Plane Waves and Planar Boundaries in FDTD Simulations

John B. Schneider
Elec. Eng. & Comp. Sci.
Washington State Univ.
Pullman, WA

Robert J. Kruhlak
Nonlinear Optics Lab.
Washington State Univ.
Pullman, WA

July 17, 2000

[Work supported in part by ONR]

Motivation/Overview

Maxwell's equations (continuous world):

- Simple problems are easy to solve
- Complex problems are hard to solve

Yee FDTD method (discrete world):

- Complex problems are easy to solve
- Simple problems are relatively hard to solve

Solutions to simple problems can yield insight into performance and limits of numerical algorithms. Addressed in this talk:

- Orthogonality of $\bar{\mathbf{E}}$, $\bar{\mathbf{H}}$, and $\tilde{\bar{\mathbf{k}}}$
- Characteristic impedance
- Reflection coefficient from planar boundaries

Yee Algorithm

Forgy notation[†]:

$$\bar{\bar{\mathbf{S}}}^{+} s_t^{+} \partial_t \epsilon \bar{\mathbf{E}}^{\bar{\mathbf{m}}} = \bar{\bar{\mathbf{S}}}^{+} s_t^{+} \bar{\bar{\mathbf{C}}} \bar{\mathbf{H}}^{\bar{\mathbf{m}}}$$
$$-\bar{\bar{\mathbf{S}}}^{-} s_x^{+} s_y^{+} s_z^{+} \partial_t \mu \bar{\mathbf{H}}^{\bar{\mathbf{m}}} = \bar{\bar{\mathbf{S}}}^{-} s_x^{+} s_y^{+} s_z^{+} \bar{\bar{\mathbf{C}}} \bar{\mathbf{E}}^{\bar{\mathbf{m}}}$$

where s_i^{+} shifts ith index by 1/2 and

$$\bar{\bar{\mathbf{S}}}^{+} = \begin{bmatrix} s_x^{+} & 0 & 0 \\ 0 & s_y^{+} & 0 \\ 0 & 0 & s_z^{+} \end{bmatrix} \text{ and } \bar{\bar{\mathbf{C}}} = \begin{bmatrix} 0 & -\partial_z & \partial_y \\ \partial_z & 0 & -\partial_x \\ -\partial_y & \partial_x & 0 \end{bmatrix}$$

Assume plane-wave propagation:

$$\bar{\mathbf{E}}^{\bar{\mathbf{m}}} = \bar{\mathbf{E}}_0 e^{j(\omega m_t \Delta_t - \tilde{k}_x m_x \Delta_x - \tilde{k}_y m_y \Delta_y - \tilde{k}_z m_z \Delta_z)}.$$

where numeric wave vector given by:

$$\tilde{\bar{\mathbf{k}}} = \left[\tilde{k}_x, \tilde{k}_y, \tilde{k}_z\right] = \tilde{k}\,[\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]$$

Finite-difference operators become

$$\partial_i \bar{\mathbf{E}}^{\bar{\mathbf{m}}} = -j\frac{2}{\Delta_i}\sin\left(\frac{\tilde{k}_i\Delta_i}{2}\right)\bar{\mathbf{E}}^{\bar{\mathbf{m}}} = -jK_i\bar{\mathbf{E}}^{\bar{\mathbf{m}}}$$
$$\partial_t \bar{\mathbf{E}}^{\bar{\mathbf{m}}} = j\frac{2}{\Delta_t}\sin\left(\frac{\omega\Delta_t}{2}\right)\bar{\mathbf{E}}^{\bar{\mathbf{m}}} = j\Omega\bar{\mathbf{E}}^{\bar{\mathbf{m}}}$$

[†]E. A. Forgy, Master's Thesis, UIUC, 1998

Orthogonality

In source-free region, Yee grid divergence-free[†]:

$$\tilde{\nabla} \cdot \bar{\mathbf{E}}^{\bar{\mathbf{m}}} = 0 \quad \Leftrightarrow \quad -j\bar{\mathbf{K}} \cdot \bar{\mathbf{E}}^{\bar{\mathbf{m}}} = 0$$

$$\tilde{\nabla} \cdot \bar{\mathbf{H}}^{\bar{\mathbf{m}}} = 0 \quad \Leftrightarrow \quad -j\bar{\mathbf{K}} \cdot \bar{\mathbf{H}}^{\bar{\mathbf{m}}} = 0$$

where $\tilde{\nabla} = [\partial_x, \partial_y, \partial_z]$.

