\mathbf{z},i} = \boxed{U_{\mathbf{z}} \begin{bmatrix} \mathbf{q}_{i,1} & \mathbf{q}_{i,2} & \cdots & \mathbf{q}_{i,n_2} \end{bmatrix}}$.
- Update $Q_{\mathbf{z},i} := \begin{bmatrix} E_{\mathbf{z},i+1} Q_{\mathbf{z},i}(:,1) & E_{\mathbf{z},i+2} Q_{\mathbf{z},i}(:,2) & \cdots & E_{\mathbf{z},i+n_2} Q_{\mathbf{z},i}(:,n_2) \end{bmatrix}^\top$.
- Compute $Q_{\mathbf{y}}(:,:,i) = E_{\mathbf{y},i} \boxed{(U_{\mathbf{y}} Q_{\mathbf{z},i})}$

end for

for $k = 1, \ldots, n_3$ **do**
- Compute $Q_{\mathbf{x}} = E_{\mathbf{x}} \boxed{U_{\mathbf{x}} \begin{bmatrix} Q_{\mathbf{y}}(:,k,1) & Q_{\mathbf{y}}(:,k,2) & \cdots & Q_{\mathbf{y}}(:,k,n_1) \end{bmatrix}^\top}$.
- Set $\mathbf{g}((k-1)n_1 n_2 + 1 : k n_1 n_2) = \frac{1}{\sqrt{n_1 n_2 n_3}} \mathrm{vec}(Q_{\mathbf{x}})$.

end for

1D backward FFT

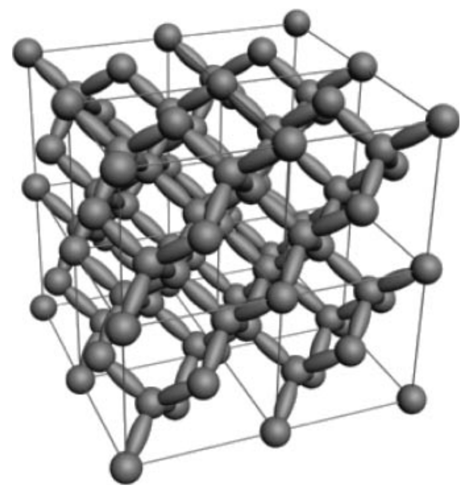
Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method

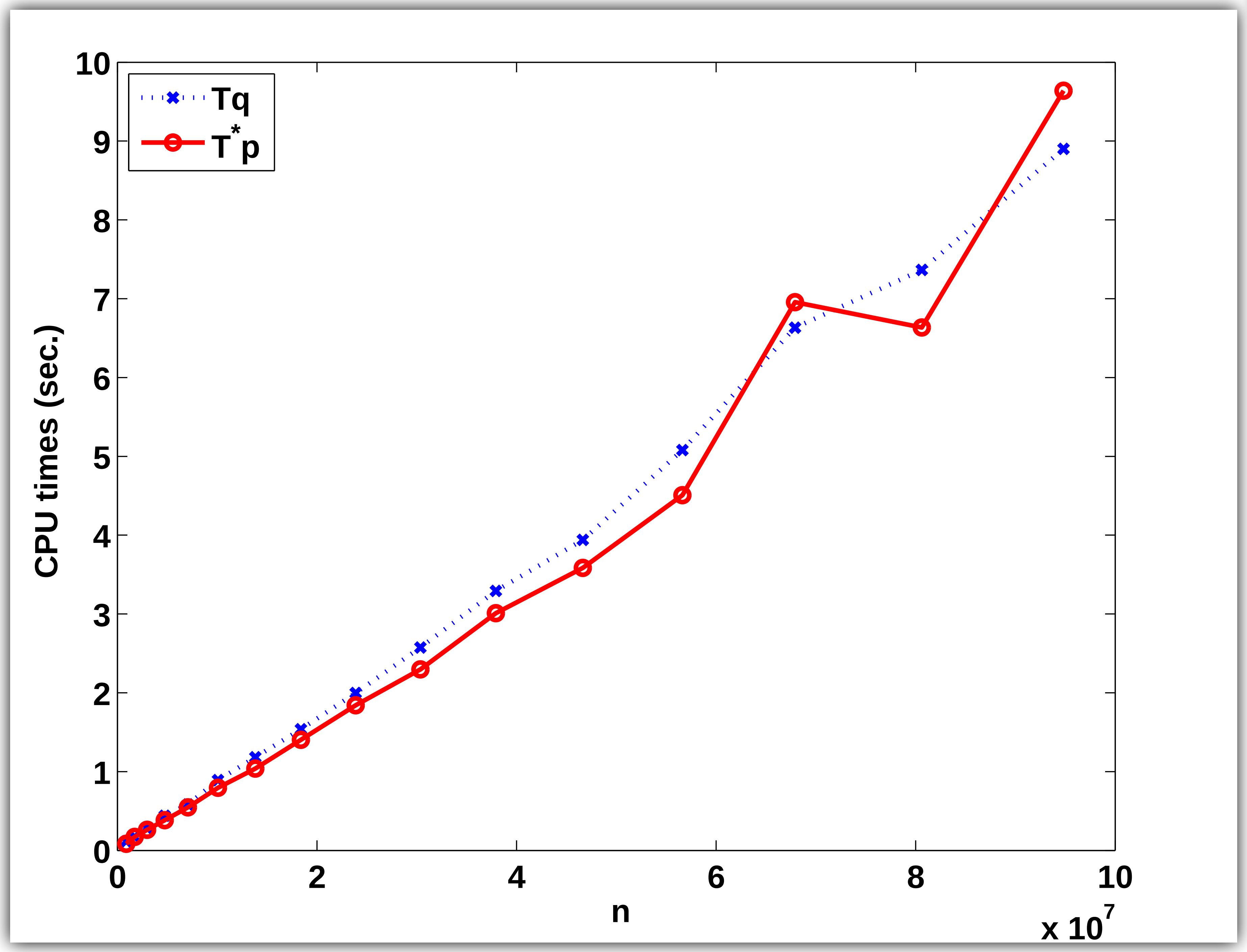
Dispersive metallic materials

Numerical results



CPU Times for T*p and Tq with FCC

MATLAB



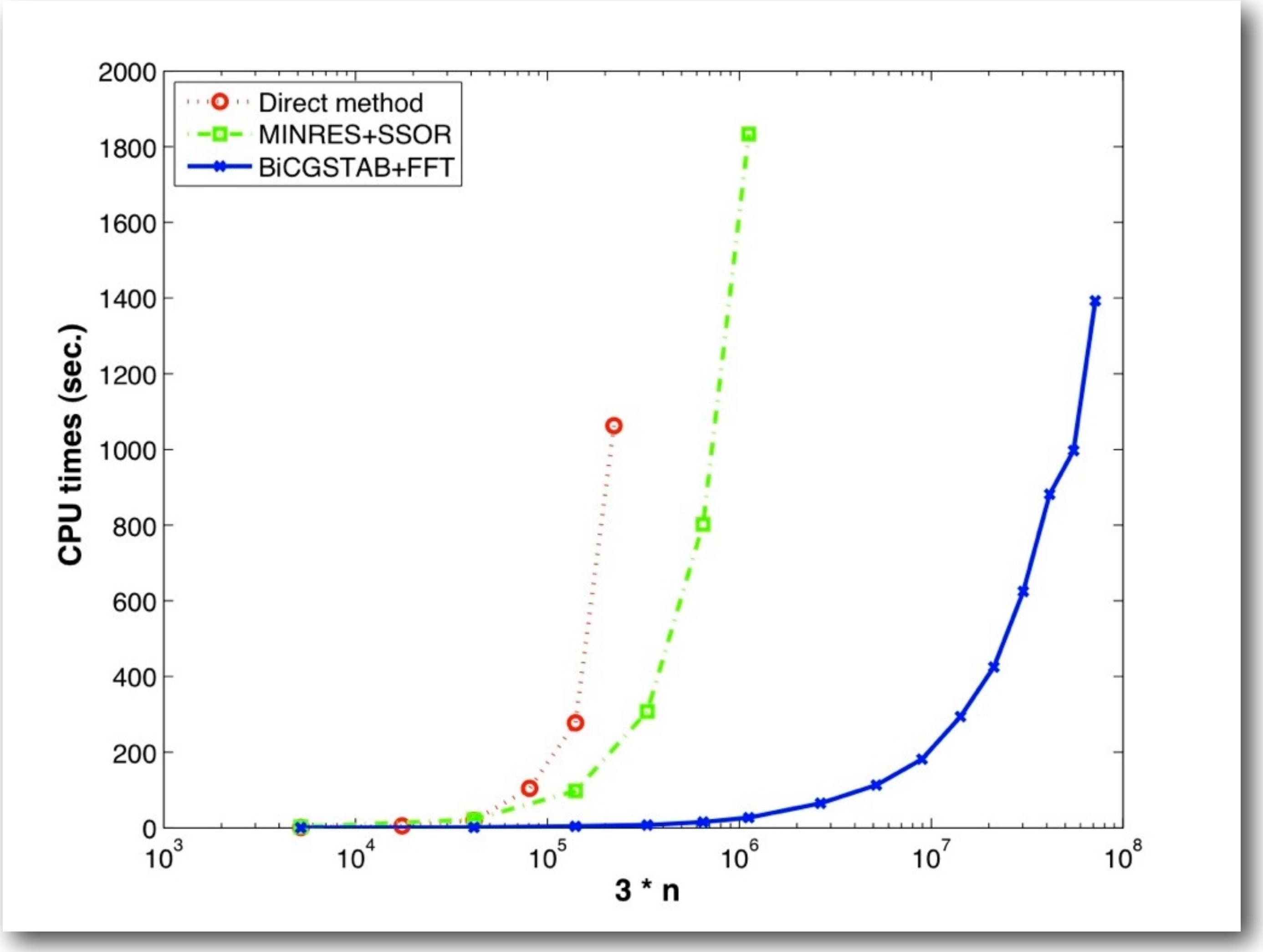
Comparison in Solving Linear System

- SC lattice (dim = 46875)

Index j	Jacobi	SSOR(0.8)	ICC(1)	ILU(1)	FFT
1	852	493	296	273	27
2	853	492	296	273	27
3	1,008	462	287	284	28

- FCC lattice

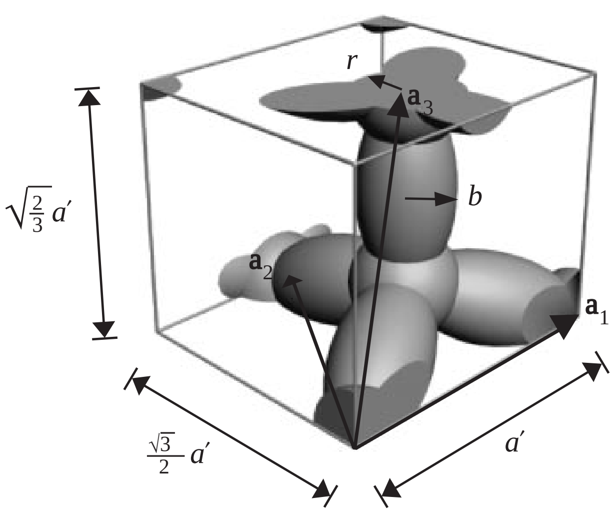
$$\boxed{(A - \sigma B)\mathbf{z} = \mathbf{b}}$$

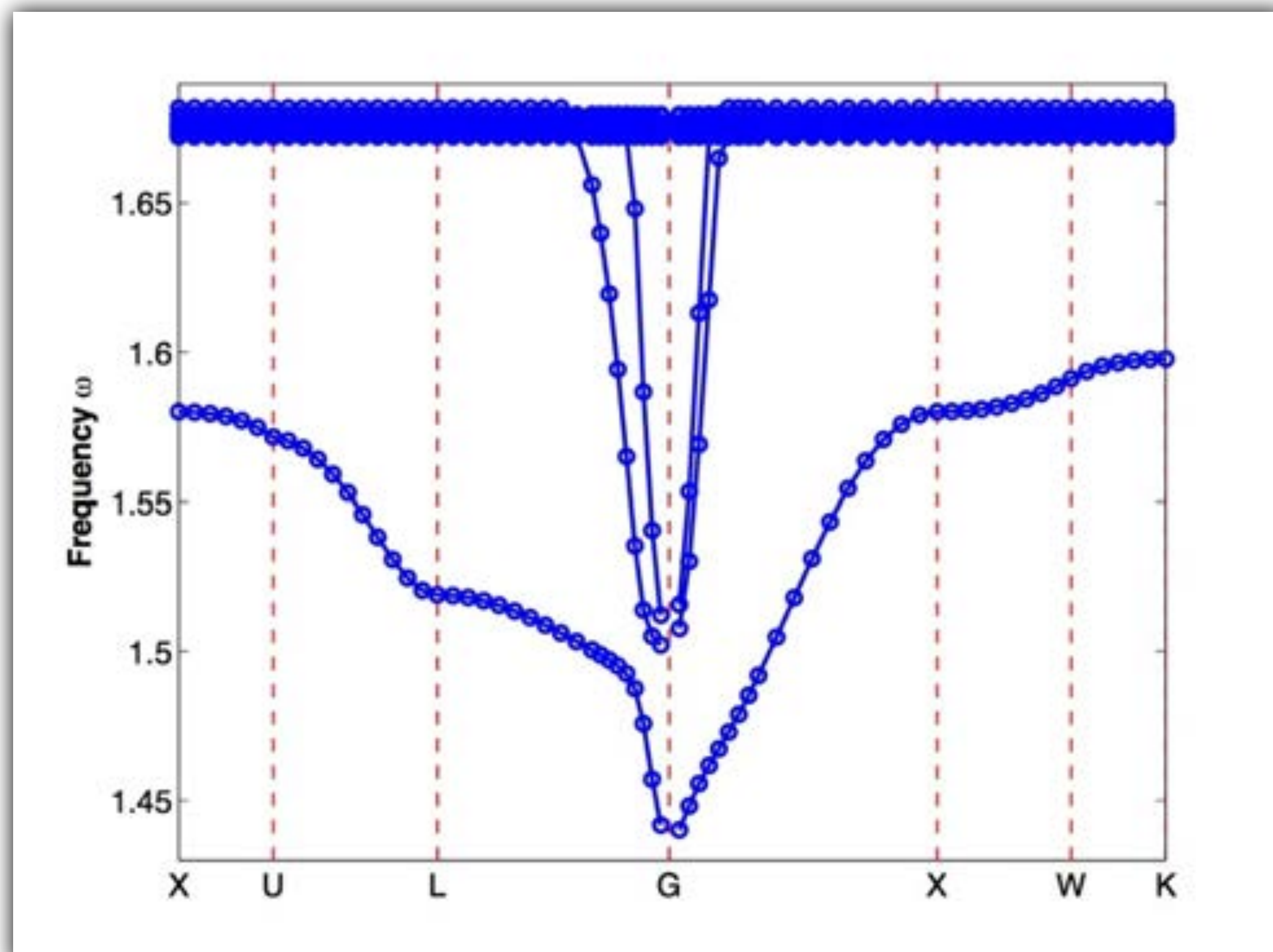


Band Structure of FCC Lattice

- Dim. of SEP: 2,654,208
- 70 test problems

$$\varepsilon(r,\omega) = \begin{cases} 1 - \dfrac{\omega_p^2}{\omega^2} & \text{in material 1} \\ 1 & \text{in material 2} \end{cases}$$



