Simulating Metal and Graphene Based Hybrid Plasmonic Devices

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LUMERICAL SOLUTIONS, INC.

Outline

Introduction to Lumerical

Key challenges when simulating metal and graphene based hybrid plasmonic devices

Some solutions

Examples

Conclusions

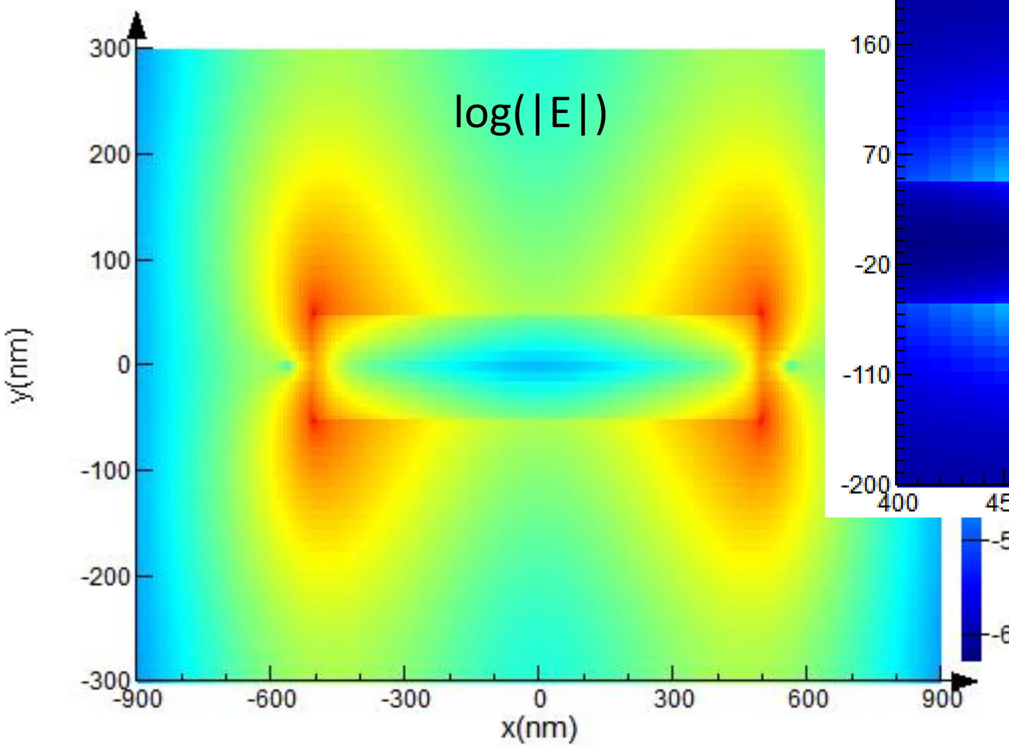
Key Challenges

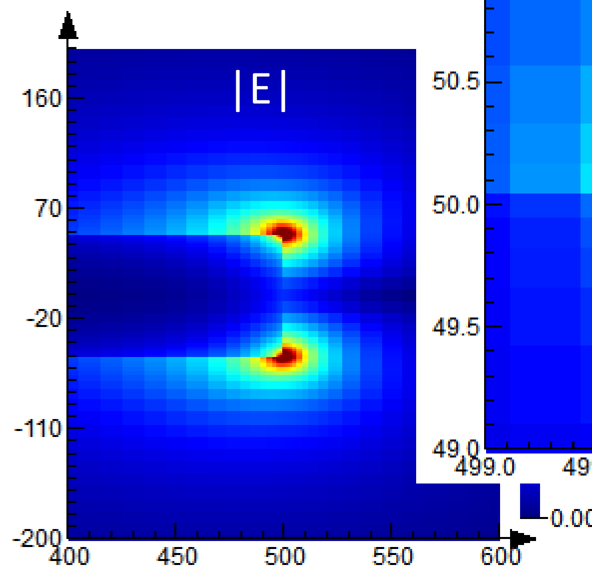
SIMULATION OF METAL AND GRAPHENE BASED HYBRID PLASMONIC DEVICES

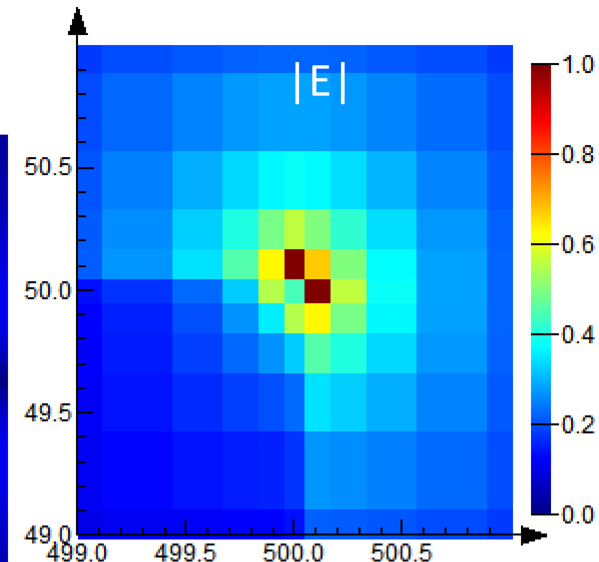
Key Simulation Challenges

Localized, discontinuous electromagnetic fields

- Example, silver waveguide (1000nm X 100 nm)
- λ_0 = 633nm





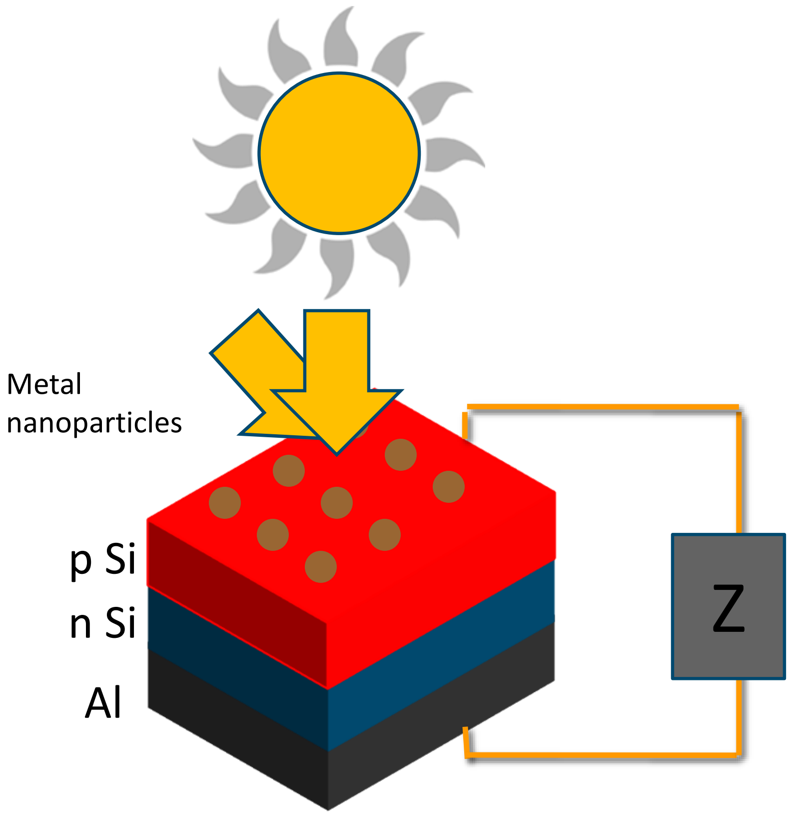


Original design from: Berini, "Plasmon-polariton waves guided by thin lossy metal films of finite width: Bound modes of symmetric structures", Phys. Rev. B, 61, 10484-10503 (2000)