Curl operator can be expressed in terms of $\bar{\mathbf{K}}$. Yee algorithm dictates

$$\begin{aligned} j\Omega\epsilon\bar{\mathbf{E}}^{\bar{\mathbf{m}}} &= -j\bar{\mathbf{K}} \times \bar{\mathbf{H}}^{\bar{\mathbf{m}}}, \\ -j\Omega\mu\bar{\mathbf{H}}^{\bar{\mathbf{m}}} &= -j\bar{\mathbf{K}} \times \bar{\mathbf{E}}^{\bar{\mathbf{m}}}. \end{aligned}$$

$\bar{\mathbf{E}}$, $\bar{\mathbf{H}}$, and $\bar{\mathbf{K}}$ are mutually orthogonal.
However, $\bar{\mathbf{K}}$ not necessarily parallel to $\tilde{\bar{\mathbf{k}}}$
(direction of wave propagation).

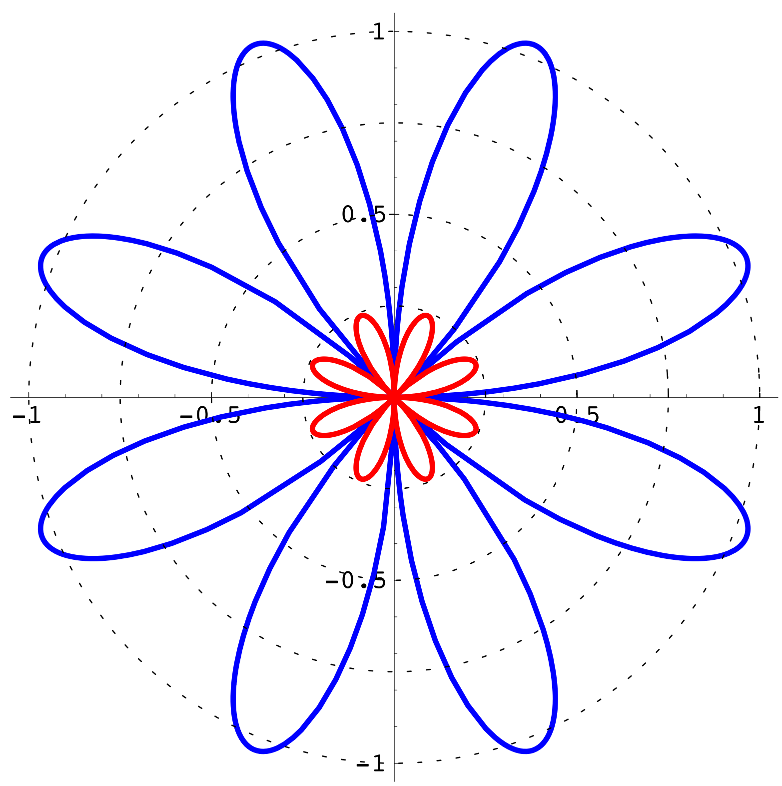
[†]A. Taflove and S. Hagness, *Computational Electrodynamics*, pp. 96–98, 2000

Angle between $\bar{\mathbf{K}}$ and $\bar{\tilde{\mathbf{k}}}$

Using dispersion relation, one can solve for angle between $\bar{\mathbf{K}}$ and $\bar{\tilde{\mathbf{k}}}$.

Angle is function of direction of propagation, discretization, and Courant number (weakly).

