Higher-order Methods for Simulating Light Propagation and Light-Matter Interaction in Nano-Photonic Systems

Kurt Busch
Institut für Theoretische Festkörperphysik
Universität Karlsruhe, 76128 Karlsruhe, Germany

Karlsruhe Institute of Technology

DFG-Center for
Functional Nanostructures
and
Karlsruhe School of
Optics & Photonics

Kurt Busch, Universität Karlsruhe, kurt@tfp.physik.uni-karlsruhe.de

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Martin Pototschnig*
Kai Stannigel

CFN DFG

KSOP
Karlsruhe School of Optics & Photonics

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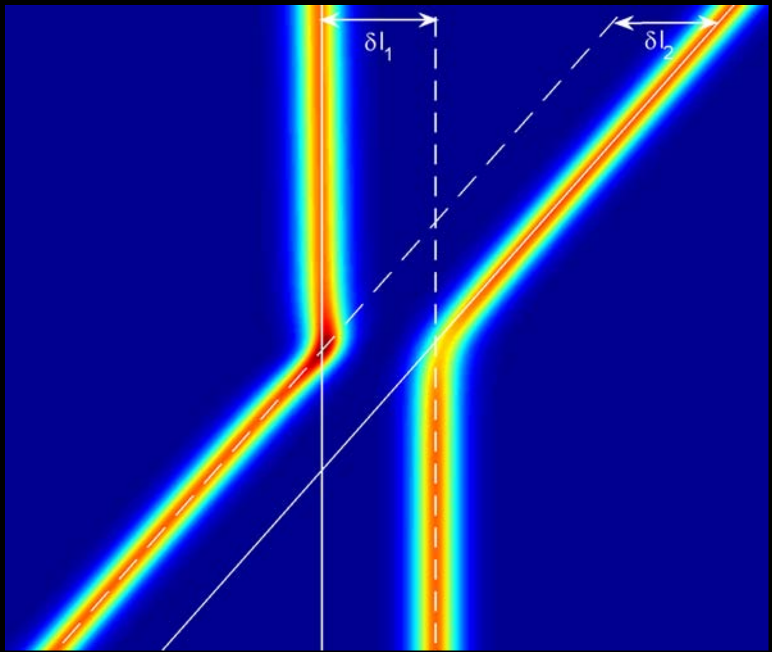
Motivation



Soliton collision in a fiber Bragg grating

- Linear, nonlinear and quantum optical problems in nano-photonic systems involve multiple time and length scales
- This requires accurate, stable, and efficient solvers for linear and nonlinear Maxwell's equation and coupled systems

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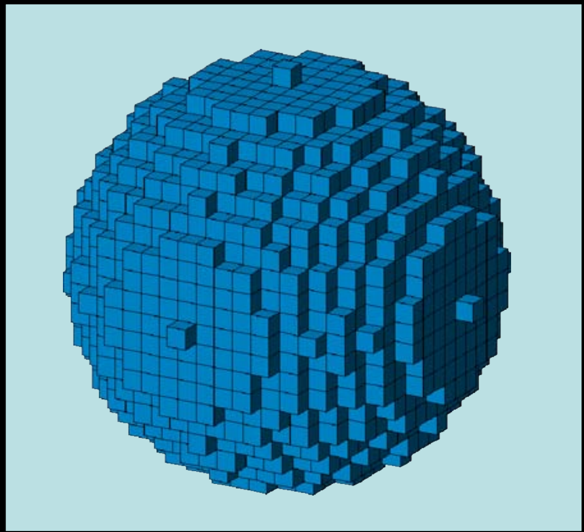
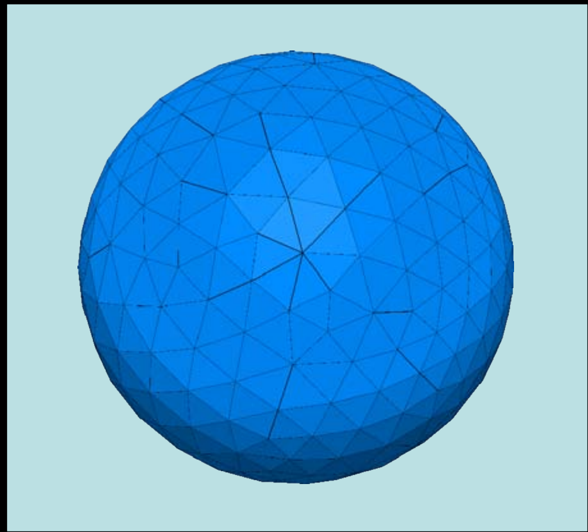
Motivation: Standard Approaches



FDTD-Method

- Discretization on Yee-grid
- 2nd order in space and time
- Efficient and easy to implement



Finite-Element-Method

- Discretization on unstructured grids
- Higher-order in space
- Frequency-domain preferred

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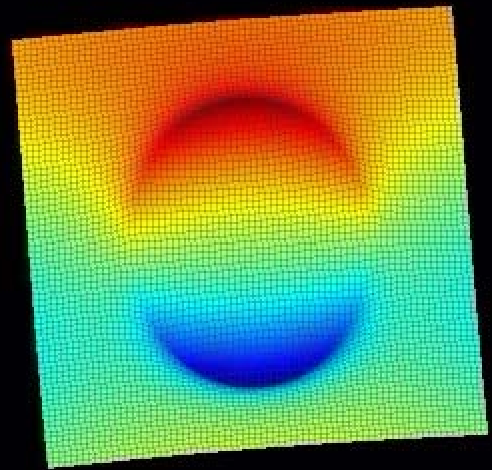
Motivation: Do not trust Computers I



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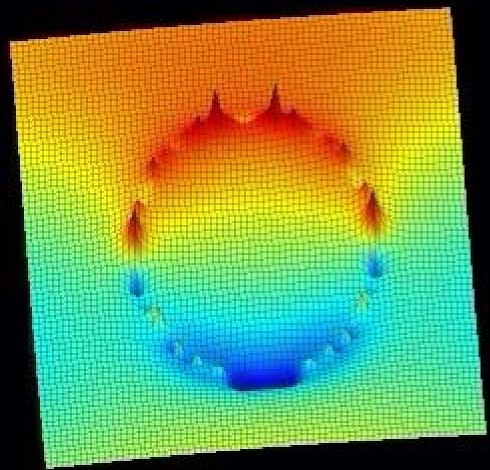
Motivation: Do not trust Computers II



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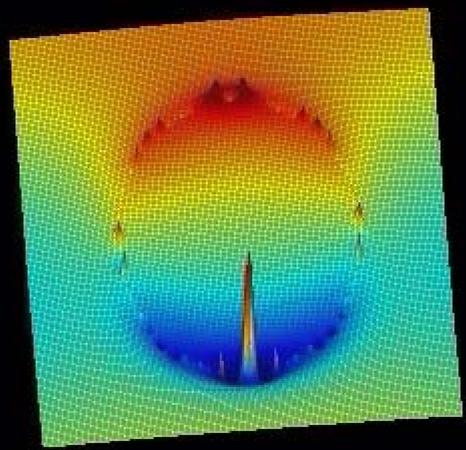
Motivation: Do not trust Computers III



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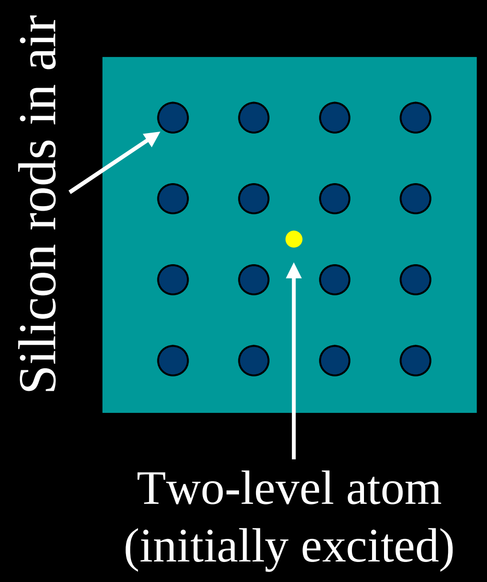
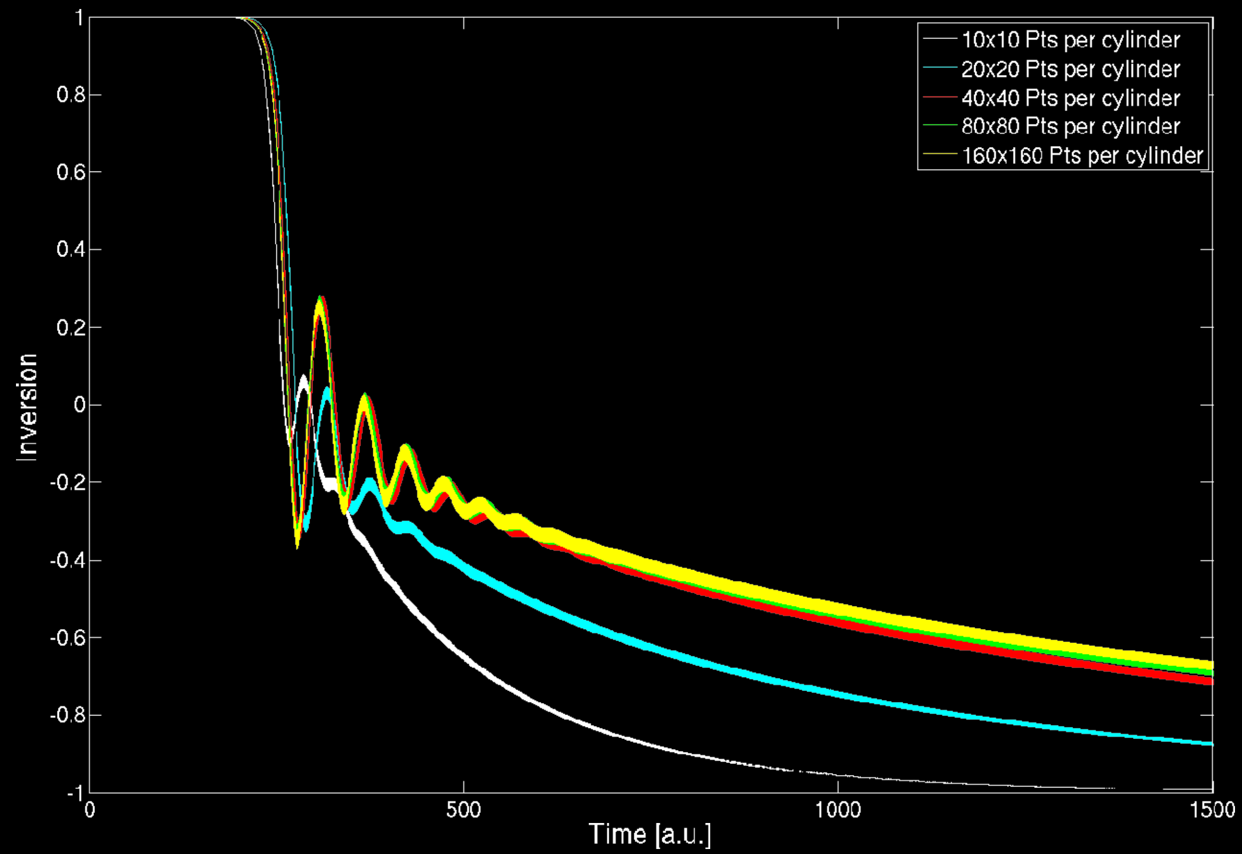
Motivation: Do not trust Computers IV





