Numerical methods in plasmonics

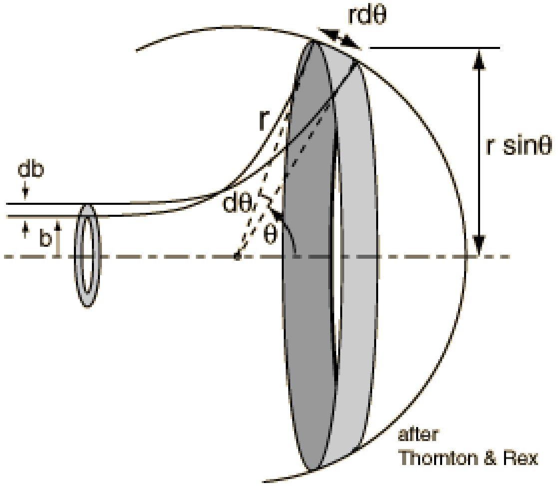
The method of finite elements

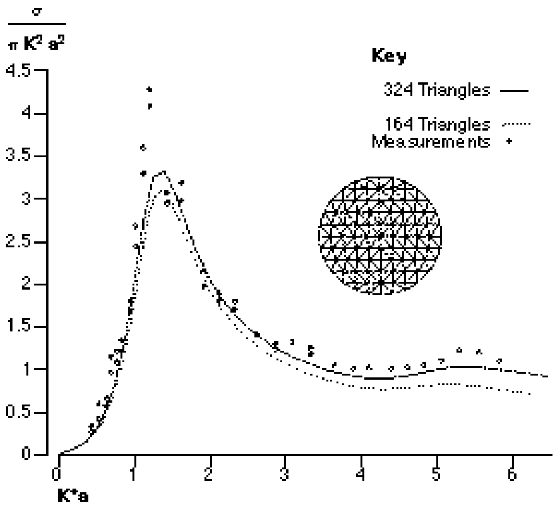
Outline

- Why numerical methods
- The method of finite elements
- FDTD Method
- Examples

How do we understand the world?

- We understand the world through scattering of waves
- Rutherford, LHC, Sonography etc.





Source upper image:http://hyperphysics.phy-astr.gsu.edu/

Source: http://www.emeraldinsight.com/content_images/fig/1740160403044.png

How do we describe the world

- Using the language of mathematics
- Understanding of Maxwell's Laws:
  - No magnetic monopoles
  - Electric charge
  - ***Changing electric fields lead to changing magnetic fields***

Maxwell's Equations

$$\nabla \cdot E = \frac{\rho}{\epsilon_0}$$

$$\nabla \cdot B = 0$$

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

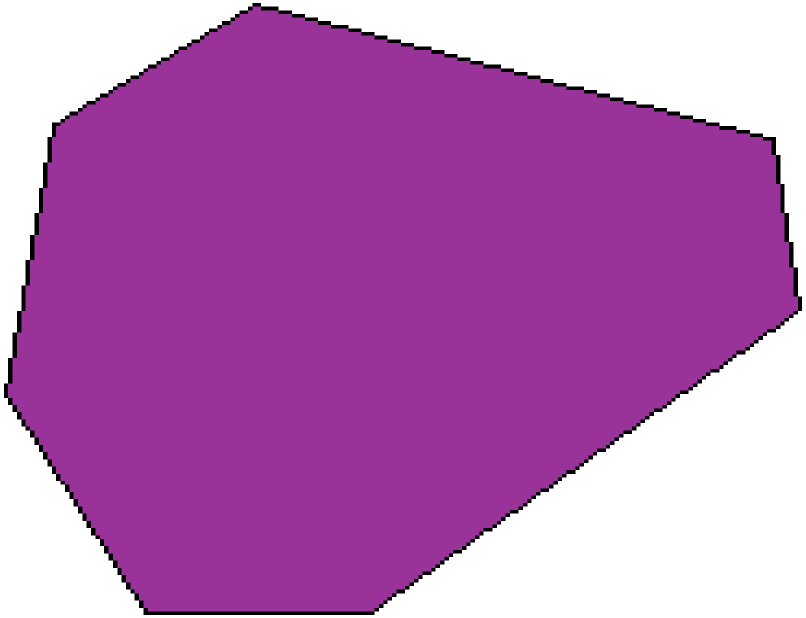
$$\nabla \times B = \mu_0 \left(J + \epsilon_0 \frac{\partial E}{\partial t} \right)$$

Source: http://en.wikipedia.org/wiki/Maxwell%27s_equations

What is the problem?

