Pseudospectral Time-Domain Method in EM Simulations

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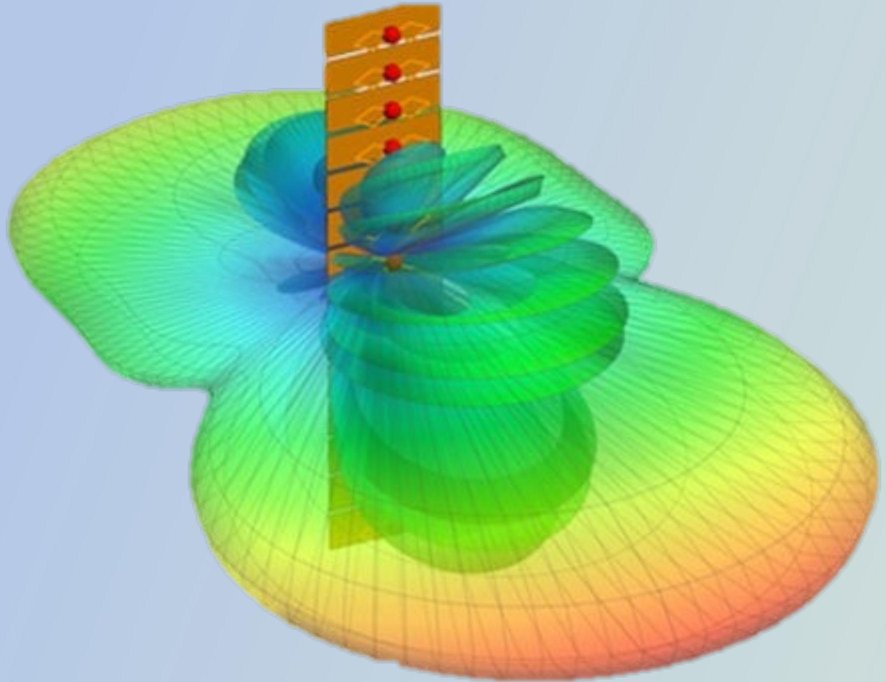
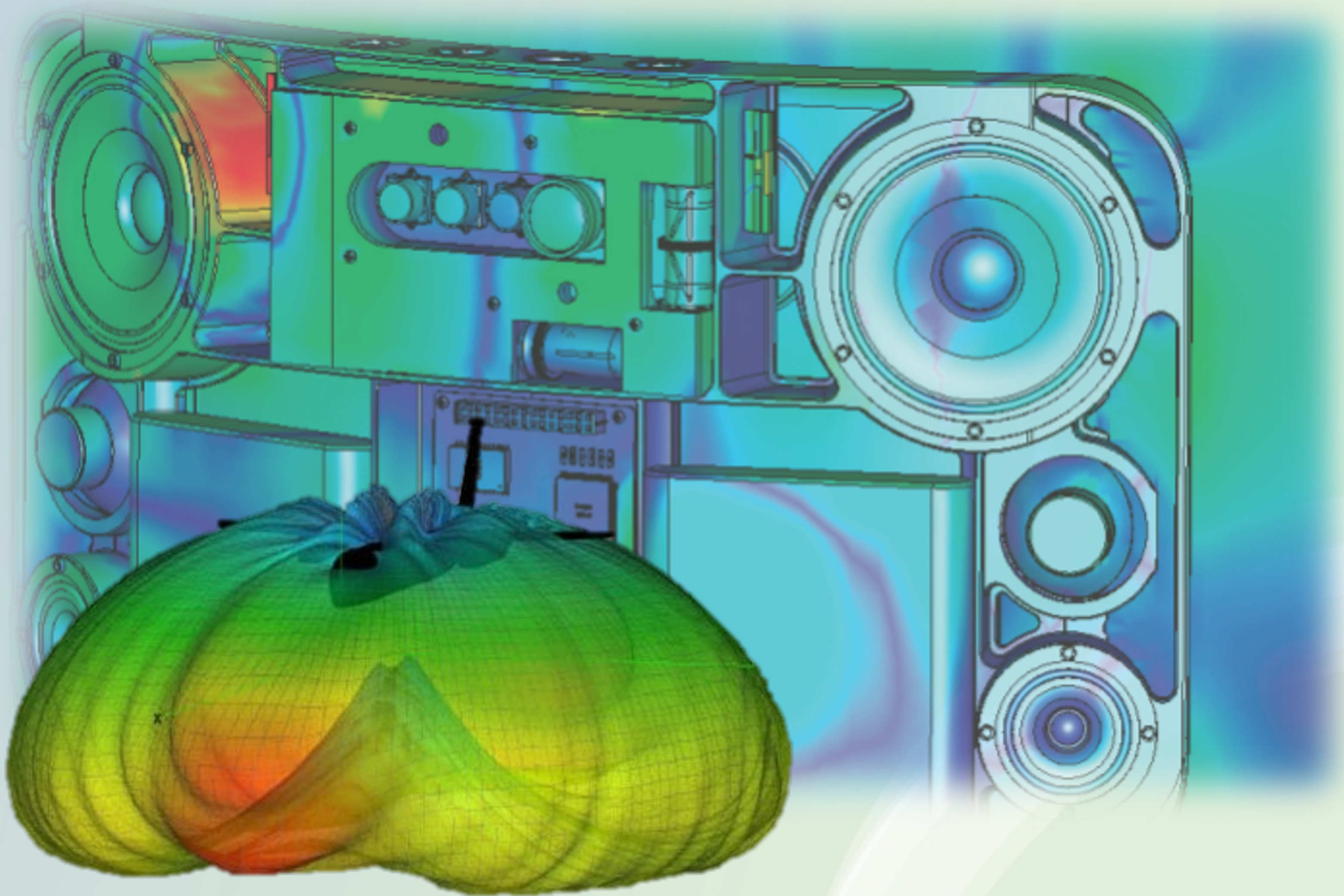
Outline