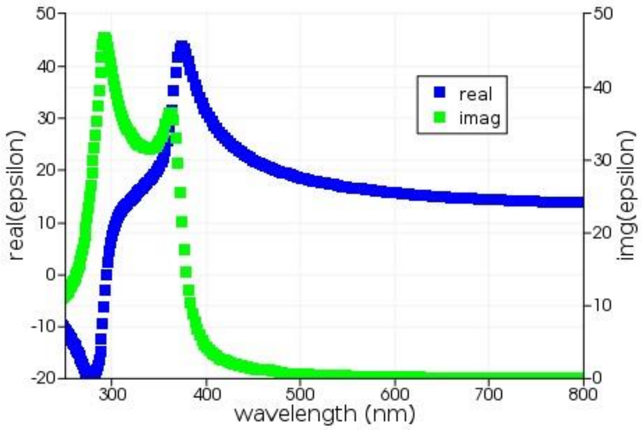
Key Simulation Challenges

Broadband results required

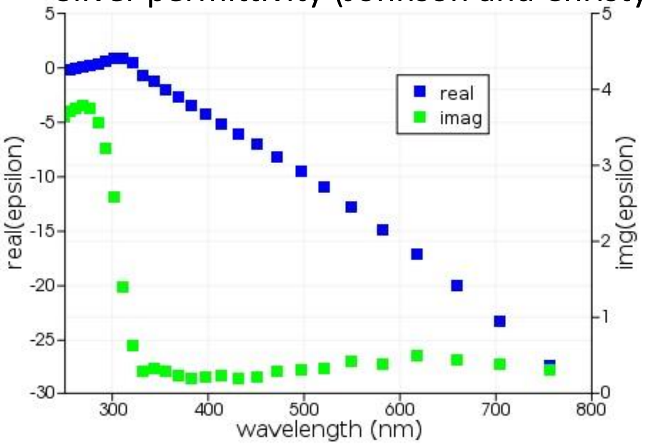
Possible oblique angle of incidence



Silicon permittivity (Palik)



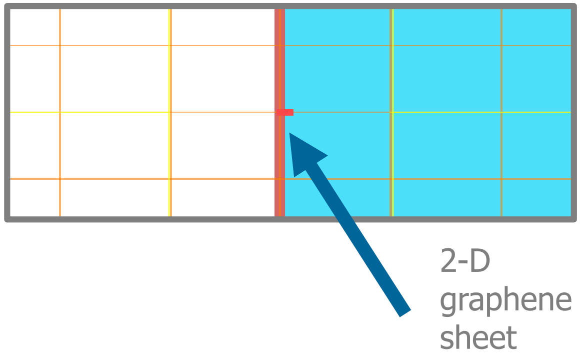
Silver permittivity (Johnson and Christy)

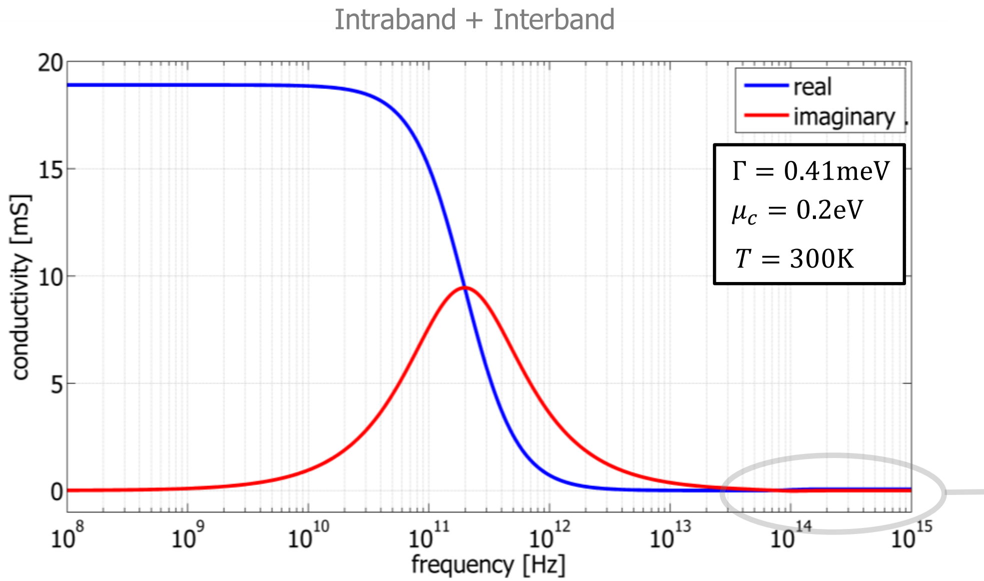


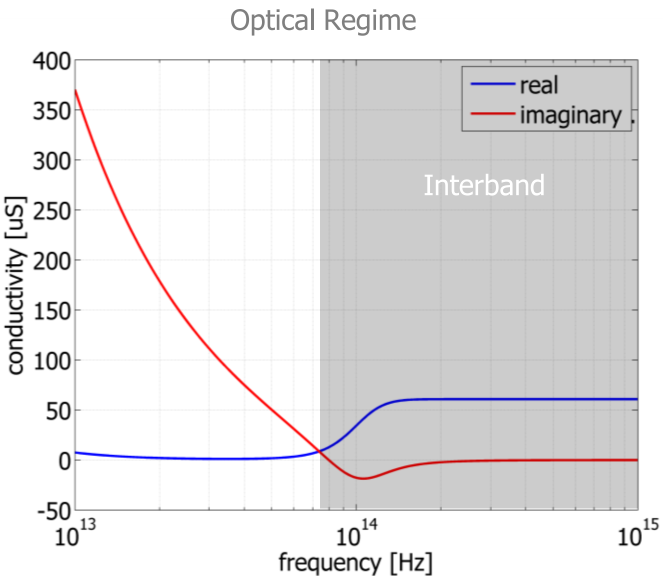
Key Simulation Challenges

2D materials such as graphene

- Challenging within a 3D mesh
- Mesh points may be in graphene and at the interface between two (dispersive) media
- Graphene surface conductivity is also dispersive







Key Simulation Challenges

Devices require a combination of electrical and optical simulation

- Tuning devices through plasma dispersion effect
- Generating distributed sources of electrons/holes through photon absorption

Solutions

Solutions

Time domain simulation

- Appealing for broadband results
- Typically involves an explicit update that is scalable through parallelization

Introduces two new challenges

- Dispersive materials in the time domain
- Oblique angles of incidence become frequency dependent in periodic structures

Solutions

Dispersive materials in the time domain

$$\vec{D}(\omega) = \varepsilon(\omega)\vec{E}(\omega)$$

$$\vec{D}(t) = \varepsilon(t) * \vec{E}(t) = \int_0^t \vec{E}(t')\varepsilon(t-t')dt'$$

