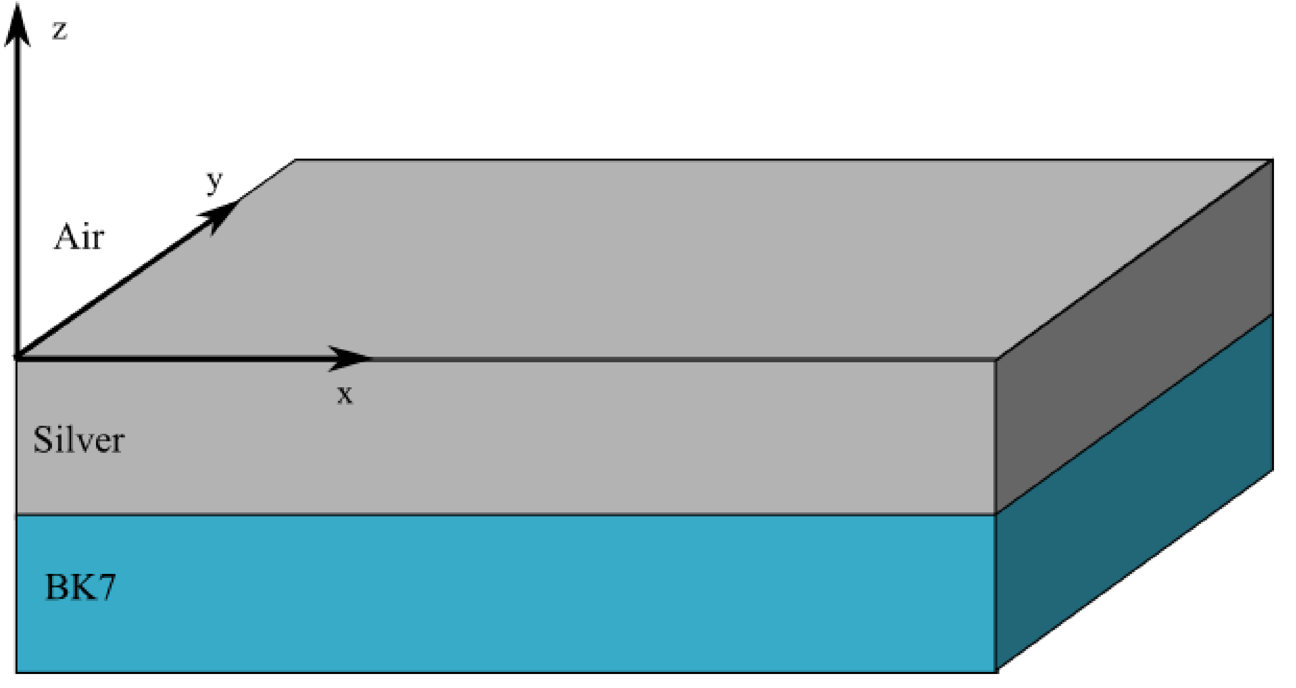
Numerical simulations of planar metal-dielectric plasmonactive systems