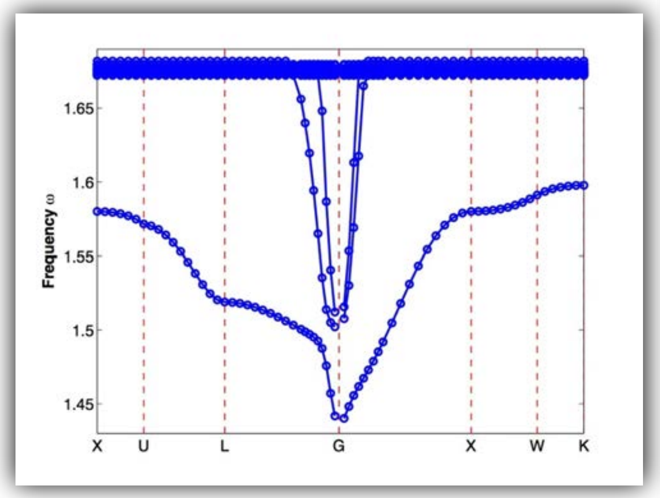


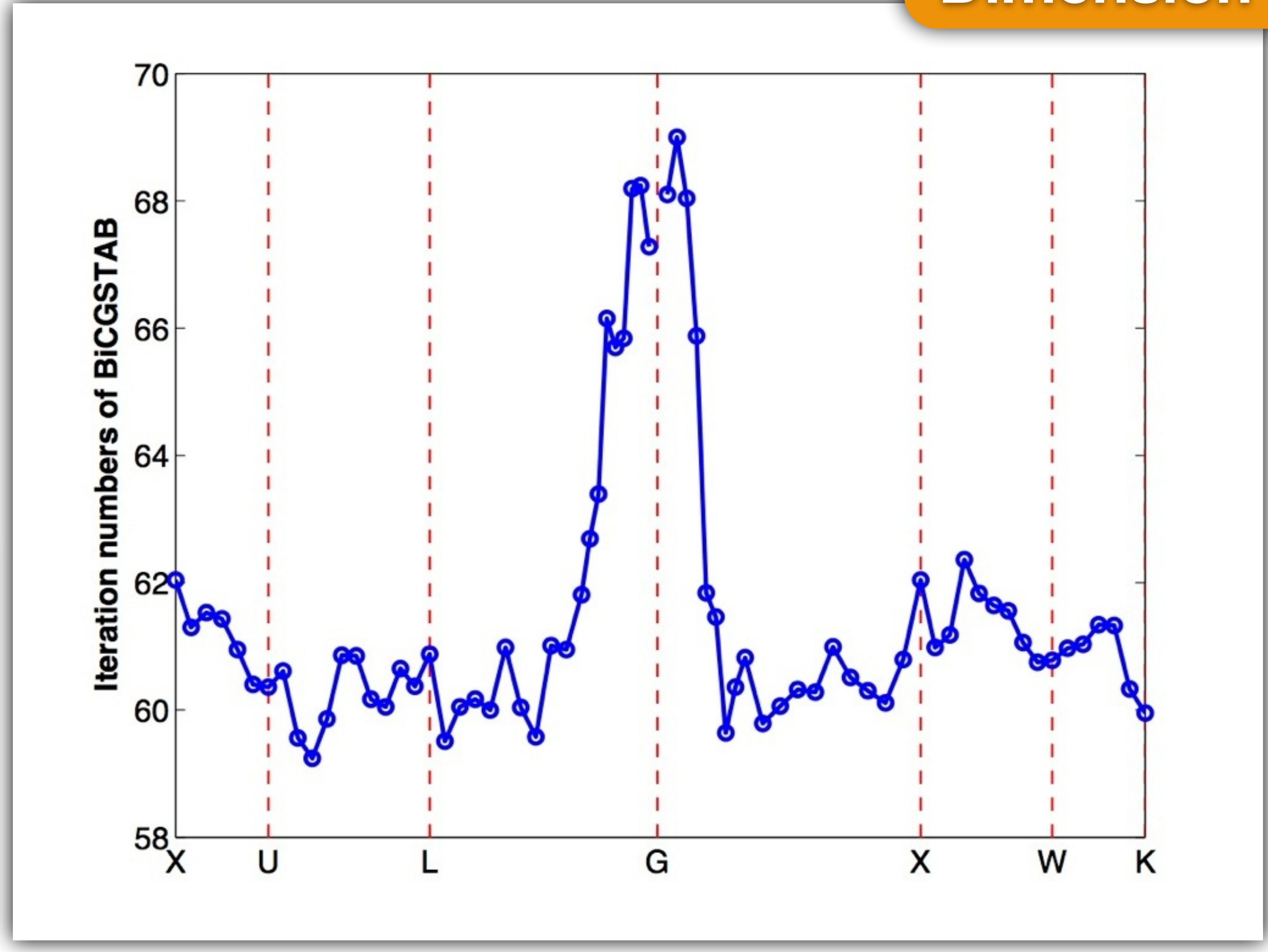
Iteration Numbers of Solving Linear Systems

$$\left(A + \omega_p^2 B_d - \sigma I\right) \mathbf{z} = \mathbf{b}$$

$$M = (A - \tau I)$$

Dimension = 2,654,208

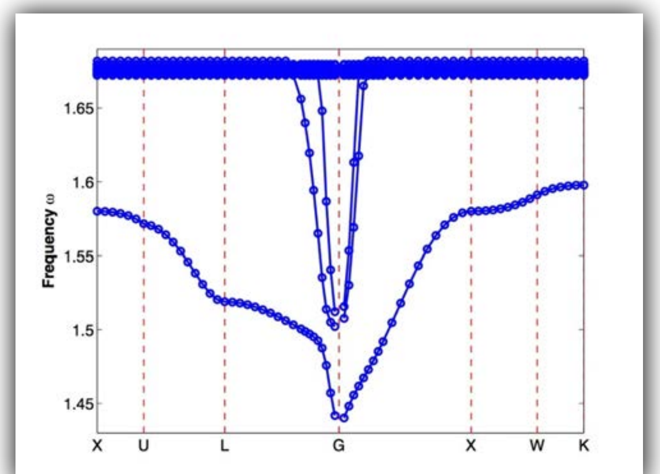


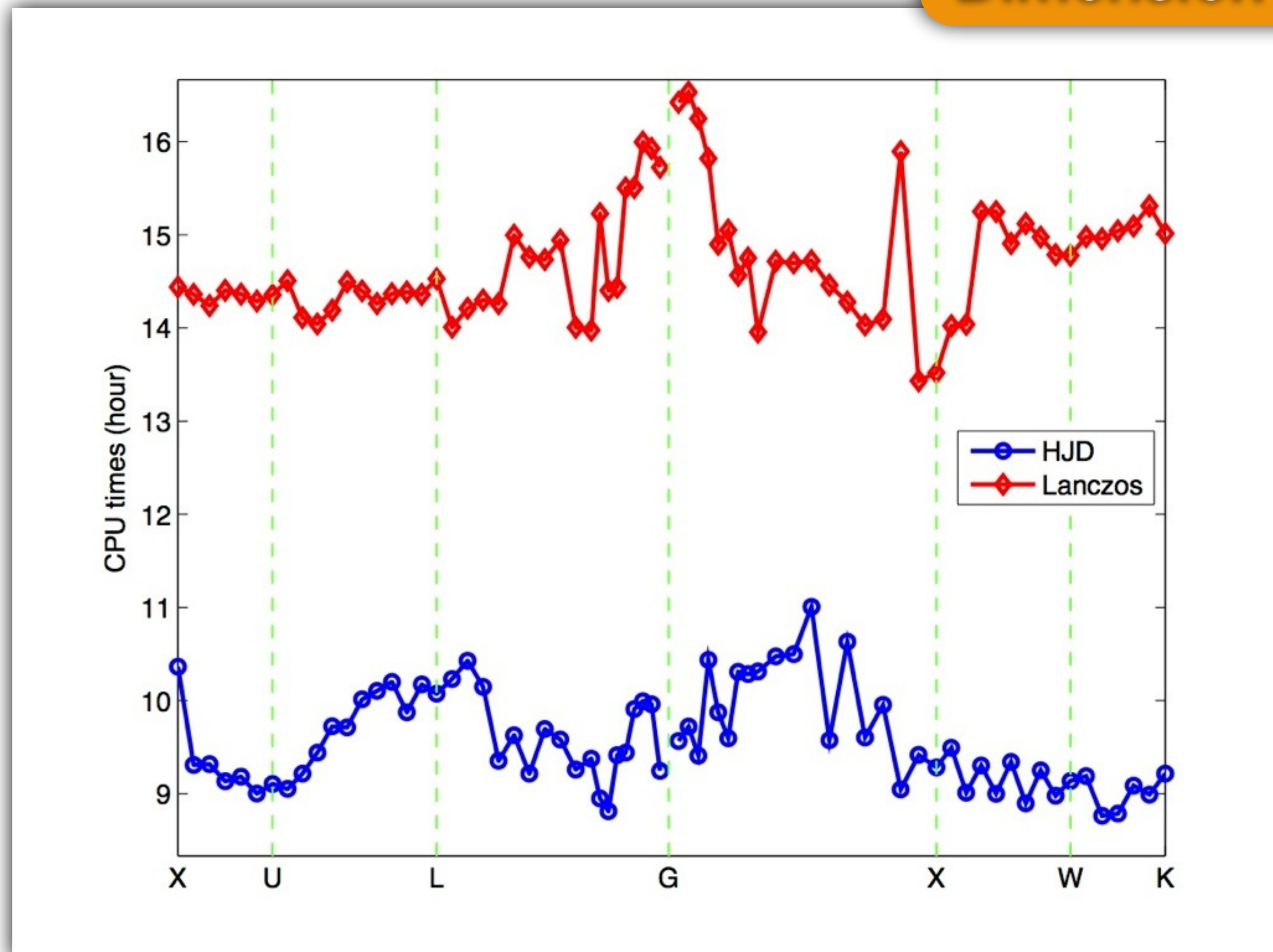


CPU times of Eigensolvers

$$\left(A + \omega_p^2 B_d\right) x = \omega^2 x = \lambda x$$

Dimension = 2,654,208





Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method

Eigen-decomposition of Discrete Double-Curl Operator and SVD of Discrete Single-Curl Operator

Null space of C^*C and CC^*

- Define

$$Q_0 = (I_3 \otimes T) \begin{bmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{bmatrix} \Lambda_q^{-1/2} \equiv (I_3 \otimes T)\,\Pi_0,$$

$$P_0 = (I_3 \otimes T)\,\overline{\Pi_0}.$$

- Then Q_0 and P_0 form orthogonal bases of the null spaces of C^*C and CC^*, respectively.

$$\boxed{C_1 T = T\Lambda_1, \quad C_2 T = T\Lambda_2, \quad C_3 T = T\Lambda_3}$$

$$\boxed{\Lambda_q = \Lambda_1^* \Lambda_1 + \Lambda_2^* \Lambda_2 + \Lambda_3^* \Lambda_3}$$

Range space of C^*C and CC^*

- Take orthogonal projection of $T_1 \equiv [\alpha T^\top, \beta T^\top, T^\top]^\top$ with respective to Q_0 and P_0 :

$$Q_1 = (I - Q_0 Q_0^*) T_1 \left(\Lambda_p^* \Lambda_p \Lambda_q^{-1}\right)^{-1/2}$$

$$\equiv (I_3 \otimes T) \Pi_1 = (I_3 \otimes T) \begin{bmatrix} \diagdown \\ \diagdown \\ \diagdown \end{bmatrix},$$

$$P_1 = (I - P_0 P_0^*) T_1 \left(\Lambda_p^* \Lambda_p \Lambda_q^{-1}\right)^{-1/2} = (I_3 \otimes T) \overline{\Pi_1}.$$

- Then Q_1 and P_1 are orthogonal, and

$$(C^*C) Q_1 = Q_1 \Lambda_q, \quad (CC^*) P_1 = P_1 \Lambda_q.$$

Range space of C^*C and CC^*

- Apply the discrete curl and dual-curl operators on T_1 , respectively:

$$Q_2 = C^* T_1 \left(\Lambda_p^* \Lambda_p\right)^{-1/2}$$

$$\equiv (I_3 \otimes T)\, \Pi_2 = (I_3 \otimes T) \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix},$$

$$P_2 = C T_1 \left(\Lambda_p^* \Lambda_p\right)^{-1/2} = (I_3 \otimes T) \left(-\overline{\Pi_2}\right).$$

- Then Q_2 and P_2 are orthogonal, and

$$(C^*C)Q_2 = Q_2 \Lambda_q, \quad (CC^*)P_2 = P_2 \Lambda_q.$$

Important Decompositions

- Define

$$Q \equiv \begin{bmatrix} Q_1 & Q_2 & Q_0 \end{bmatrix} = (I_3 \otimes T) \begin{bmatrix} \Pi_1 & \Pi_2 & \Pi_0 \end{bmatrix},$$
$$P \equiv \begin{bmatrix} P_2 & P_1 & P_0 \end{bmatrix} = (I_3 \otimes T) \begin{bmatrix} -\overline{\Pi_2} & \overline{\Pi_1} & \overline{\Pi_0} \end{bmatrix}.$$

- *Eigen-decompositions* of discrete double curl

$$C^*C = Q \operatorname{diag}(\Lambda_q, \Lambda_q, 0) Q^* = Q_r \Lambda Q_r^*,$$
$$CC^* = P \operatorname{diag}(\Lambda_q, \Lambda_q, 0) P^* = P_r \Lambda P_r^*.$$