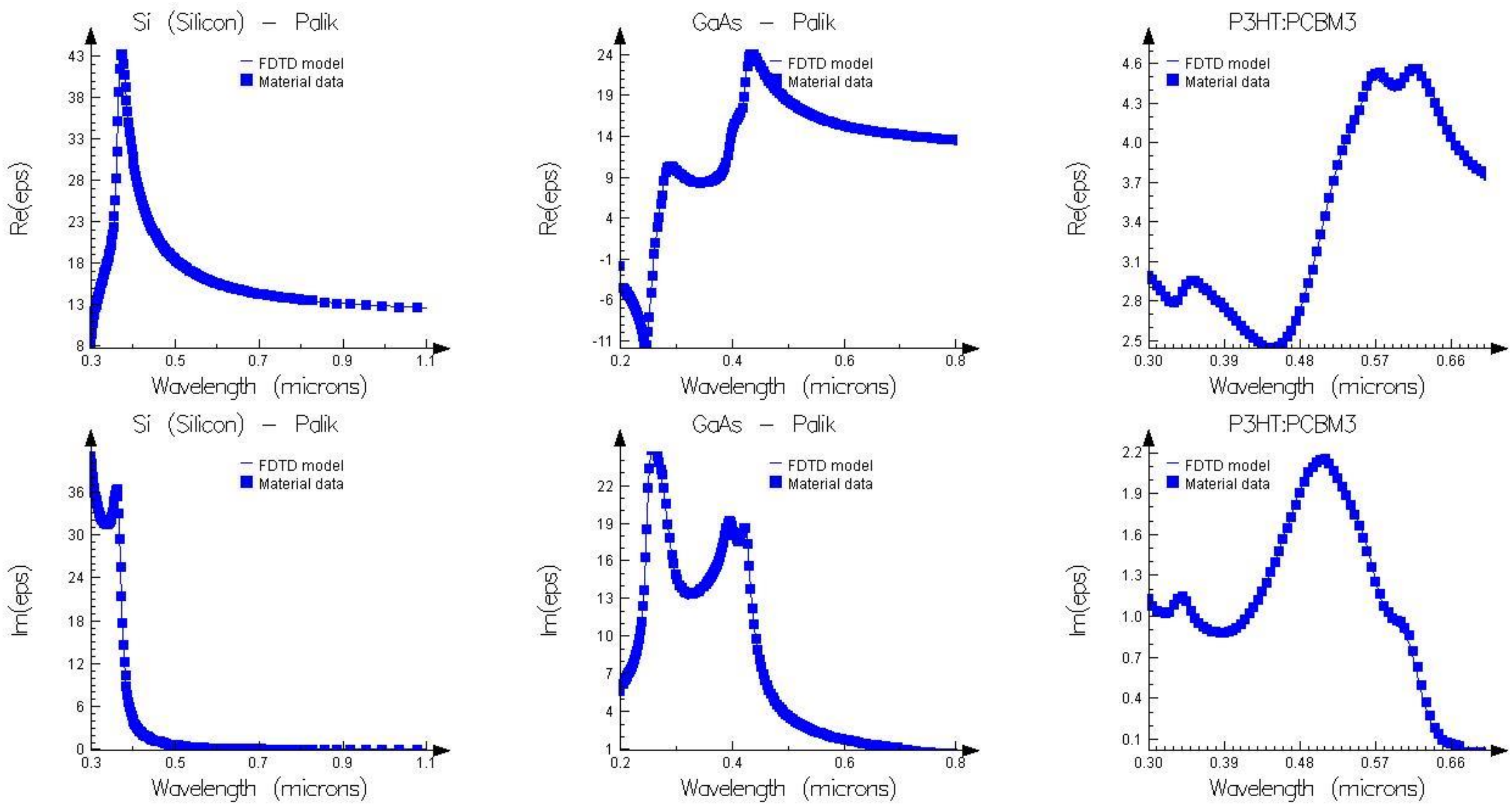
- The numerical solution of the convolution product limits the acceptable expansions for $\varepsilon(\omega)$
- Must be causal and therefore will satisfy Kramers-Kronig relations!