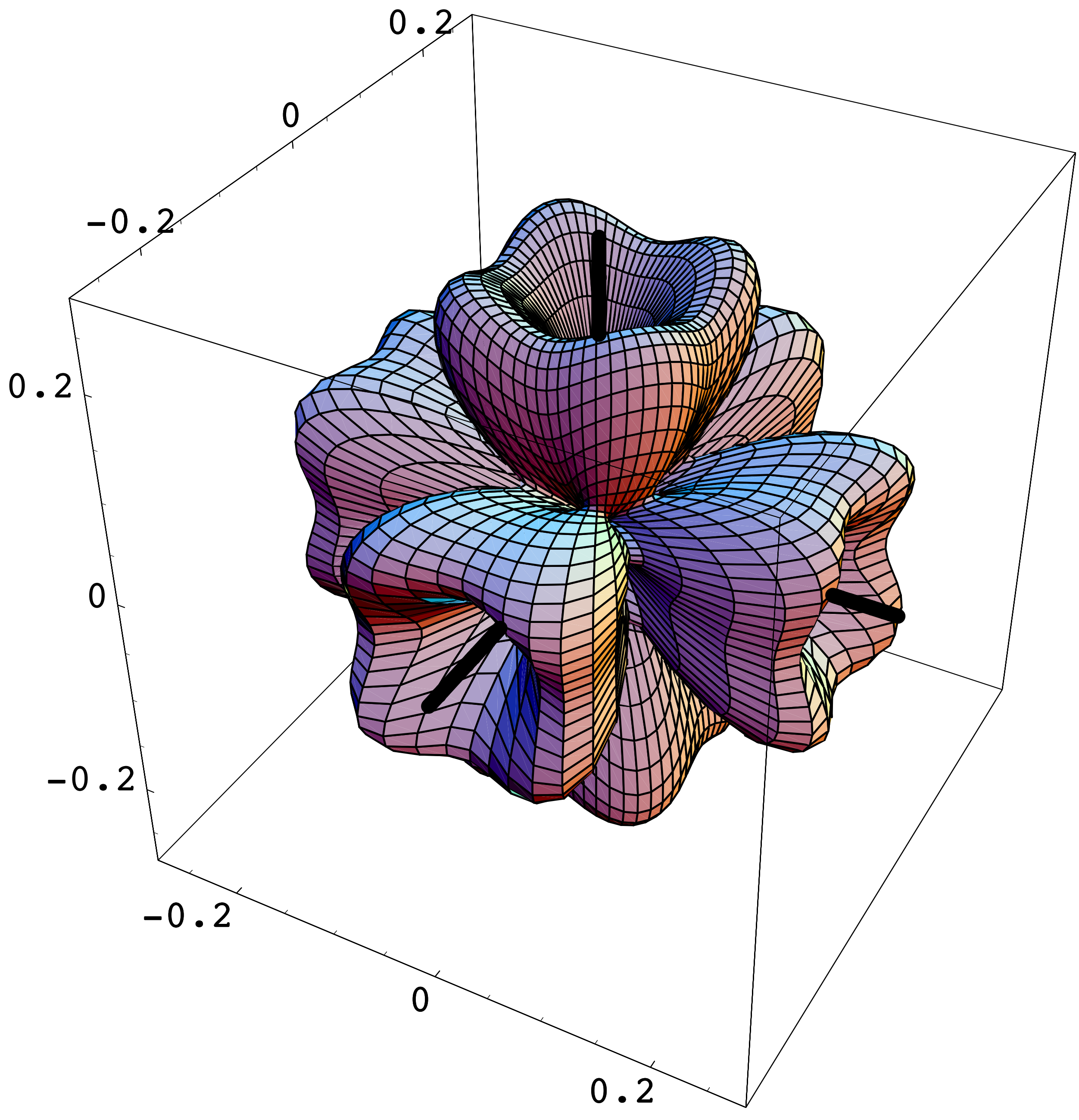
Courant number: $1/\sqrt{3}$
Discretization: 5 or 10 cells/λ
$\bar{\tilde{\mathbf{k}}} = \tilde{k}[\cos\phi, \sin\phi, 0]$
Angle between $\mathbf{K}$ and $\tilde{\mathbf{k}}$ [degrees]



$\Rightarrow$ Second-order behavior

Angle between $\bar{\mathrm{K}}$ and $\tilde{\bar{\mathrm{k}}}$: 3D

Courant number: $1/\sqrt{3}$
Discretization: 10 cells/λ
Angle between $\bar{\mathrm{K}}$ and $\tilde{\bar{\mathrm{k}}}$ [degrees]



Characteristic Impedance

Take magnitude of both sides of governing equation:

$$\left|j\Omega\epsilon\bar{\mathbf{E}}\right| = \left|-j\bar{\mathbf{K}} \times \bar{\mathbf{H}}\right|$$

Because $\bar{\mathbf{K}}$ and $\bar{\mathbf{H}}$ are orthogonal and all fields have same spatial dependence, this becomes:

$$\Omega\epsilon\left|\bar{\mathbf{E}}_0\right| = \left|\bar{\mathbf{K}}\right| \left|\bar{\mathbf{H}}_0\right|$$