- A few systems can be analytically solved
  - Via Artful neglect, Transformations etc.
- YET this does not suffice
  - For all other problems we need numerical methods

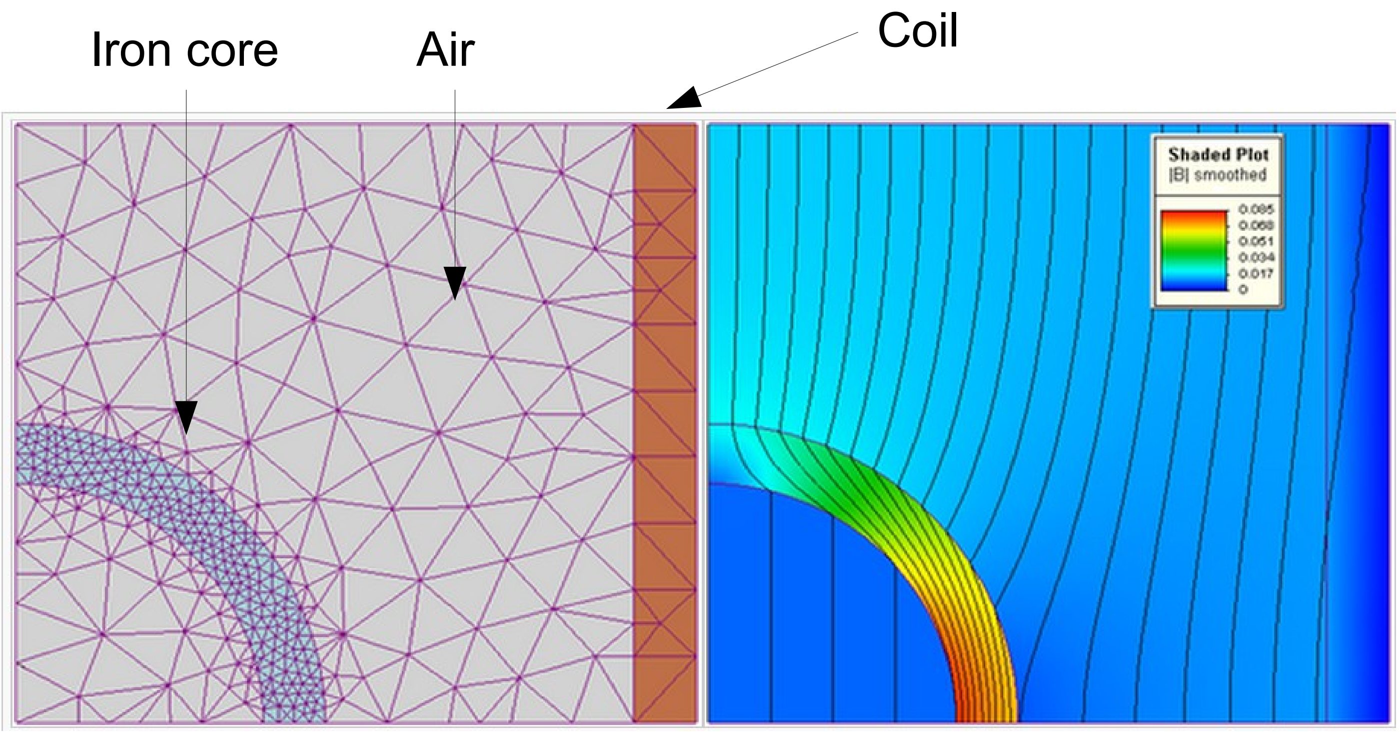
What does this mean for plasmons?