Lumerical's multi-coefficient model (MCM) provides an easy solution

- Fitting to experimental data for n,k is fully automated

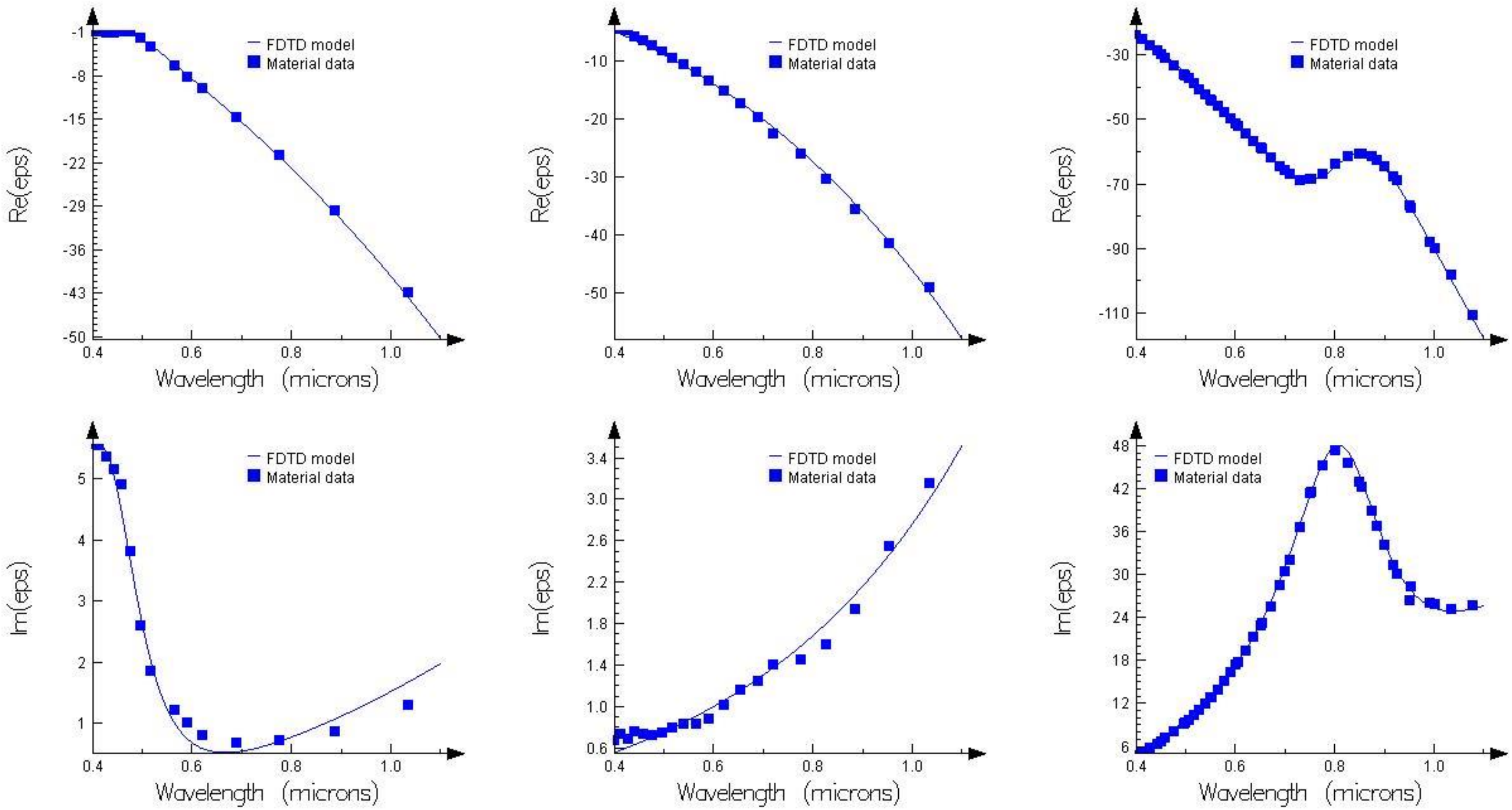
MCM fitting

Silicon | **GaAs** | **P3HT:PCBM**

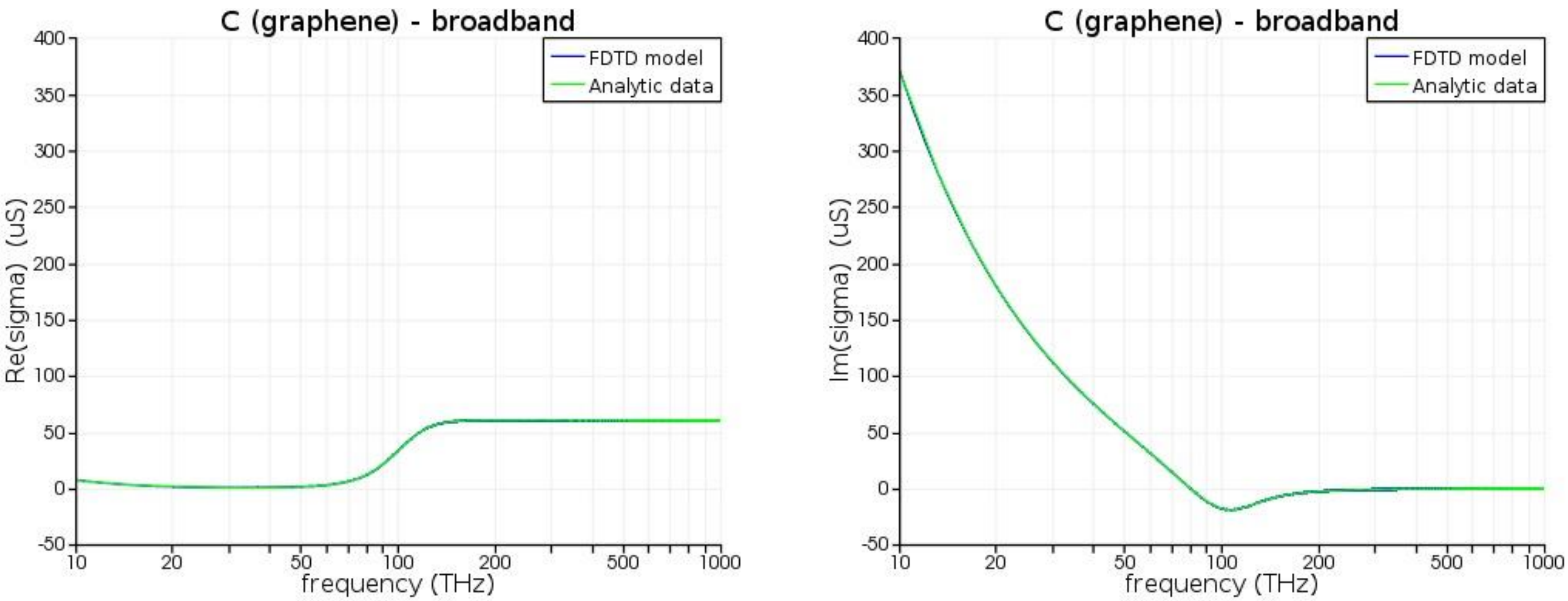


MCM fitting

Gold **Silver** **Aluminum**



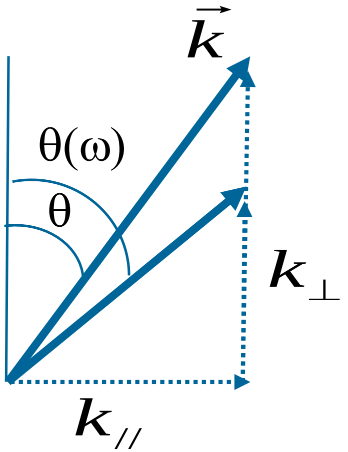
MCM fitting of graphene



Solutions

Second challenge for time domain simulations

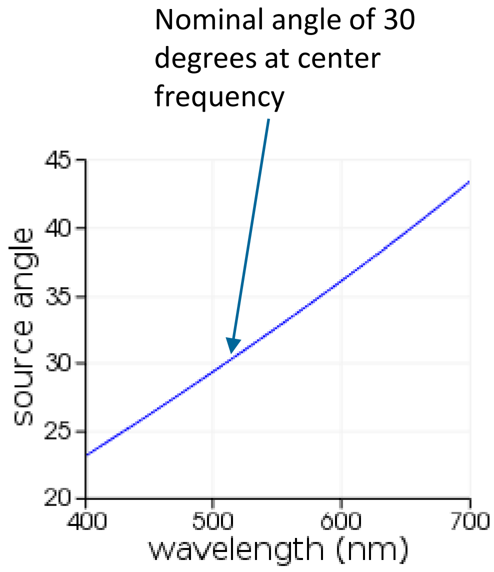
- Oblique angles of incidence on periodic structures
- Common solution is Bloch-Periodic boundaries
- Angles of incidence become frequency dependent



$$k = \omega / c$$

$$k_{//} = k_{Bloch} = \text{constant}$$

$$k_\perp = \sqrt{k(\omega)^2 - k_{Bloch}^2}$$



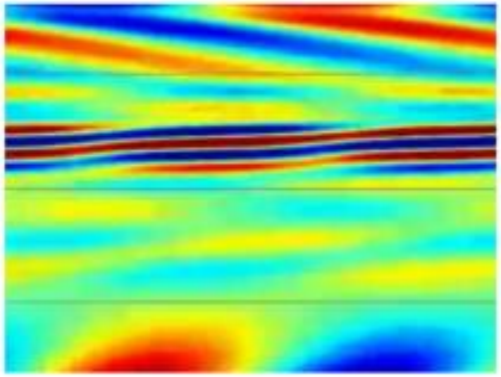
BFAST - Example

For oblique angles, we introduce BFAST

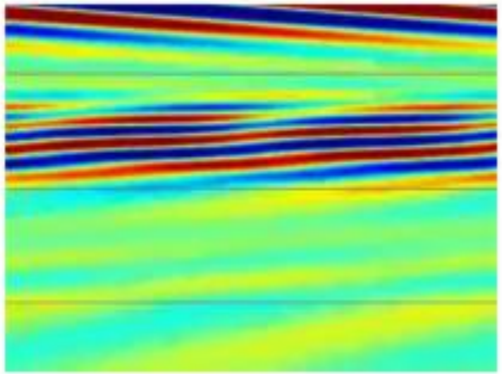
- Broadband fixed angle source technique, based on the split-field method
- Works for arbitrary dispersive media
- There is a big penalty to pay in the time step, Δt, but it is worth it for broadband simulations
- Number of frequency points recorded can be increased without increasing simulation time

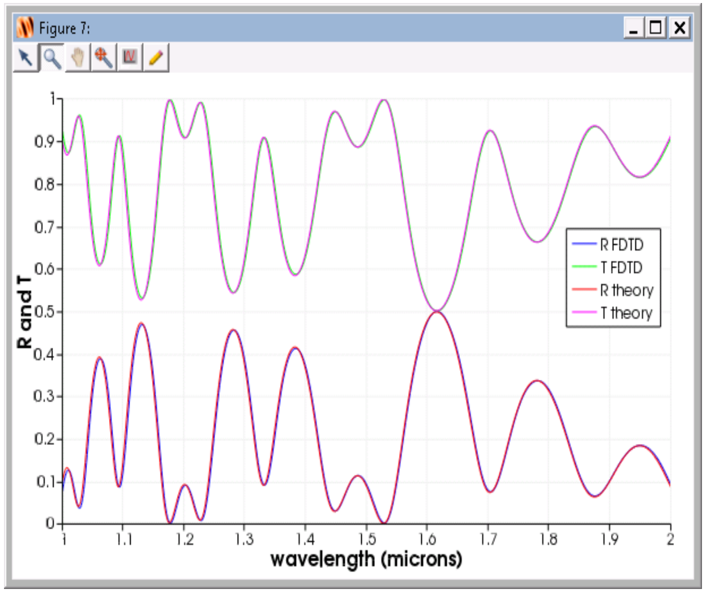
Transmission/reflection spectra compared to theoretical results calculated by transfer matrix

Bloch-Periodic



BFAST





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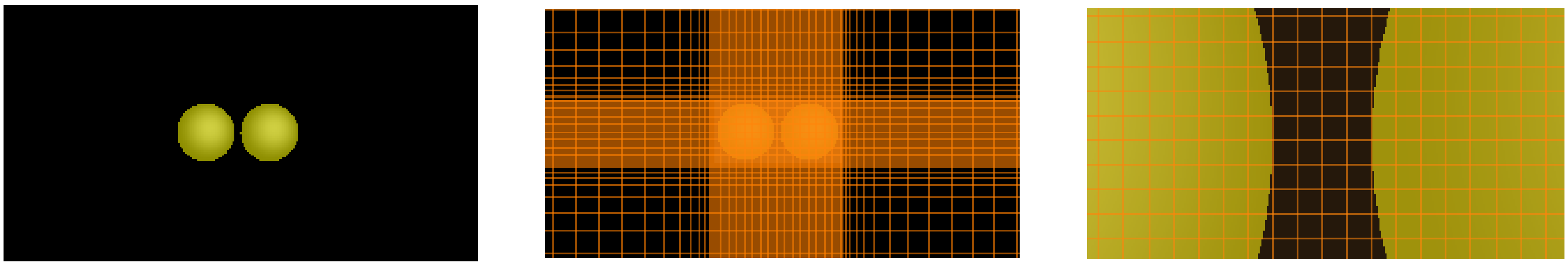
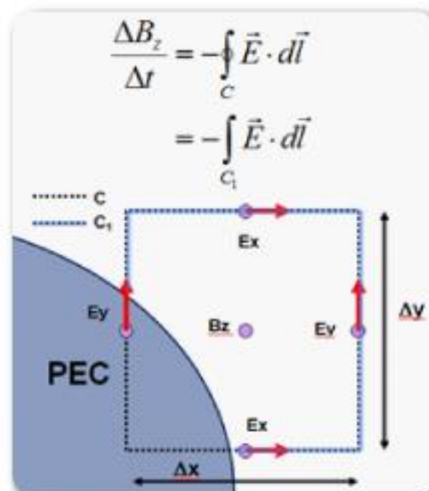
Solutions