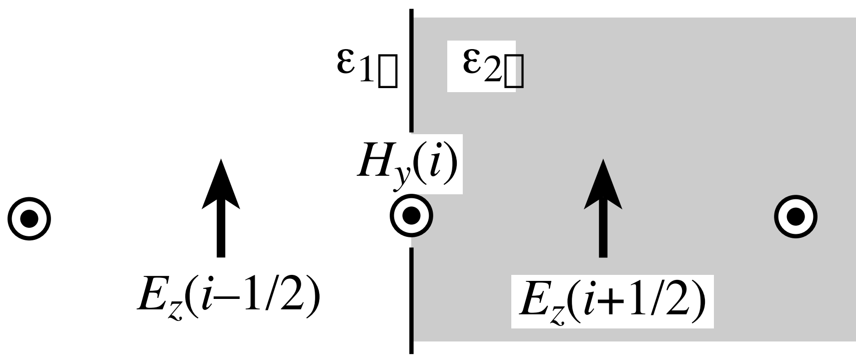
From dispersion relation $\left|\bar{\mathbf{K}}\right| = \sqrt{\epsilon\mu}\Omega$. Thus,

$$\frac{\left|\bar{\mathbf{E}}_0\right|}{\left|\bar{\mathbf{H}}_0\right|} = \frac{E_0}{H_0} = \sqrt{\frac{\mu}{\epsilon}}$$

Grid characteristic impedance is exact independent of direction of propagation.

Reflection Coefficient

Consider plane wave normally incident on planar interface:



Assume incident, reflected, and transmitted electric field.

Via update equation, can express H at interface in terms of neighboring E's.

H related to E via impedance relation. "Boundary condition" implied by H being common to medium 1 and 2:

$$\frac{1}{Z_1}\left[1-\tilde{\Gamma}\right]=\frac{1}{Z_2}\tilde{T}$$

Combine and solve for reflection coefficient $\tilde{\Gamma}$.

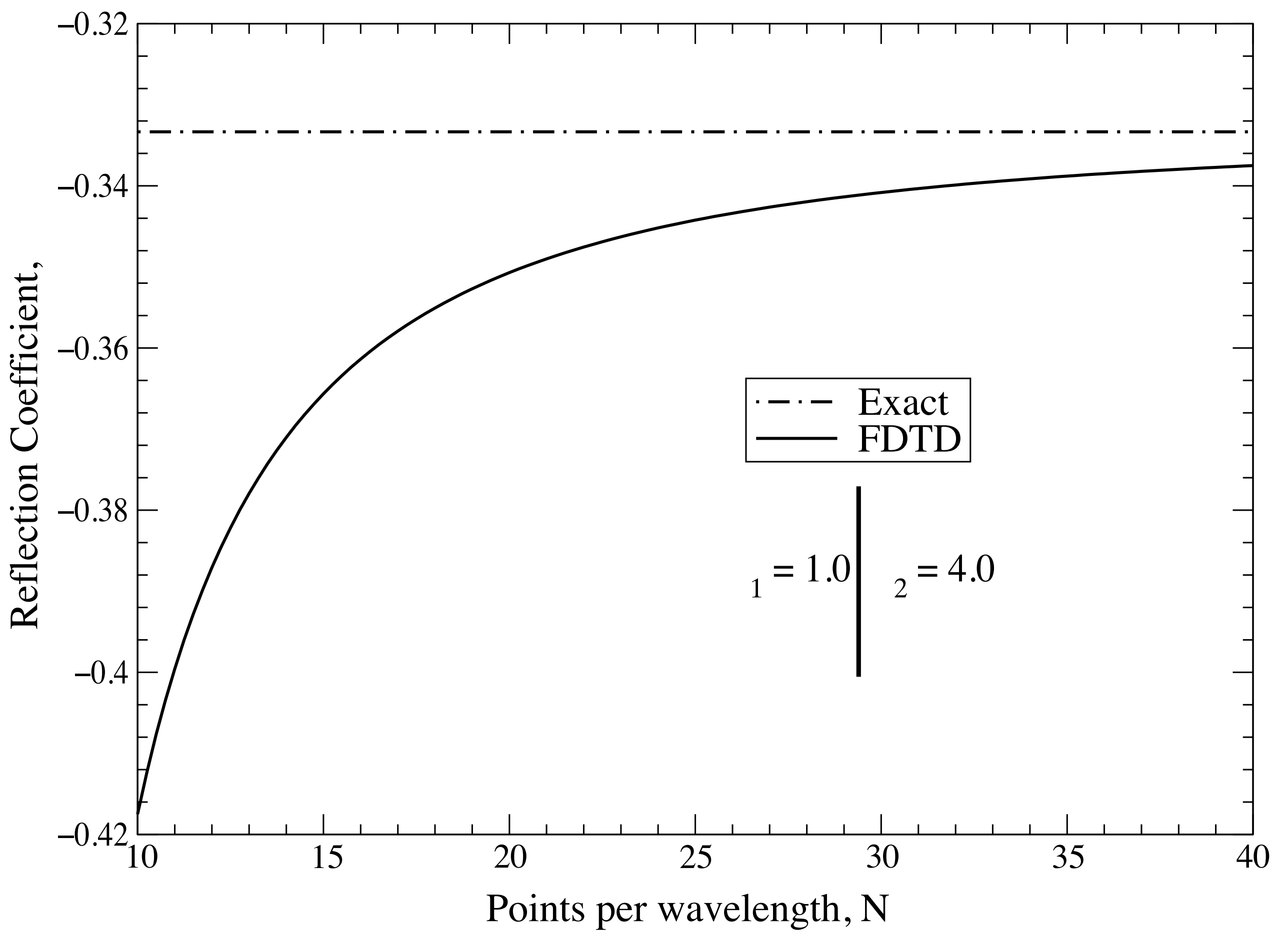
Reflection Coefficient (cont.)

