



DFG Research Center MATHEON
mathematics for key technologies
and
Zuse Institute Berlin



Finite Element Methods for Optical Device Design

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Computational **CNO**
Nano-Optics

<http://www.zib.de/nano-optics>

JCM wave

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Outline

1. Finite Element Method

- Variational Formulation
- Vectorial Finite Elements (Nedelec's Edge Elements)
- Adaptivity

2. Scattering Problems

- Metamaterials
- Photomasks

3. Eigenvalue/Resonance Problems

- Photonic Crystals
- Resonators

Time Harmonic Maxwell's Equations

$$\begin{aligned}\mathbf{H}(\vec{x}, t) &= e^{-i\omega t} \mathbf{H}(\vec{x}), \\ \mathbf{E}(\vec{x}, t) &= e^{-i\omega t} \mathbf{E}(\vec{x})\end{aligned}$$

yield:

$$\begin{aligned}\nabla \times \frac{1}{\epsilon} \nabla \times \mathbf{H} &= \omega^2 \mu \mathbf{H}, \\ \nabla \cdot \mu \mathbf{H} &= 0 \\ \nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} &= \omega^2 \epsilon \mathbf{E} \\ \nabla \cdot \epsilon \mathbf{E} &= 0\end{aligned}$$

Variational Formulation

Simple example:

$$\begin{aligned}\nabla \times \frac{1}{\varepsilon_r} (\nabla \times \mathbf{H}) - \mu_0 \varepsilon_0 \omega^2 \mathbf{H} &= \mathbf{F} \\ \mathbf{n} \times \mathbf{H} &= 0 \quad \text{on } \Gamma = \partial\Omega\end{aligned}$$

Define quantities:

$$\begin{aligned}a(\mathbf{u}, \mathbf{v}) &= \int_{\Omega} \frac{1}{\varepsilon_r} (\nabla \times \mathbf{u}) \cdot \overline{(\nabla \times \mathbf{v})} \, dx - \mu_0 \varepsilon_0 \omega^2 \int_{\Omega} \mathbf{u} \cdot \overline{\mathbf{v}} \, dx \\ (\mathbf{u}, \mathbf{v}) &= \int_{\Omega} \mathbf{u} \cdot \overline{\mathbf{v}} \, dx \\ d(\mathbf{u}, q) &= \int_{\Omega} \mathbf{u} \cdot \overline{\nabla q} \, dx.\end{aligned}$$

Variational Formulation

Simple example:

$$\begin{aligned}\nabla \times \frac{1}{\varepsilon_r} (\nabla \times \mathbf{H}) - \mu_0 \varepsilon_0 \omega^2 \mathbf{H} &= \mathbf{F} \\ \mathbf{n} \times \mathbf{H} &= 0 \quad \text{on } \Gamma = \partial\Omega\end{aligned}$$

Variational form:

Find $\mathbf{u} \in V^0$ such that $a(\mathbf{u}, \mathbf{v}) = (\mathbf{F}, \mathbf{v})$ for all $\mathbf{v} \in H(\text{curl}, \Omega)$

$$\begin{aligned}H(\text{curl}, \Omega) &= \{\mathbf{v} \in \mathbf{L}^2(\Omega) \mid \text{curl } \mathbf{v} \in \mathbf{L}^2(\Omega)\} \\ V^0 &= \{\mathbf{w} \in H(\text{curl}, \Omega) \mid d(\mathbf{w}, q) = 0 \quad \forall q \in H^1\}.\end{aligned}$$

Galerkin Method

$\psi_1, \dots, \psi_N \in H(\text{curl})$ ansatz functions. Approximate solution:

$$u = \sum_{i \leq N} c_i \psi_i$$

Galerkin method: Project variational problem onto subspace V spanned by the ansatz functions $\psi_1, \dots, \psi_N$:

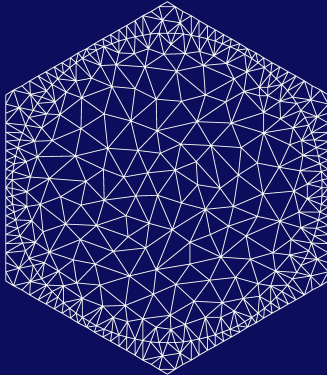
$$a(u, \psi_j) = (\mathbf{F}, \psi_j) \quad \forall \psi_j \in V$$

$$\begin{aligned} A_{i,j} &= a(\psi_i, \psi_j) \\ b_j &= (\mathbf{F}, \psi_j) \end{aligned}$$

Algebraic problem:

$$\implies Au = b, \quad u = [c_1, \dots, c_N]$$

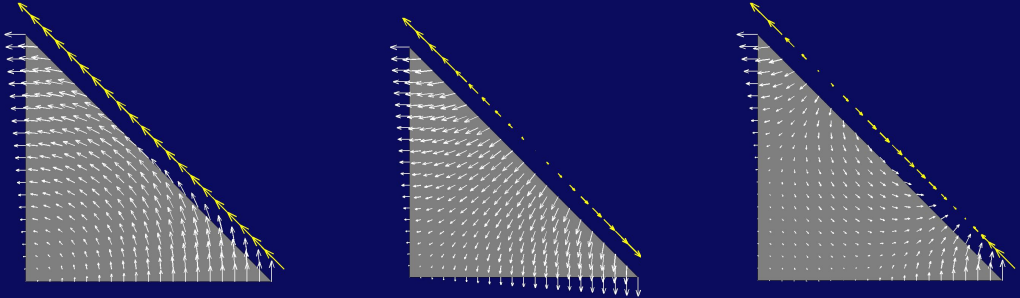
Triangulation



Decomposition of the computational domain (triangles, tetrahedra, etc.)

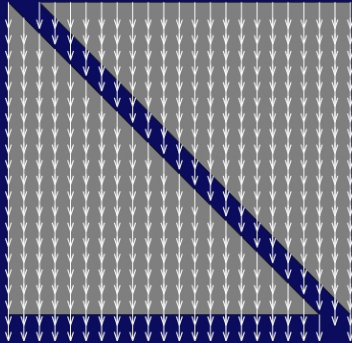
- $\mathbf{H}$ and $\mathbf{E}$ are only tangentially continuous on material boundaries.
- Normal component jumps across material interfaces.

Edge Elements



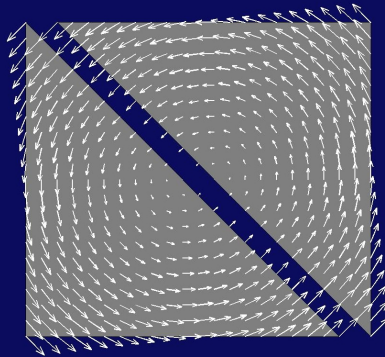
- Edge elements (Nedelec 1980)
- Elements of order 0, 1, 2 with respect to the **tangential** component of the “diagonal” edge

Curl-Free and Div-Free Fields



curl-free field:

$$\begin{aligned}\text{curl } \mathbf{E} &= 0 \\ \mathbf{E} &= -\nabla\phi\end{aligned}$$