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Outline

- The Krylov-Subspace/Discontinuous Galerkin Approach
  - How the method works and performs
  - Advanced spatial discretization
- Extension to Nonlinear & Coupled Systems
  - Lawson-Transformation and Rosenbruck-Wanner solvers
  - Performance
- Examples and Applications
  - Spontaneous emission in photonic crystals
  - Plasmonic structures

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The Krylov-Subspace Method

- Maxwell equations in Schrödinger form

$$\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}}_{\mathbf{\Psi}(t)} = \underbrace{\begin{pmatrix} -\sigma_{\mathrm{el}} & \frac{1}{\epsilon(\vec{r})}\nabla\times \\ -\frac{1}{\mu(\vec{r})}\nabla\times & -\sigma_{\mathrm{mag}}\end{pmatrix}}_{\mathcal{H}}\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix} - \underbrace{\begin{pmatrix}\vec{J}_{\mathrm{el}}(t)\\ \vec{J}_{\mathrm{mag}}(t)\end{pmatrix}}_{\mathbf{J}(t)}$$

- A formal solution of is given by

$$\mathbf{\Psi}(t) = e^{t\mathcal{H}}\mathbf{\Psi}(0) + \int_0^t e^{(\tau-t)\mathcal{H}}\mathbf{J}(s)\,d\tau$$

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The Krylov-Subspace Method

- Discretization of $\Psi(t)$ and $\mathcal{H}$ (e.g. on a Yee-Grid)
  à Very large but sparse matrix H

- Matrix-Vector-Products $H\Psi$ are feasable

- We do not require the full matrix e^{tH}, only its action on a vector: $e^{tH}\Psi$

- We do not want any restrictions on the properties of the matrix H (such as skew-symmetry etc.)

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The Krylov-Subspace Method

- Build up the Krylov Subspace

$$K_m = \mathrm{span}\{\Psi_0, H\Psi_0, H^2\Psi_0, \ldots, H^{m-1}\Psi_0\}$$

- Ortho-normalize the basis by Arnoldi-method

à Orthogonal Basis V_m

- Obtain projection of H onto V_m

$$H_m = V_m^T \mathcal{H} V_m$$

- The number of basis vectors can be small (m ~10)

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The Krylov-Subspace Method

- The key approximation then is

$$e^{tH}\mathbf{\Psi} \approx \|\mathbf{\Psi}_0\| V_m e^{tH_m}\mathbf{e}_1$$

- Works for arbitrary matrices H
- The accuracy of the method is at least $O(t^m)$
- Memory usage: (m+1)/2 relative to FDTD

J. Niegemann, L. Tkeshelashvili, and K. Busch,
J. Comput. Theor. Nanosci. 4, 627 (2007)

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Comparison of Performance (1D)

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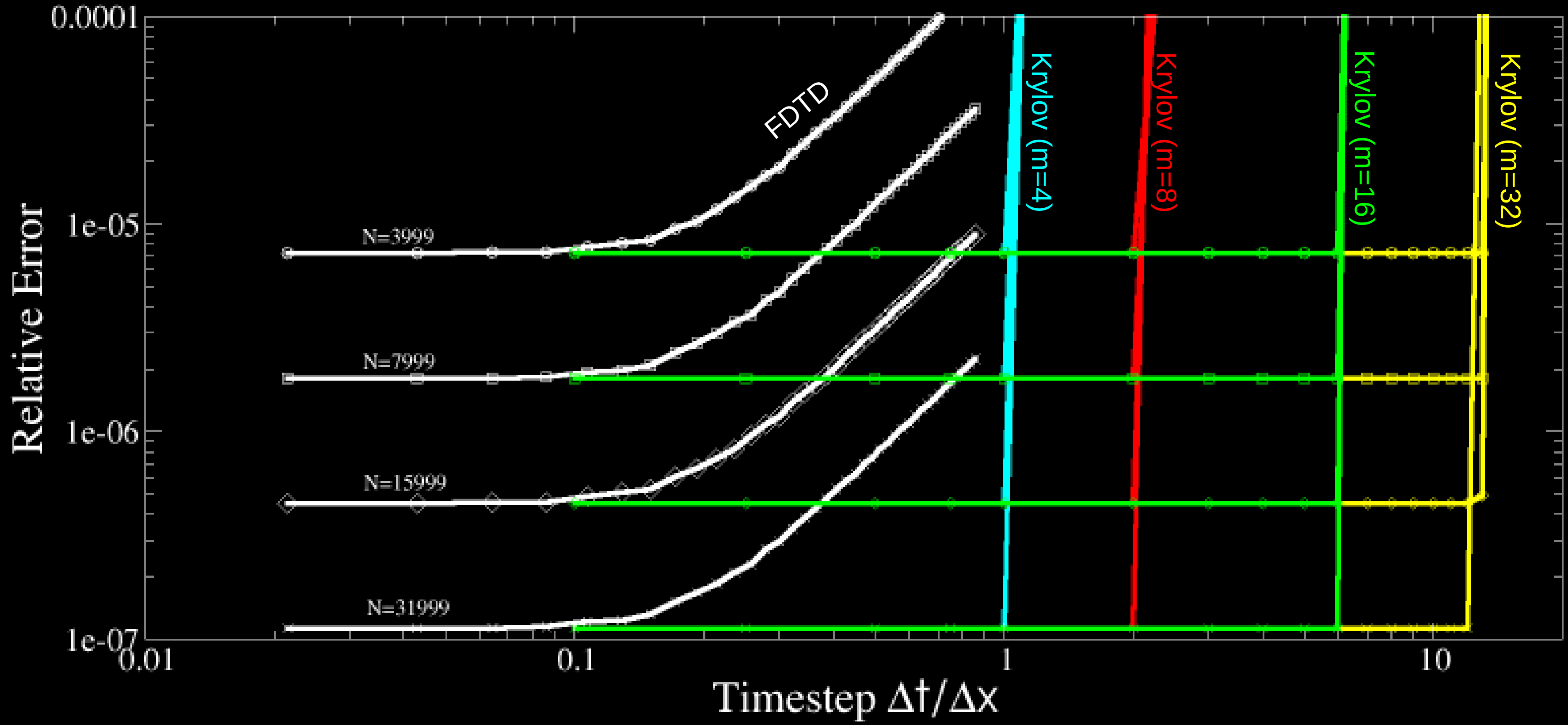
- The method allows much larger time steps