Solving for $\tilde{\Gamma}$ yields

$$\tilde{\Gamma} = \frac{\epsilon_1 \cos\left(\frac{\tilde{k}_2 \Delta_x}{2}\right) - \epsilon_2 \cos\left(\frac{\tilde{k}_1 \Delta_x}{2}\right)}{\epsilon_1 \cos\left(\frac{\tilde{k}_2 \Delta_x}{2}\right) + \epsilon_2 \cos\left(\frac{\tilde{k}_1 \Delta_x}{2}\right)}$$

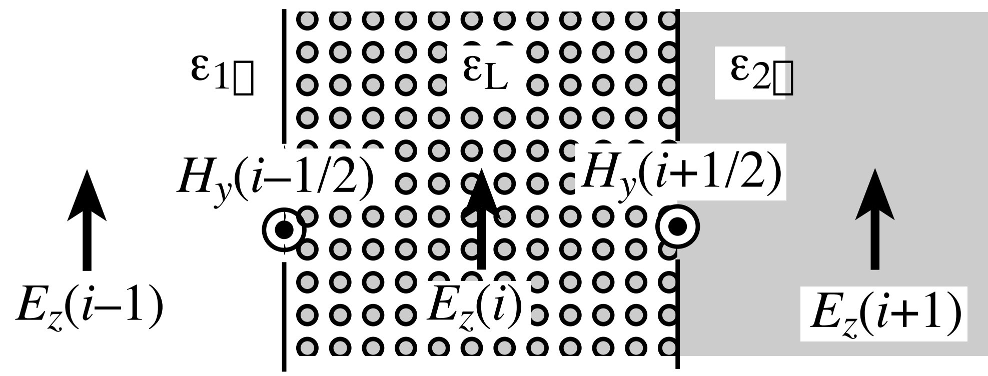
Compare to continuous world:

$$\Gamma = \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2}$$



Reflection Coefficient—One Cell Layer

Plane wave normally incident on planar interface:



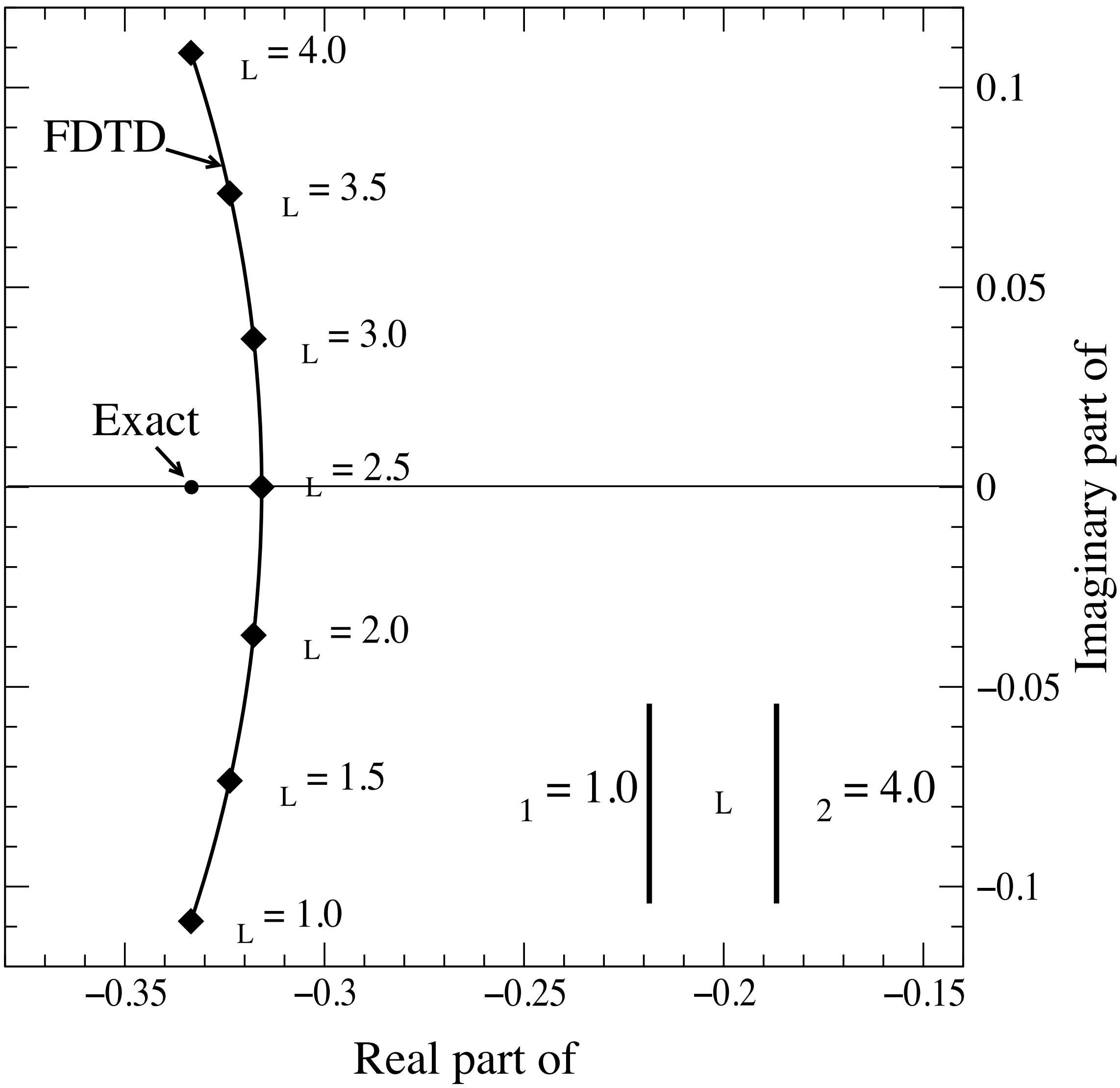
Solving for $\tilde{\Gamma}$ yields

$$\tilde{\Gamma} = e^{j\tilde{k}_1\Delta_x}\frac{\tilde{\Gamma}_{1L} + \tilde{\Gamma}_{L2}\exp\left(-j2\tilde{k}_L\Delta_x\right)}{1 + \tilde{\Gamma}_{1L}\tilde{\Gamma}_{L2}\exp\left(-j2\tilde{k}_L\Delta_x\right)}$$

where $\tilde{\Gamma}_{1L}$ and $\tilde{\Gamma}_{1L}$ are single-interface reflection coefficients.