T. Repän, S. Pikker, L. Dolgov
University of Tartu
Estonia

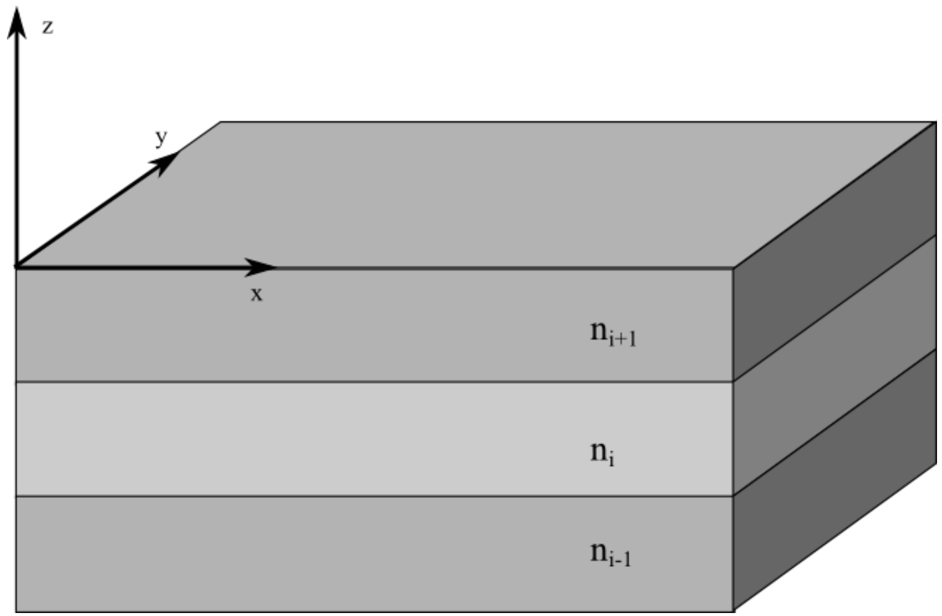
taavi.repan@ut.ee

Thin-film structures



Transfer matrix method (TMM)

- Analytical method
- For 1D structures
- Computationally cheap

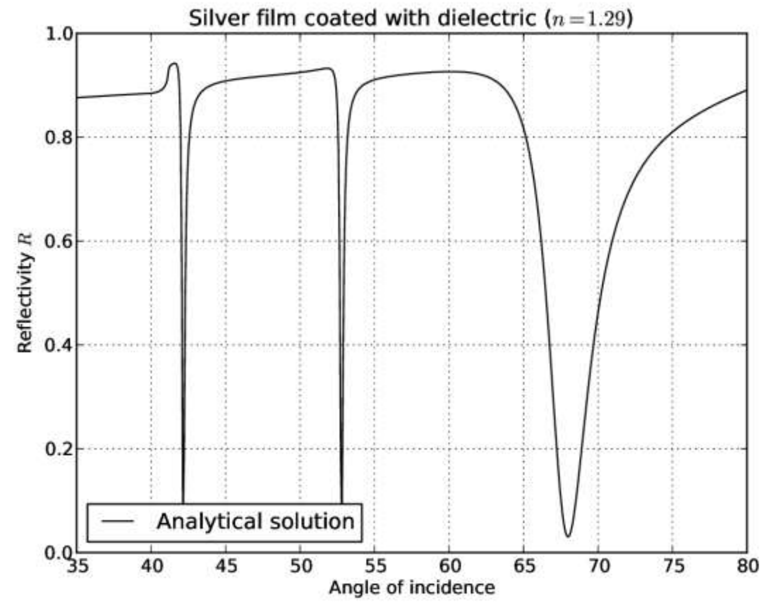


TMM for reflectivity calculations

- Fields in layer i:

$$E_i(x) = A_i exp\{-ik(x - x_i)\} + B_i exp\{ik(x - x_i)\}$$

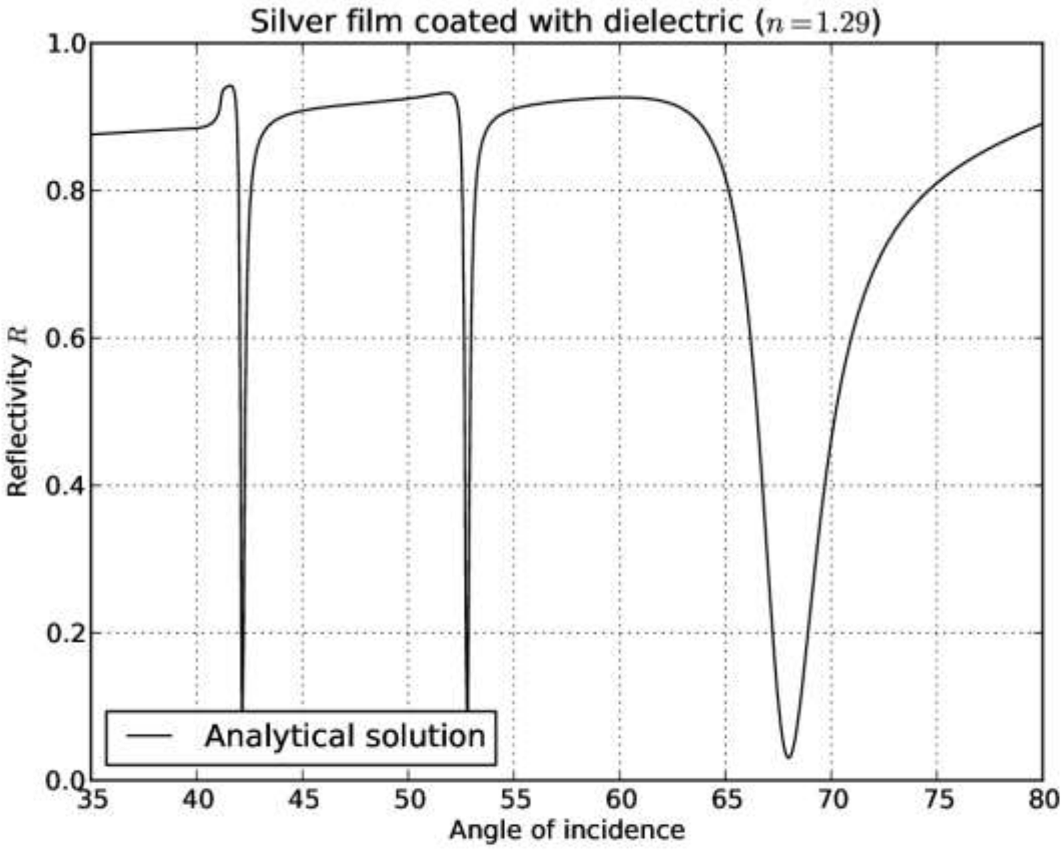
- Obtain 2x2 matrix for each layer
- Multiply matrices to get system matrix
- R and T are expressed as functions of M