- Solve for irregular shapes
- determine scattering cross/sections

Source: http://tx.english-ch.com/teacher/aisa/irreg-hepta.gif

The method of finite elements

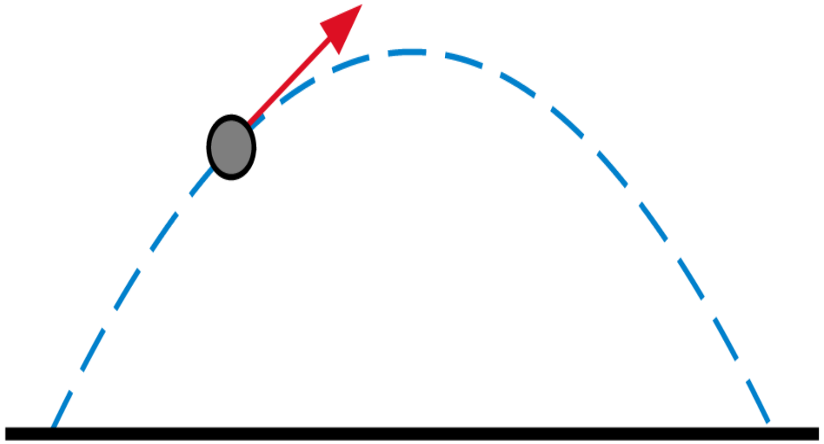


- Use continuous equations
- Solve problems in discrete steps

http://en.wikipedia.org/wiki/Finite_element_method

Preconditions

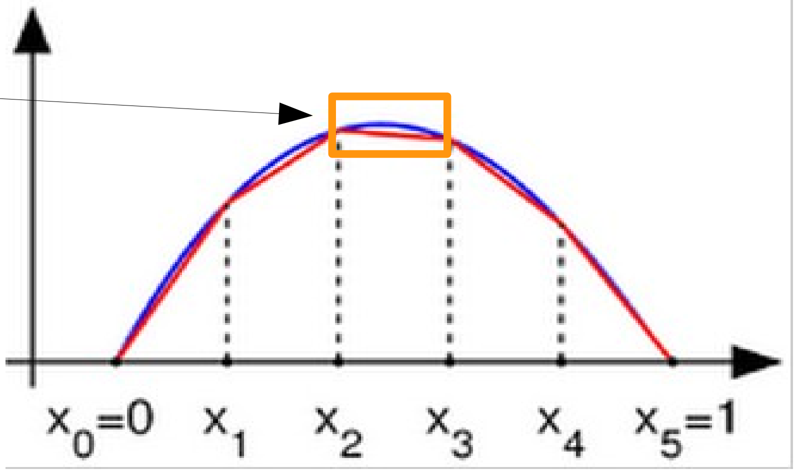
- Uniqueness of solutions
- Well-defined boundary conditions
- Reasonable computation time



Source: http://upload.wikimedia.org/wikipedia/commons/a/a4/Parabolic_trajectory.svg

The art of discretization

- discretization error
- Errors propagate
- Smaller discretization error will not always lead to more precise results
  - computational complexity
  - linear behavior

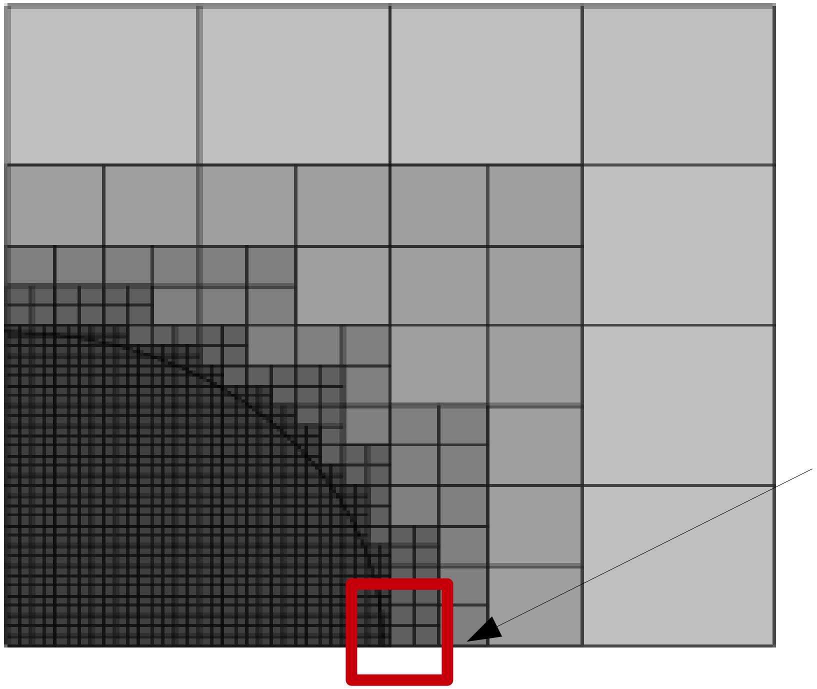


$$\frac{\partial f}{\partial x} \approx \frac{f(x+h) - f(x)}{h}$$

http://upload.wikimedia.org/wikipedia/commons/8/85/Finite_element_method_1D_illustration1.png