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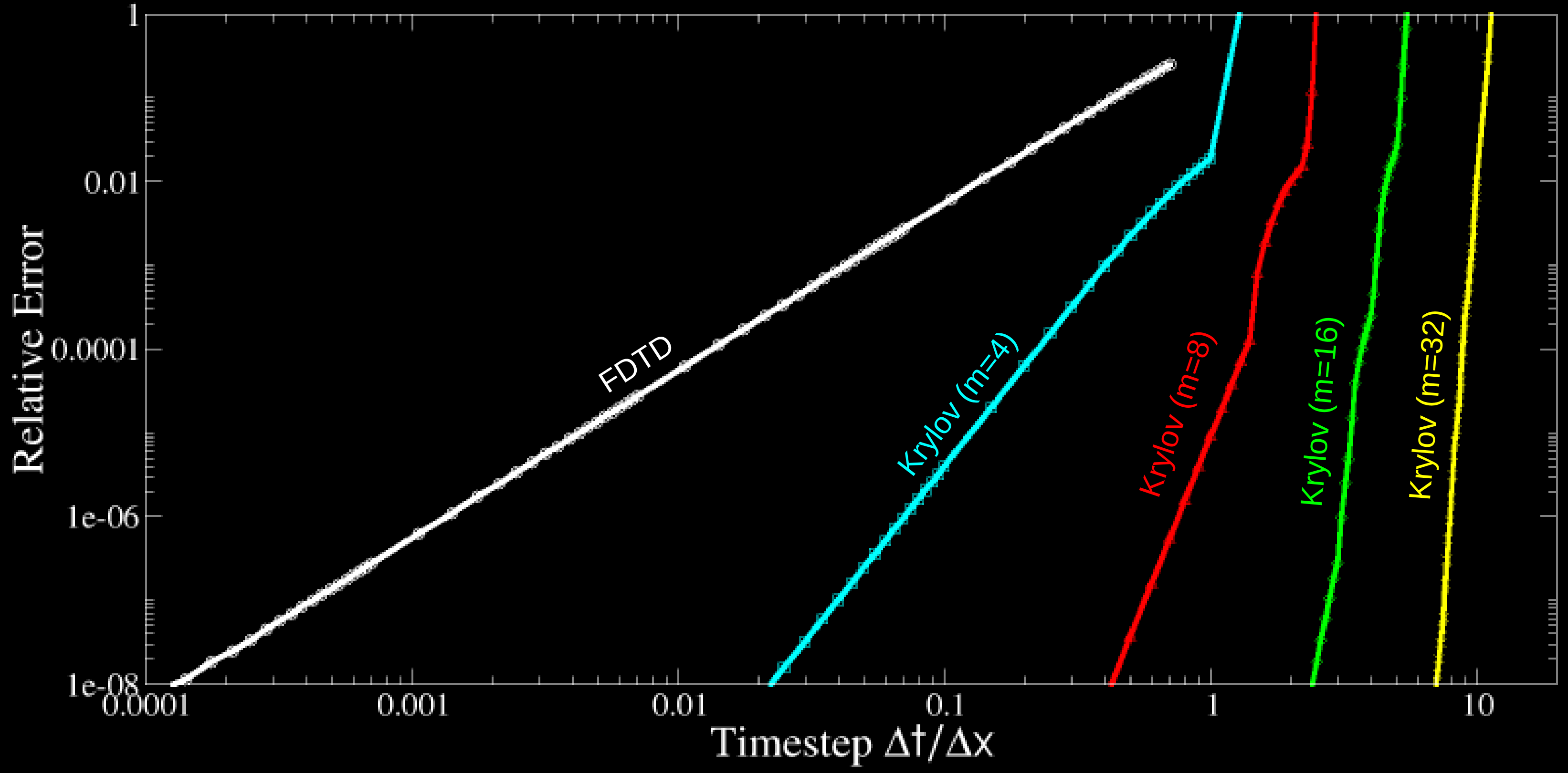
Comparison of Performance (2D)

- In a 2D system, the effect is even more pronounced



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Important Add-Ons - Via ADEs

- Dispersive Materials
  - Drude-, Lorentz-, Debye-Model
  - Sellmaier-type Models
- Sources
- Open Systems: Complex frequency shifted PMLs

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Material Dispersion via ADEs

- All typical analytic dispersion relations (Drude, Lorentz, Debye) can be implemented via ADEs.
- Experimental dispersion fitted by combined (multiple) Lorentz- or Drude-terms.
- Example: $\epsilon(\omega) = \epsilon_\infty + \frac{\omega_0^2 \Delta\epsilon}{\omega_0^2 + 2i\omega\delta - \omega^2}$ (Single Lorentz-term)

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{E}\\ \mathbf{H}\\ \mathbf{j}\\ \mathbf{k}\end{pmatrix} = \begin{pmatrix} -\sigma_e & \frac{1}{\epsilon_\infty}\nabla\times & -\frac{1}{\epsilon_\infty} & 0 \\ -\frac{1}{\mu}\nabla\times & -\sigma_m & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{\omega_0^2\Delta\epsilon}{\epsilon_\infty}\nabla\times & -\omega_0^2\left(1+\frac{\Delta\epsilon}{\epsilon_\infty}\right) & -2\delta \end{pmatrix}\begin{pmatrix}\mathbf{E}\\ \mathbf{H}\\ \mathbf{j}\\ \mathbf{k}\end{pmatrix}$$

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Advanced Spatial Discretization

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- With the Krylov-subspace method, accuracy of time-integration can be chosen arbitrarily
- Problem: Error from the spatial discretization is limiting the total accuracy
  - à Higher order stencils
  - à Still only 2nd order in the presence of boundaries
- Possible solution: Adaptive grid refinement around boundaries

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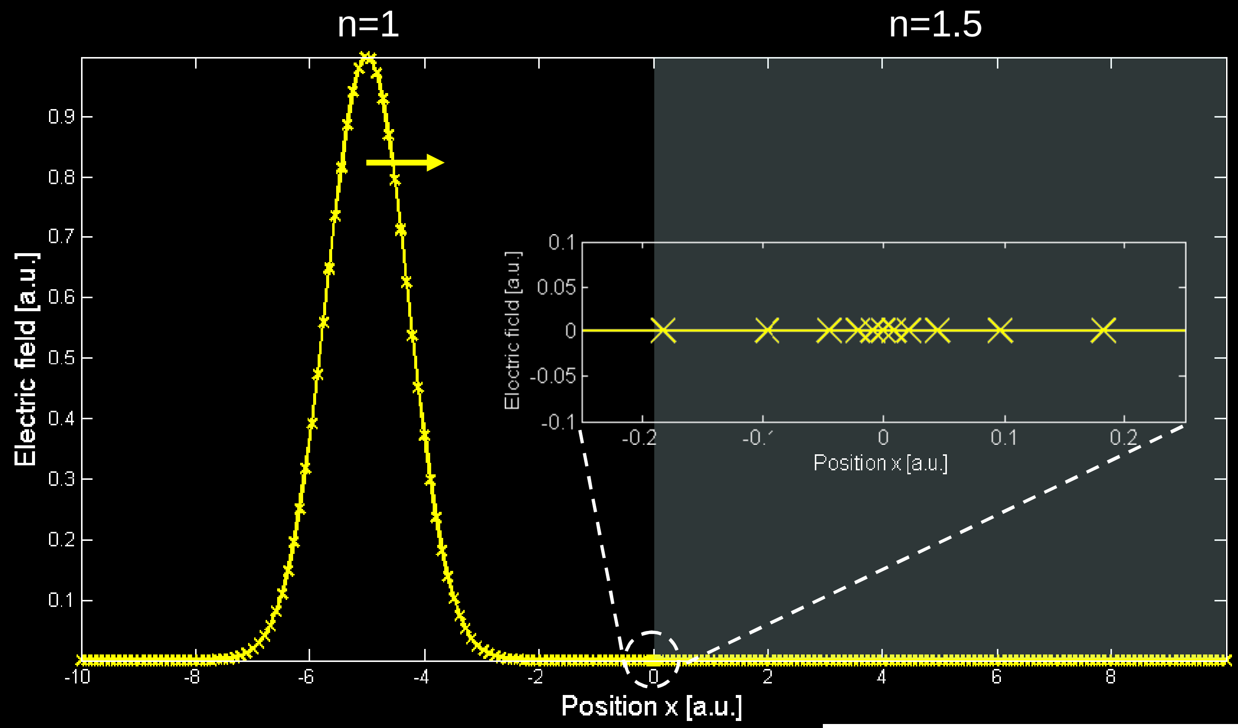
Unstructured Grid in 1D

- Adapt the grid so the point density is higher around the material boundaries



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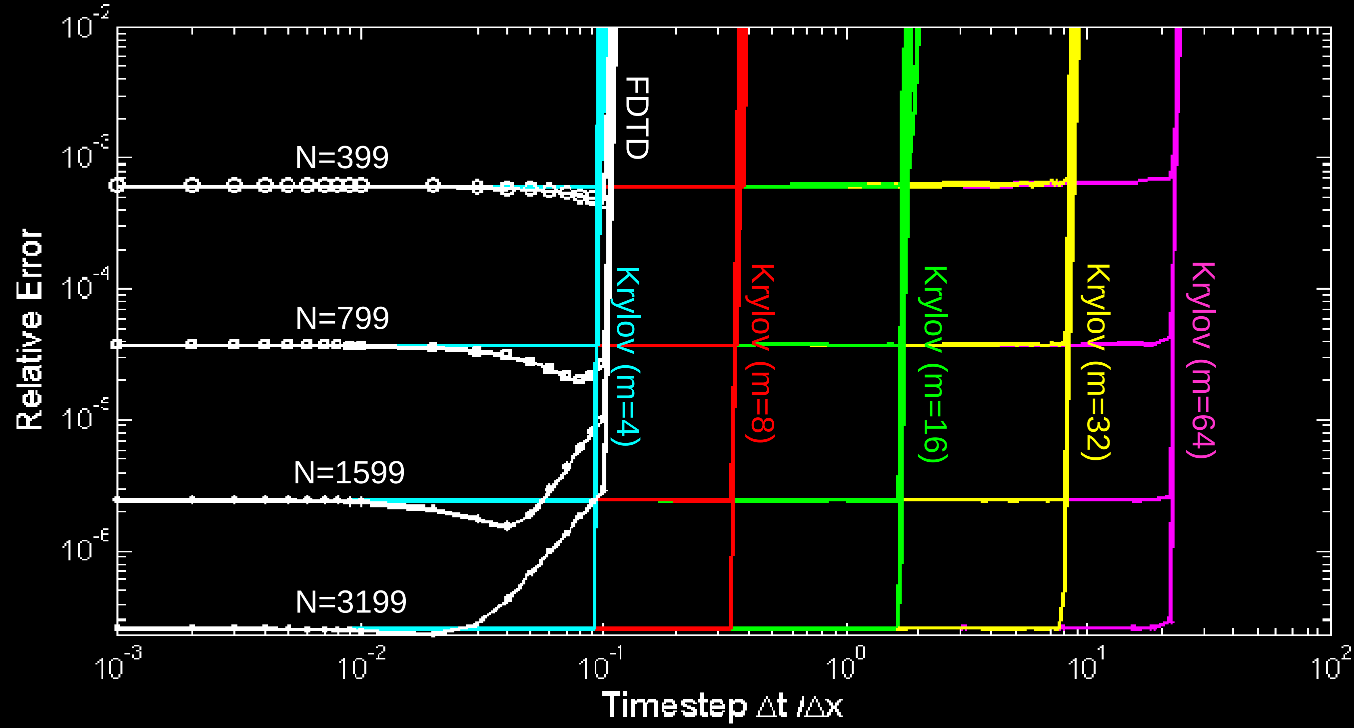
Unstructured Grid Performance (1D)