- *Singular value decomposition* of single curl

$$C = P \operatorname{diag}\left(\Lambda_q^{1/2}, \Lambda_q^{1/2}, 0\right) Q^* = P_r \Sigma_r Q_r^*$$

where

$$P_r = [P_2,\ P_1],\ Q_r = [Q_1,\ Q_2],\ \Sigma_r = \operatorname{diag}\left(\Lambda_q^{1/2}, \Lambda_q^{1/2}\right)$$

Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method

Null Space Free Method

Resulting Eigenvalue Problems

- Discretized 3D photonic crystals (Dielectric materials):

$$\nabla \times \nabla \times E = \mu_0 \omega^2 \varepsilon(\mathbf{x}) E$$

leads to the generalized eigenvalue problem

$$A\mathbf{x} = \lambda B \mathbf{x} \qquad A = C^* C$$

B is a positive diagonal matrix.

$$\boxed{C^* C = Q \operatorname{diag}(\Lambda_q, \Lambda_q, 0) Q^*}$$

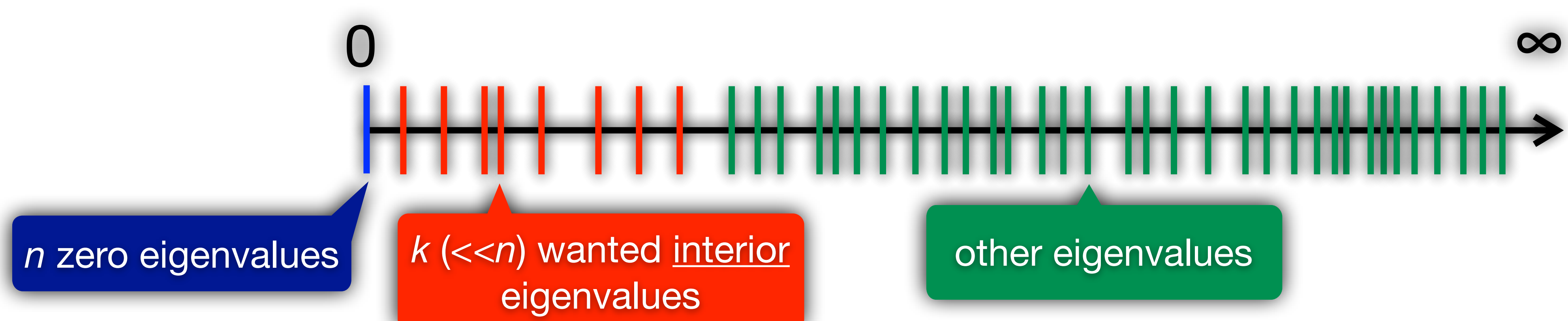
- The discretization of

$$\begin{bmatrix} \nabla\times & 0 \\ 0 & \nabla\times \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \imath\omega \begin{bmatrix} \zeta & \mu \\ -\varepsilon & -\xi \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix}$$

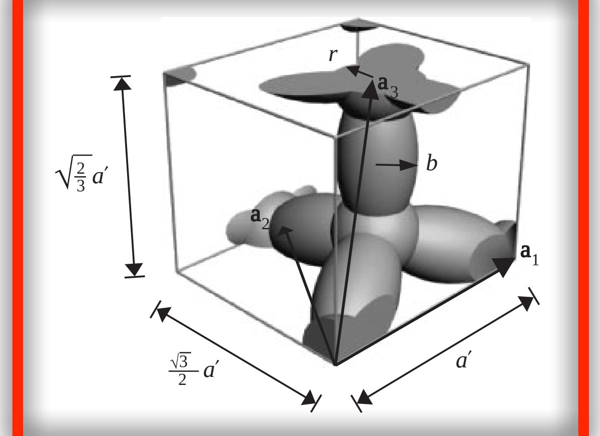
leads to the generalized eigenvalue problem:

$$\boxed{C = P \operatorname{diag}\left(\Lambda_q^{1/2}, \Lambda_q^{1/2}, 0\right) Q^*}$$

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \omega \left(\imath \begin{bmatrix} \zeta_d & \mu_d \\ -\varepsilon_d & -\xi_d \end{bmatrix} \right) \begin{bmatrix} E \\ H \end{bmatrix} \equiv \omega B \begin{bmatrix} E \\ H \end{bmatrix}$$



Explicit Represent. of matrices



Photonic crystals

Eigen-decomposition of double-curl and SVD of single-curl

Numerical results

Complex materials

Null-space free method

Numerical results

3D Photonic Crystals (Dielectric materials)

$$\nabla \times \nabla \times E = \mu_0 \omega^2 \varepsilon(\mathbf{x}) E$$

$$\boxed{A\mathbf{x} = \lambda B\mathbf{x}, \qquad A = Q_r \Lambda Q_r^*}$$

$$\boxed{\operatorname{span}\left\{B^{-1} Q_r \Lambda^{1/2}\right\} = \{\mathbf{x} | A\mathbf{x} = \lambda B\mathbf{x},\ \lambda > 0\}}$$

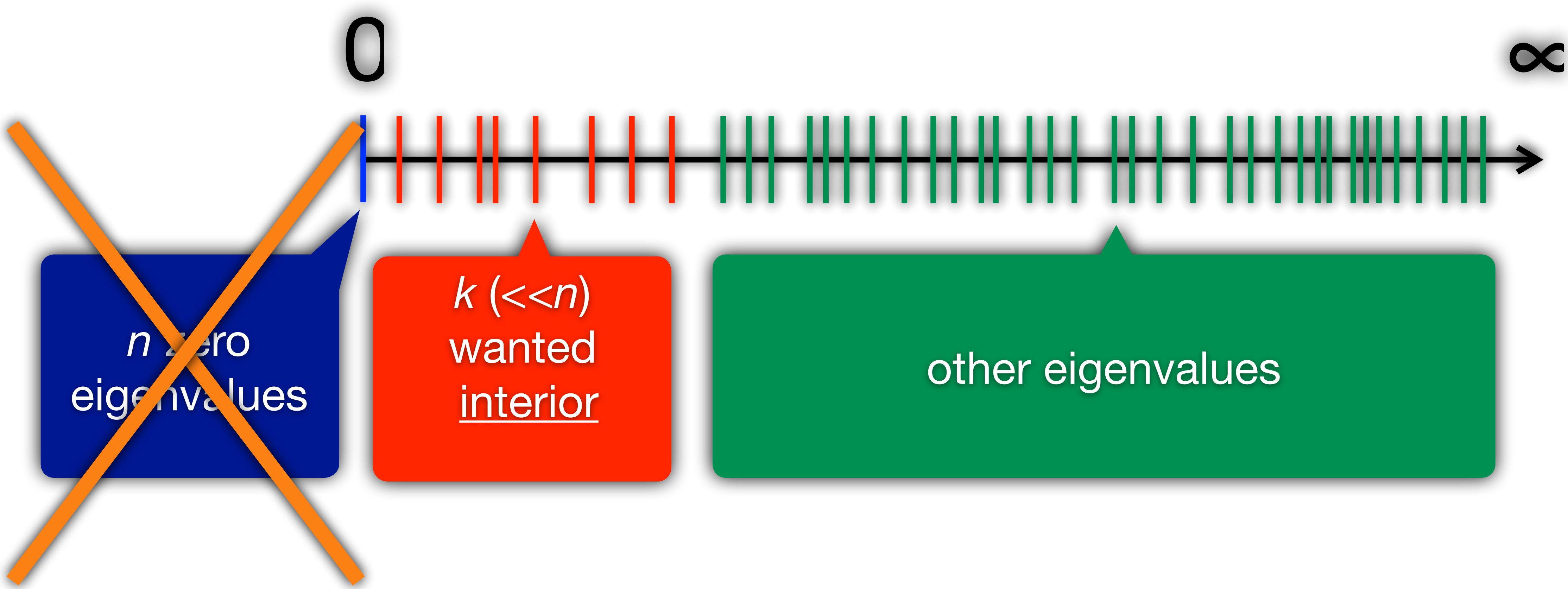
$$\boxed{\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}, \quad \mathbf{x} = B^{-1} Q_r \Lambda^{\frac{1}{2}} \mathbf{y}}$$

Advantages of SEVP

$$\boxed{A\mathbf{x} = \lambda B\mathbf{x}}$$

$$\boxed{\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}}$$

- Dim. of GEVP and SVEP are 3n and 2n, respectively
- GEVP and SEVP have same 2n positive eigenvalues.
  SEVP has no zero eigenvalues.
  SEVP can be solved by inverse Lanczos.



Advantages of SEVP

- As the SEVP

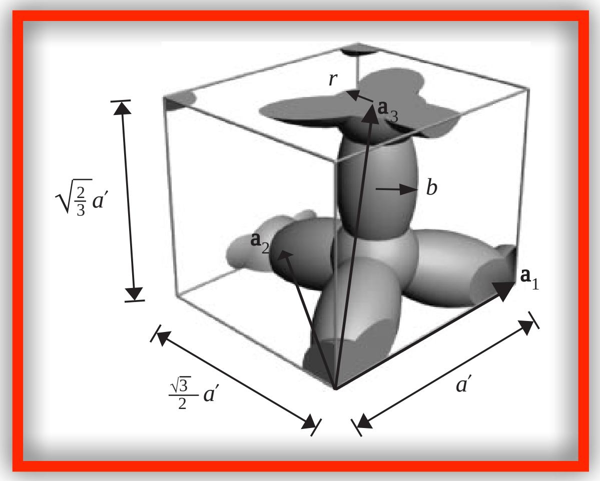
$$A_r \mathbf{y} = \lambda \mathbf{y} \qquad A_r \equiv \Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}$$

in inverse Lanczos, we need to solve

$$Q_r^* B^{-1} Q_r \mathbf{u} = \mathbf{c} \qquad \boxed{\Lambda_r^{\frac{1}{2}} \left(Q_r^* B^{-1} Q_r \right) \Lambda_r^{\frac{1}{2}} \tilde{\mathbf{u}} = \tilde{\mathbf{c}}}$$

- Well-conditioned system
  - Can show that $\kappa \left(Q_r^* B^{-1} Q_r \right) \leq \kappa \left(B^{-1} \right)$
  - Conditioning number of B^{-1} is 13
  - $Q_r^* \hat{\mathbf{p}}_2$ and $Q_r \hat{\mathbf{q}}_2$ can be computed efficiently by the FFT-based schemes
  - Can be efficiently solved by CG method

$$\boxed{Q_r = (I_3 \otimes T) \begin{bmatrix} \ddots & \ddots \\ \ddots & \ddots \\ \ddots & \ddots \end{bmatrix}}$$



Explicit Represent. of matrices

Photonic crystals

Eigen-decomposition of double-curl and SVD of single-curl

Numerical results

Complex materials

Null-space free method

Numerical results

Bandgap Diagram of FCC Lattice

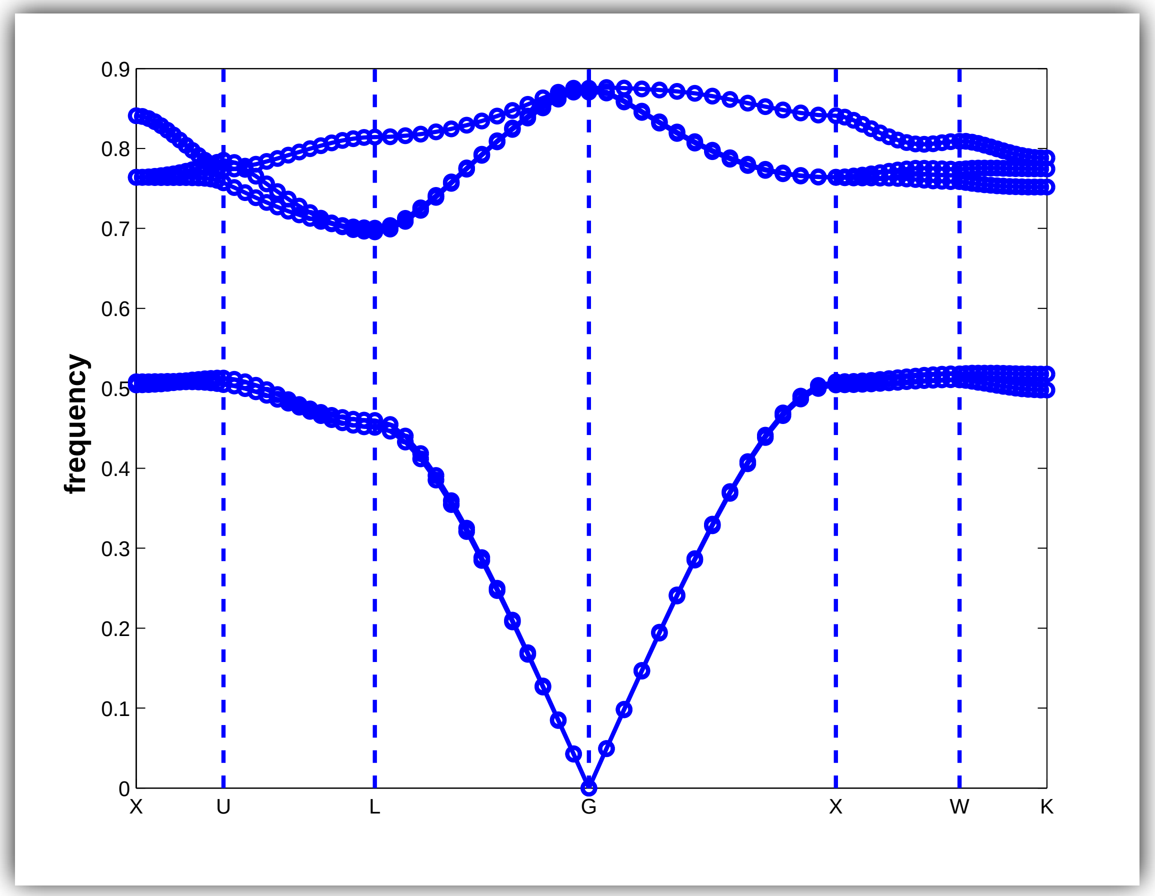
- Dim. of GEVP: 5,184,000

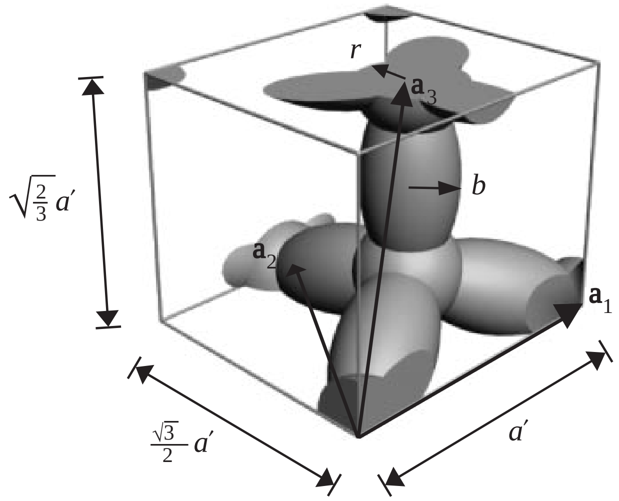
  Dim. of SEVP: 3,456,000

- 90 test problems

$$A\mathbf{x} = \lambda B\mathbf{x}$$

$$\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}$$





Comparison for Solving Linear Sys.