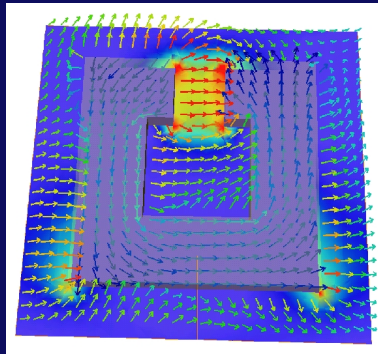


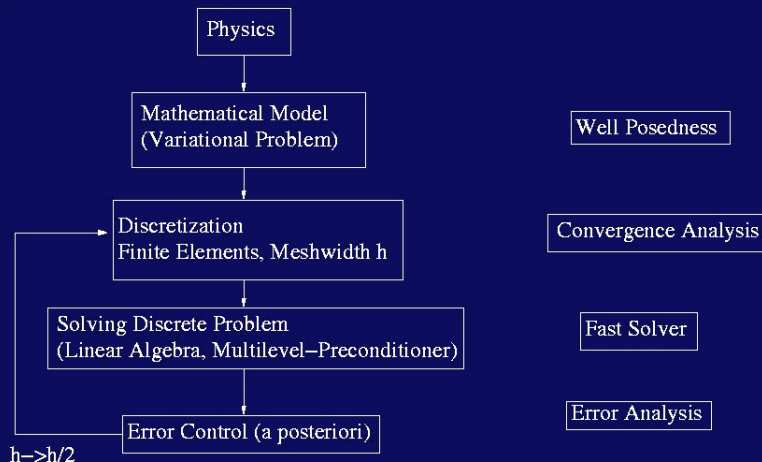
div-free field:

$$\begin{aligned}\text{div } \mathbf{E} &= 0 \\ \mathbf{E} &= \nabla \times \mathbf{W}\end{aligned}$$

Field on Elementary Ring Resonator

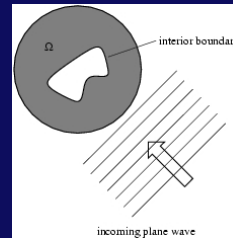
Global field composed from fields on local patches:





Scattering Problem

Scattering of a plane wave
on a bounded obstacle



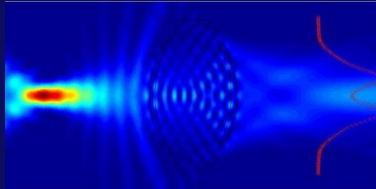
Task: Compute $\mathbf{H}$ on Ω from

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \omega^2 \mu \mathbf{H} = 0,$$

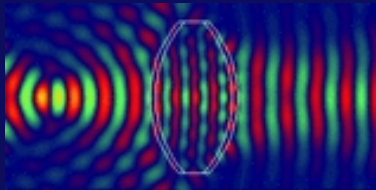
$$\nabla \cdot \mu \mathbf{H} = 0$$

- + incident field and its normal derivative on $\partial\Omega$
- + inner boundary conditions
- + (quasi periodic boundary conditions)
- + transparent boundary conditions

Beam Passing a Plane Lens



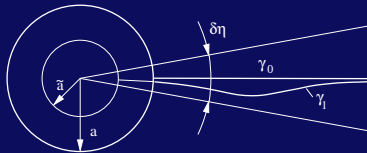
Micro lens embedded in free space: intensity



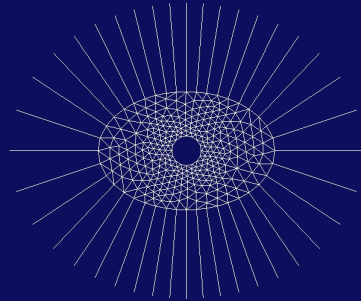
Micro lens embedded in free space: phase

Basic idea: PML and Pole Condition

PML: Consider complex continuation
on exterior rays



Curved ray

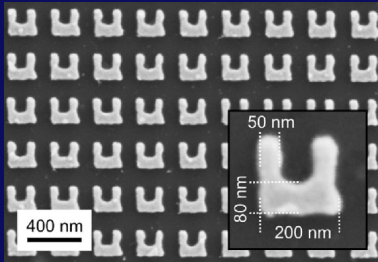


Straight rays

Pole condition: Consider Laplace transform
on exterior rays

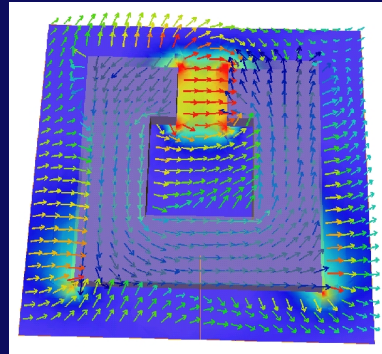
Scattering Problems: Metamaterials

Periodic array:

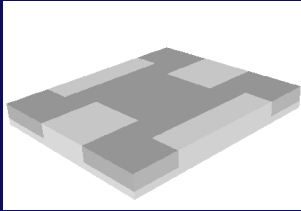


SEM of miniaturized gold split-ring resonators with dimension smaller than optical wavelength (courtesy of CFN Karlsruhe).