- 4^{th}-order stencil and adaptive grids: 4^{th} order is maintained in the presence of material boundaries



K. Busch et al.,
physica status solidi (b) 244, 3479 (2007)

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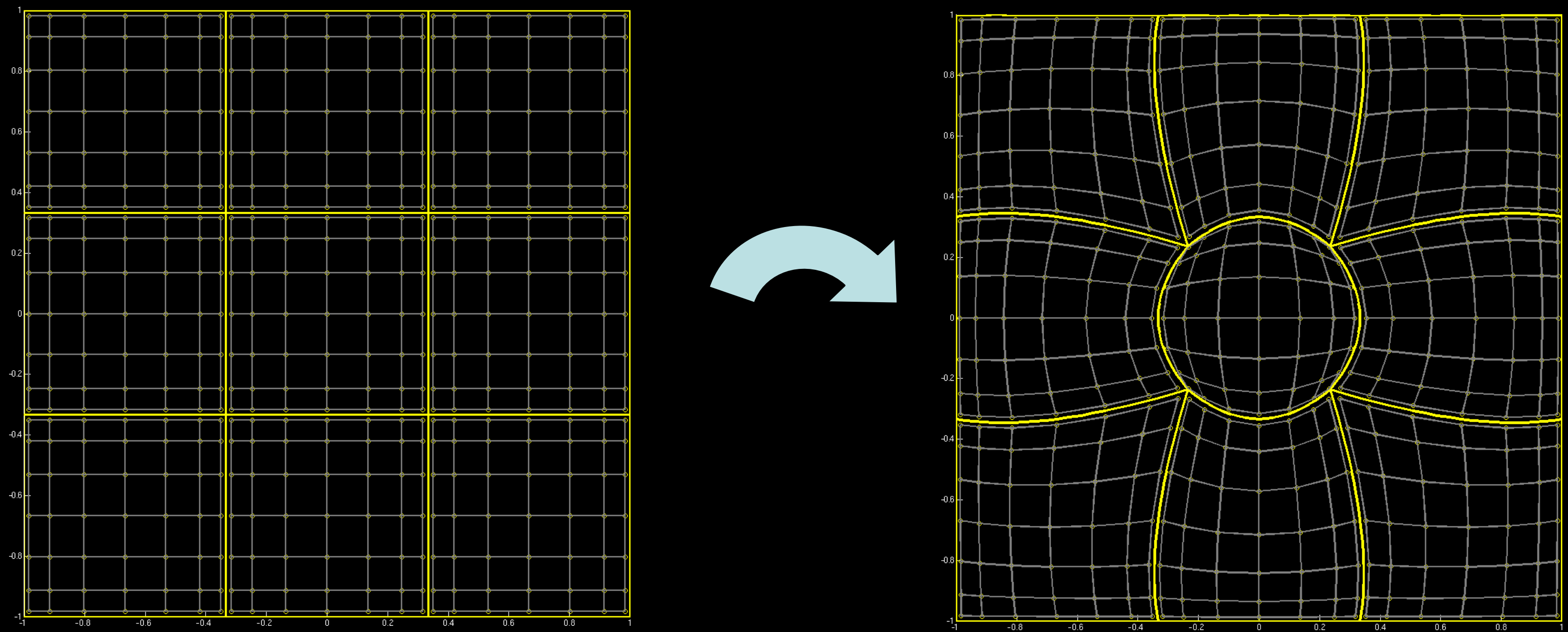
Unstructured Grids in 2D/3D



- Discontinuous Galerkin finite element technique (borrowed from hydrodynamics)

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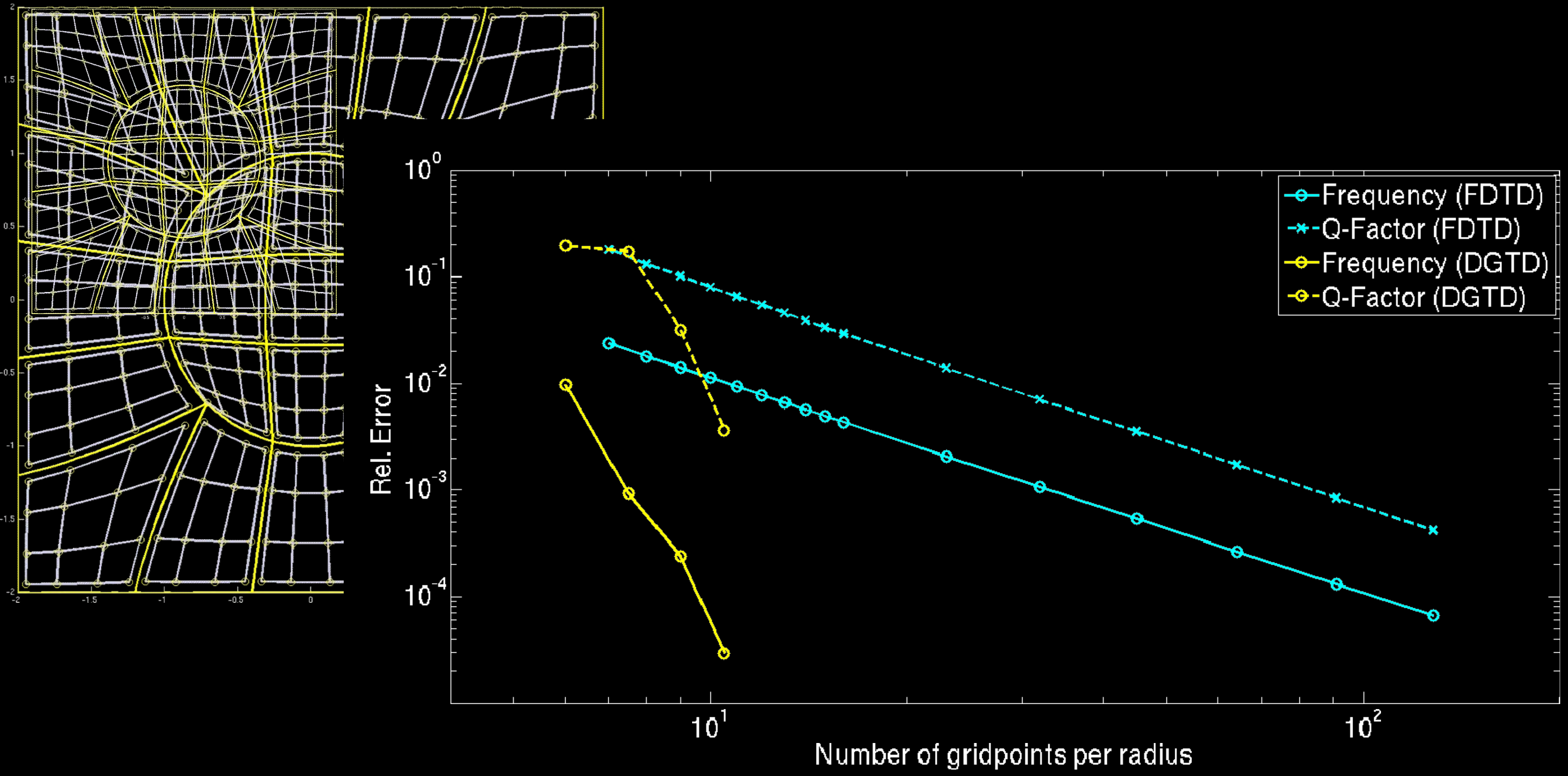
Results on Unstructured Grids (2D)



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Extension to Nonlinear Systems

- The method can be extended to nonlinear systems

$$\frac{\partial}{\partial t}\Psi = H\Psi + N[\Psi]$$

- Lawson-Transformation:

  à *H* is the linear part of the nonlinear system

- Rosenbruck-Wanner solvers:

  à *H* is the Jacobian of the nonlinear system

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Extension to Nonlinear Systems

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$$\frac{\partial}{\partial t}\Psi = H\Psi + N\left[\Psi\right]$$