- Basics of Computational Electromagnetics
- Recap of FDTD
- Introduction to PSTD
- Advanced topics in PSTD

Numerical Simulations in EM

What are the applications?





- https://altair.com/feko-applications
- https://www.3ds.com/fileadmin/PRODUCTS-SERVICES/SIMULIA/PRODUCTS/CST/CST_Brochure_A4.pdf

Some Applications

- Antenna radiation modeling
- Device modeling (SIPI / EMC)
- Metamaterials and nanostructures
- Wave propagation and scattering
- …

Based on the application requirements, we select an appropriate computational electromagnetics (CEM) method for modeling.

🙃	IE	DE
TD	$\oint \boldsymbol{E} \cdot d\boldsymbol{l} = -\frac{d}{dt}\int \boldsymbol{B} \cdot d\boldsymbol{s}$ $\oint \boldsymbol{H} \cdot d\boldsymbol{l} = \int (\boldsymbol{J} + \frac{d}{dt}\boldsymbol{D}) \cdot d\boldsymbol{s}$ $\oint \boldsymbol{D} \cdot d\boldsymbol{s} = \int q \, dv$ $\nabla \cdot \boldsymbol{B} = 0$	$\nabla \times \boldsymbol{E} = -\partial \boldsymbol{B}/\partial t$ $\nabla \times \boldsymbol{H} = \boldsymbol{J} + \partial \boldsymbol{D}/\partial t$ $\nabla \cdot \boldsymbol{D} = q$ $\nabla \cdot \boldsymbol{B} = 0$
FD	$\oint \boldsymbol{E} \cdot d\boldsymbol{l} = -i\omega \int \boldsymbol{B} \cdot d\boldsymbol{s}$ $\oint \boldsymbol{H} \cdot d\boldsymbol{l} = \int (\boldsymbol{J} + i\omega \boldsymbol{D}) \cdot d\boldsymbol{s}$ $\oint \boldsymbol{D} \cdot d\boldsymbol{s} = \int q \, dv$ $\nabla \cdot \boldsymbol{B} = 0$	$\nabla \times \boldsymbol{E} = -i\omega \boldsymbol{B}$ $\nabla \times \boldsymbol{H} = \boldsymbol{J} + i\omega \boldsymbol{D}$ $\nabla \cdot \boldsymbol{D} = q$ $\nabla \cdot \boldsymbol{B} = 0$

Computational Electromagnetics

- Well known numerical methods are listed

	IE	DE
TD	**TDIE**	**FDTD**
FD	**MOM**	**FEM**

These are called full-wave methods

Asymptotic Methods

- Asymptotic methods can be applied for the electrically-large cases:

$\Rightarrow$ Geometrical optics (GO)

$\Rightarrow$ Physical Optics (PO)

- And their advanced version:

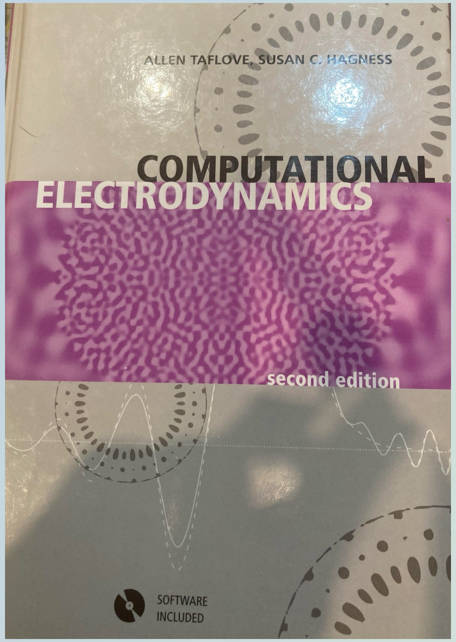
$\Rightarrow$ Geometrical Theory of Diffraction (GTD)

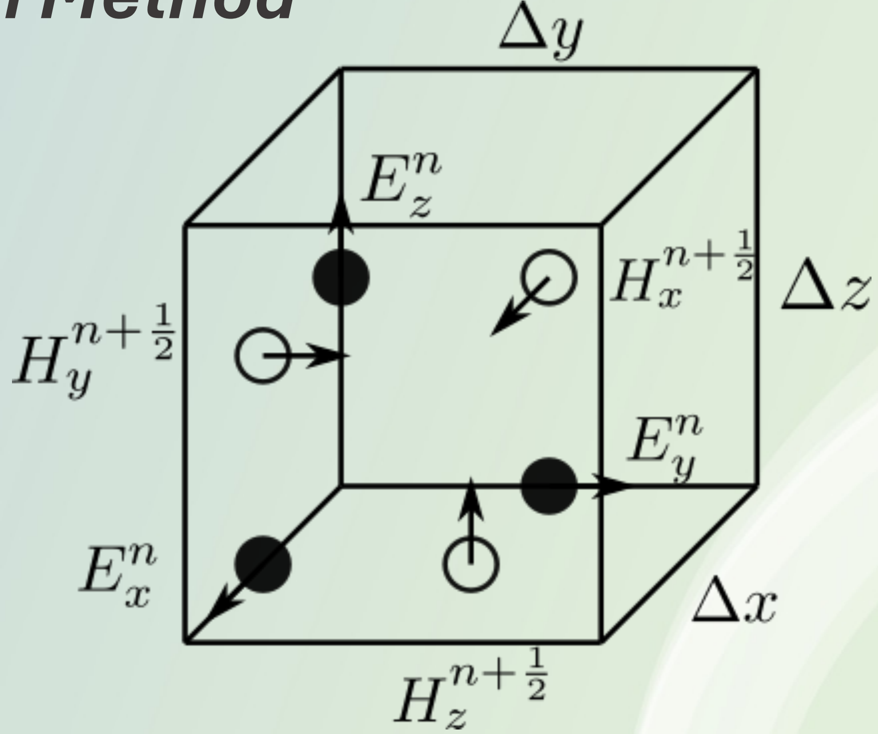
$\Rightarrow$ Physical Theory of Diffraction (PTD)

Finite-Difference Time-Domain Method

- Kane Yee, 1966, "***Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media***"
- Allen Taflove, 1995, ***Computational Electrodynamics: The Finite-Difference Time-Domain Method***

This is my 2nd edition.
I got my 3rd edition recently😁





FDTD Formulation

- Discretization in time => **FD**
- Discretization in space => **FD**

2nd order accuracy

$$\boxed{\frac{E_{x,k}^{n+1/2} - E_{x,k}^{n-1/2}}{\Delta t} = -\frac{H_{y,k+1/2}^{n} - H_{y,k-1/2}^{n}}{\varepsilon \Delta z}}$$

2nd order accuracy

Topics in FDTD

- Discretization
- Material
- Perfectly Matching Layer (PML)
- Hard Source / Soft Source
- Pure Scattered-Field (SF) / Total-Field Scattered-Field (TFSF)
- Near-to-Far Field Transformation (NTFF)

Pseudospectral Time-Domain Method

- Q. H. Liu, 1997, “***The PSTD algorithm: A time-domain method requiring only two cells per wavelength***”
- Discretization in time => **FD**
- Discretization in space => **PS**
  - using global basis function to approximate differential operations
    - **Fourier** => uniform collocated points
    - **Multi-domain** => non-uniform collocated points

Fourier PSTD Formulation

- Denoting the Fourier transform operator as

$$\Psi(\vec{k}) = \mathfrak{F}_\eta(\psi) = \int_{-\infty}^{\infty} \psi(\vec{r}) e^{-ik_\eta \eta} d\eta$$

$$\psi(\vec{r}) = \mathfrak{F}_\eta^{-1}(\Psi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi\left(\vec{k}\right) e^{ik_\eta \eta} dk_\eta$$