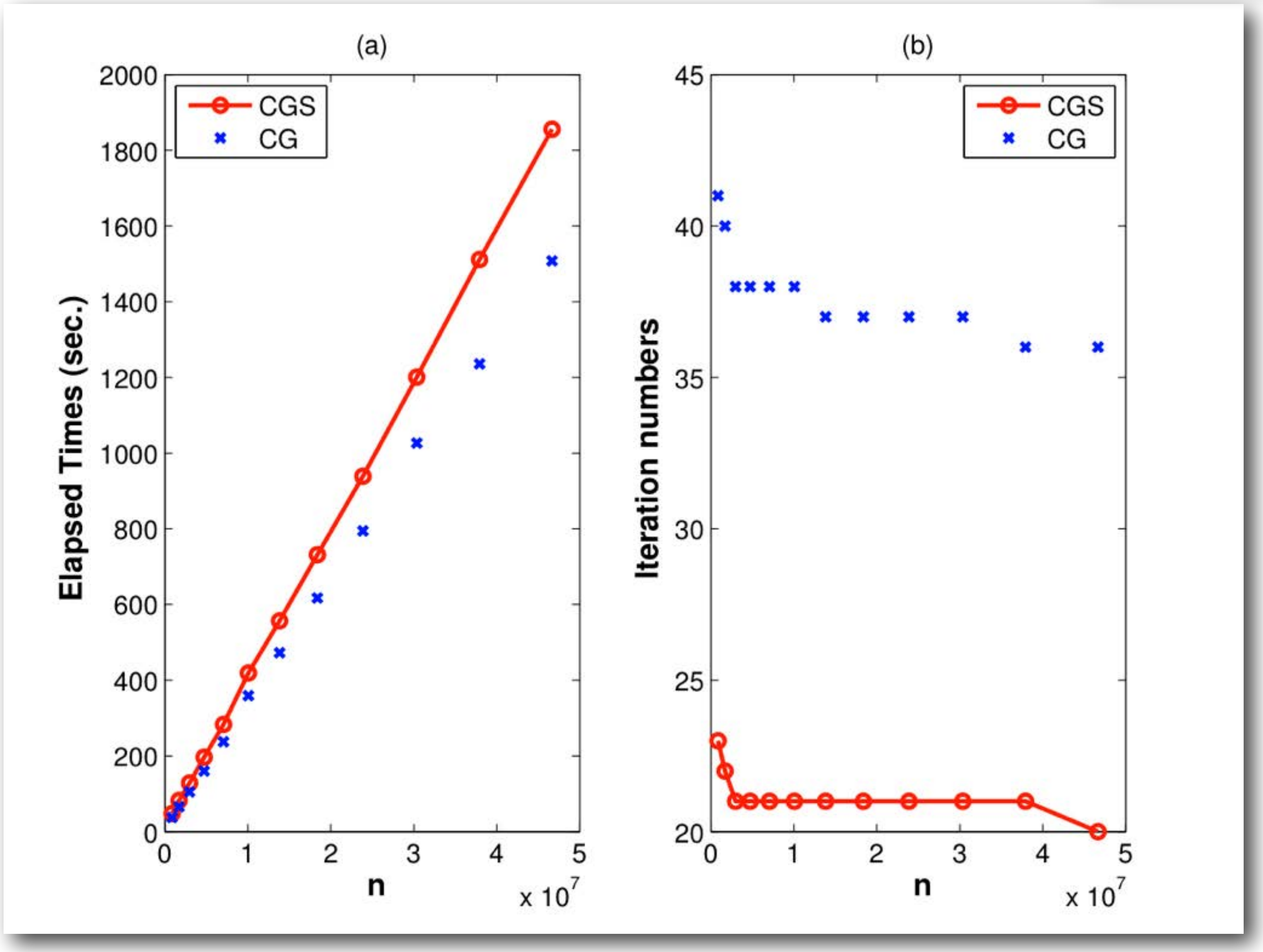
$$(A - \sigma B)\mathbf{z} = \mathbf{b}$$

$$Q_r^* B^{-1} Q_r \mathbf{u} = \mathbf{c}$$

$$A\mathbf{x} = \lambda B\mathbf{x}$$

$$M = (A - \tau I)$$

$$\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}$$

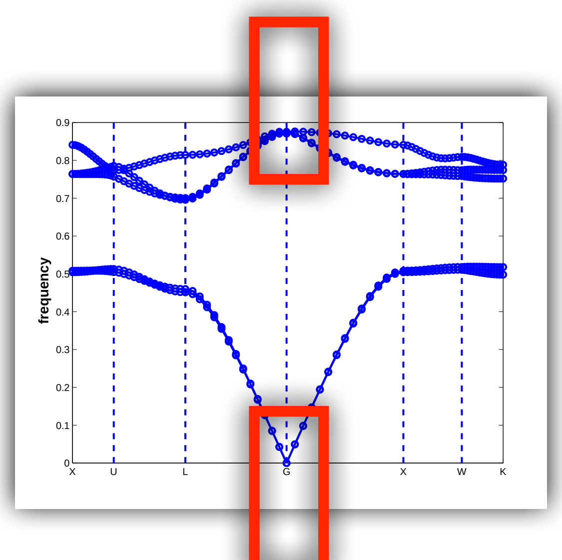


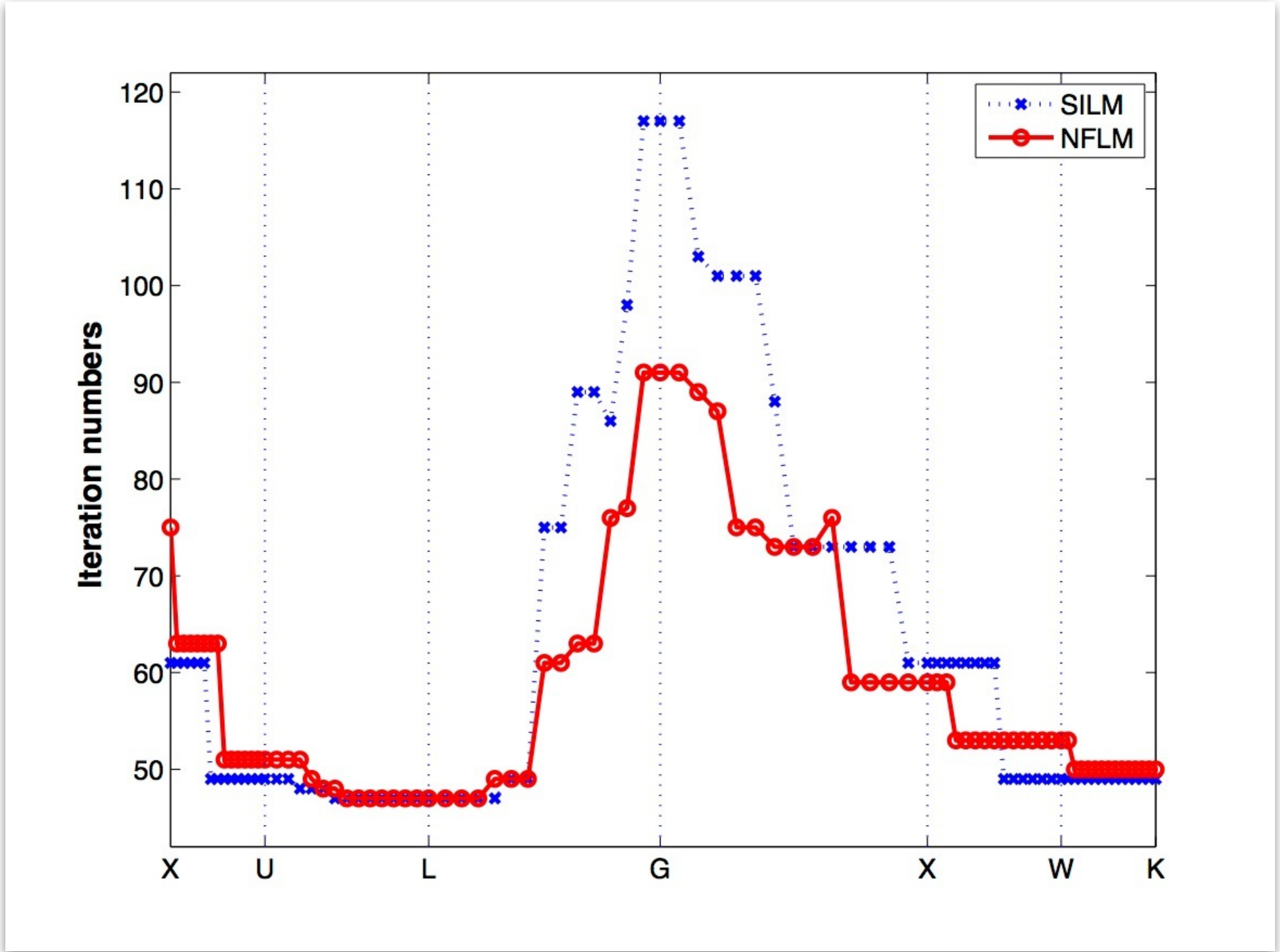
Iteration Numbers

$$A\mathbf{x} = \lambda B\mathbf{x}$$

$$\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}$$

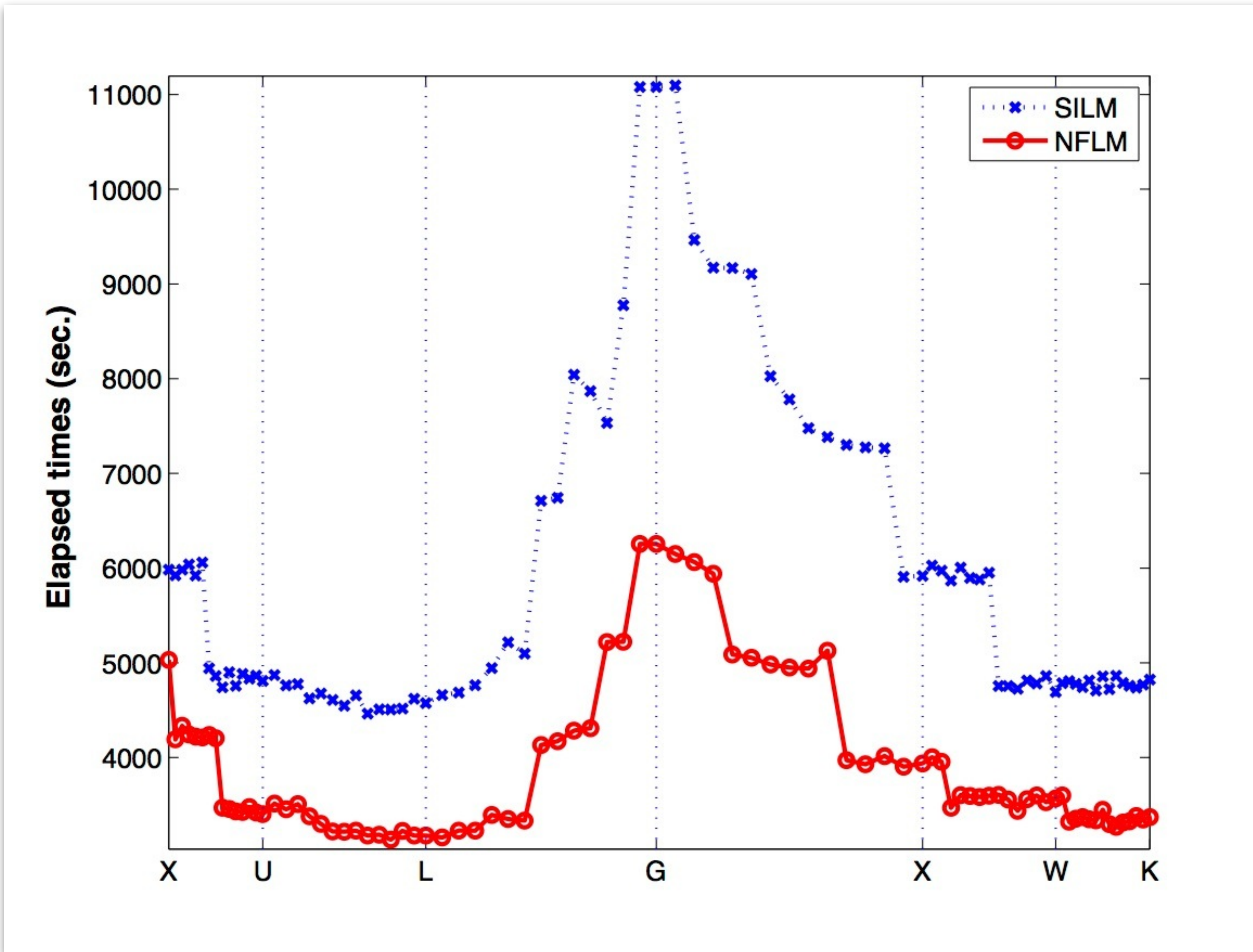
$$(A - \sigma B)\mathbf{z} = \mathbf{b}$$



