Nanophotonic Modeling Lecture 1.17: Targeted Eigensolvers

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Targeted Eigensolvers

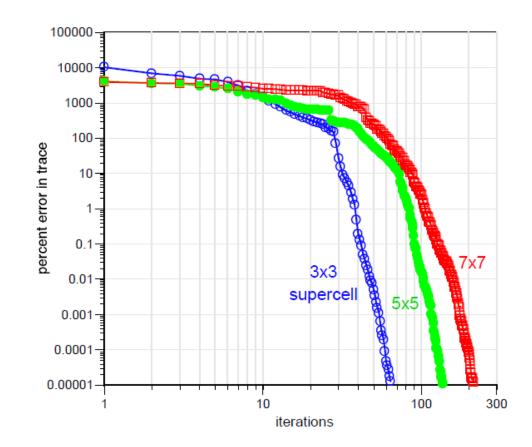
 To find a single defect state in a photonic crystal, use a supercell and shift the target of the eigensolver via:

$$\hat{A}'_{\vec{k}} = \left(\hat{A}_{\vec{k}} - \frac{\omega_m^2}{c^2}\right)^2$$

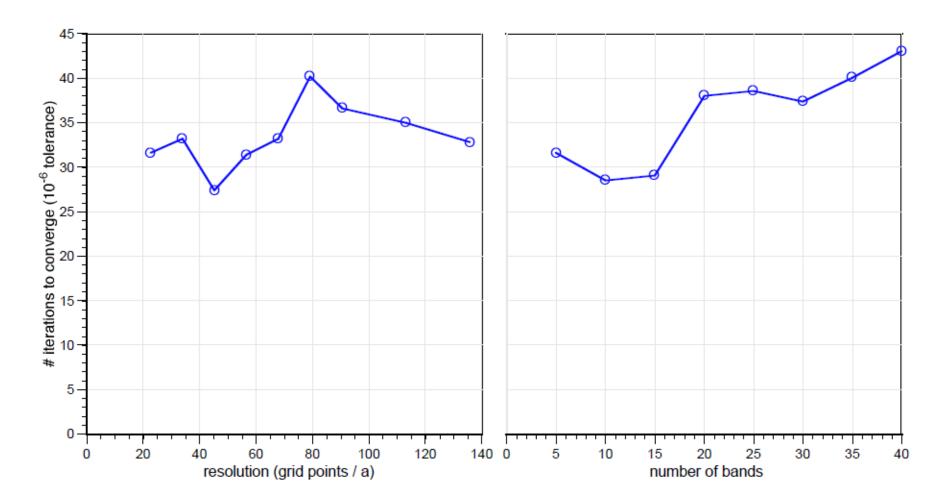
• This yields the same eigenvectors, but shifted eigenvalues-can easily return to original basis

Targeted Eigensolvers

Convergence of targeted eigensolver as the supercell grows still reasonable



Eigensolver Performance



PurdueX 540: Nanophotonic Modeling, Prof. Bermel

Reformulating the Eigenproblem

• Magnetic field in planewave basis:

$$|H_{\vec{k}}\rangle \cong \sum_{\{m_j\}} \vec{h}_{\{m_j\}} e^{i\sum_{j,k} m_j \vec{G}_j \cdot n_k \vec{R}_k / N_k} = \sum_{\{m_j\}} \vec{h}_{\{m_j\}} e^{2\pi i \sum_j m_j n_j / N_j}$$

• Operator scales like $\mathcal{O}(N \log N)$:

$$A_{\ell m} = -\left(\vec{k} + \vec{G}_{\ell}\right) \times \cdots \operatorname{IFFT} \cdots \widetilde{\varepsilon^{-1}} \cdots \operatorname{FFT} \cdots \left(\vec{k} + \vec{G}_{m}\right) \times$$

- Tensor-based averaging aids in convergence: $\widetilde{\varepsilon^{-1}} = \overline{\varepsilon^{-1}}P + \overline{\varepsilon}^{-1}(1-P) \qquad P_{ij} = n_i n_j$
- MPB performs conjugate-gradient minimization of Block Rayleigh quotient