- Then

$$\partial_\eta \psi = \partial_\eta \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi\left(\vec{k}\right) e^{ik_\eta \eta} dk_\eta\right] = \frac{ik_\eta}{2\pi} \int_{-\infty}^{\infty} \Psi\left(\vec{k}\right) e^{ik_\eta \eta} dk_\eta = \mathfrak{F}_\eta^{-1}\left(ik_\eta \Psi\right) = \mathfrak{F}_\eta^{-1}\left[ik_\eta \mathfrak{F}_\eta(\psi)\right]$$

$$\boxed{\frac{E_{x,\Bbbk}^{\mathrm{n}+1/2} - E_{x,\Bbbk}^{\mathrm{n}-1/2}}{\Delta t} = -\frac{1}{\varepsilon} \mathfrak{F}_z^{-1}\left[ik_z \mathfrak{F}_z\left(H_y^{\mathrm{n}}\right)\right]|_{\Bbbk}}$$

Implementation of PSTD

- **FFT** can be applied to compute the derivatives.
- Be aware of the use of **fftshift/ifftshift** if k vector is defined as zero-centered.
- To avoid numerical errors, taking the real part of the computed result is necessary!

```
dF = real.(ifft(im .* K .* fft(F, dim), dim))
```

Advantages and Disadvantages of PSTD

- Advantages
    - Requires only two cells per wavelength according to Nyquist theorem (theoretically speaking…)
    - Computations for E and H fields are collocated*
- Disadvantages
    - Difficult to deal with field discontinuities
        - → Source
        - → TFSF formulation
        - → Metallic surfaces
        - → High-contrast dielectrics

Topics in PSTD (vs. FDTD)

- Discretization
- Material
- Perfectly Matching Layer (PML)
- Hard Source / Soft Source
- Pure Scattered-Field / Total-Field Scattered-Field (TFSF)
- Near-to-Far Field Transformation (NTFF)

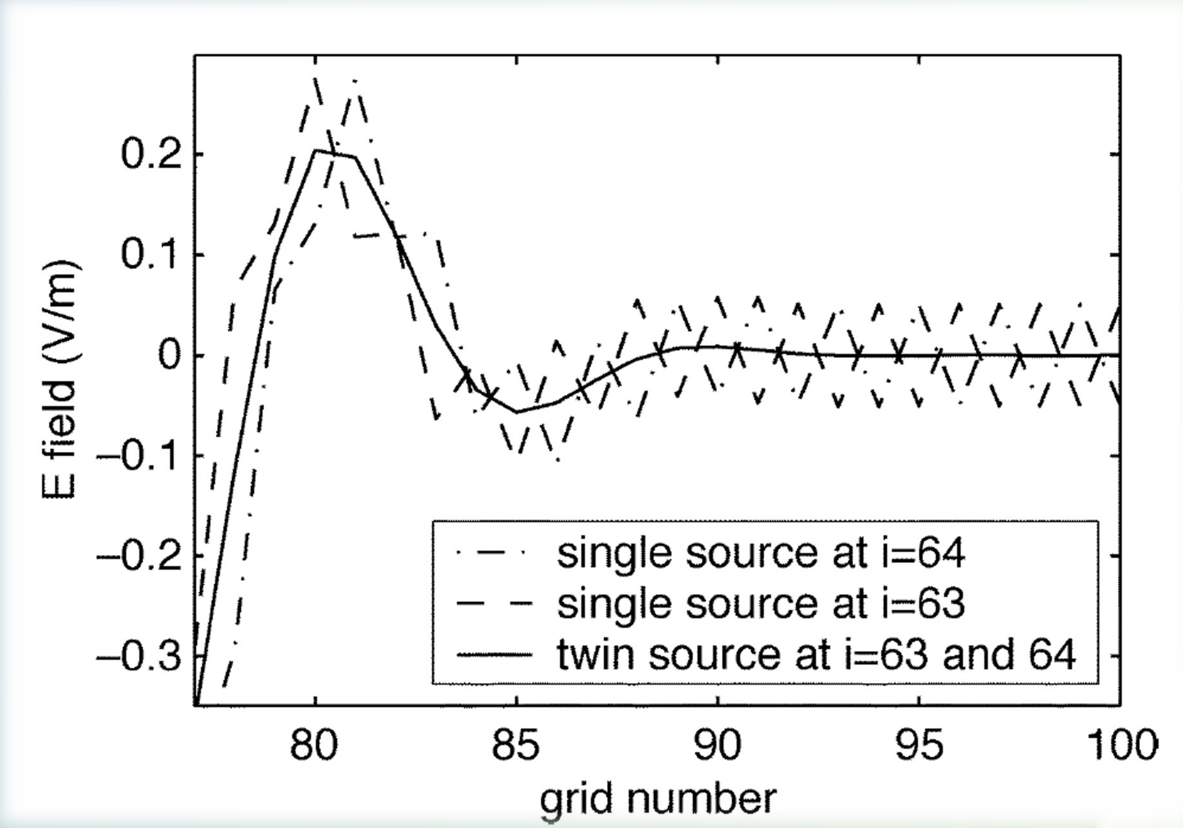
How does the topic differ from that of FDTD?