FDTD is a good tradeoff between mesh accuracy and performance for many applications

- Key is to use a graded mesh for plasmonics



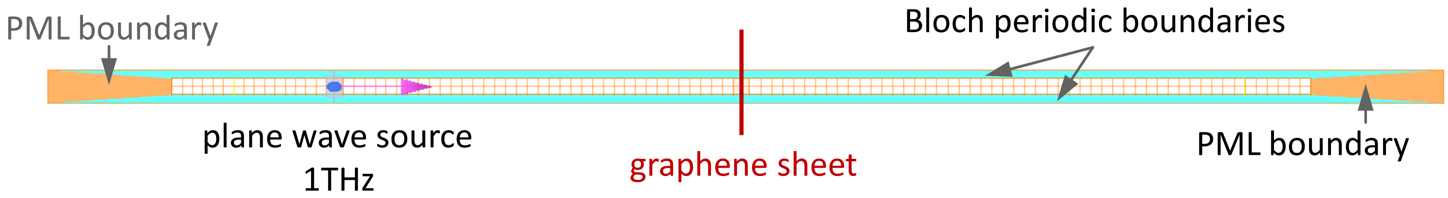
- And a conformal mesh
  - Integral solution to Maxwell's equations
  - Extended to arbitrary dispersive media
  - Caution when using with metals

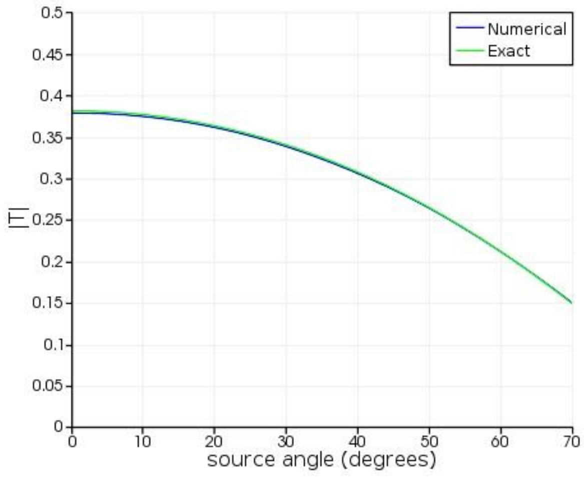


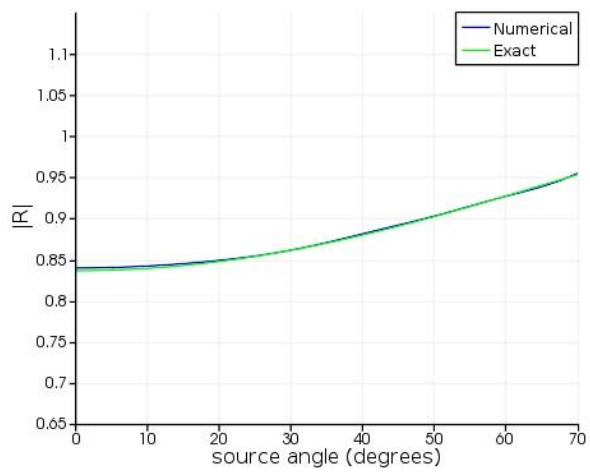
Solutions

Conformal mesh approach can be extended to include graphene

- 2D conductivity within the 3D mesh
- Graphene can be at the interface of dispersive media



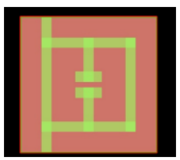


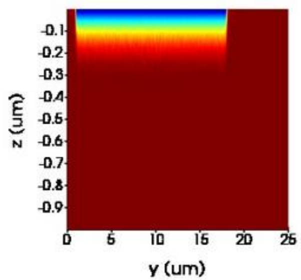


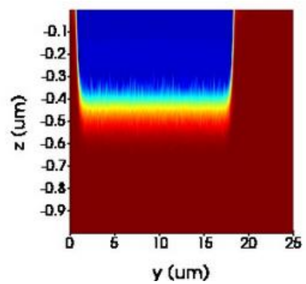
Solutions

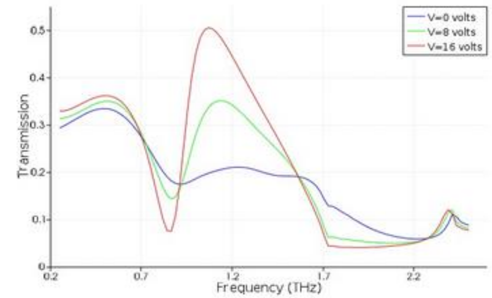
Electrical and optical simulations

- Run electrical simulation, calculate charge density, import to optical solvers

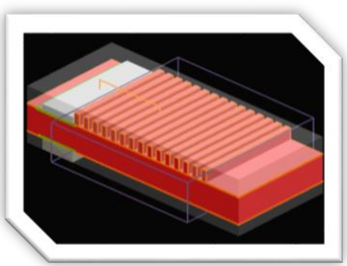


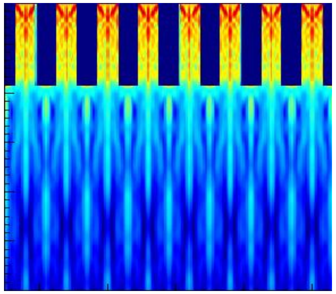


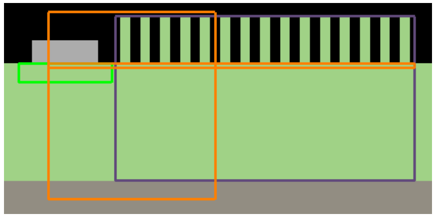


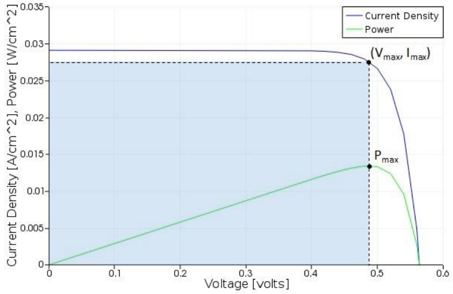


- Run optical simulation, calculate optical generation rate of electrons and holes, import to electrical simulator