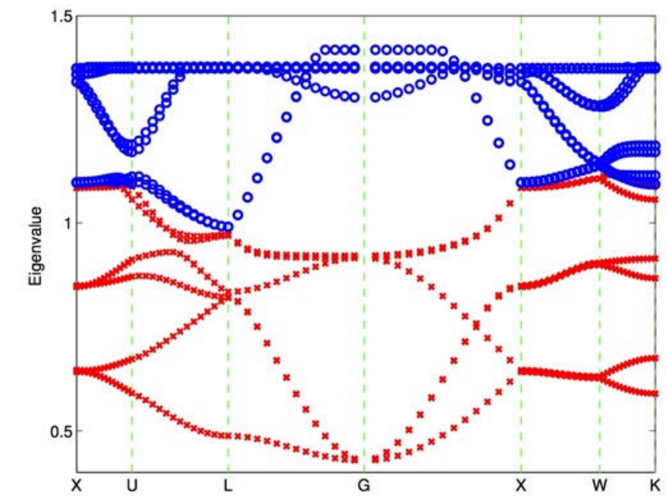


CPU Time Comparison

$$\boxed{A\mathbf{x} = \lambda B\mathbf{x}} \longleftrightarrow \boxed{\left(\Lambda^{\frac{1}{2}} Q_r^* B^{-1} Q_r \Lambda^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y}}$$



Remarks



- Dispersive metallic materials

$$\left(A-\omega^2 B_n-\omega^2\varepsilon(\omega)B_d\right)x=0$$

$$\Rightarrow\quad Ax=\omega\left(\omega B_n+\omega\varepsilon(\omega)B_d\right)x\equiv\omega B(\omega)x$$

$$\Rightarrow\quad \beta(\omega)Ax=B(\omega)x,\quad \beta(\omega)=\frac{1}{\omega}$$

- Linearization

$$\beta Ax=B(\omega_k)x$$

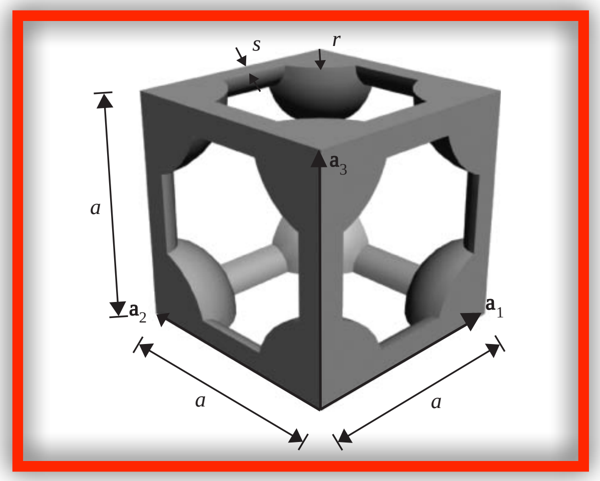
- Newton's method

$$\omega_{k+1}=\omega_k-\left(\beta'(\omega_k)+\omega_k^{-2}\right)^{-1}\left(\beta(\omega_k)-\omega_k^{-1}\right)$$

Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method



Photonic crystals

Numerical results

Complex materials

Numerical results

Complex Materials

- The discretization of

$$\begin{bmatrix} \nabla\times & 0 \\ 0 & \nabla\times \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \imath\omega \begin{bmatrix} \zeta & \mu \\ -\varepsilon & -\xi \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix}$$

leads to the generalized eigenvalue problem:

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \omega \left(\imath \begin{bmatrix} \zeta_d & \mu_d \\ -\varepsilon_d & -\xi_d \end{bmatrix} \right) \begin{bmatrix} E \\ H \end{bmatrix} \equiv \omega B \begin{bmatrix} E \\ H \end{bmatrix}$$

- Singular value decomposition:

$$C = P_r \Sigma_r Q_r^*, \quad C^* = Q_r \Sigma_r P_r^*$$

Null space free eigenvalue problem

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \omega B \begin{bmatrix} E \\ H \end{bmatrix}$$

$$C = P_r \Sigma_r Q_r^* \qquad C^* = Q_r \Sigma_r P_r^*$$

$$\operatorname{span}\left\{ B^{-1}\mathsf{diag}\left(P_r \Sigma_r^{\frac{1}{2}}, Q_r \Sigma_r^{\frac{1}{2}} \right) \right\} = \left\{ \mathbf{x};\ \begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \mathbf{x} = \omega B \mathbf{x}, \omega \neq 0 \right\}$$

$$\operatorname{diag}\left(\Sigma_r^{\frac{1}{2}} Q_r^*, \Sigma_r^{\frac{1}{2}} P_r^* \right) B^{-1} \operatorname{diag}\left(P_r \Sigma_r^{\frac{1}{2}}, Q_r \Sigma_r^{\frac{1}{2}} \right) y = \omega y$$

Null space free generalized eigenvalue problem

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \omega \left(\imath \begin{bmatrix} \zeta_d & \mu_d \\ -\varepsilon_d & -\xi_d \end{bmatrix} \right) \begin{bmatrix} E \\ H \end{bmatrix} \equiv \omega B \begin{bmatrix} E \\ H \end{bmatrix}$$

$$\Phi \equiv \varepsilon_d - \xi_d \mu_d^{-1} \zeta_d \succ 0,$$
$$\mu_d \succ 0, \quad \xi_d^* = \zeta_d.$$

All eigenvalues are real

$$\operatorname{diag}\left(\Sigma_r^{\frac{1}{2}} Q_r^*, \Sigma_r^{\frac{1}{2}} P_r^*\right) B^{-1} \operatorname{diag}\left(P_r \Sigma_r^{\frac{1}{2}}, Q_r \Sigma_r^{\frac{1}{2}}\right) y = \omega y$$

$$\left(\imath \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix} \right) y_r = \omega^{-1} A_r y_r$$

$$A_r \equiv \operatorname{diag}(P_r^*, Q_r^*) \begin{bmatrix} \mu_d^{-1}\zeta_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & \mu_d^{-1} \end{bmatrix} \begin{bmatrix} \xi_d \mu_d^{-1} & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \operatorname{diag}(P_r, Q_r)$$

Advantages

$$\left(\imath \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix}\right) y_r = \omega^{-1} A_r y_r$$

- A_r is Hermitian and positive definite
- We can use the generalized Lanczos method to solve NFGEP
- In each step, we need to solve the linear system

$$\begin{bmatrix} P_r^* & \\ & Q_r^* \end{bmatrix} \begin{bmatrix} \zeta_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & \mu_d^{-1} \end{bmatrix} \begin{bmatrix} \zeta_d^* & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \begin{bmatrix} P_r & \\ & Q_r \end{bmatrix} u = b$$

- Because A_r is Hermitian positive definite, the linear system can be solved by the conjugate gradient method efficiently.

Chiral and pseudochiral media

- Two important complex media with positive ε and $\mu = I_3$
- Isotropic Chiral medium:

$$\xi = \imath\gamma I_3, \quad \zeta = -\imath\gamma I_3$$

- Pseudochiral medium:

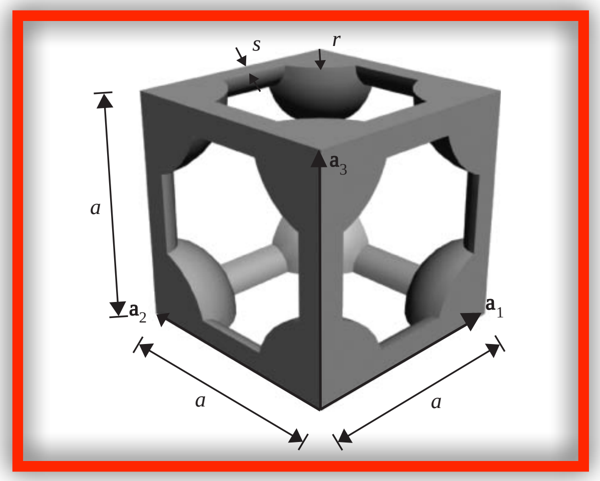
$$\xi = \begin{bmatrix} 0 & 0 & \imath\gamma \\ 0 & 0 & 0 \\ \imath\gamma & 0 & 0 \end{bmatrix}, \quad \zeta = \begin{bmatrix} 0 & 0 & -\imath\gamma \\ 0 & 0 & 0 \\ -\imath\gamma & 0 & 0 \end{bmatrix}$$

- $\Phi = \varepsilon_d - \xi_d\mu_d^{-1}\zeta_d = \varepsilon_d - \xi_d\zeta_d$ is a positive diagonal matrix provided $\gamma \in (0, \sqrt{\varepsilon_i})$
- All eigenvalues are real

Explicit Represent. of matrices

Eigen-decomposition of double-curl and SVD of single-curl

Null-space free method



Photonic crystals

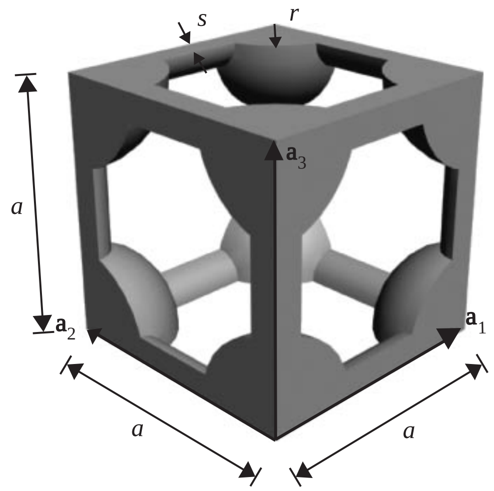
Numerical results

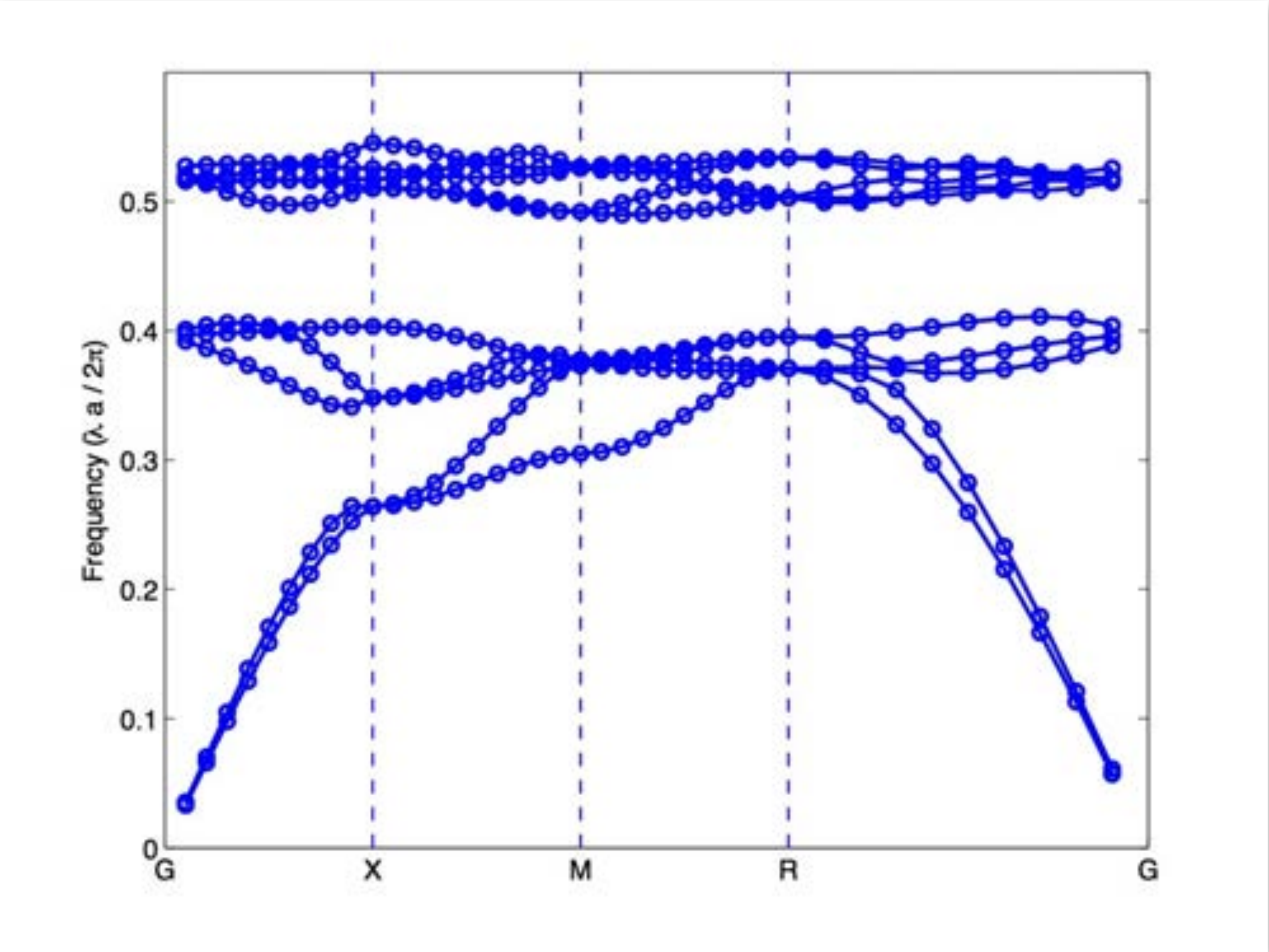
Complex materials

Numerical results

Bandgap Diagram of SC Lattice

- Dim. of coefficient matrix A_r : 8,388,608
- 39 test problems with $(\varepsilon_i, \varepsilon_o, \gamma) = (13, 1, 0.5)$
- Chiral medium