- Few
- Medium
- High

Compact Wave Source Condition

- Tae-Woo Lee and Susan C. Hagness, 2004, "***A Compact Wave Source Condition for the Pseudospectral Time-Domain Method***"

Discontinuity introduced by point sources



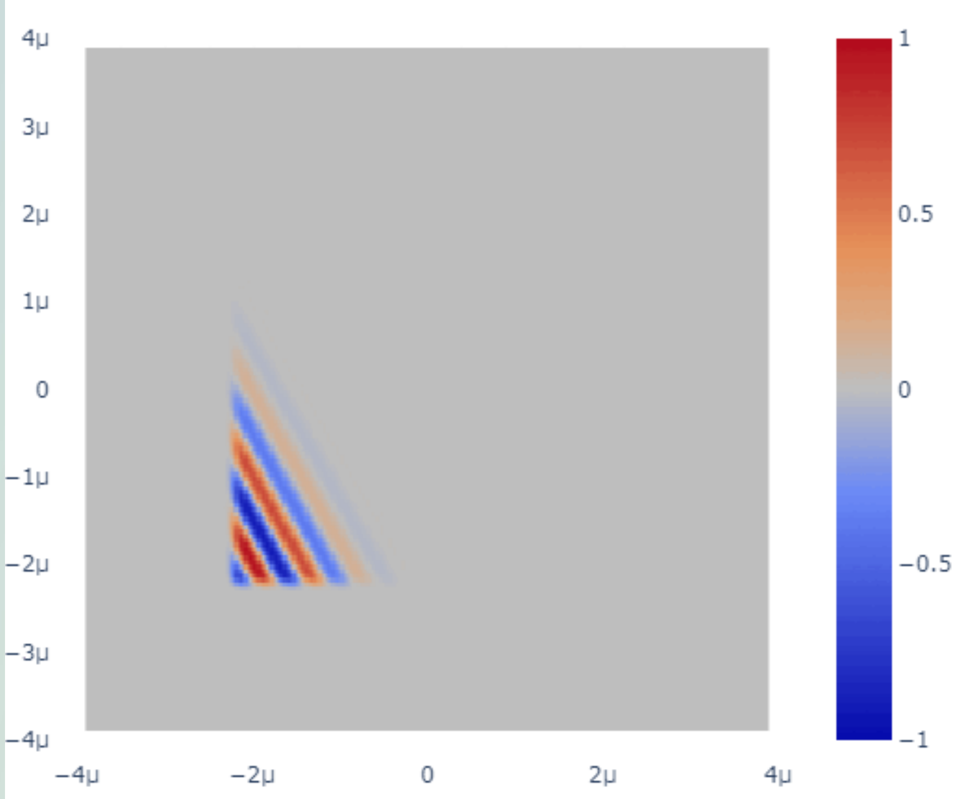
SF / TFSF Formulation

- SF / TFSF are techniques to introduce plane wave into the space
- Decompose the total field into incident field and scattered field as