- Lawson-Transformation

$$e^{-tH}\frac{\partial}{\partial t}\Psi = e^{-tH}\left(H\Psi + N\left[\Psi\right]\right)$$

$$\frac{\partial}{\partial t}\underbrace{\left(e^{-tH}\Psi\right)}_{\mathbf{A}} = e^{-tH}N\left[\Psi\right]$$

$$\frac{\partial}{\partial t}\mathbf{A} = \underbrace{e^{-tH}N\left[e^{tH}\mathbf{A}\right]}_{F[\mathbf{A}]}$$

Extension to Nonlinear Systems

- With a standard Euler scheme, one obtains the "Lawson-Euler Scheme":

$$\Psi(t+\Delta t) = e^{\Delta t H}\Psi(t) + \Delta t e^{\Delta t H} N[\Psi(t)]$$

- In practice, we use a 4th-order Runge-Kutta scheme instead of Euler: "Lawson4"

- Rosenbruck-Wanner solver proposed by Hochbruck and Lubich:"Hochbruck4"

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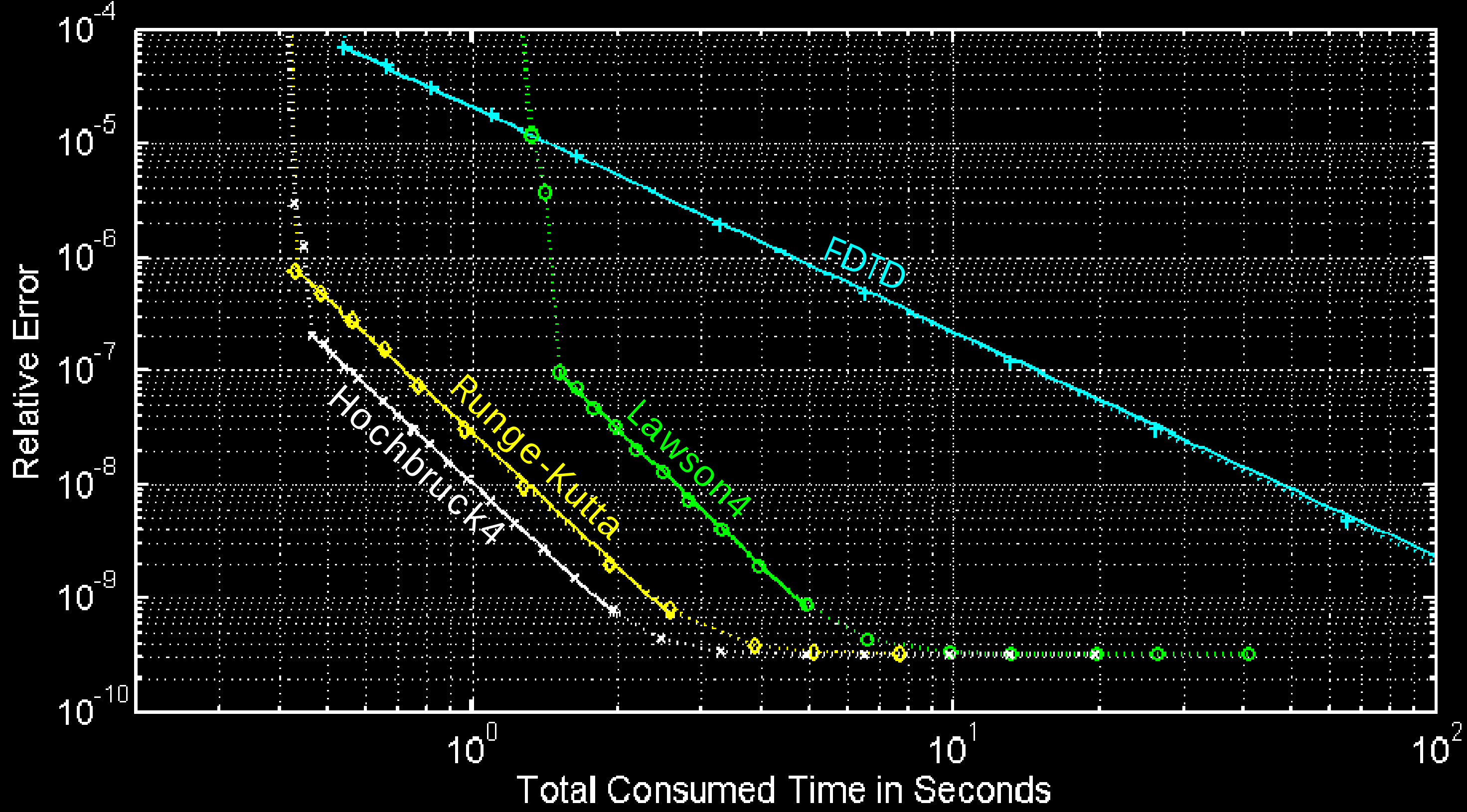
Performance Comparison

- Dispersion-free 1D system with Kerr-Nonlinearity



M. Pototschnig et al., submitted (2007)

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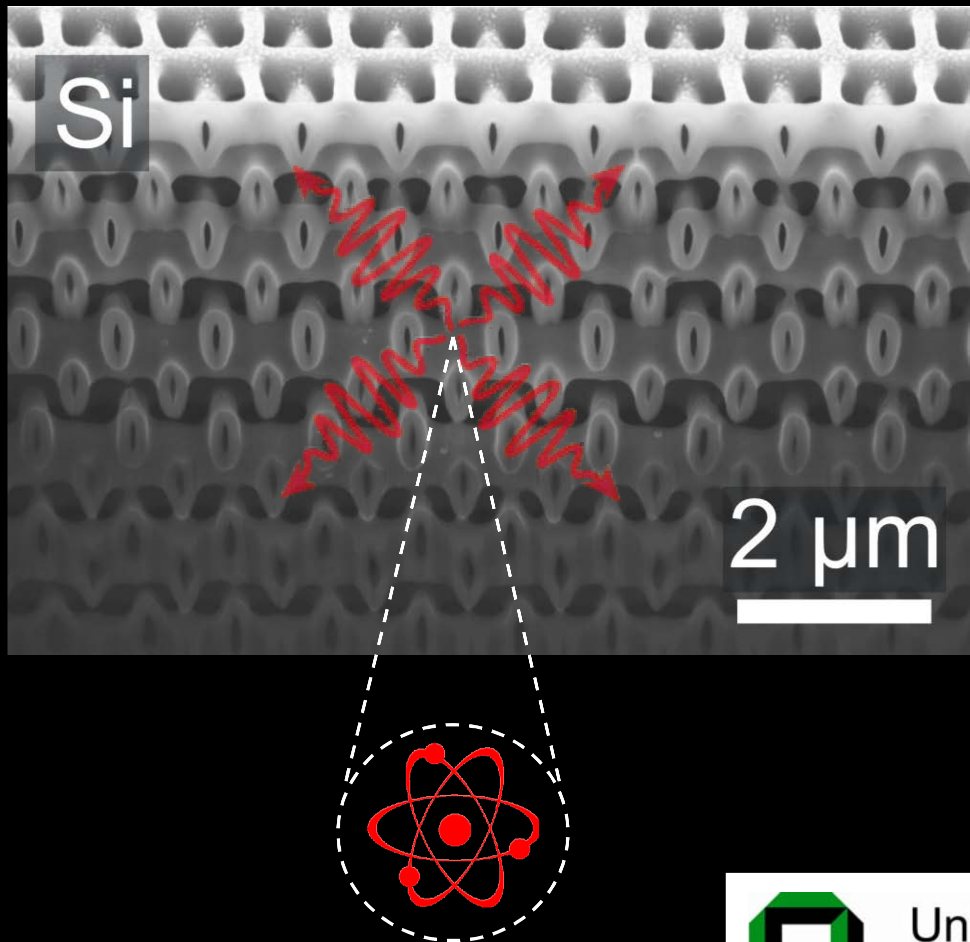
Modified Radiation Dynamics



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Semi-classical Description

- Full Hamiltonian: $\mathcal{H} = \mathcal{H}_{Atom} + \mathcal{H}_{Field} + \mathcal{H}_{Int}$

$$\mathcal{H}_{Atom} = E_0 |0\rangle \langle 0| + E_1 |1\rangle \langle 1|$$

$$\mathcal{H}_{Int} = -e\mathbf{r}\mathbf{E}$$

- Field is treated classically via Maxwell's Equations with polarization

$$\mathbf{P} = -n_{Atom} e \langle \mathbf{r} \rangle$$

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Semi-classical Description

- Introducing the density matrix ρ which obeys

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho]$$

$$\rho_1 = 2\mathrm{Re}(\rho_{12}), \quad \rho_2 = 2\mathrm{Im}(\rho_{21}), \quad \rho_3 = \rho_{22} - \rho_{11}$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho_1\\ \rho_2\\ \rho_3\end{pmatrix} = \begin{pmatrix}0 & \omega_0 & 0\\ -\omega_0 & 0 & 2\Omega_R\\ 0 & -2\Omega_R & 0\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\\ \rho_3\end{pmatrix} - \begin{pmatrix}\frac{1}{T_2} & 0 & 0\\ 0 & \frac{1}{T_2} & 0\\ 0 & 0 & \frac{1}{T_1}\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\\ \rho_3 - \rho_{30}\end{pmatrix}$$