Reflection Coefficient vs. Layer Permittivity

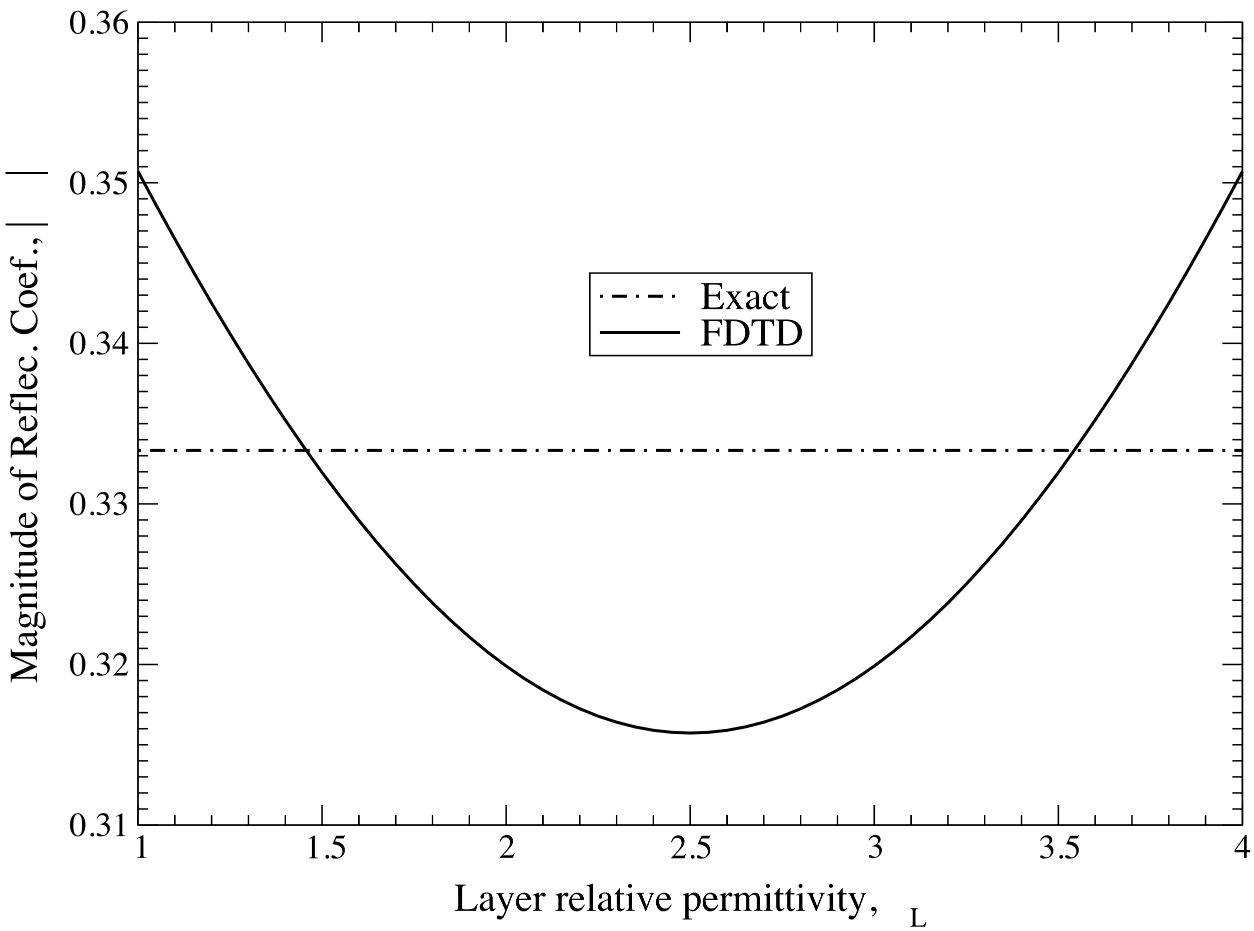
Let $\epsilon_1 = 1$ and $\epsilon_2 = 4$. What is optimum ϵ_L?