TMM for finding waveguide modes

- Additional conditions for derivative of electric field are enforced
- From those conditions relation $F(\beta) = 0$ is obtained
- Zeros of F correspond to available modes in structure
- In case of metals β is complex

TMM for finding waveguide modes

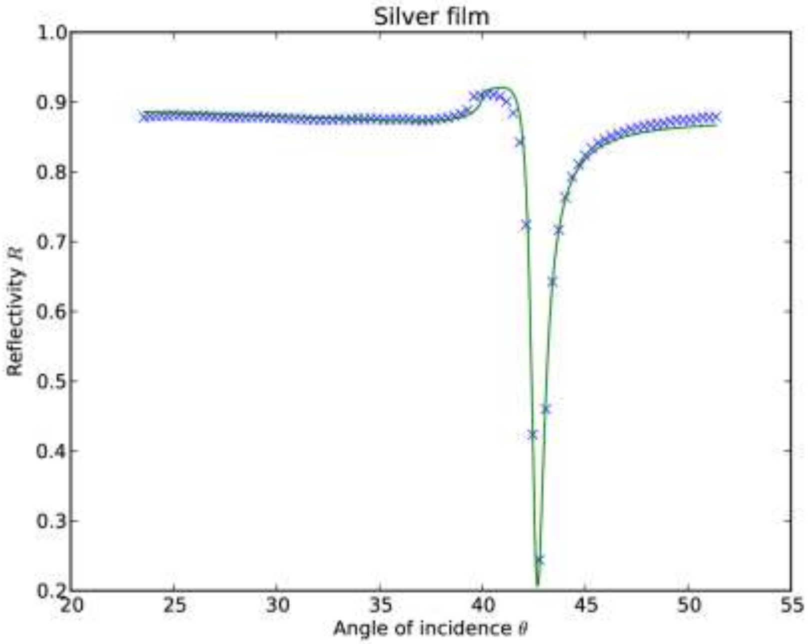


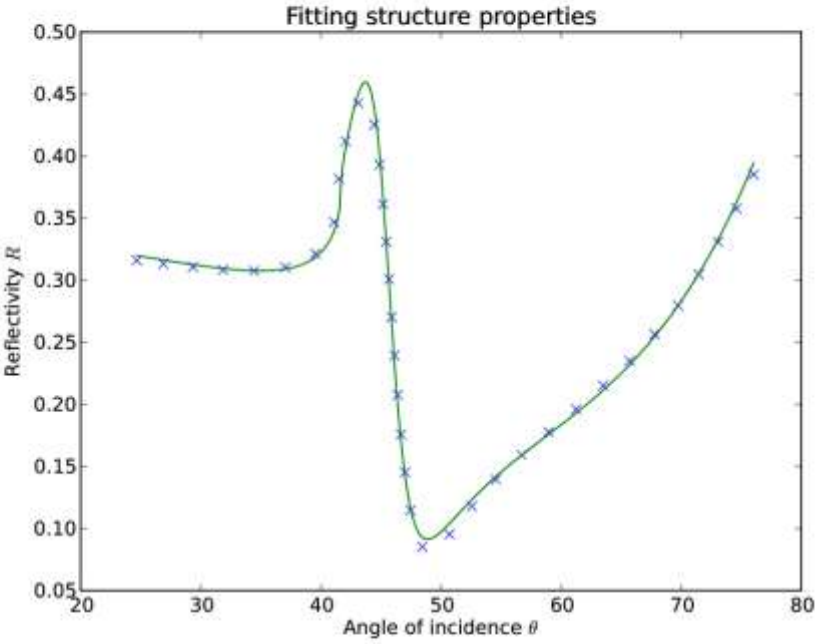
TM_0	1.40837861961600062+0.0030912124514507725j	67.98°
TM_1	1.2098157689478155+0.00024205017343937 46j	52.78°
TM_2	1.0196667874711303+0.0002481782550071288 5j	42.16°