Initial population difference (ρ_{30})

$$\Omega_R = \frac{\gamma}{\hbar}E$$

T_1: Relaxation

T_2: Dephasing

γ : Dipole moment

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Semi-classical Description

- Maxwell-Boch-Equations in 1D

$$\frac{\partial H}{\partial t} = -\frac{1}{\mu}\frac{\partial E}{\partial x}$$

$$\frac{\partial E}{\partial t} = -\frac{1}{\epsilon(x)}\frac{\partial H}{\partial x} - \frac{N\gamma}{\epsilon(x)T_2}\rho_1 + \frac{N\gamma\omega_0}{\epsilon(x)}\rho_2$$

$$\frac{\partial \rho_1}{\partial t} = -\frac{1}{T_2}\rho_1 + \omega_0\rho_2$$

$$\frac{\partial \rho_2}{\partial t} = -\frac{1}{T_2}\rho_2 - \omega_0\rho_1 + 2\frac{\gamma}{\hbar}E\rho_3$$

$$\frac{\partial \rho_3}{\partial t} = -2\frac{\gamma}{\hbar}E\rho_2 - \frac{1}{T_1}(\rho_3 - \rho_{30})$$

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Spontaneous Emission in 2D PhCs

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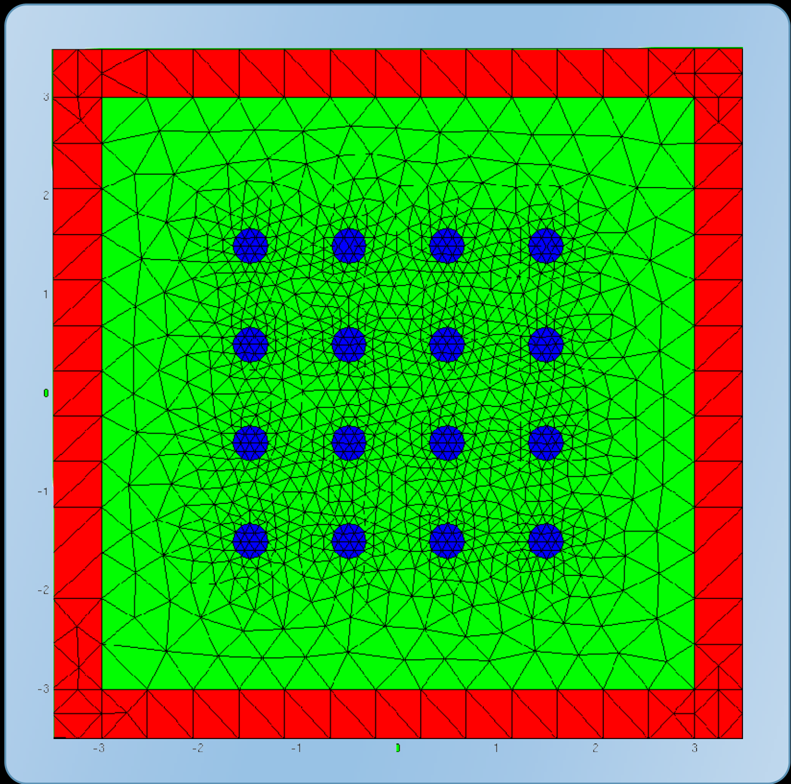
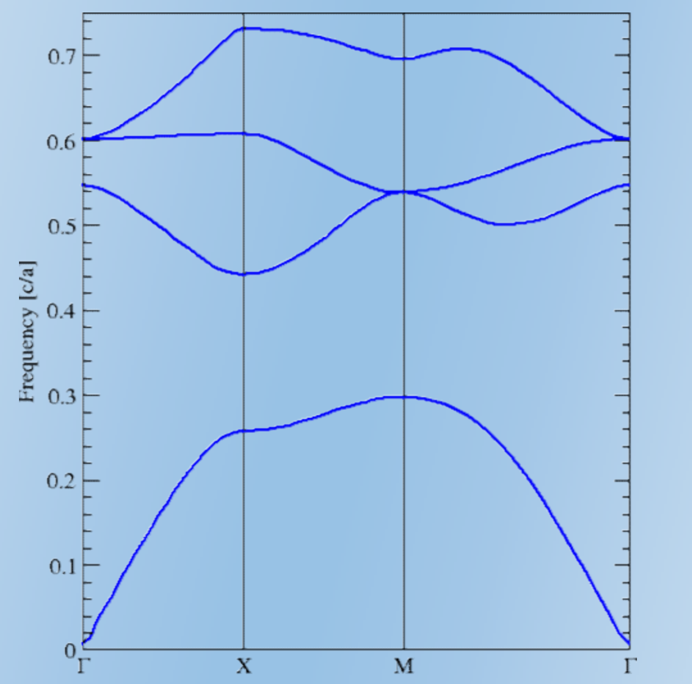


Corresponding bandstructure



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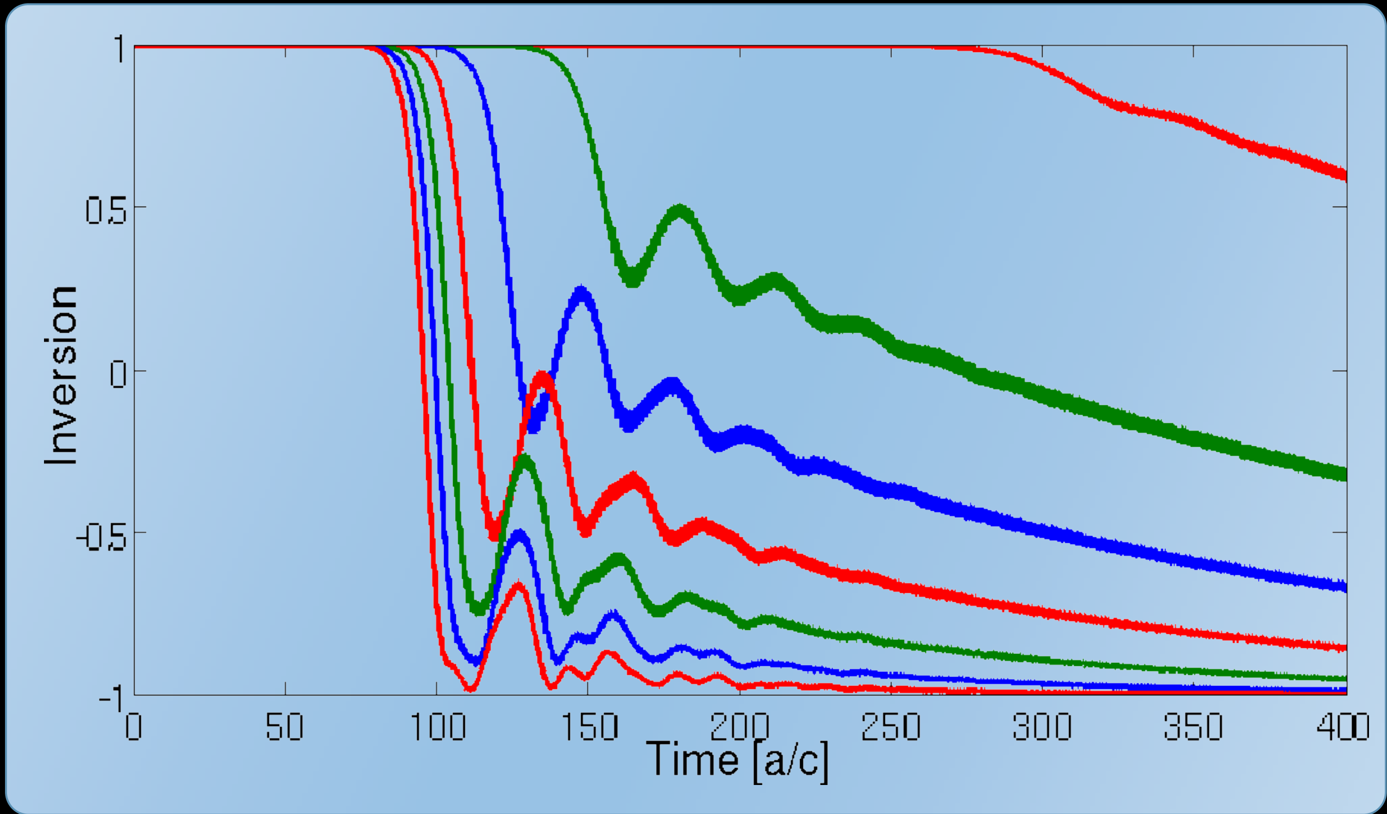

