MMP simulations of plasmonic optical waveguides and antenna structures

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Overview

• Motivation
  – Concentration of the optical field on ultra-small spots
  – Applications: Telecomm and optical sensors based on CPP effects

• Numerical field solvers
  – Time domain versus frequency domain
  – Domain discretization versus boundary discretization
  – The Multiple Multipole Program (MMP) and related methods

• Numerical eigenvalue analysis of lossy, dispersive waveguides
  – Analytic methods: Zeros of the determinant
  – Measurement, FDTD, etc.: Resonance peaks
  – The Multiple Multipole Program (MMP)

• Simulations of metallic optical waveguide structures
  – Channel Plasmon-Polariton (CPP) waveguides
  – Ultra-small CPP waveguides

• Simulations of optical antenna structures
  – Two rectangles with a gap vs. single rectangle with a V-groove
  – 2D structures on a substrate
  – 3D axi-symmetric structures

• Conclusions and Outlook
Motivation: Concentration of the optical field

The diffraction limit of classical lenses limits the optical resolution of microscopes and optical storage devices. Similarly, the packaging density of integrated optics is limited.

Ways towards sub-wavelength resolution

- **Negative index (Veselago) slab** → “Pendry lens”:
  - Not perfect, no magnification, super-resolution only in the *near* field
- **Optical nano jets** (*near* micro lenses, when the focus is on the surface)
- **Hypothetical high index lenses** (focus *near* the surface): very high n not available!
- **Nearfield optics, SNOM**:
  - The optical field may be concentrated in a sub-wavelength area as any electromagnetic field, but only *near* the surface of a material!
- **Optical antennas**:
  - Low frequencies: lightning rod effect near metal tips and wedges, but:
  - Metals loose conductivity at optical frequencies, but:
    - **Plasmon-polariton effects occur**: strong even for feature size $<< \lambda$!

Applications: sensors (single molecule detection, bio), laser output modification, ...
Plasmon-polariton effects

Plane wave scattered at a circular wire with complex permittivity, H field parallel to the wire axis
Plot: scattered field intensity as a function of the complex permittivity $\varepsilon$, white line: trace of silver
• Strong impact of material loss ($\text{Im}(\varepsilon)$) and size (diameter $D$)
• Small size ($<<\lambda$):
  • one strong resonance peak visible (dipole resonance),
  • higher order resonances usually invisible because of losses
• Large size:
  • Additional resonances visible
  • original plasmon-dipole resonance may become invisible because of losses
Application example: Micro-size telecom

Grooves in metallic surfaces support Channel Plasmon-Polariton (CPP) waveguide modes

Very simple material system: Air-metal

Problems:
• Losses
• Dispersion
• Cutoff
• Excitation
• Size > 1μ?
• Simulation!

Fig. 3. (Color online) Modal shape of the CPP fundamental mode for increasing wavelength λ: (a) λ = 0.6 μm, (b) λ = 1.0 μm, (c) λ = 1.4 μm (close to cutoff). These panels display the time averaged electric field. (d) Instantaneous transverse electric field at λ = 1.4 μm for a structure with groove edges rounded with a 100 nm radius of curvature. All panels have a lateral size of 2 μm.
Application example: Optical analysis of nanoparticles

Possible configuration

Molecule or nanoparticle in a groove of a silver patch on a dielectric substrate

Illumination from the substrate side causes very strong field in the groove

Detection of the scattered light: SNOM tip moving along the groove

Alternative: Detection of the light at the ends of the grooves
Application example: Optical analysis of nanoparticles

Possible configuration

Molecule or nanoparticle in a groove of a silver patch on a dielectric substrate

Illumination by a Channel Plasmon-Polariton (CPP) waveguide mode with very strong field in the groove

Detection of the scattered light: SNOM tip moving along the groove

Alternative: Detection of the transmitted light at the end of the grooves

Scattered light

Groove size $\ll \lambda$!

Incident light (CPP waveguide mode)
Numerical field solvers: TD vs. FD

Time domain
- Lossy and dispersive materials problematic (Drude-Lorenz approximations)
- Small features in resonant structures → very fine discretization of space and time → long computation time!
- Unstructured grids (FE, FVTD) difficult
- Adaptive discretization difficult
- Convergence and accuracy limited
- Frequency characteristics: Fourier transform not really easy

Frequency domain
- Lossy and dispersive materials easy
- Speed-up techniques for frequency characteristics available
- Convergence and accuracy depends on discretization technique

Domain methods
- Large sparse matrices
- Iterative solvers with preconditioners
- Mesh generators important

Boundary methods
- Small dense matrices → Direct matrix solvers
- Fast convergence and high accuracy possible (semi-analytic: MMP, MAS,...)
- Adaptive discretization easy
- Small features in resonant structures not difficult
Principles of MMP/GMT, MAS, etc.

Superposition: Field = Sum $Amplitude_k \times Basis_k + Error$

- **Select Basis$_k$**: Maxwell’s field equations hold in at least one domain
  - Simple: plane waves
  - Most useful: monopoles, dipoles, ... , multipoles, complex origin multipoles
  - Advanced: Analytic solutions, waveguide modes, superpositions...