Optimum value = average of permittivities to either side

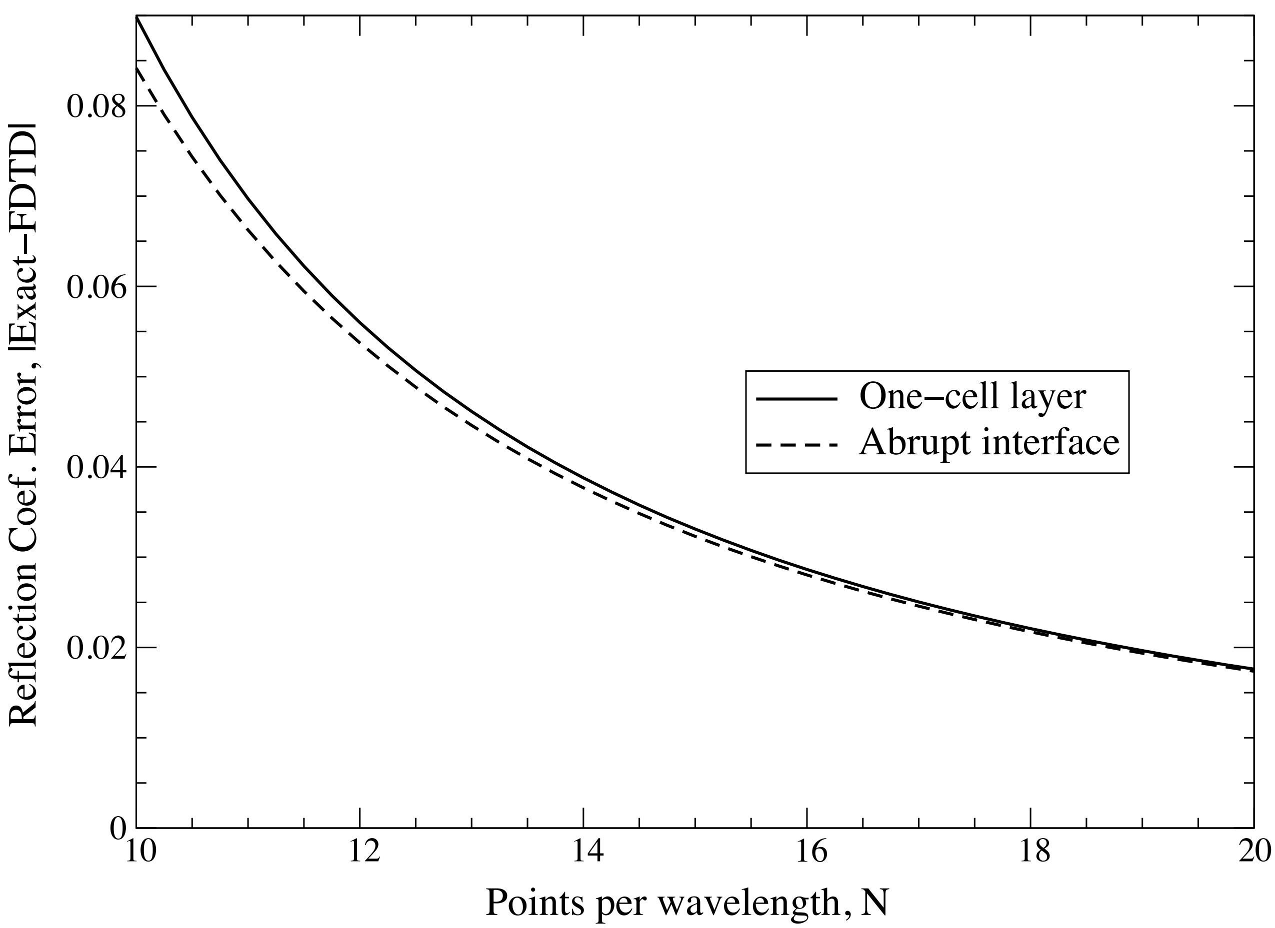
Reflection Coefficient vs. Layer Permittivity (cont.)

Considering only magnitude of reflection coefficients will lead to wrong conclusions. For example:



Abrupt Interface vs. One-Cell Layer

Error vs. points per wavelength for abrupt or layered realization of interface.
$\epsilon_1 = 1.0$ ($\epsilon_L = 2.5$) $\epsilon_2 = 4.0$



Abrupt realization of boundary superior (slightly) to layered one.

Additional Remarks

- Have derived reflection & transmission coefficients for obliquely incident waves.
  - TE and TM polarization
  - Layered and abrupt boundaries
- Have derived reflection coefficients for changes in permittivity and permeability.
  - Results depend on order in which discontinuities introduced.
- Have performed numerical simulations to confirm analytic results.

Conclusions

- $\bar{\mathbf{E}}$, $\bar{\mathbf{H}}$, and $\tilde{\bar{\mathbf{k}}}$ are not mutually orthogonal
  - $\bar{\mathbf{E}}$, $\bar{\mathbf{H}}$, and $\bar{\mathbf{K}}$ are orthogonal
  - Second-order dependence for angle between $\bar{\mathbf{K}}$ and $\tilde{\bar{\mathbf{k}}}$
- Characteristic impedance exact for all angles of propagation
- Reflection coefficient from planar boundaries can be analyzed via harmonic techniques
  - Reflection coefficient error dependent on discretization in both (all) media
  - Average permittivity is optimum when layered realization required
  - Abrupt realization slightly better than layered

Postscript

- Upcoming MGWL by Hirono *et al.* considers slightly different problem (geometric mean for "normal" permittivities optimal when boundary offset from grid-aligned position).
- Because $\bar{\mathbf{E}}$, $\bar{\mathbf{H}}$, and $\tilde{\bar{\mathbf{k}}}$ not mutually orthogonal, may not make sense to study general 3D problems in terms of TE and TM polarization.