TMM for estimating material properties

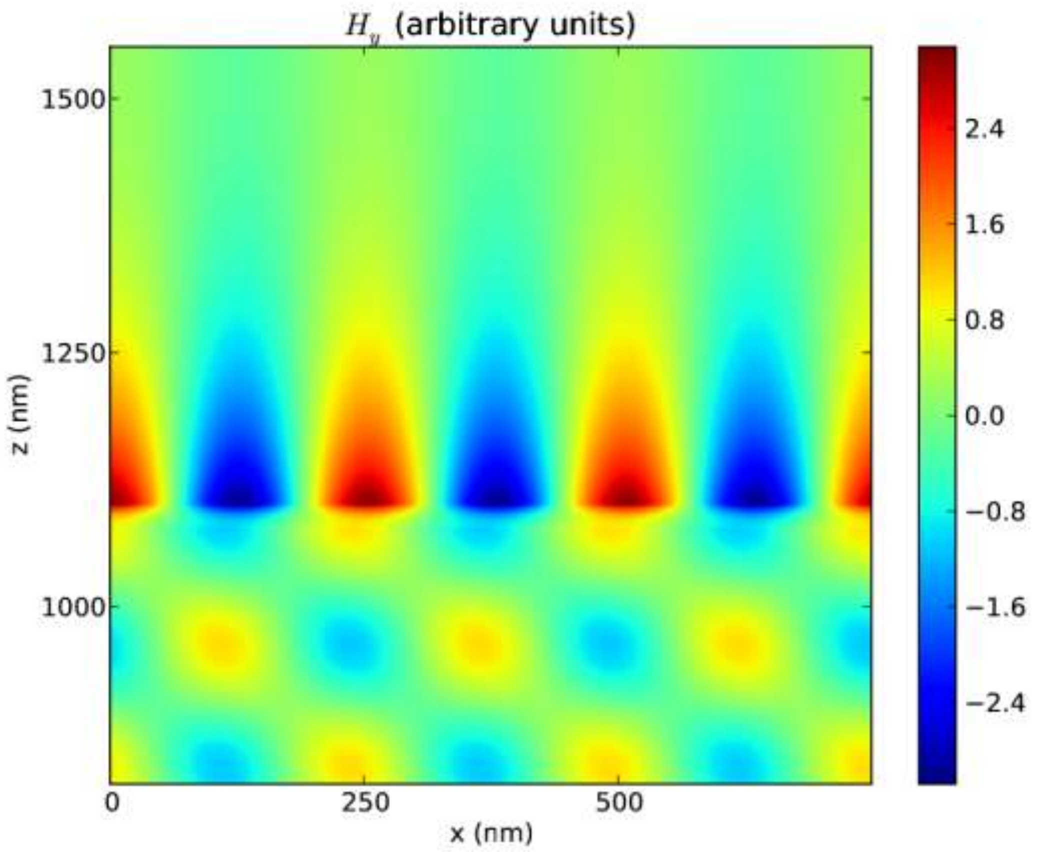
- Possible to fit experimental data and estimate system properties
- Implemented using Python and SciPy