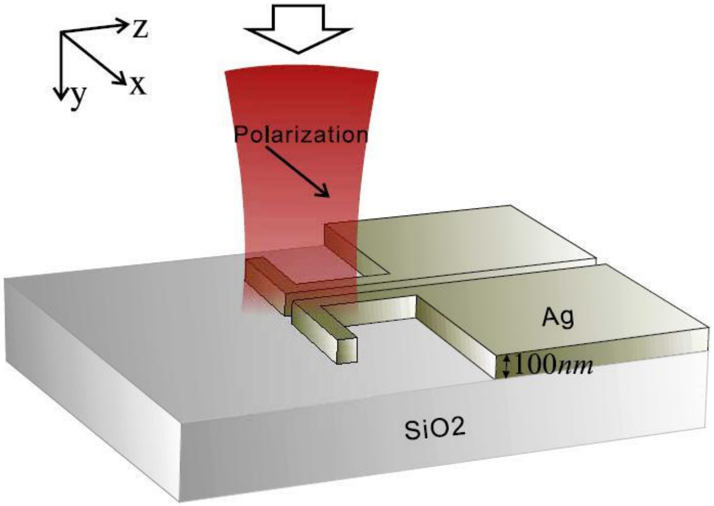


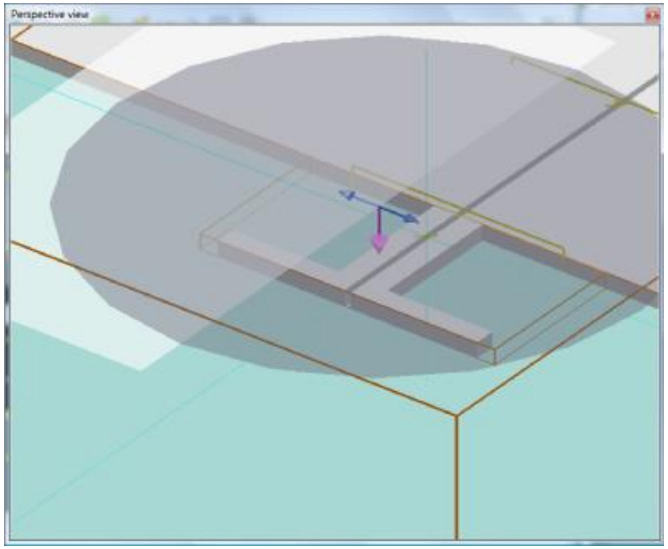


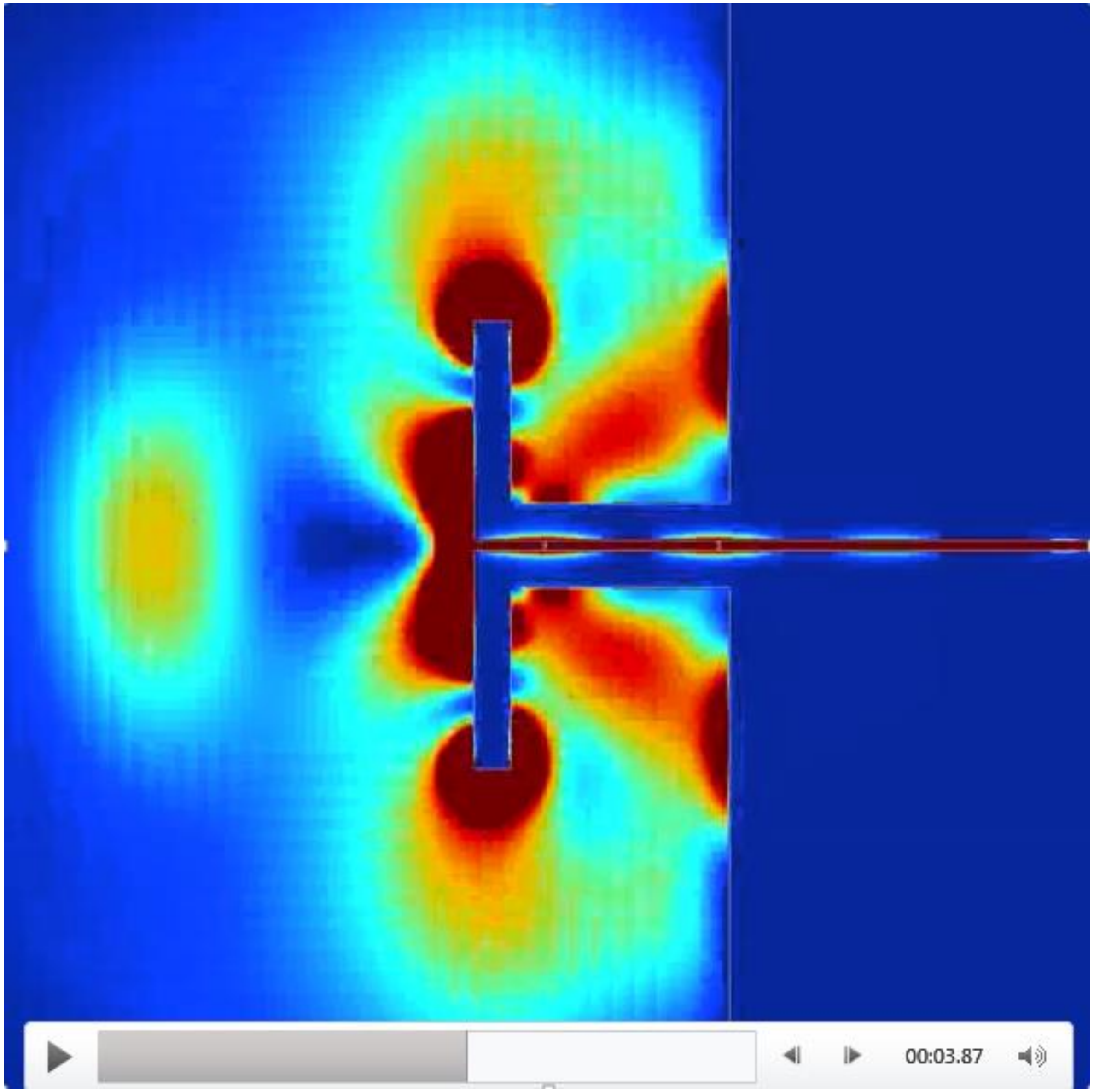
Examples

Gap SPR waveguide nano-antenna

We'll consider the structure in Jing Wen, Sergei Romanov, and Ulf Peschel, "Excitation of plasmonic gap waveguides by nanoantennas," Opt. Express 17, 5925-5932 (2009)



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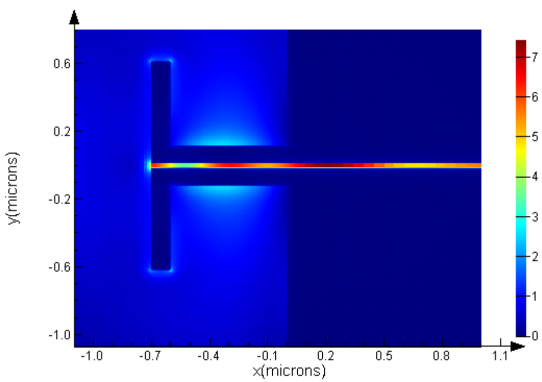
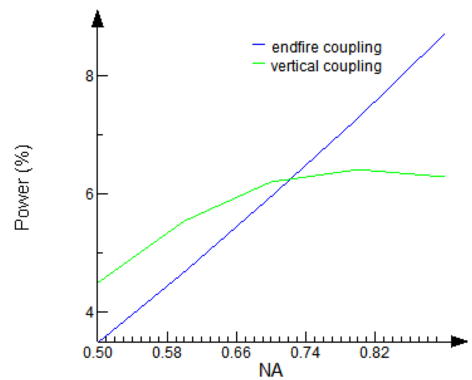
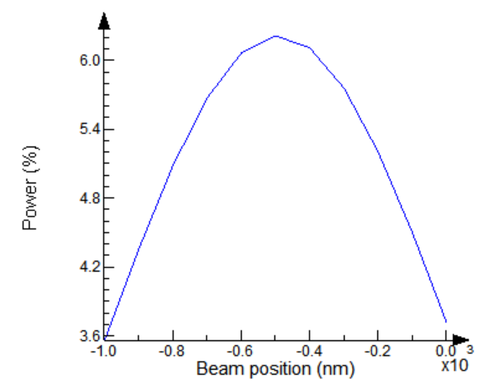
Gap SPR waveguide nano-antenna