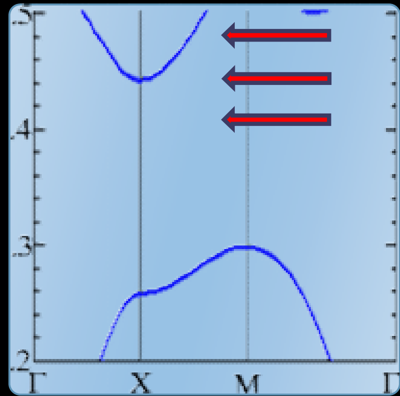

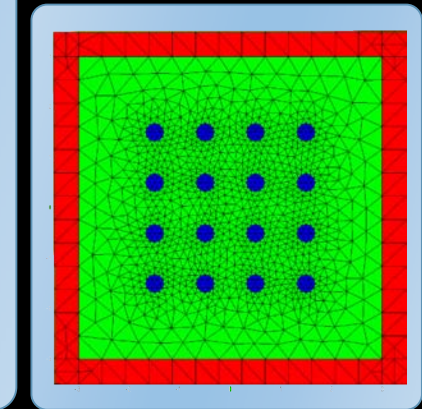

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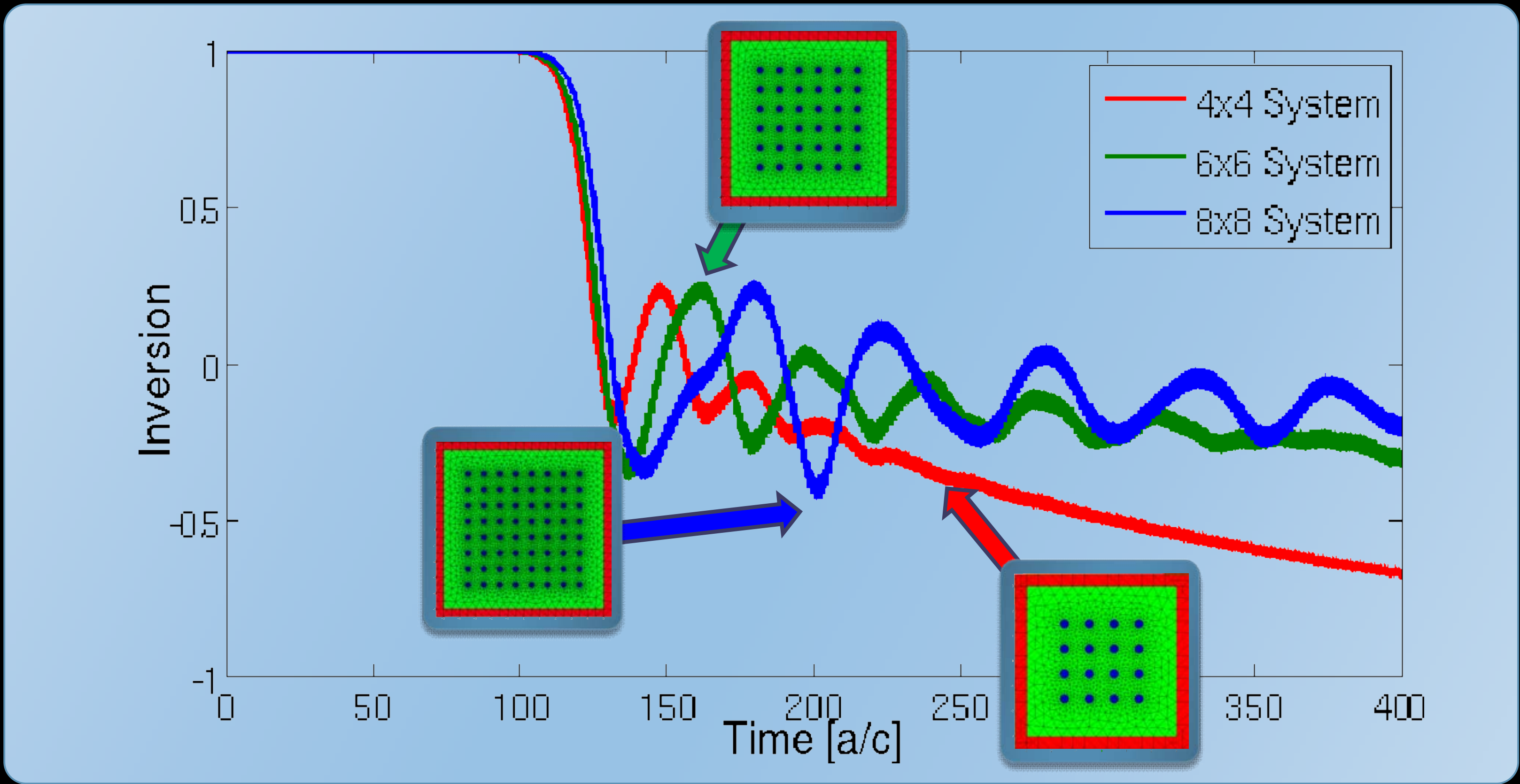

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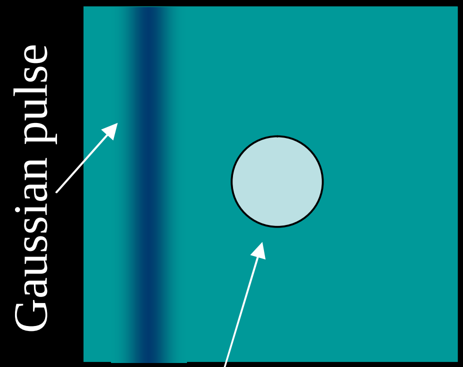
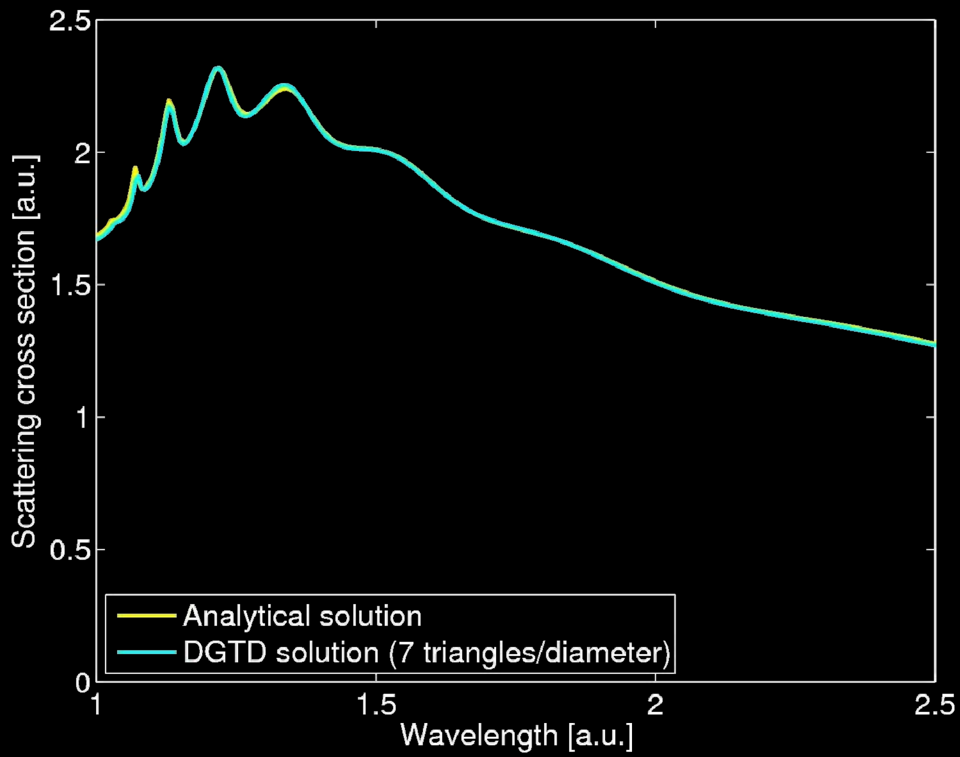
Resonances of Plasmonic Structures



Metallic cylinder
(r=25nm, Ag)



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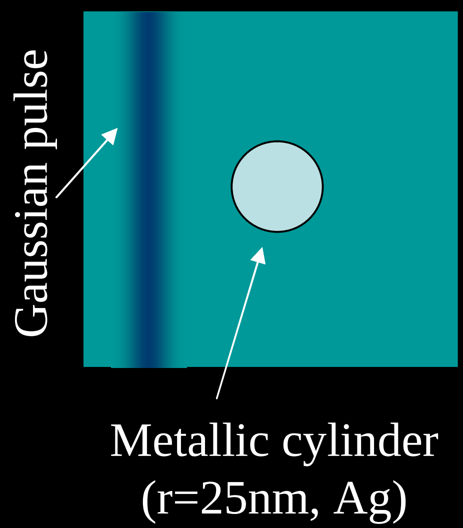