TMM for estimating material properties



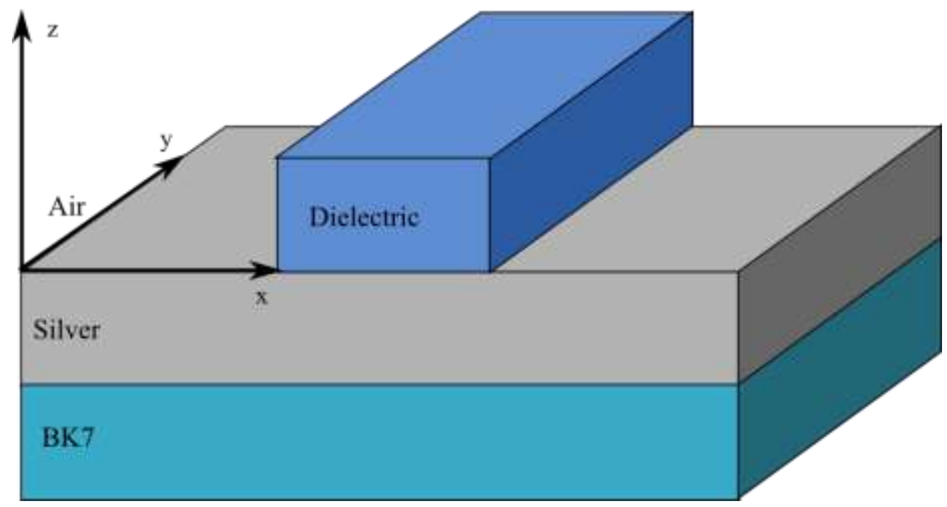


TMM for calculating fields



Effective index method

- Extension of TMM for 2D structures
- Approximate solution



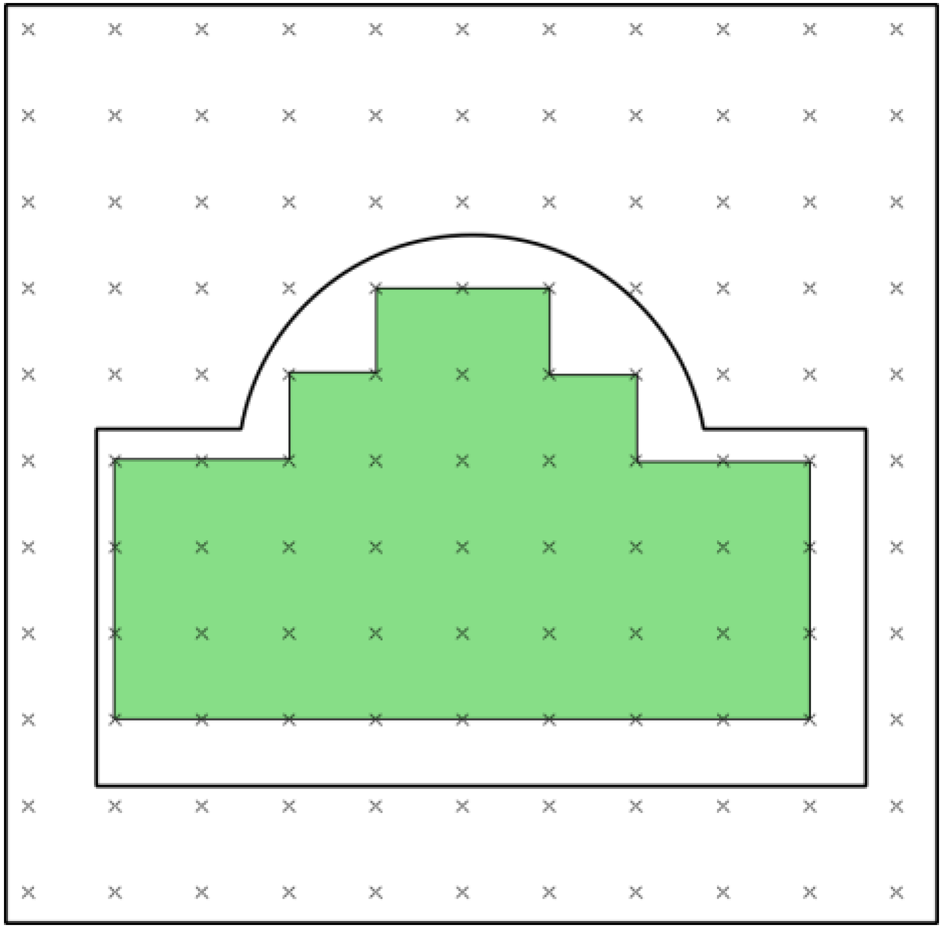
Finite difference time domain

- Arbitrary geometry
- Time and spatial derivatives are approximated using 1st order Taylor expansion:

$$\frac{dF(x)}{dx} = \frac{f(x+\delta) - f(x)}{\delta}$$

- Leapfrog time stepping
- Spatial discretization using regular grid: staircase approximation