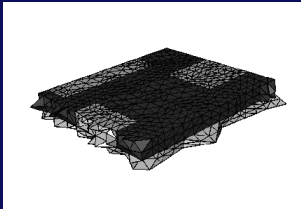
Field on elementary cell:



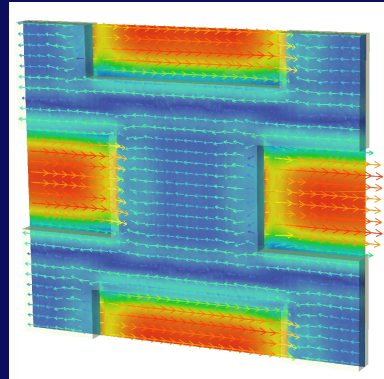
Photomask Simulation



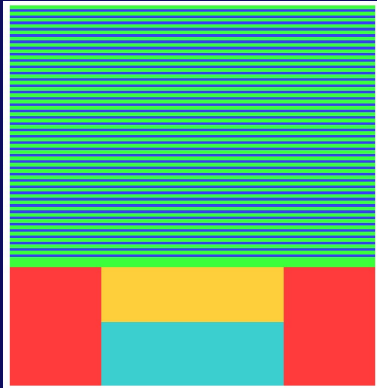
3D geometry



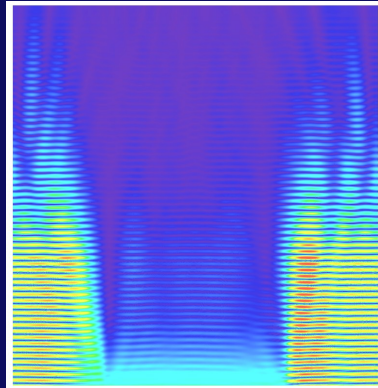
Triangulation



Scattering Problems: EUV Lithography

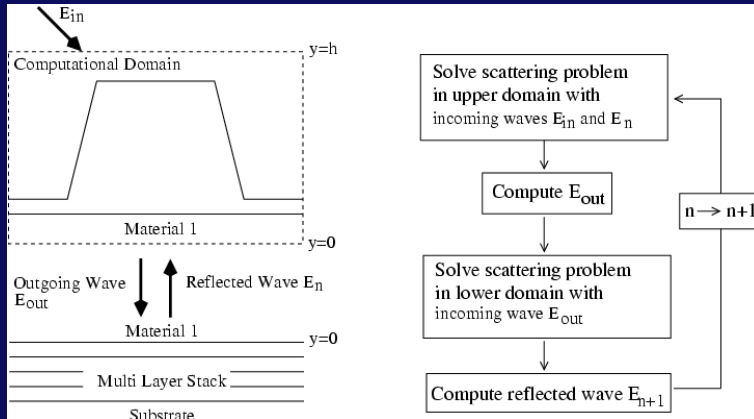


Line mask with EUV grating



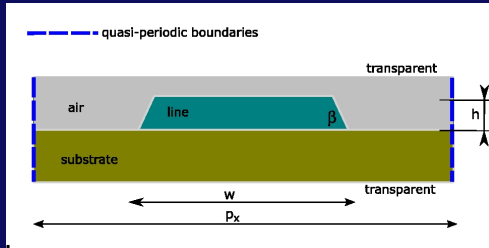
Field distribution

EUV Domain Decomposition

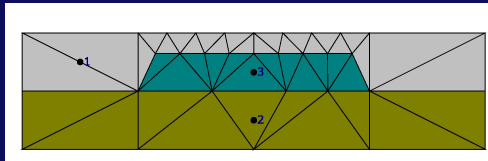


→ Talk by Lin Zschiedrich this morning!