Can study optimal beam alignment and NA to maximize coupling

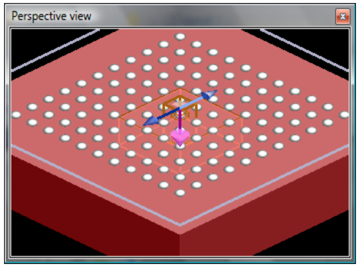




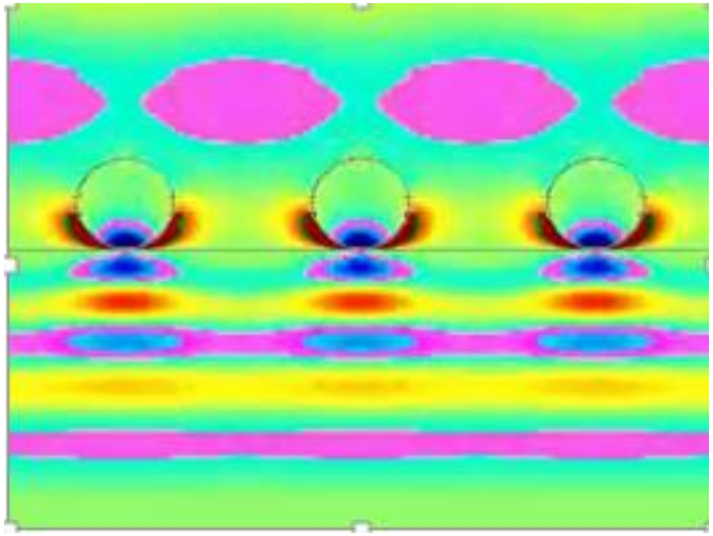


Dimensions (μm)	3 x 3 x 2
Symmetries	2 x reduction
Minimum mesh size	2 nm
Materials	Silver, SiO_2
Wavelength	1.5 μm
Simulation time (Workstation, 4 cores)	90 seconds
Simulation time (Laptop, 4 cores)	2 minutes, 40 seconds

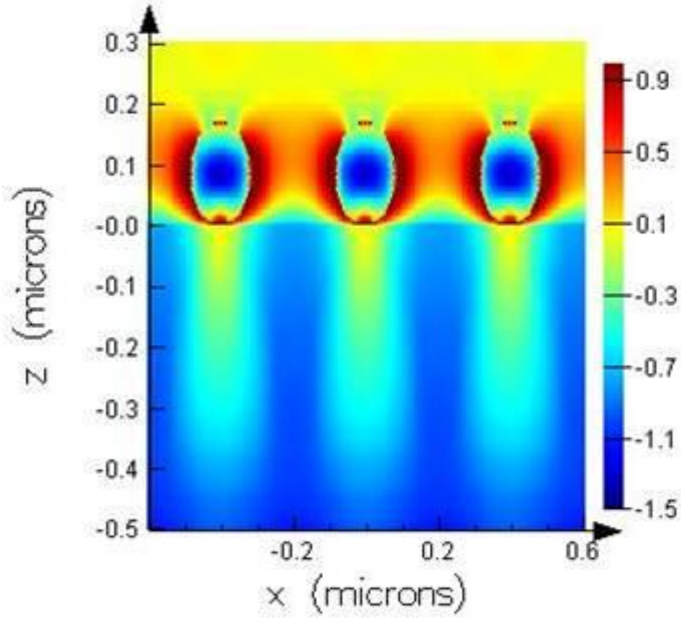
Plasmonic enhanced solar cell



E(t)

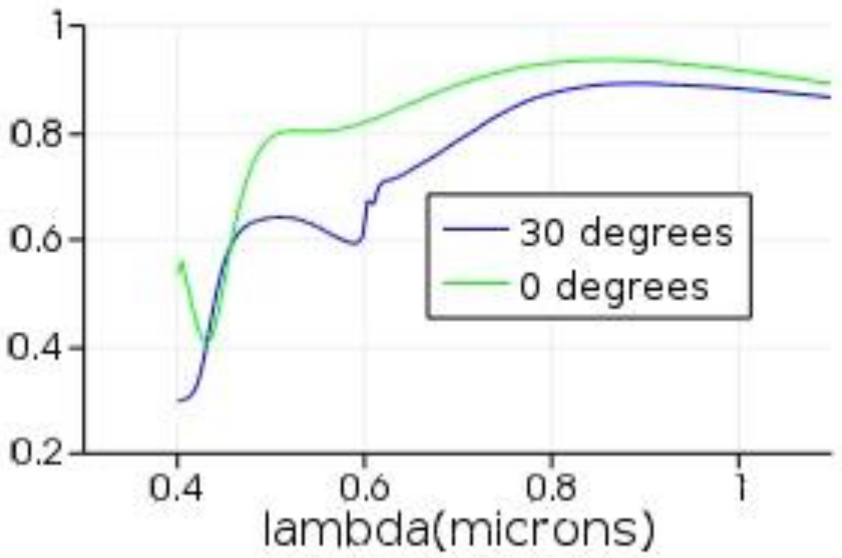


|**E**(w)|^2



Plasmonic enhanced solar cell

Normal incidence vs 30 degree (P polarized)



Next step – export electron/holes generation rate anc calculate J-V curves, maximum power

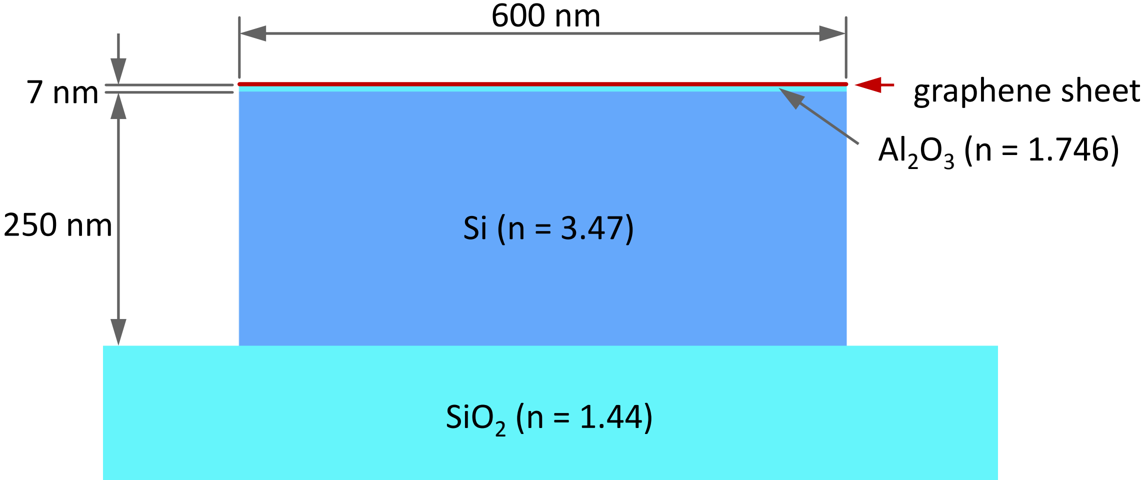
Normal incidence, standard FDTD

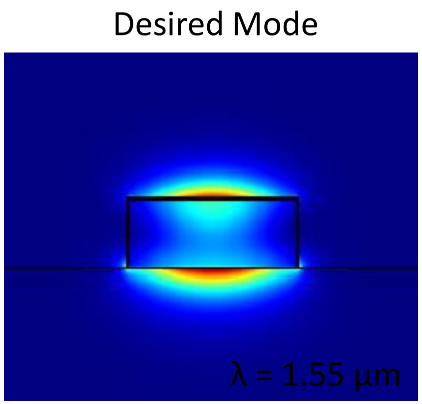
Dimensions (μm)	0.4 x 0.4 x 1.3
Symmetries	4 x reduction
Minimum mesh size	1 nm
Materials	Silicon, Silver
Wavelength	400 – 1000 nm (500 points)
Simulation time (Workstation, 4 cores)	1.3 minutes