Adaptive meshes

- Optimize via the mesh
- Change resolution with complexity



Change the grid structure at curved interfaces

http://www.cita.utoronto.ca/~ljdursi/research/curve-region-oct.png

Summary

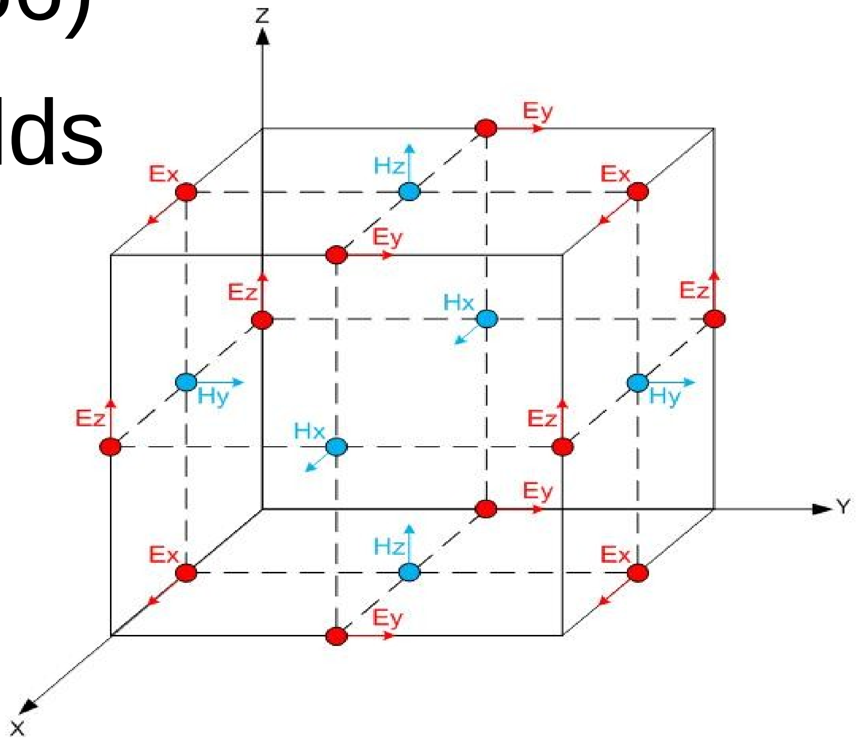
- We have two principle domains of changes
  - Discretization
  - Mesh structure
  - And the method, i.e. the number of grid points we connect or the type of grid points (i.e. in time)....

Computational electrodynamics

- Naturally, you do not reinvent the wheel
  - Open Source solvers (like MEEP from MIT)
- Finite Difference **Time** Domain (FDTD)
  - Time Evolution of Waves
  - Transmission
  - Reflection
- Finite Difference Frequency Domain(FDFD)