Photomask simulation - geometry 2D

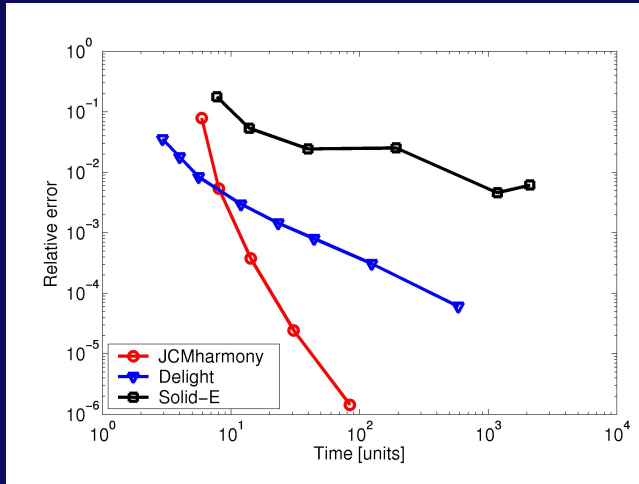


2D geometry

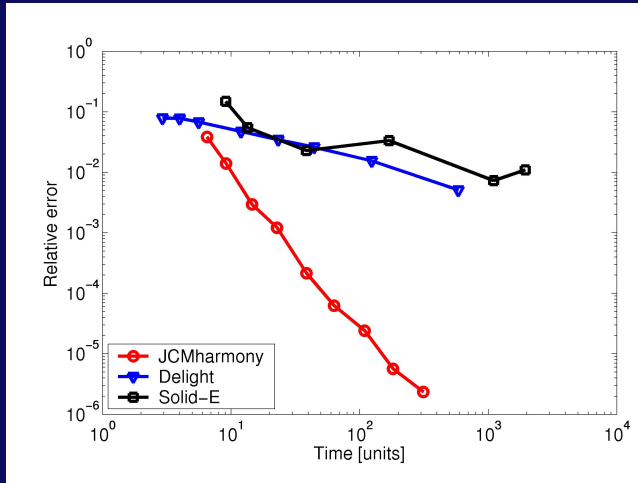


Triangulation

Benchmark Photomask Simulation 2D - TE

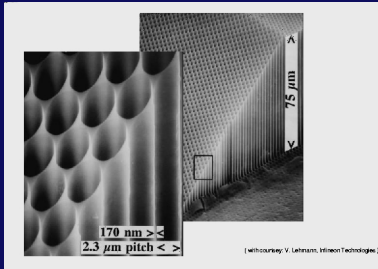


Benchmark Photomask Simulation 2D - TM



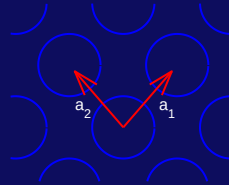
Eigenvalue Problems: Bloch Modes

Periodic materials:



2D Photonic crystal (courtesy of V. Lehmann, Infineon Technologies).

Bloch periodicity:



$$\vec{a}_{mn} = m\vec{a}_1 + n\vec{a}_2, m, n \in \mathbb{Z}$$

$$\epsilon(\vec{x}) = \epsilon(\vec{x} + \vec{a}_{mn}),$$

$$\mu(\vec{x}) = \mu(\vec{x} + \vec{a}_{mn})$$

$$\mathbf{H}(\vec{x} + \vec{a}_{mn}) = e^{i\vec{k} \cdot \vec{a}_{mn}} \mathbf{H}(\vec{x}).$$

Eigenvalue Problems: Bloch Modes

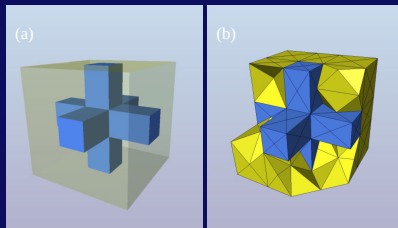
Lattice periodic field: $\mathbf{h}(\vec{x}) = e^{-i\vec{k}\cdot\vec{x}}\mathbf{H}(\vec{x})$

$$\begin{aligned} \Rightarrow \left(\nabla \times + i\vec{k} \times\right) \frac{1}{\varepsilon} \left(\nabla \times + i\vec{k} \times\right) \mathbf{h} &= \omega^2 \mu \mathbf{h}, \\ \left(\nabla \cdot + i\vec{k} \cdot\right) \mu \mathbf{h} &= 0 \\ &+ \text{quasi-periodic boundary conditions} \\ &+ \text{(transparent boundary conditions).} \end{aligned}$$