30 degree incidence, BFAST FDTD

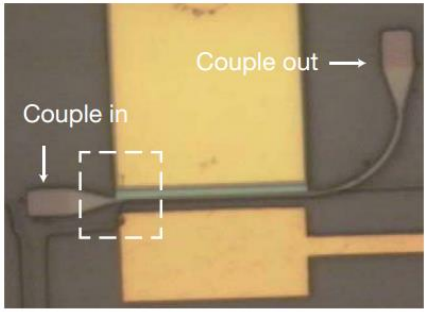
Symmetries	None
Simulation time (Workstation, 4 cores)	30 minutes << 1.3 minutes * 500

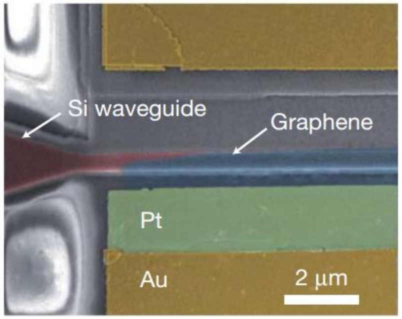
Graphene modulator





- Chemical potential of the graphene layer can be tuned using a voltage source





M. Liu, X. Yin, E. Ulin-Avila, B. Geng, T. Zentgraf, L. Ju, F. Wang and X. Zhang , “A graphene-based broadband optical modulator”, *Nature Letters*, vol. 474, pp. 64-67, 2011.

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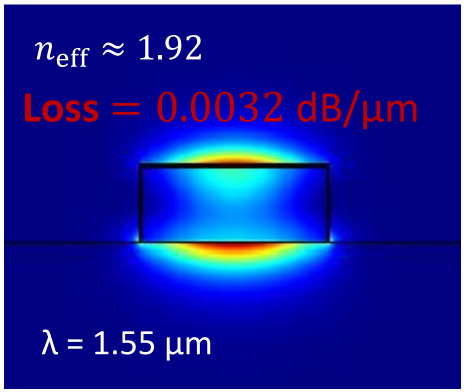
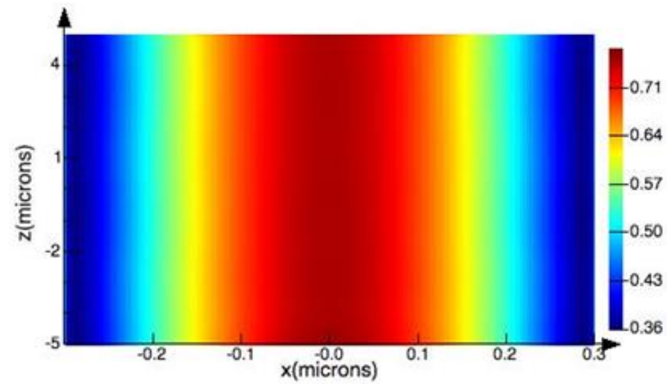
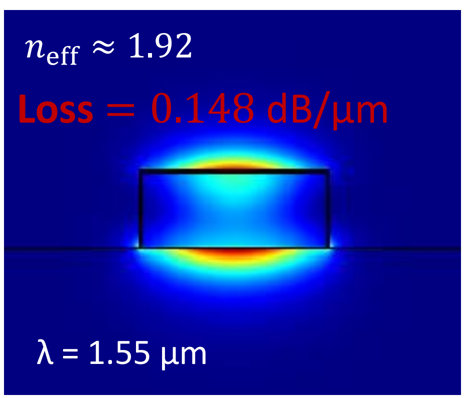
Graphene modulator

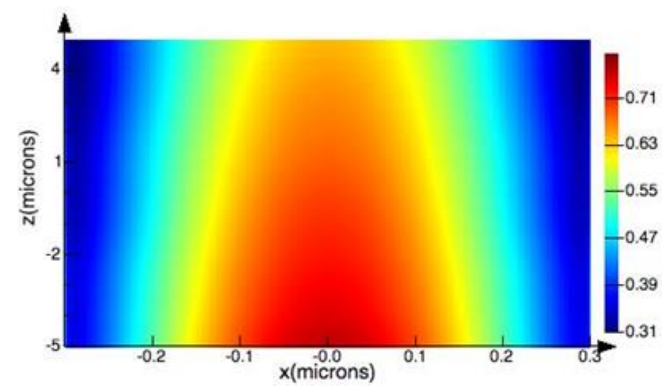
On state (μ_c = 0.8 eV)





Off state (μ_c = 0)

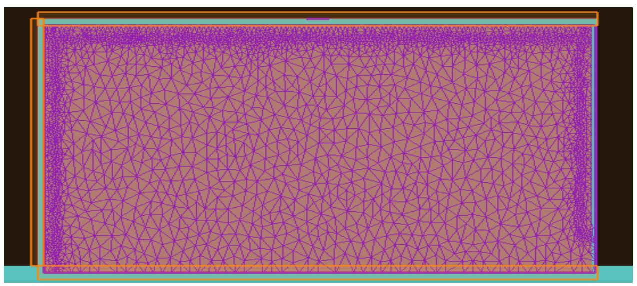


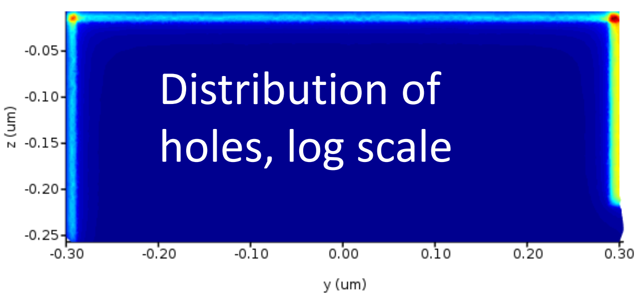


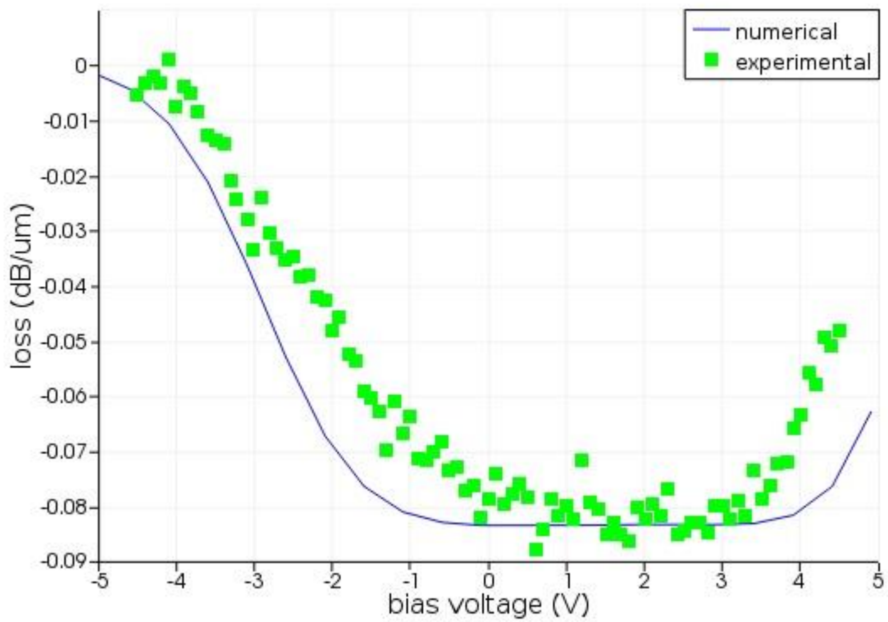
Graphene modulator

We can combine optical and electrical simulation results

- Electron-hole distribution in Si (depends on bias voltage)
- Relationship between bias voltage and chemical potential







Conclusions

Metal and graphene based devices present many opportunities

But…

- These leading edge materials and devices present many simulation challenges

The challenges can be overcome with continual improvements to implement start-of-the art algorithms

- MCM dispersive materials in time domain simulations
- Graded and conformal meshes
- Contour path integral approaches to two-dimensional materials
- Novel split-field FDTD methods
- Efficient use of modern HPC resources
- Combination of electrical and optical simulations

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