FDTD: Staircasing



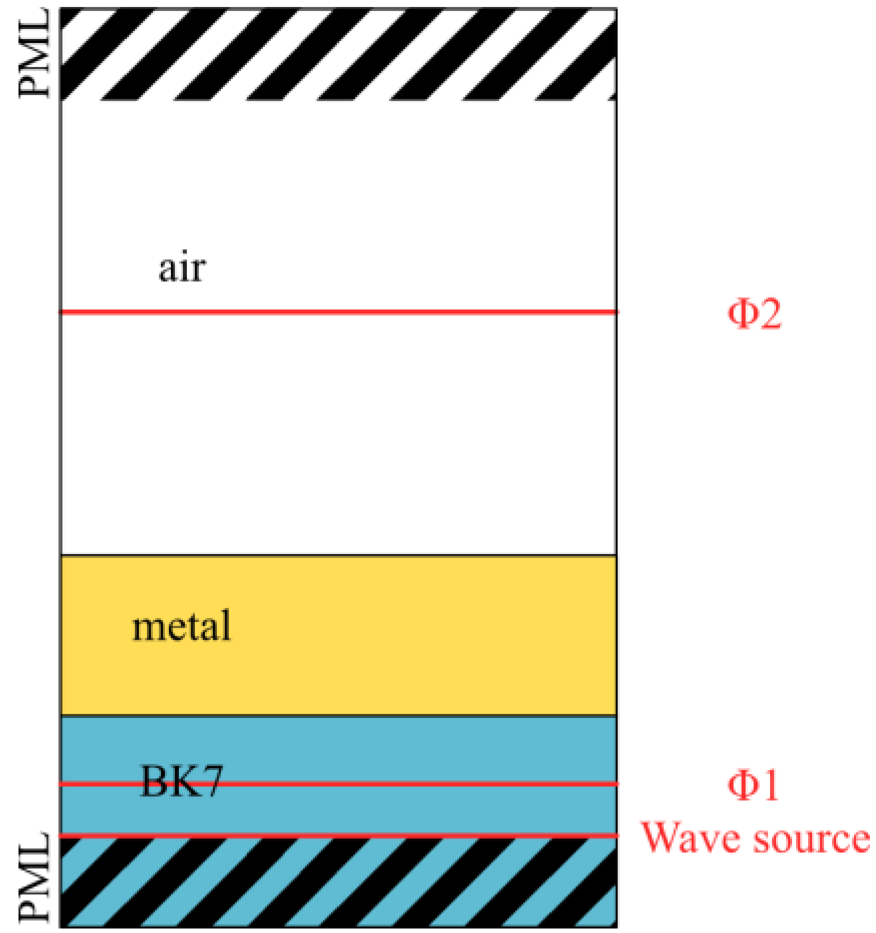
FDTD package Meep

- Open-source FDTD package from MIT
- 2D/3D simulations (regular grid)
- Tools for Fourier transform
- Drude-Lorentz model

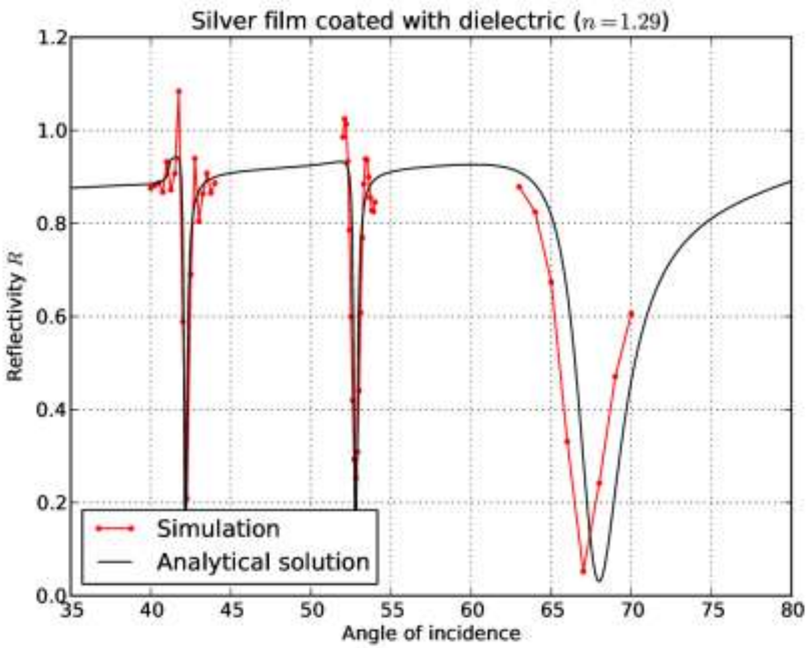
$$\varepsilon(\omega) = \left(1 + \frac{i\sigma_D}{\omega}\right)\left[\varepsilon_\infty + \sum_n \frac{\sigma_n \omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n}\right]$$