Tasks:

- Given $\vec{k}$, compute the Blochvector $\mathbf{h}$ and the positiv real number ω^2 , or,
- Given ω^2 , compute the Blochvector $\mathbf{h}$ and the complex wavevector $\vec{k}$

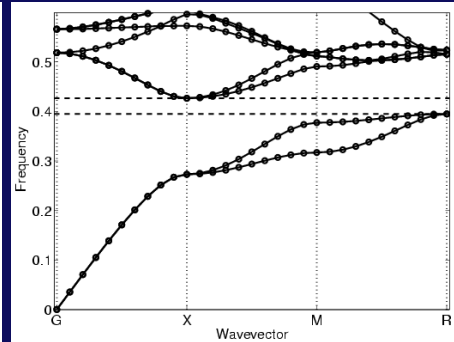
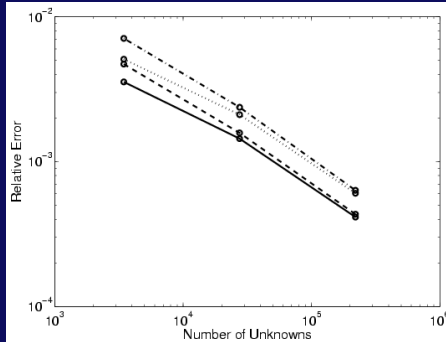
Example: Scaffold (3D)



First eigenvalues at X -Point

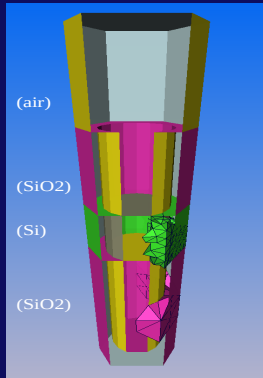
Step	N° DOF	CPU time	$\tilde{\omega}_1$	$\tilde{\omega}_2$	$\tilde{\omega}_3$	$\tilde{\omega}_4$
0	3450	00:00:22.95	2.73648e-01	2.73967e-01	4.27901e-01	4.28753e-01
1	27572	00:07:36.46	2.73074e-01	2.73113e-01	4.26632e-01	4.26746e-01
2	220520	01:04:18.70	2.72794e-01	2.72801e-01	4.25991e-01	4.26006e-01
3	1764048	08:48:01.65	2.72681e-01	2.72683e-01	4.25734e-01	4.25737e-01

Example: Scaffold (3D) continued

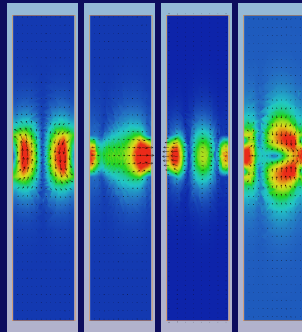


→ Talk by Roland Klose this afternoon!

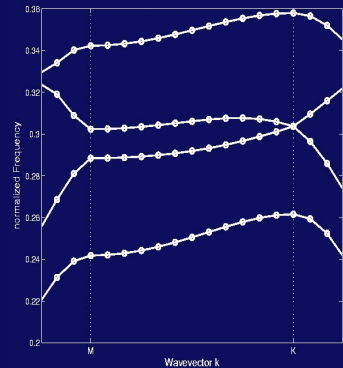
Photonic crystal from MPI Halle with measured data



Unit cell with hole



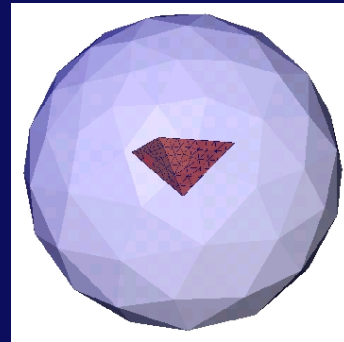
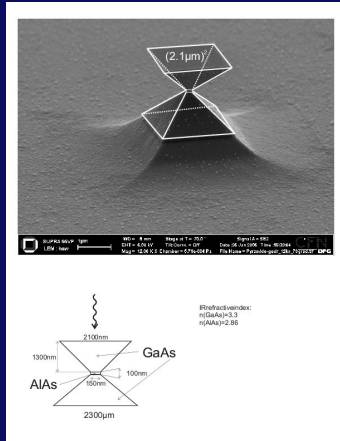
Optical fields