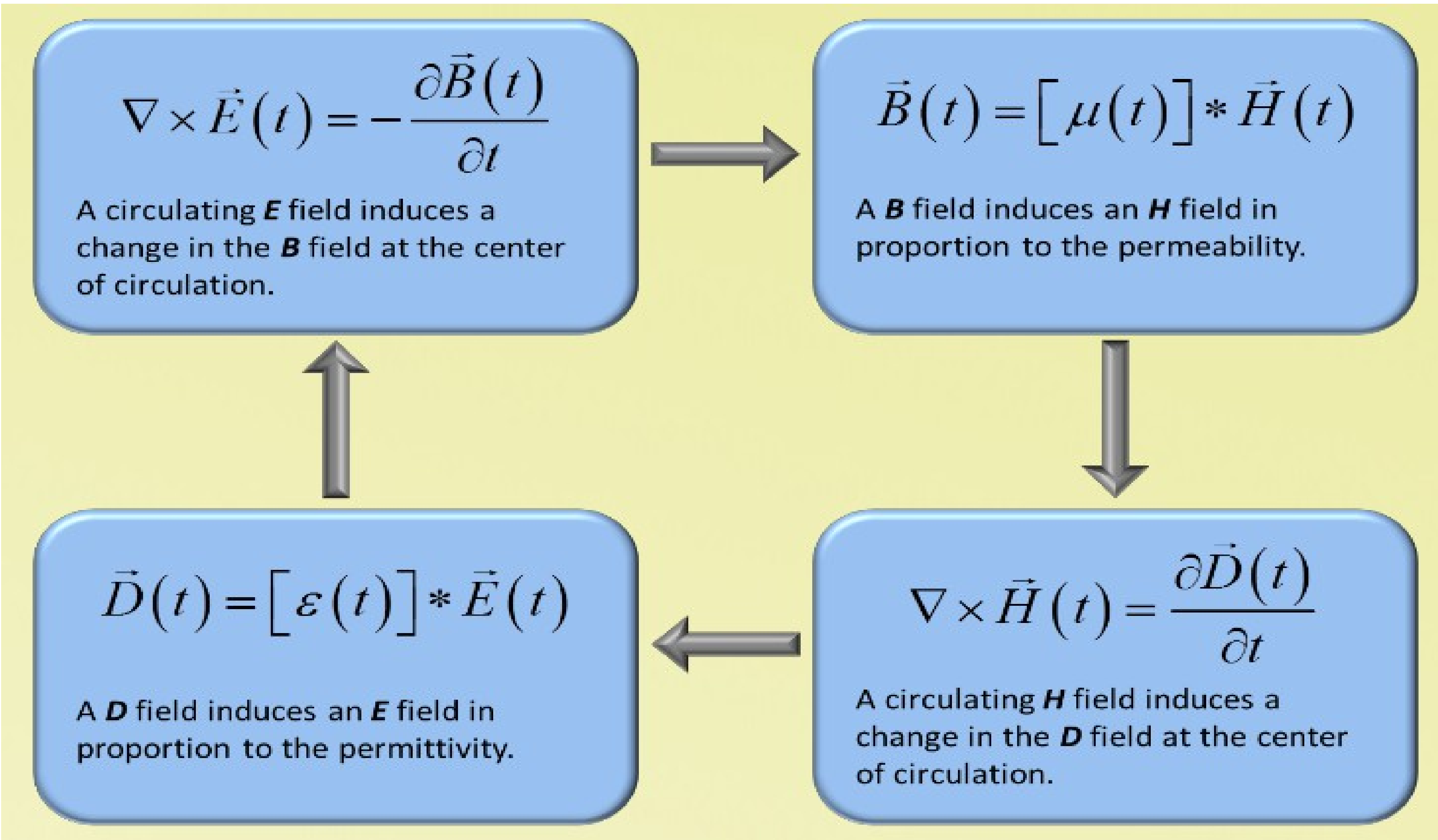
Yee Grid

- Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media (May 1966)
- Two staggered vector fields