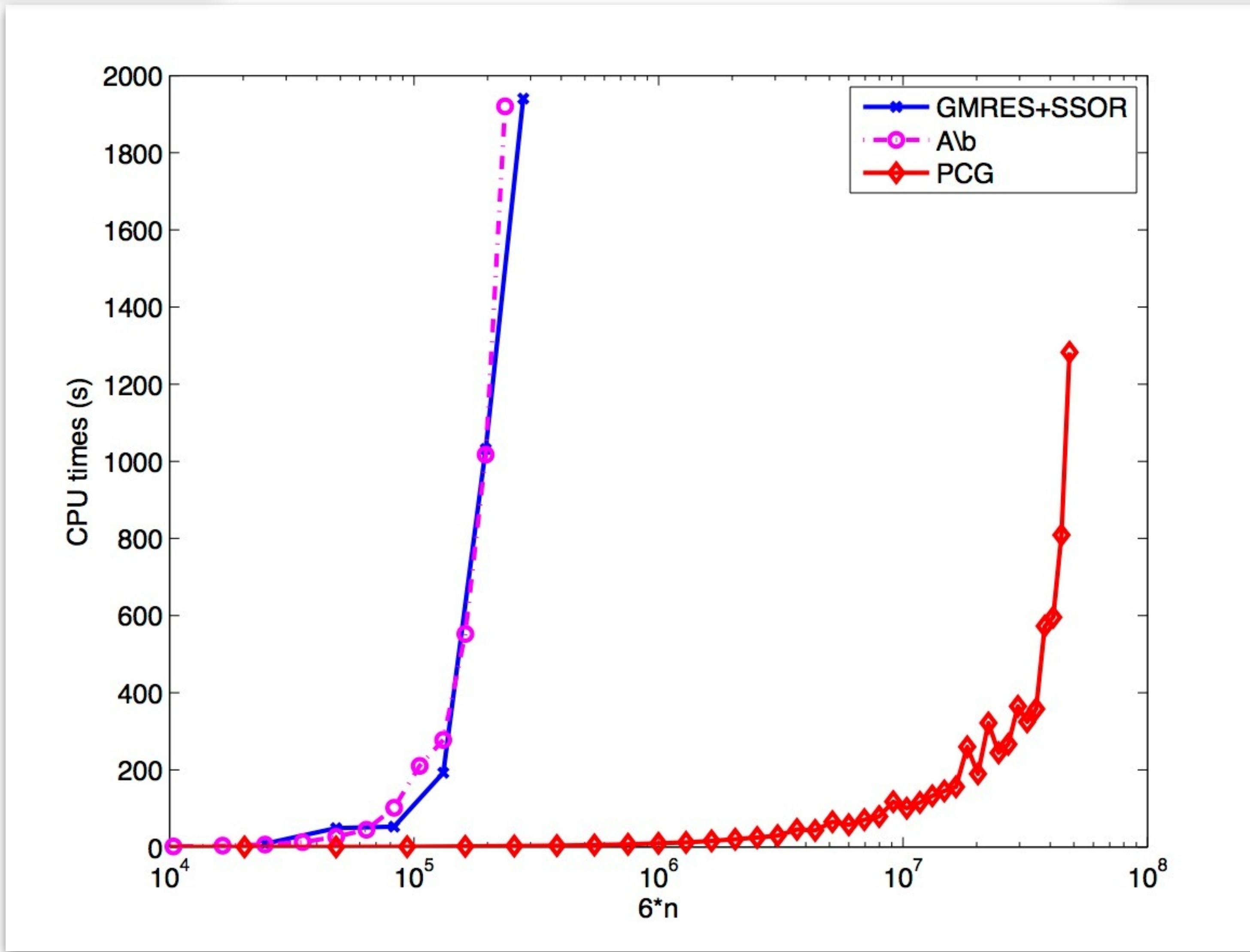
Comparison for Solving Linear Sys.

$$\left(\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} - \sigma \begin{bmatrix} \zeta_d & I_{3n} \\ -\varepsilon_d & -\xi_d \end{bmatrix}\right) y = b$$

$$\begin{bmatrix} P_r^* & \\ & Q_r^* \end{bmatrix} \begin{bmatrix} \zeta_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & \mu_d^{-1} \end{bmatrix} \begin{bmatrix} \zeta_d^* & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \begin{bmatrix} P_r & \\ & Q_r \end{bmatrix} u = b$$

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \omega B \begin{bmatrix} E \\ H \end{bmatrix}$$

$$\left(\imath \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix}\right) y_r = \omega^{-1} A_r y_r$$



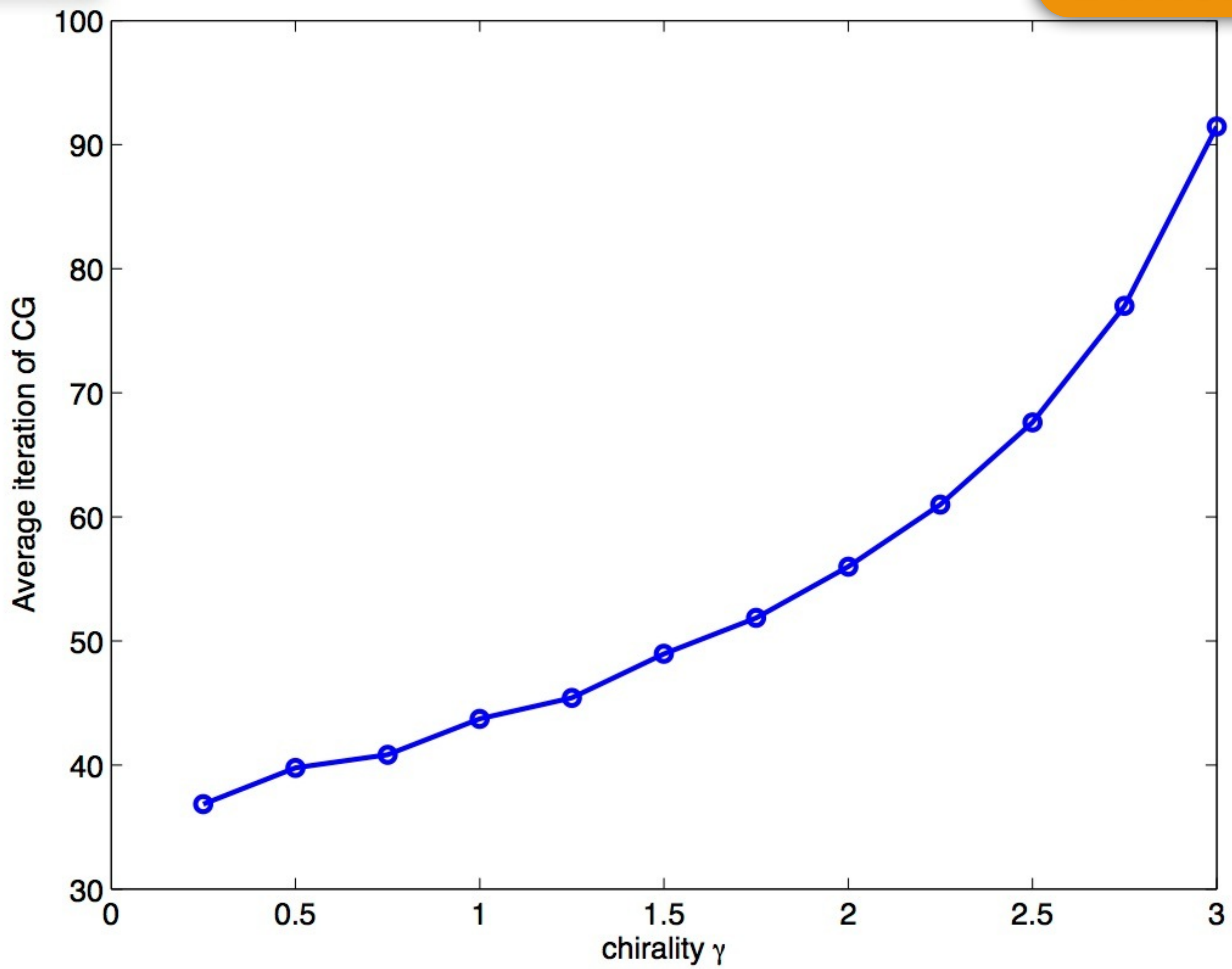
Iteration Numbers of Solving Linear Systems

$$\begin{bmatrix} P_r^* & \\ & Q_r^* \end{bmatrix} \begin{bmatrix} \zeta_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & \mu_d^{-1} \end{bmatrix} \begin{bmatrix} \zeta_d^* & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \begin{bmatrix} P_r & \\ & Q_r \end{bmatrix} u = b$$

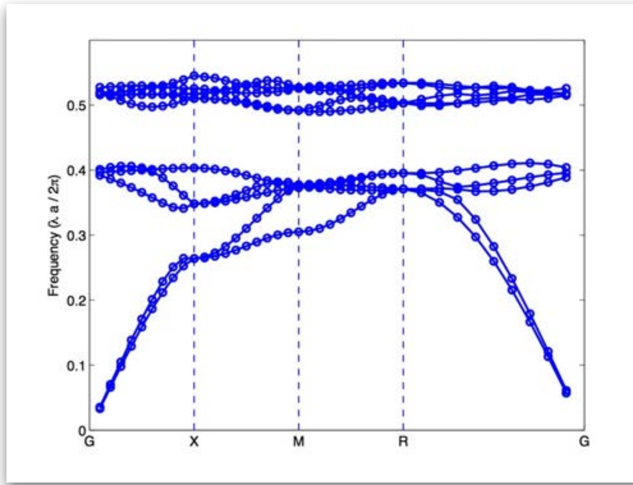
$$(\varepsilon_i, \varepsilon_o, \gamma) = (13, 1, \gamma)$$

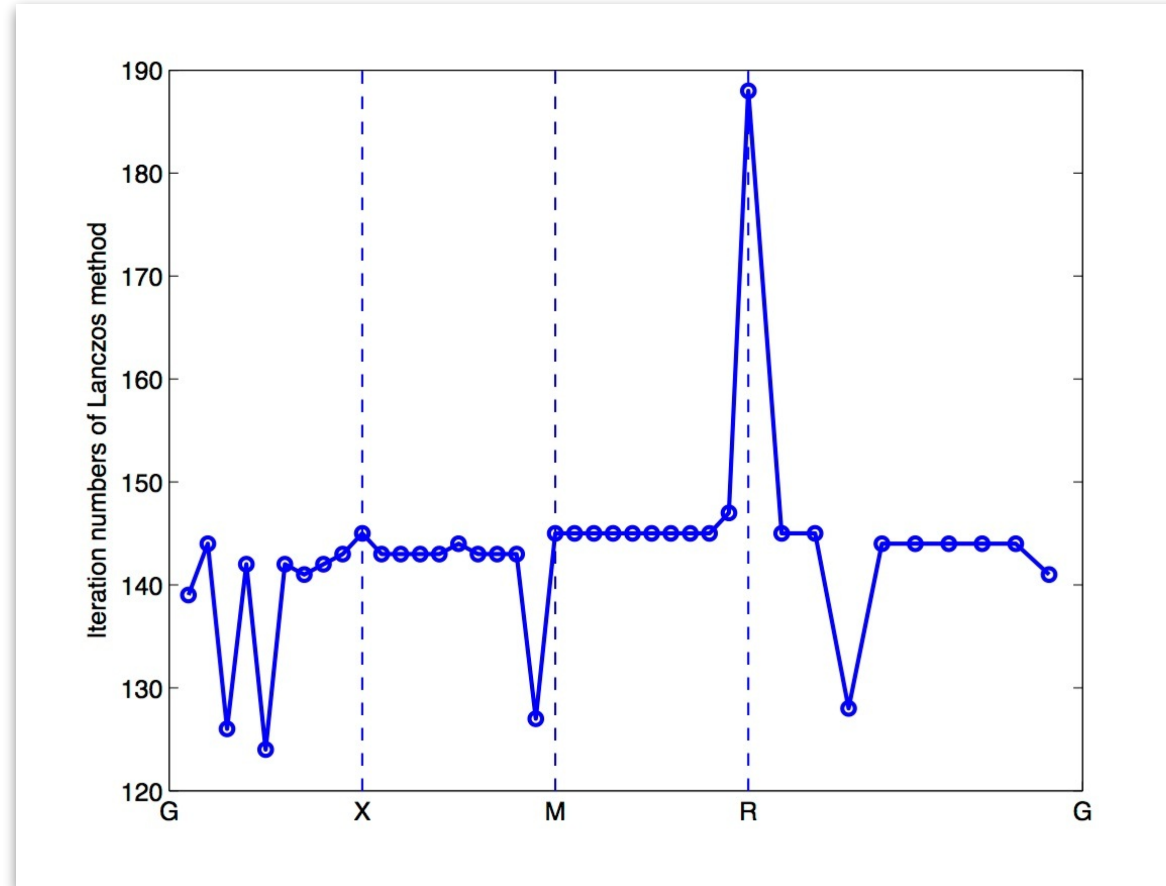
$$\xi = \imath\gamma I_3, \quad \zeta = -\imath\gamma I_3$$

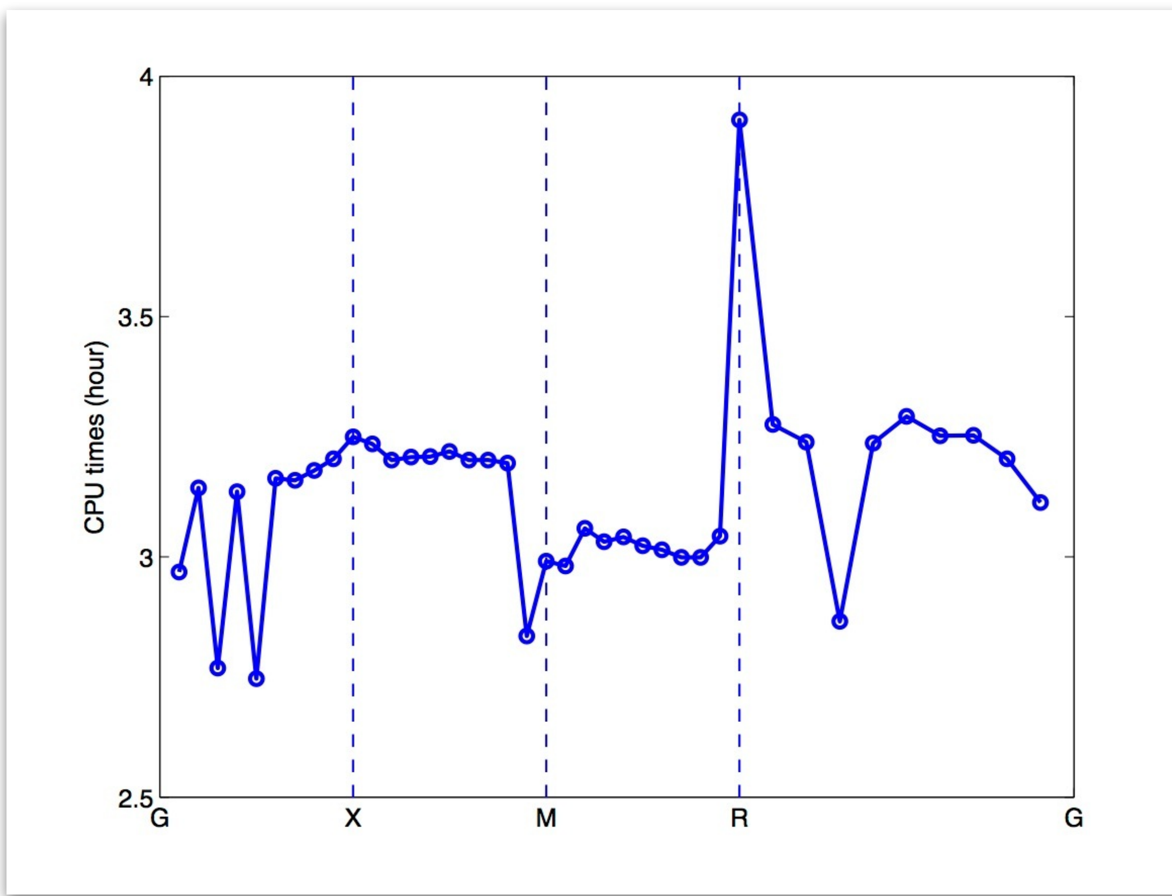
Dimension = 8,388,608



CPU Time for Solving Eig. Prob.