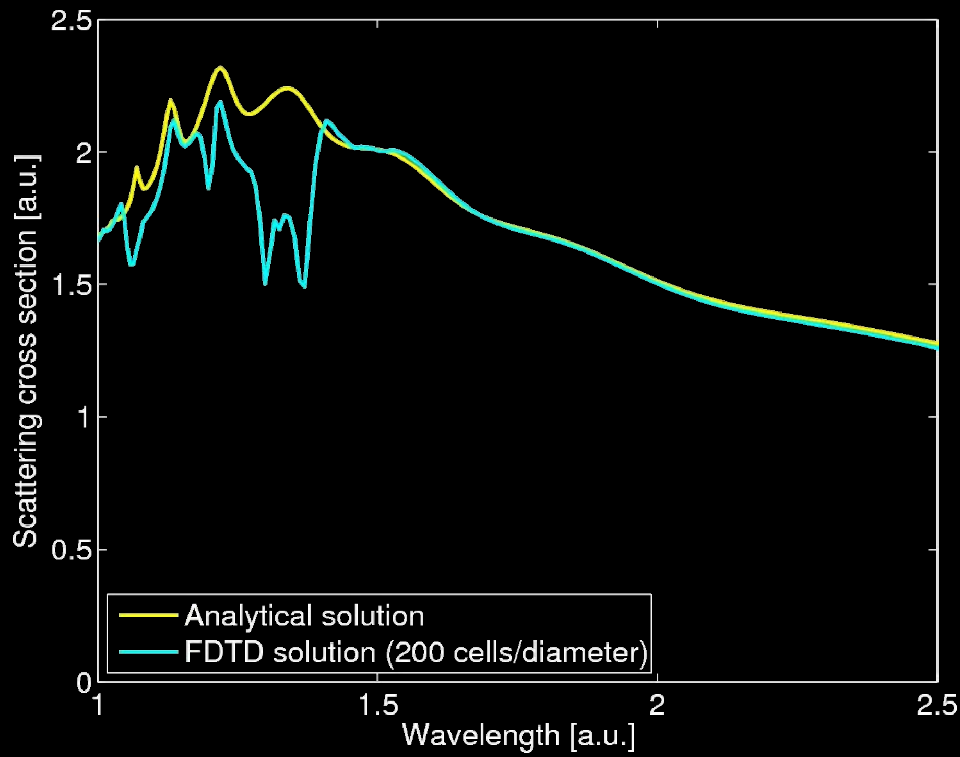

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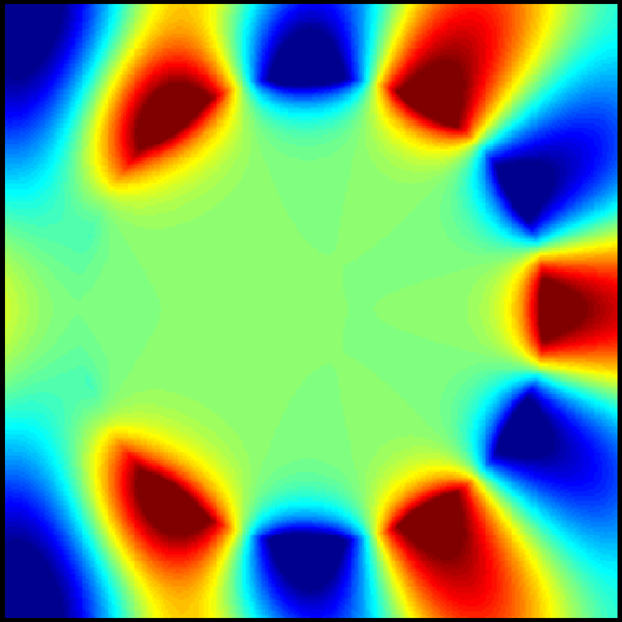

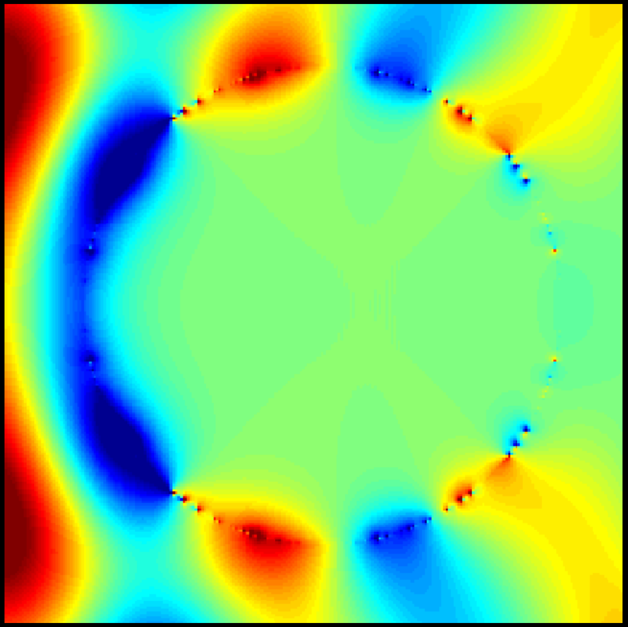

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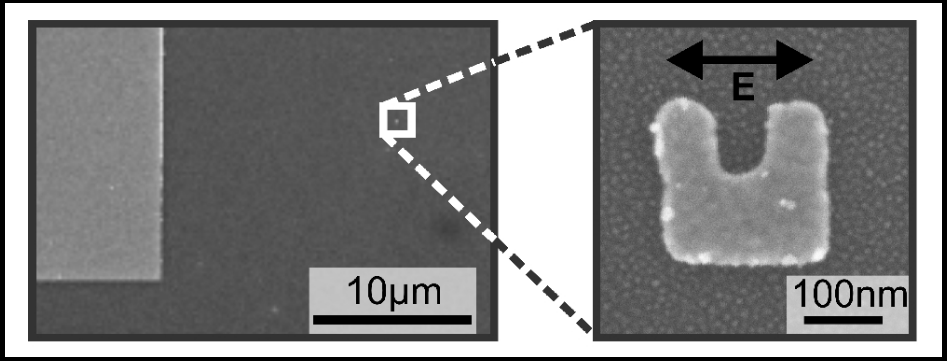
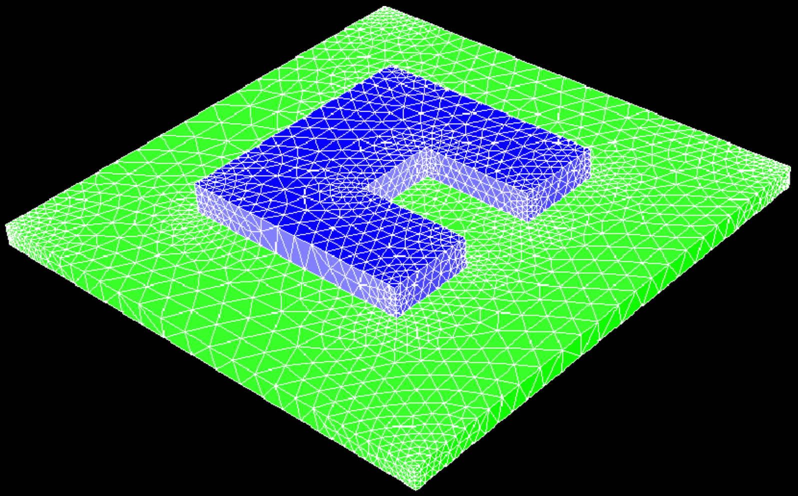


Courtesy of Martin Husnik



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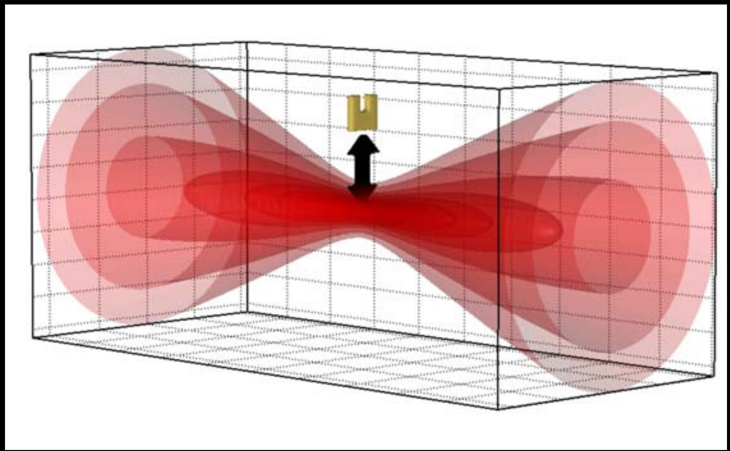
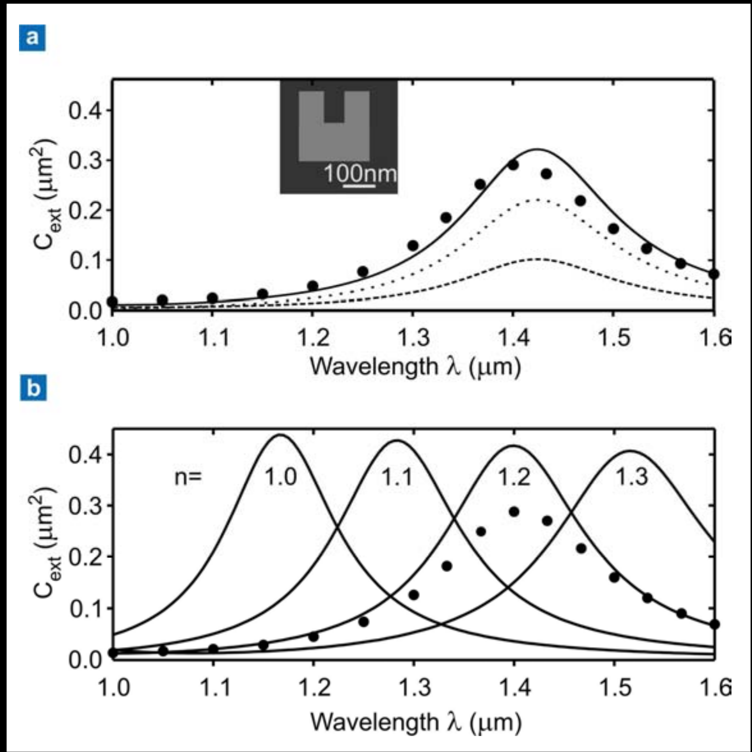


M. Husnik et al., submitted



Kurt Busch, Universität Karlsruhe, kurt@tfp.physik.uni-karlsruhe.de

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Summary and Outlook

- Higher-order time-domain simulation of the Maxwell equations using Krylov-subspace methods
- Sources, UPMLs/CPML and dispersive materials (Sellmeier-type) via auxiliary fields
- Discontinous Galerkin technique for "conformal" spatial discretization
- Extension to nonlinear and coupled systems' dynamics
- Future work:
  - Parallelization
  - Application to complex photonic systems

Kurt Busch, Universität Karlsruhe, kurt@tfp.physik.uni-karlsruhe.de