- **Compute Amplitude$_k$** from boundary conditions: Point Matching, Projection techniques, Galerkin, MoM, Generalized Point Matching: Minimize weighted norm of Error, overdetermined systems of equations

**Special cases:**
- Analytic: Mie, Rayleigh, Yasuura
- **Generalized Multipole Technique (GMT) / Multiple Multipole Program (MMP)**
- Monopoles/dipoles: Auxiliary Sources, Fictitious Sources
- Multipoles only: Discrete Sources, Spherical Expansions
- Static: Image Charges, Charge Simulation
Eigenvalue analysis of lossy, dispersive waveguides

Resonances: Electromagnetically closed system

Analytic
Electromagnetic system described by a homogeneous matrix equation \( M(e)X(e) = 0 \)
Nontrivial solutions for \( \text{Det}(M(e)) = 0 \)
\( \rightarrow \) Eigenvalue \( e \) obtained from search for zeros

Measurement
Resonator must be opened for inserting energy and for detecting modes: Input/output ports
Frequency-response at the output port for constant input power: “scattering problem”
\( M(e)X(e) = I \)
\( \rightarrow \) Eigenvalue \( e \) obtained from search for maxima

Numerical
Search for zeros / maxima (resonance peaks) / minima (residual error minimization)
Note: \( R(e)X(e) = E(e), \|E\|^2 = \text{min.} \rightarrow R^*RX = 0 \rightarrow \text{Det}(R^*R) = 0 \)
More advanced: \( \|E\|^2/\text{Amplitude(output port)} = \text{min.}, \text{error integral minimization} \ldots \)

Waveguide modes: Resonator problem in the transverse plane
Eigenvalue search in the complex eigenvalue plane

Either the **frequency** or the **propagation constant** may be considered as eigenvalue
1. Fix propagation constant, search for frequency (Physicist)
2. Fix frequency, search for propagation constant (Engineer)

Lossy structures: Eigenvalue becomes complex → 2. is more natural

Complex eigenvalue search is very demanding!

Separation evanescent/guided/radiating modes difficult
- Fast transition from “guided” to “evanescent”
- Reasonable start points for search?
- Only solutions with low attenuation of practical value
- Almost degenerate modes
- Smart eigenvalue definitions
- Long computation time
- **Eigenvalue tracing** (Parameter Estimation Technique)
Eigenvalue tracing

Start at a certain frequency $f_0$
Search the propagation constant $g_0$

$f_1 = f_0 + df$, df small increment
Start search for $g_1$ at $g_0$

$f_2 = f_1 + df$
Start search for $g_2$ at $2g_1 - g_0$ (linear extrapolation)

$f_3 = f_2 + df$
Use quadratic extrapolation for start point…

- Higher order extrapolations are risky!
- Smart extrapolations (similar task: trace field lines)
- Adaptive increment size…
Channel Plasmon-Polariton waveguides, Au

CPP modes in deep grooves (>1000nm) well-known
Cutoff near 1400nm!
No modes for tiny grooves?

Simulation: Rectangular metallic wires with tiny grooves support modes with strong field localization in the groove but with some field also near the wedges
WPP-CPP modes

Au: strong loss
Frequency band with Reasonable performance
Channel Plasmon-Polariton waveguides, Ag

Ag has considerably lower loss than Au at shorter wavelength → Numerically more demanding!

WPP-CPP modes of Ag structures
• Narrower frequency band with low attenuation
• Shorter wavelengths: around 450nm (Au: around 600nm)
• Smaller dimensions of the wire
2D simulations of optical antennas: Gap-based

Design different from design of RF and microwave antenna (much more demanding)!
- Strong material dispersion → optimal material depends on desired resonance frequency
- Plasmon resonances → only very narrow frequency range for a given metal, only few metals with sufficiently low loss
- Surface plasmon propagation → larger antenna structures (still considerably shorter than half wavelength!) allow tuning of the resonance frequency within a broader range
- The narrower the gap, the stronger the field in the gap
- Quality factor depends on material properties and wavelength
2D simulations of optical antennas: Groove-based

Design even more demanding than for gap-based antennas (Channel Plasmon-Polariton)
- Very strong field may be obtained in the groove
- Two resonance peaks (groove in the center) instead of a single one (in the center)
- Higher Q factor, stronger resonance peaks than gap-based antennas
- For a certain antenna length, the peaks have the same size
- The narrower the groove, the stronger the field inside

Problems: Validity of „macroscopic“ Maxwell description, Simulation, Fabrication
Influence of substrates

2D structures on a substrate
• red shift (with increasing $\varepsilon$)
• reduced field enhancement
• reduced Q factor
• triple points with extreme impact! (compare T1 with T2)

Substrate $\varepsilon = 1, 2, \ldots, 10$

V-groove Ag

Substrate $\varepsilon = 1, 2, \ldots, 10$
3D simulations of optical antennas

3D very time-consuming!

Axisymmetric 3D structures:
- Symmetry-decomposition important: ring multipoles
- Symmetry-adapted excitation: ring-dipole
- Pseudo-2D simulation possible (matrix size same as for 2D)

Circular rod $r=10\text{nm}$, $L=20\ldots60\text{nm}$

Ring-dipole excitation in the groove
Conclusions and Outlook

Even simple configurations may turn out to be difficult!

Simulation-based investigation of new physical effects:
• Difficulties to understand the effects when no analytic models are available
• Fabrication demanding → Simulation important
• Simulation demanding (many tuning parameters) → Optimizers important
• Software for simulation and optimization must be accurate and reliable

Maxwell solvers:
• Many years of development, no “optimal” method, room for improvement
• Selection of “appropriate” method: knowledge of available methods
• Special requirements for successful combination with optimizers:
  Boundary discretization methods well suited

Nanotechnology reaches limitations of Maxwell theory!