$$\left(\imath \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix} \right) y_r = \omega^{-1} A_r y_r$$

Dimension = 8,388,608

Summary

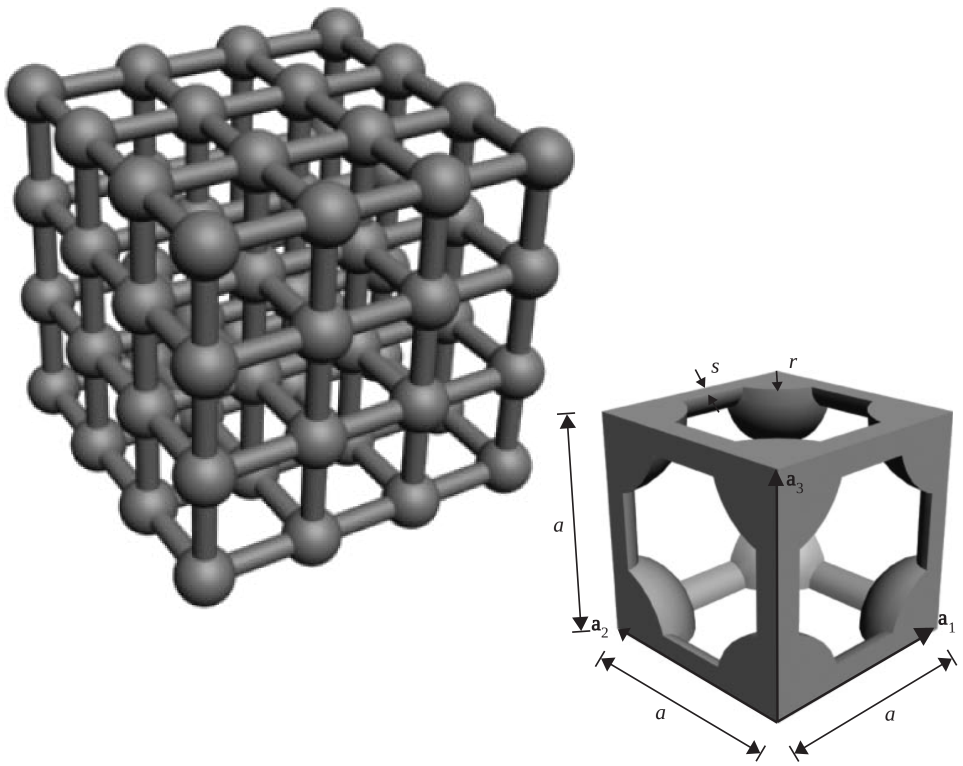
Conclusion

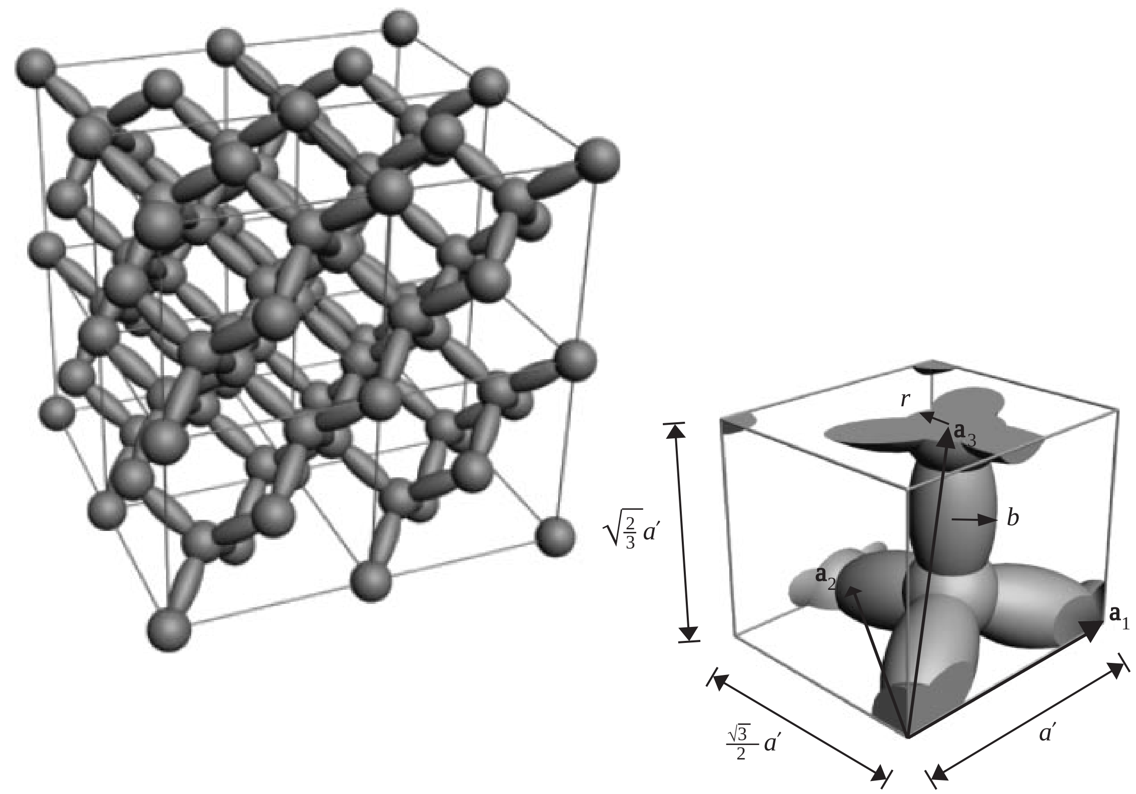
- Explicit representation and eigen-decomposition of the discrete double-curl matrix A
- FFT-based preconditioner for metallic materials
- Singular value decomposition of discrete single-curl operator
- Null-space free methods
  - The $3n \times 3n$ GEVP is reduced to $2n \times 2n$ SEVP for photonic crystals
  - The $6n \times 6n$ GEVP is reduced to $4n \times 4n$ GEVP for complex media
  - No zero eigenvalues in the reduced eigenvalue problems
    - Well-conditioned linear systems
    - Efficient FFT based algorithms

Thank you.

Photonic Crystals

- Periodic lattice composed of dielectric or metallic materials





- If we design a three-dimensional photonic crystal appropriately, there appears a frequency range where no electromagnetic eigenmode exists. Frequency ranges of this kind are called photonic band gaps.

- Light waves can be reflected, trapped, transported in photonic crystals.

Bandgap Maximization

- For SC, depends on radius of “ball” & “cylinder”
- $\max_{r,s}(\min(\lambda_{i+1})-\max(\lambda_i))$.
- Many eigenvalue problems for the band structure

Silicon-Air ($\epsilon : \epsilon_0 = 13 : 1$)

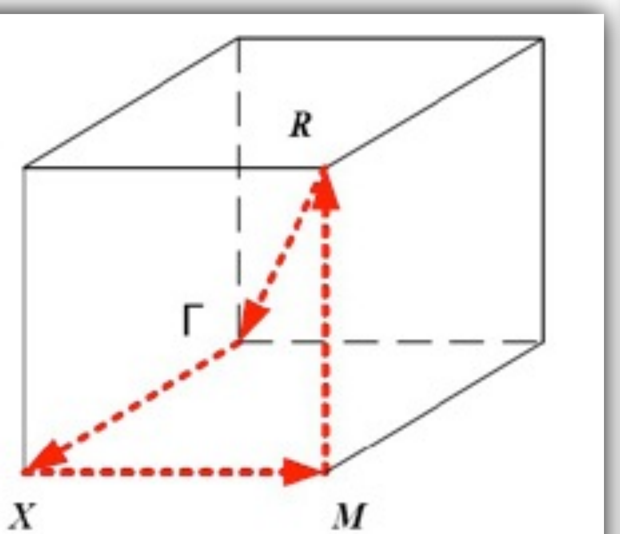
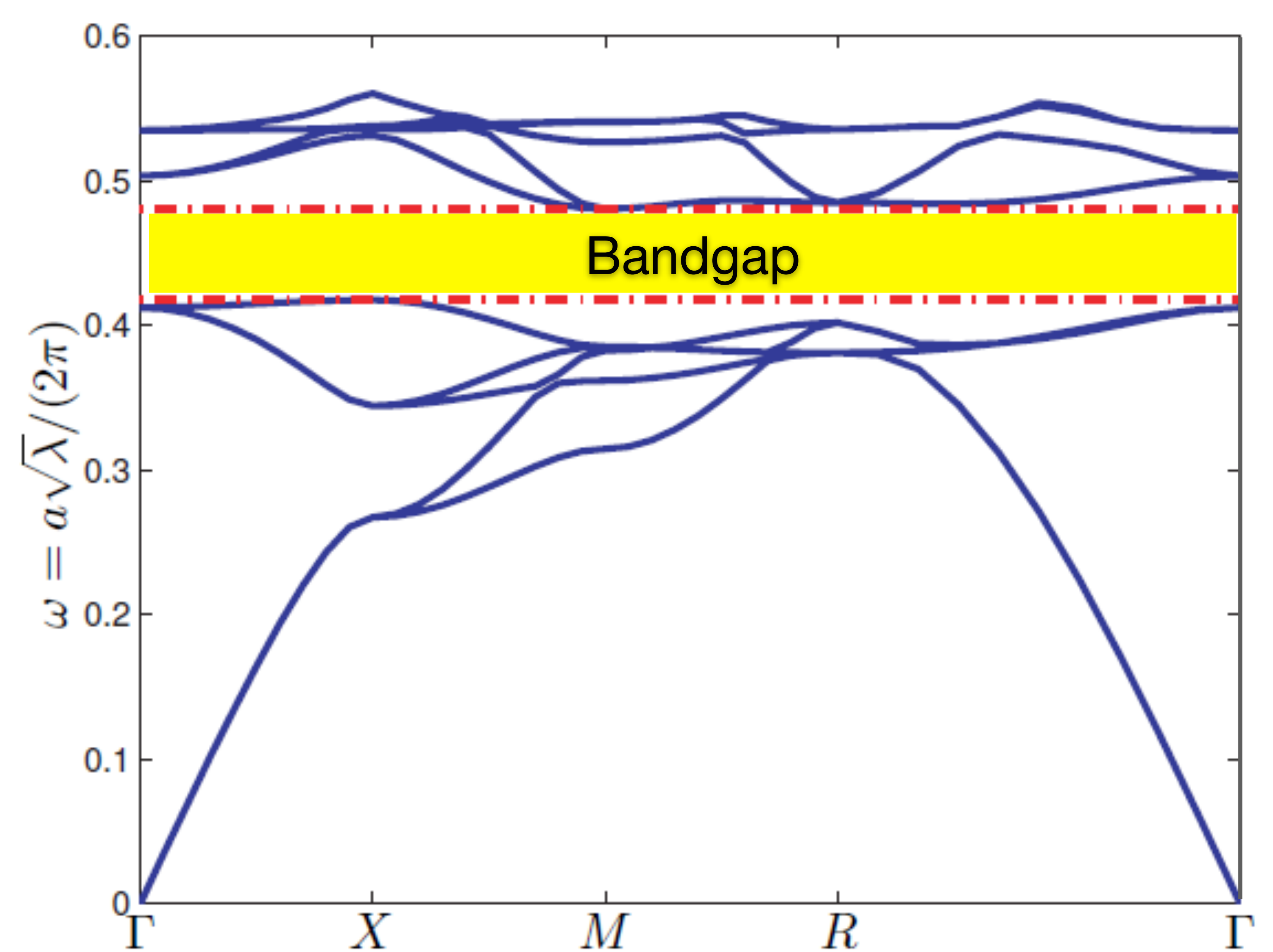


Figure: The varying of the wave vector k



Numerical Challenges

- Yee's scheme discretizes the equation

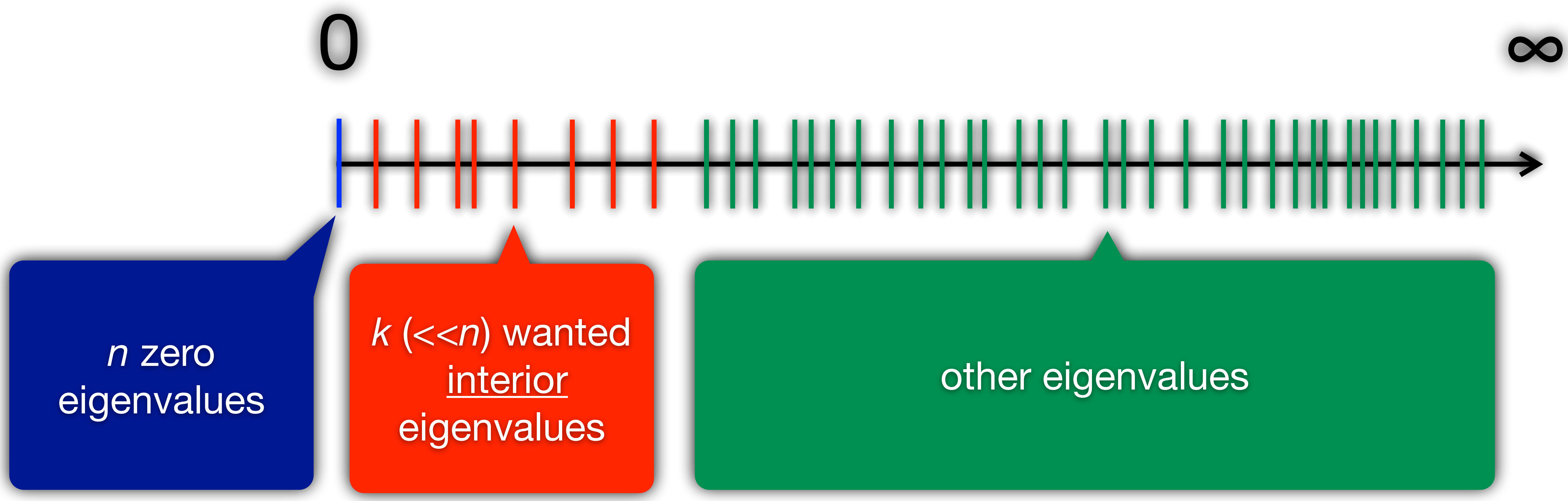
$$\boxed{\nabla \times \nabla \times} \tilde{E}(\mathbf{x}) = \boxed{\mu_0 \omega^2} \boxed{\varepsilon(\mathbf{x})} \tilde{E}(\mathbf{x})$$