Source:http://fdtd.wikispaces.com/file/view/YeeCell01.jpg/51844909/YeeCell01.jpg

How the EM fields interact



Source: http://emlab.utep.edu/

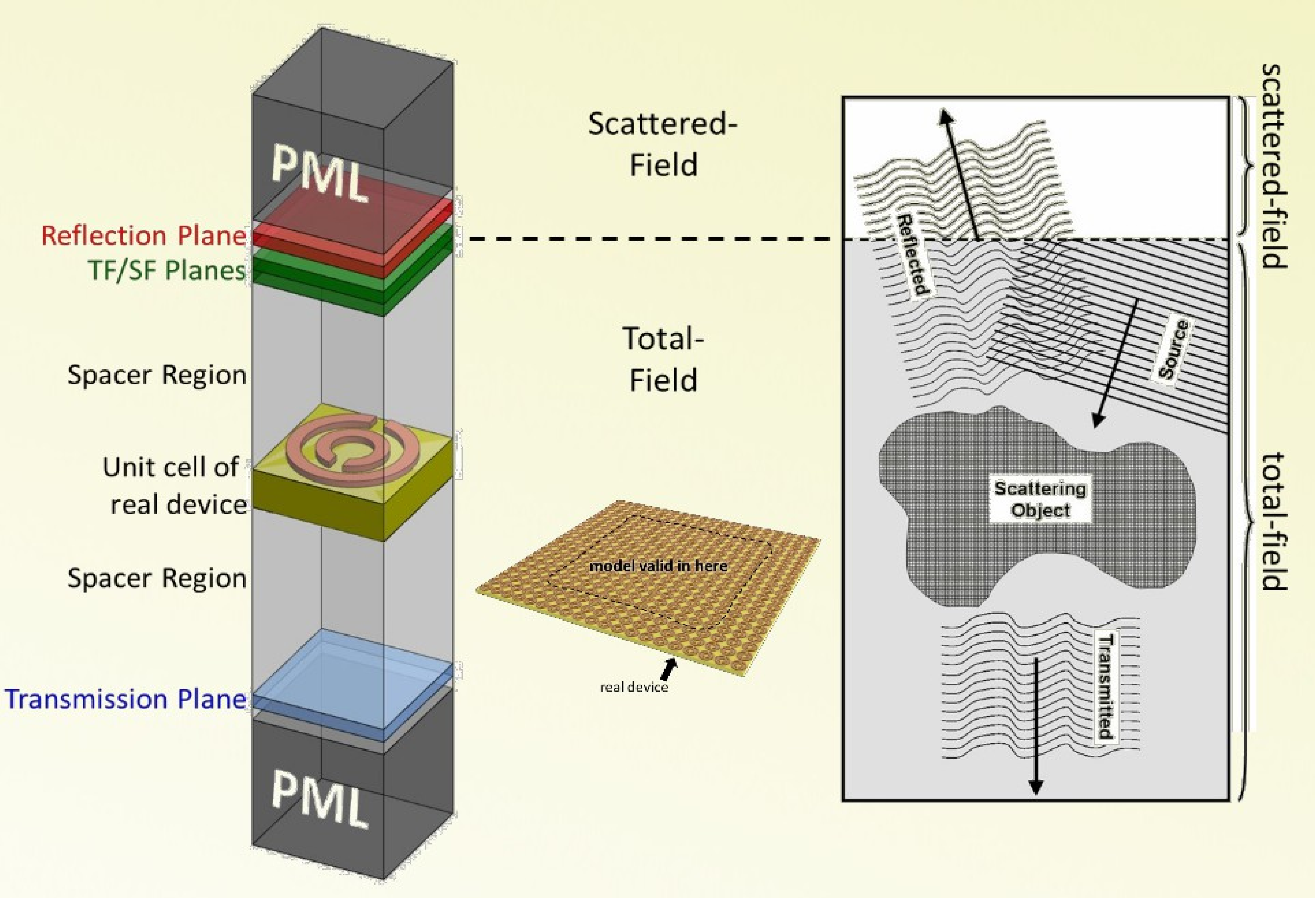
Update equations

$$\nabla \times \vec{H}\Big|_{t+\frac{\Delta t}{2}} = \epsilon \frac{\vec{E}|_{t+\Delta t} - \vec{E}|_{t}}{\Delta t}$$

$$E|_{t+\Delta t} = E|_{t} + \frac{\Delta t}{\epsilon}\left(\nabla \times H|_{t+\frac{\Delta t}{2}}\right)$$

Source: http://emlab.utep.edu/

Sample setup



Sourece: http://emlab.utep.edu/

Software Packages

- Commercial Lumerical
  - Electrical detection of confined gap plasmons in metal–insulator–metal waveguides (>100 citations)
- Open Source MEEP (Examples)
  - Python-meep (Python interface to meep)

MEEP

- Materials are implemented via
  - Differing permeability and permittivity

$$\epsilon(\omega) = \epsilon_\infty + \sum_n \frac{\sigma_n \omega_n^2}{\omega_n^2 - \omega^2 - \mathrm{i}\omega\Gamma_n}$$

$$\epsilon_{LD} = \epsilon_D + \epsilon_L$$

$$\epsilon_D = 1 - \frac{f_1 \omega_p'^2}{\omega(\omega - \mathrm{i}\Gamma_1')}$$

$$\epsilon_L = \sum_n \frac{f_n \omega_p'^2}{\omega_n'^2 - \omega^2 + \mathrm{i}\omega\Gamma_n'}$$

Free electron gas

Bound electrons

```
(set! default-material
      (make dielectric (epsilon 2.25)
            (E-susceptibilities
             (make lorentzian-susceptibility
               (frequency 1.1) (gamma 1e-5) (sigma 0.5))
             (make lorentzian-susceptibility
               (frequency 0.5) (gamma 0.1) (sigma 2e-5))
             )))
```

$$\epsilon(\omega) = \epsilon_\infty + \sum_n \frac{\sigma_n \omega_n^2}{\omega_n^2 - \omega^2 - \mathrm{i}\omega\Gamma_n}$$

Conclusion

- We can use numerical methods such as the FDTD method to simulate plasmons
- Or determine the near field structrue of irregular shapes
- Or determine the cross sections (transmission and reflection) in a setup using numerical methods.