Band diagram

Problem: Off plane radiation $\rightarrow$ transparent boundary conditions

Micro Cavity

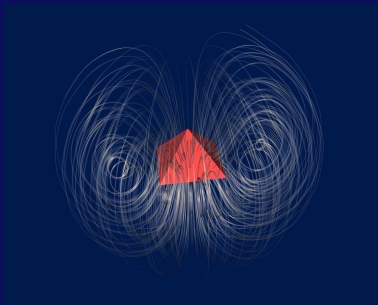


Micro resonator embedded in free space

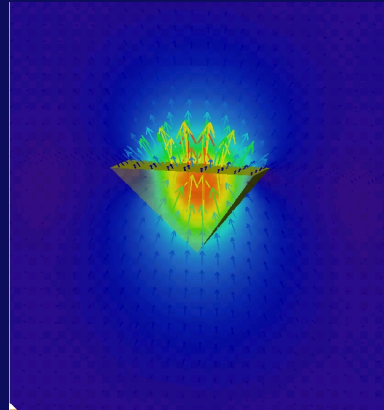
Resonating mode

Problem: Radiation in all directions $\rightarrow$ transparent boundary conditions

Micro Cavity



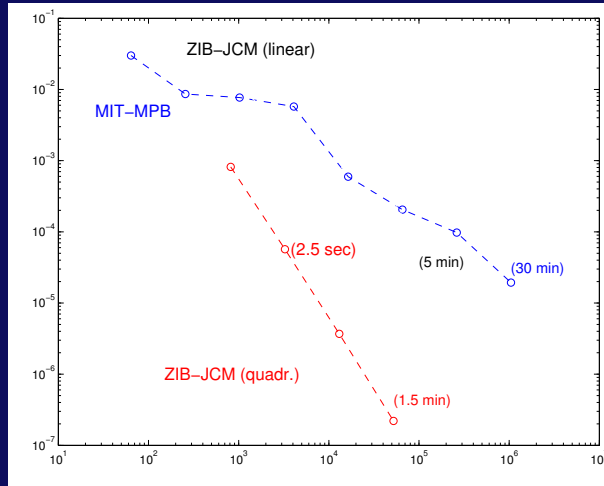
Micro resonator embedded in free space



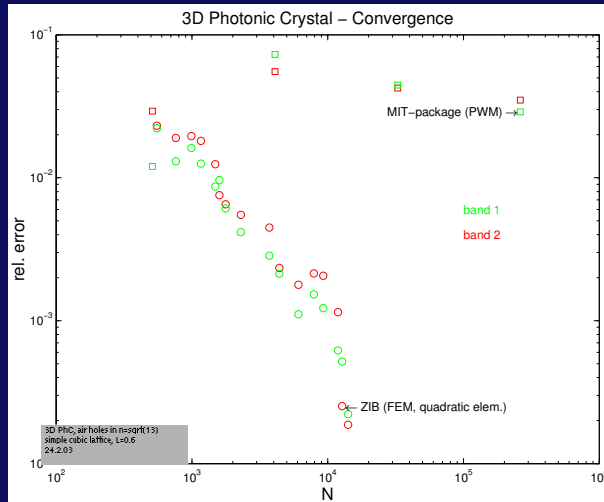
Resonating mode

Problem: Radiation in all directions → transparent boundary conditions

Comparison between PWM (MIT) and FEM (ZIB) 2D



Comparison between PWM (MIT) and FEM (ZIB) 3D



Conclusions

- FEM for time-harmonic Maxwell's equations is a versatile method to solve problems from optics.
- It is both applicable to eigenvalue problems as well as scattering problems.
- Numerical methods with optimal complexity are available.
- Adaptivity helps to overcome complexity barriers.