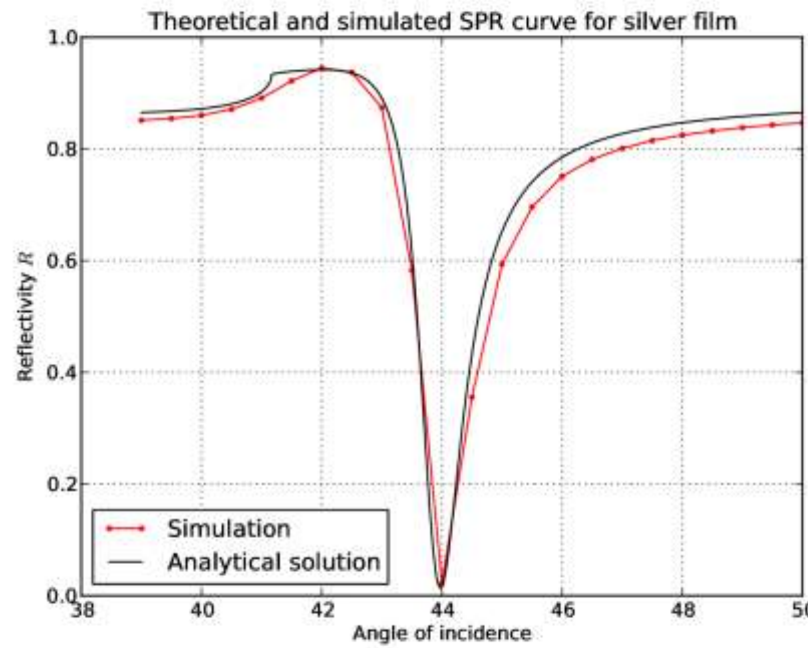
Simulation configuration

- ~ 100x1000 nm
- 50 nm metal layer
- 5 nm resolution
- Simulation time is about 200 fs



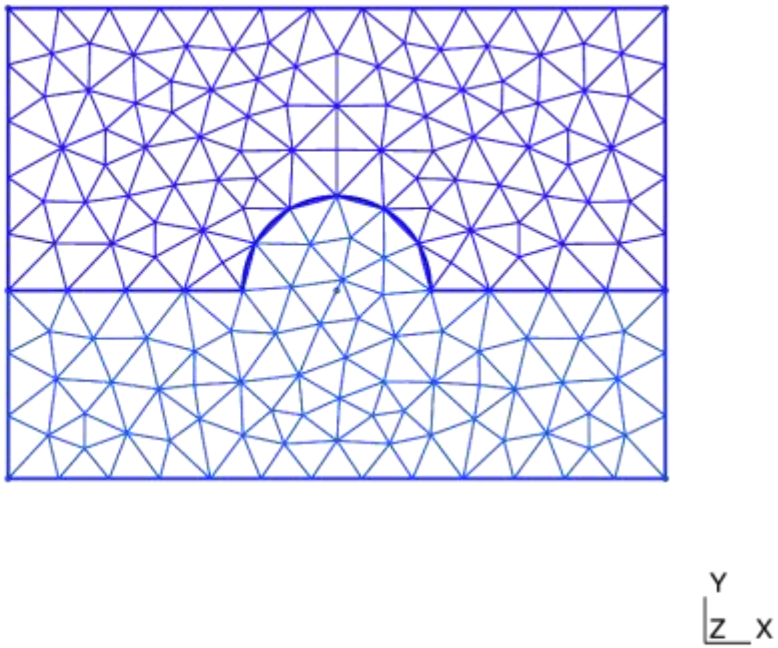
Basic FDTD simulations





Extensions to FDTD

- Higher-order FDTD
- Unstructured grid FDTD



Conclusions

- TMM codes for analyzing 1D/2D structures were developed
- FDTD simulations with Meep were investigated
- Future interest is to create codes for unstructured grid FDTD

Finite element method

- Unstructured grids
- Larger computational costs
- Used mostly for frequency-domain simulations
- Better accuracy due to higher-order basis functions