$$\boldsymbol{E}_{tot} = \boldsymbol{E}_{scat} + \boldsymbol{E}_{inc}$$

→ assumed known

Illustration of the TFSF technique



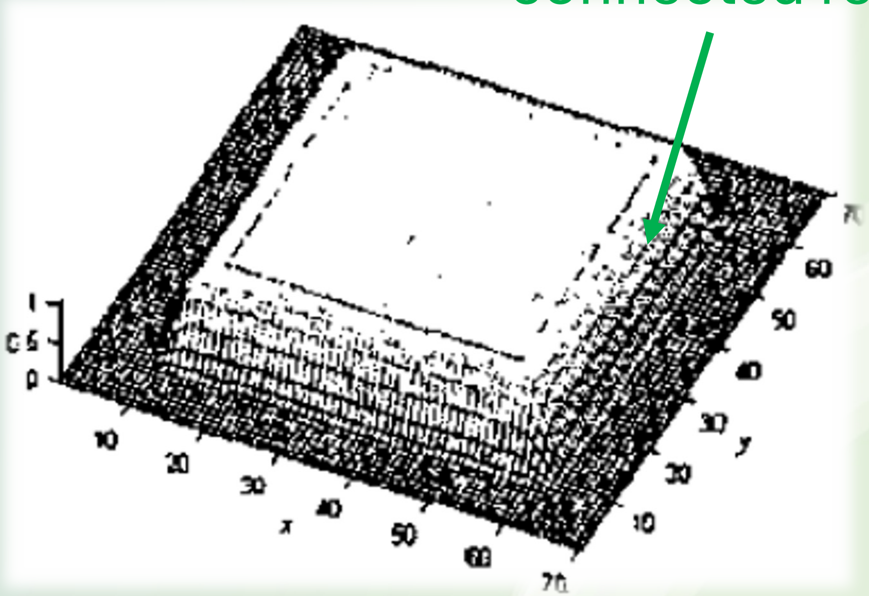
TFSF Formulation in PSTD

- Xiang Gao, Mark S. Mirolznik and Dennis W. Prather, 2004, "***Soft Source Generation in the Fourier PSTD Algorithm***"

Discontinuity introduced by TFSF boundaries

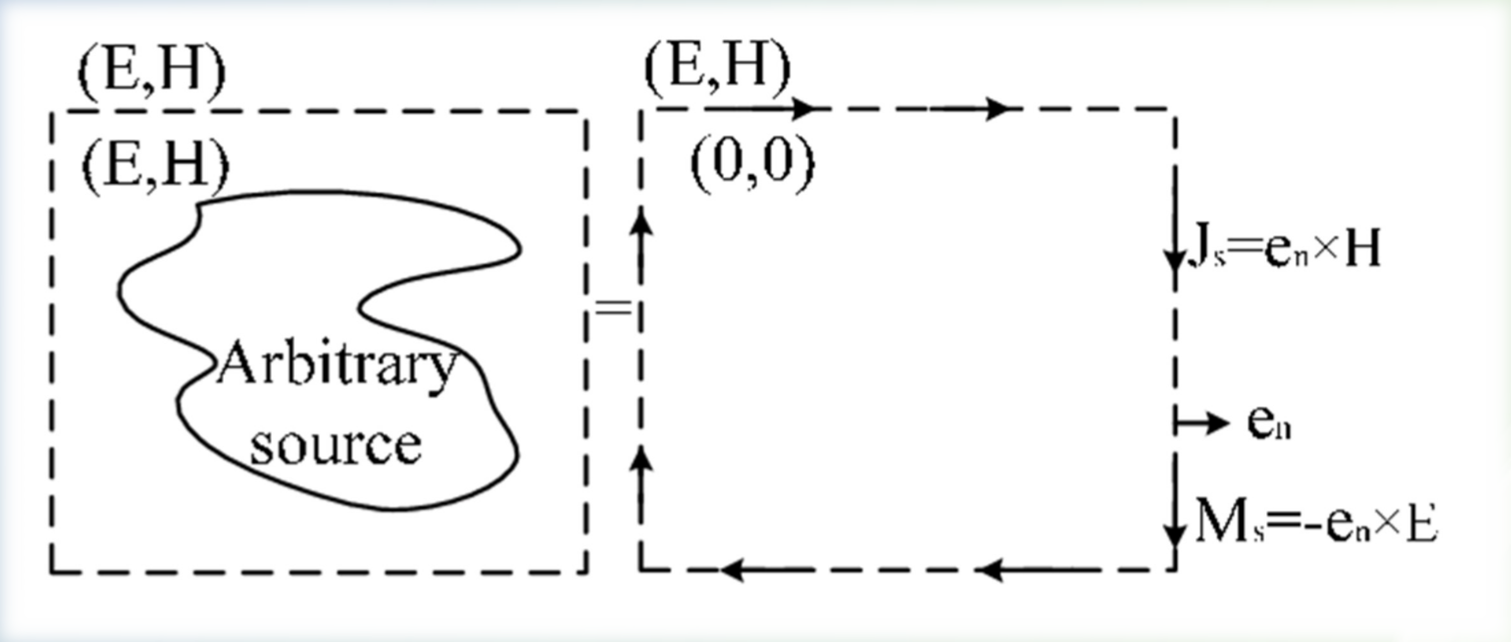
$$
\begin{cases}
\hat{\vec{E}}_{tot} = \hat{\vec{E}}_{inc} + \vec{E}_{scat} = \zeta \vec{E}_{inc} + \vec{E}_{scat} \\
\hat{\vec{H}}_{tot} = \hat{\vec{H}}_{inc} + \vec{H}_{scat} = \zeta \vec{H}_{inc} + \vec{H}_{scat}
\end{cases}
$$