to get the generalized eigenvalue problem (GEVP)

$$A\mathbf{x} = \lambda B\mathbf{x} \quad Ax = \lambda Bx$$

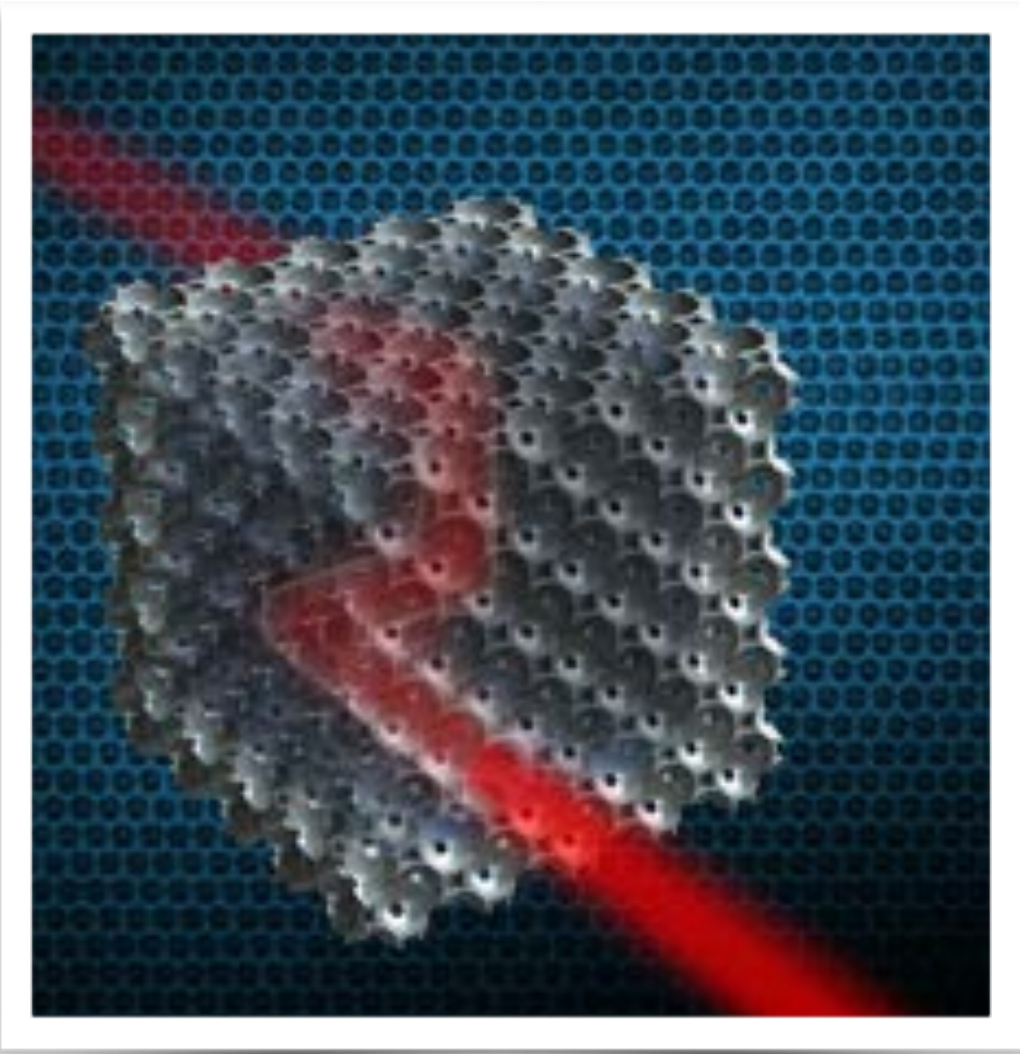
- A: complex Hermitian positive semi-definite
- B: positive diagonal (containing magnetic constant, frequency, material dependent permittivity)
- Dimension: 3n ($n=n_1 n_2 n_3$, i.e. order 3)
- Need a few of smallest (interior) positive eigenvalues

Challenge: Multiple Zero Eigenvalues



Backup Slides

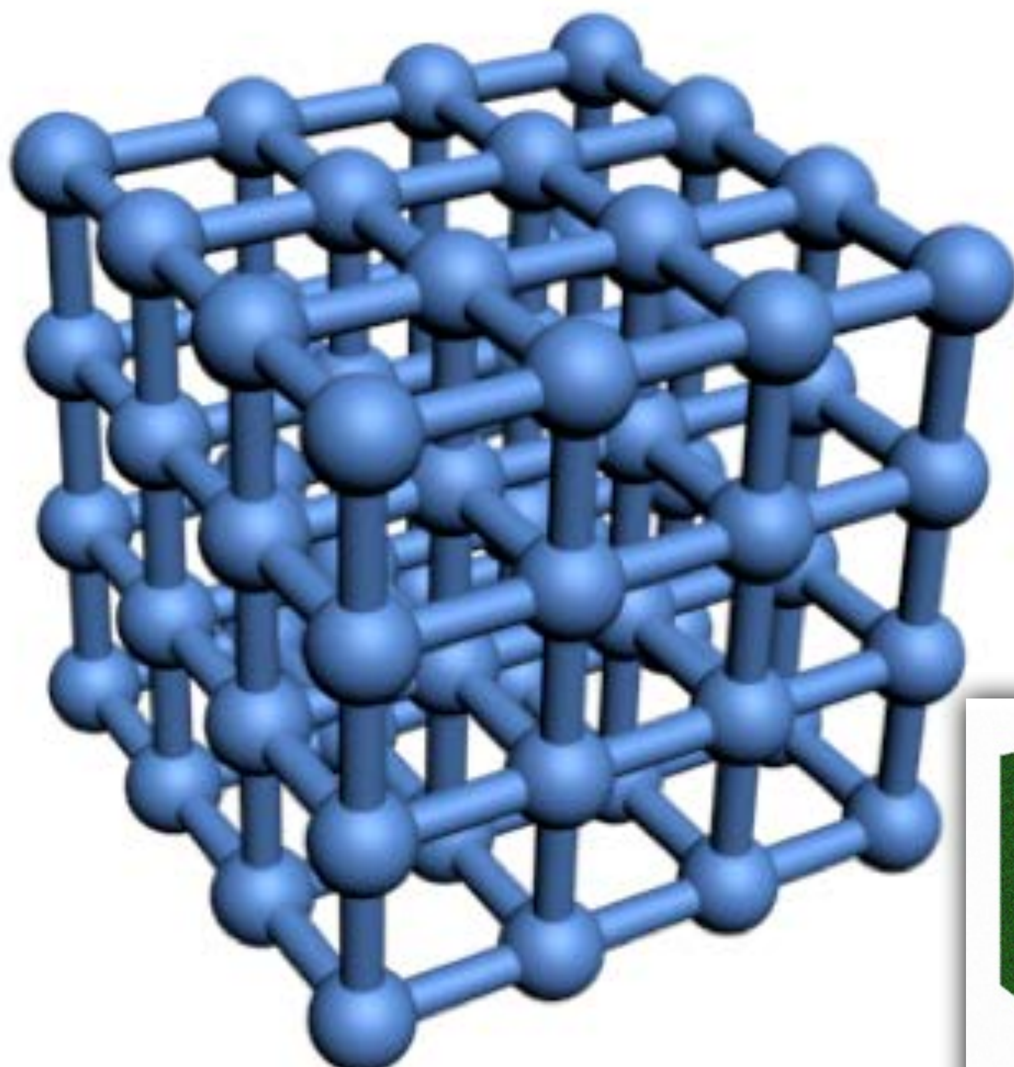
Perodic Lattice

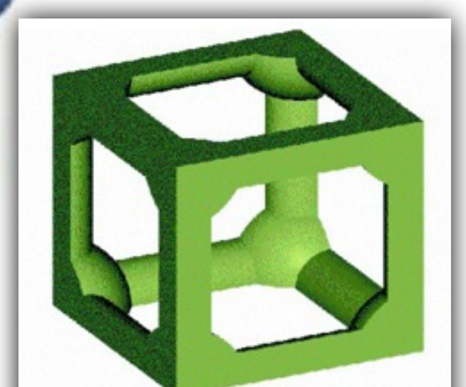


Preconditioning in SC

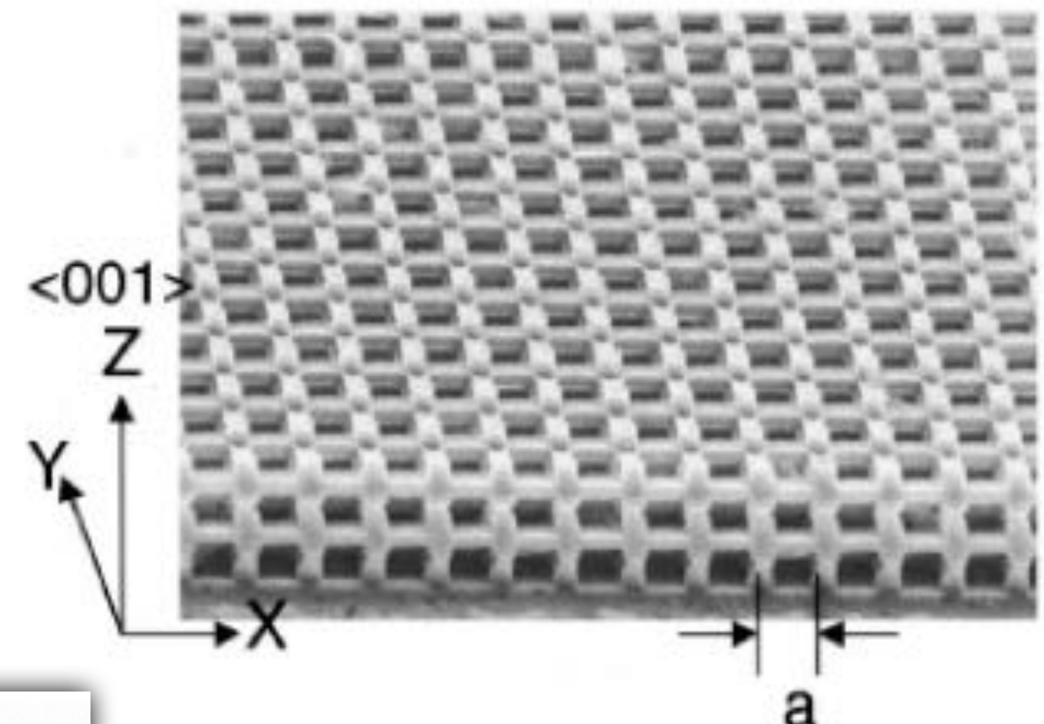
Simple Cubic Photonic Crystal

- Spheres (radius r) connected with cylinders (radius s)



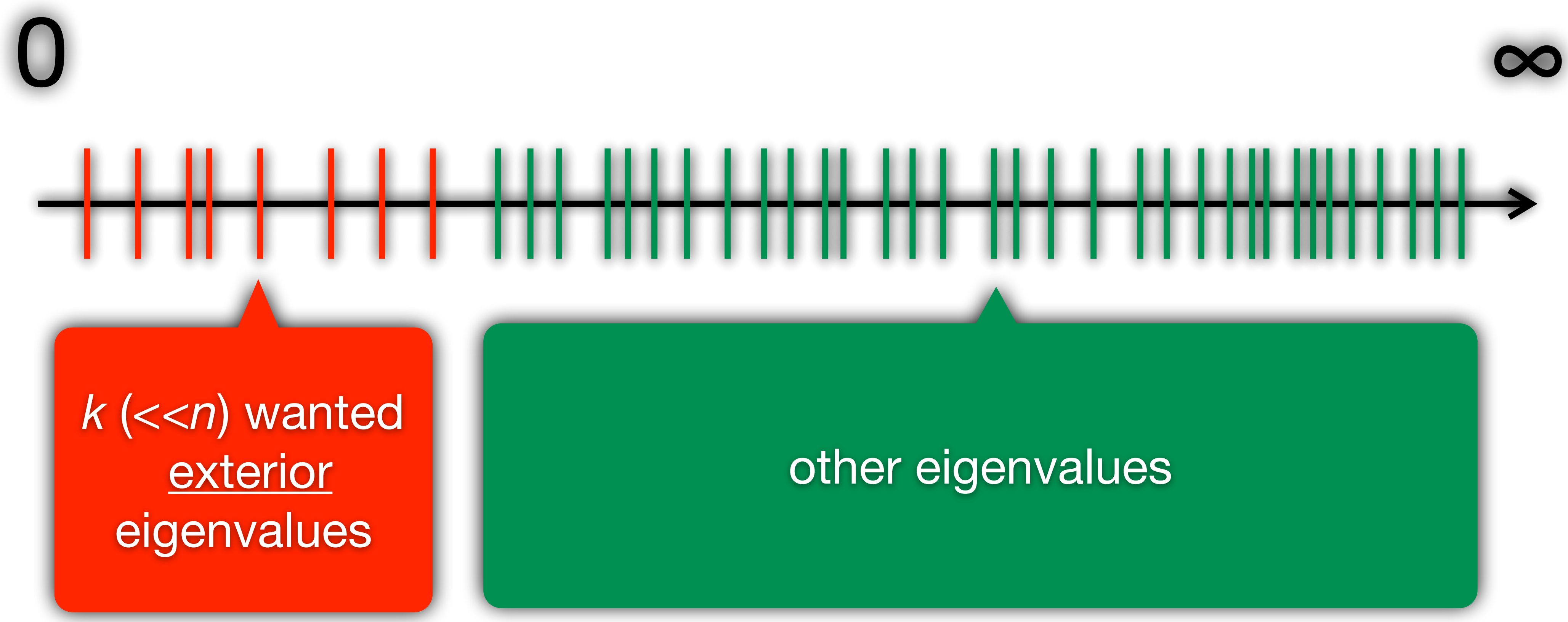


Silicon-Air ($\epsilon : \epsilon_0 = 13 : 1$)



Microfabrication
Size: 1μm

Biswas et al. (PRB, 2002)


0
∞
k (<<n) wanted exterior eigenvalues
other eigenvalues