connected region



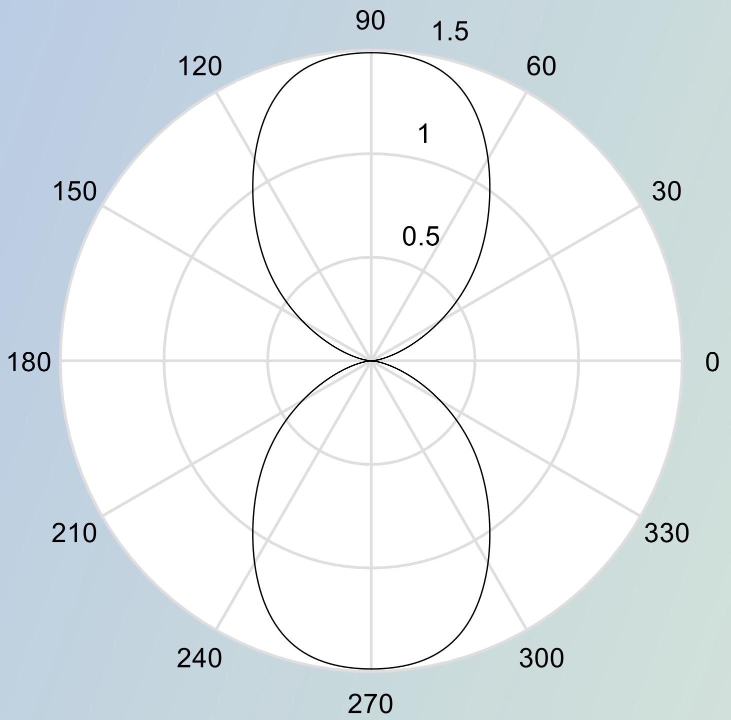
NTFF Transformation

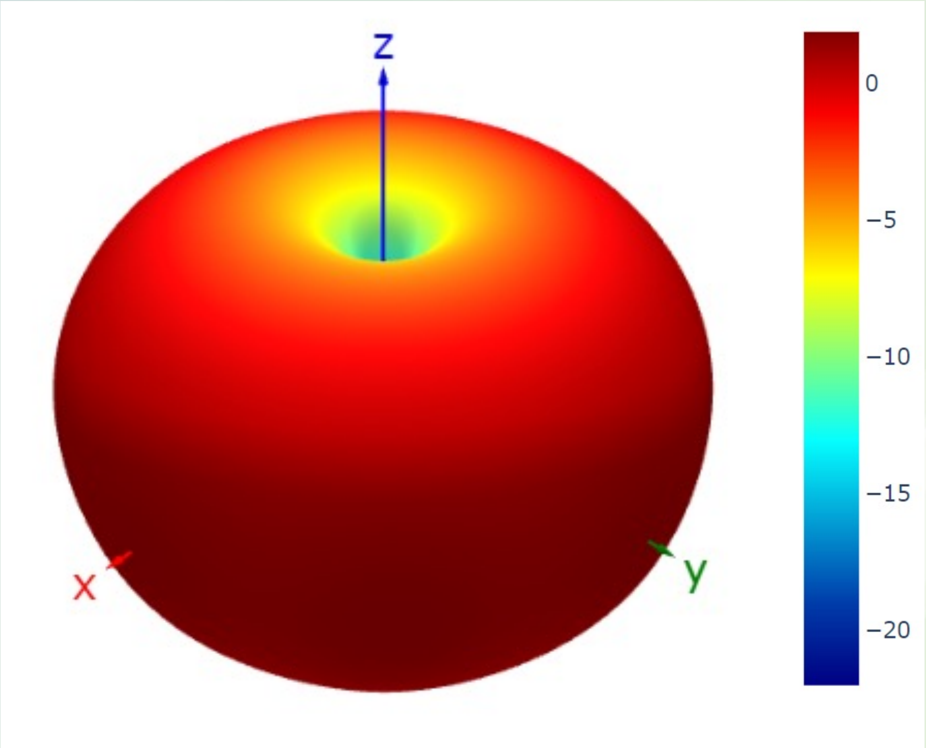
- From equivalence principle, when the surface currents on a selected imaginary surface are known, the fields inside the surface or outside the surface can be deduced from the imaginary currents.



NTFF Transformation

- From the imaginary currents, one can compute the far field of the source with NTFF transformation.





Staggered PSTD

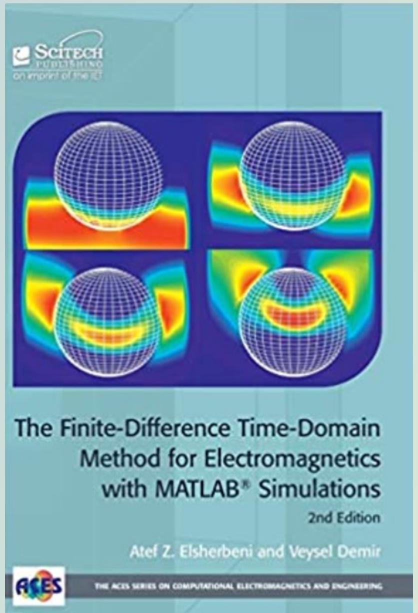
- M. Ding and K. Chen, 2010, "***Staggered-grid PSTD on local Fourier basis and its applications to surface tissue modeling***"
- Set PSTD grid to Yee grid.
- Advantages include mitigation of discontinuities and least modification of original FDTD code.

Some Advices on Implementing Your Own Code…

- FDTD (or PSTD) is relatively easy to implement as compared to other CEM methods (there are lots of "toy" codes out there…)
- Start with the basics, progressing from 1D to 2D to 3D. This approach helps avoid getting bogged down in details.
- Find some simple problems to model (dipole radiation, reflection from a plane, etc.) → open your college EM book

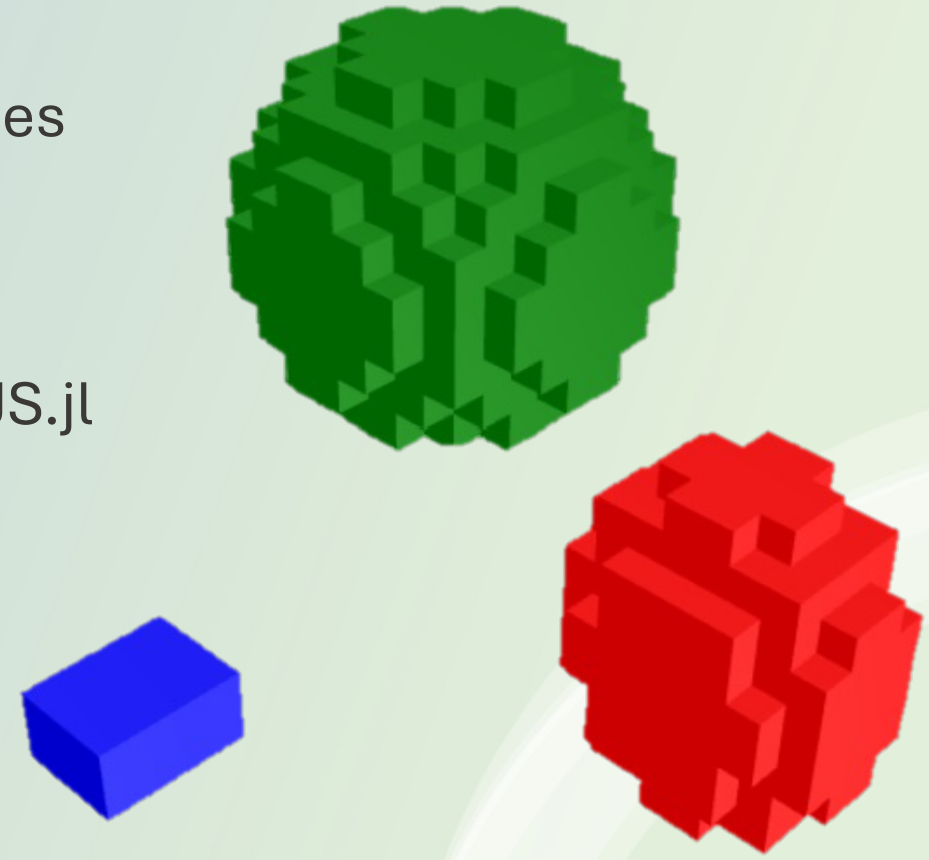
Some Useful References For You to Start

- John B. Schneider, ***Understanding the FDTD Method***
- Atef Z. Elsherbeni and Veysel Demir, ***The Finite-Difference Time-Domain Method for Electromagnetics with MATLAB® Simulations***



Some Interesting Tools I Made (in Julia)

- VoxelModel.jl
  - Create voxel models with simple geometries
- RadiationPatterns.jl
  - Plot 2D/3D radiation patterns using PlotlyJS.jl



Exercises

- Try to modify your 1D FDTD code into PSTD formulation
- Find out the differences in the implementation
- Compare results of both methods with different simulation scenarios

Thank You!