Computational Science:
Introduction to Finite-Difference Time-Domain

Implementation of Two-Dimensional FDTD

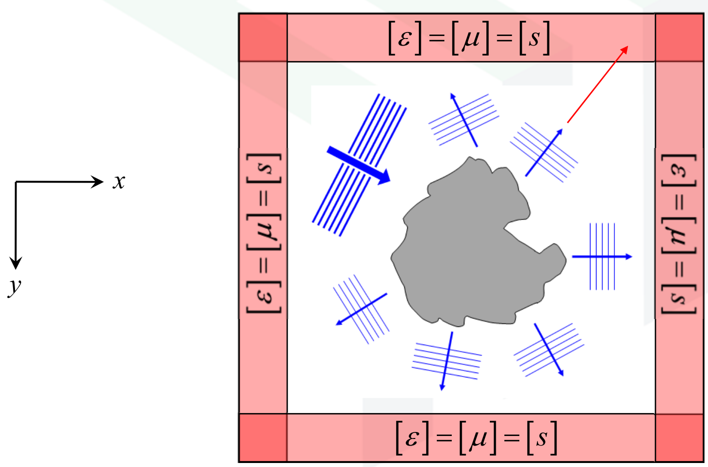
Lecture Outline

- Review
  - Update equations with PML
  - Code development sequence
- Numerical Boundary Conditions for 3D
- Reduction to Two-Dimensions
- Calculating the PML Parameters
- Implementation for Ez Mode
- Implementation for Hz Mode
- Total-Field/Scattered-Field Source

Review

Uniaxial PML

Reflections can be prevented at all angles, all frequencies, and for all polarizations if the absorbing material is made to be diagonally anisotropic.



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Derivation of Update Equation for H_x

$$\mathbf{F}\{g(t)\} = G(\omega)$$
$$\mathbf{F}\{ag(t)\} = aG(\omega)$$
$$\mathbf{F}\left\{\frac{d^a}{dt^a}g(t)\right\} = (j\omega)^a G(\omega)$$
$$\mathbf{F}\left\{\int_{-\infty}^{t} g(\tau)\,d\tau\right\} = \frac{1}{j\omega}G(\omega)$$

1. Start with governing equation in the frequency-domain.

$$j\omega\left(1+\frac{\sigma'_x}{j\omega\varepsilon_0}\right)^{-1}\left(1+\frac{\sigma'_y}{j\omega\varepsilon_0}\right)\left(1+\frac{\sigma'_z}{j\omega\varepsilon_0}\right)H_x(\omega) = -\frac{c_0}{\mu_{xx}}\left[\frac{\partial\tilde{E}_z(\omega)}{\partial y}-\frac{\partial\tilde{E}_y(\omega)}{\partial z}\right]$$

2. Prepare equation for conversion to the time-domain. Want all terms multiplied by $(j\omega)^a$.

$$j\omega H_x(\omega)+\frac{\sigma'_y+\sigma'_z}{\varepsilon_0}H_x(\omega)+\frac{1}{j\omega}\frac{\sigma'_y\sigma'_z}{\varepsilon_0^2}H_x(\omega) = -\frac{c_0}{\mu_{xx}}C_x^E(\omega)-\frac{1}{j\omega}\frac{c_0\sigma'_x}{\varepsilon_0\mu_{xx}}C_x^E(\omega)$$

3. Convert each term to the time-domain one at a time.

$$\frac{\partial H_x(t)}{\partial t}+\frac{\sigma'_y+\sigma'_z}{\varepsilon_0}H_x(t)+\frac{\sigma'_y\sigma'_z}{\varepsilon_0^2}\int_{-\infty}^{t}H_x(\tau)\,d\tau = -\frac{c_0}{\mu_{xx}}C_x^E(t)-\frac{c_0\sigma'_x}{\varepsilon_0\mu_{xx}}\int_{-\infty}^{t}C_x^E(\tau)\,d\tau$$

4. Approximate the equation using finite-differences and summations for numerical implementation.

$$\frac{H_x\big|_{t+\Delta t/2}^{i,j,k}-H_x\big|_{t-\Delta t/2}^{i,j,k}}{\Delta t}+\frac{\sigma_y^H\big|^{i,j,k}+\sigma_z^H\big|^{i,j,k}}{\varepsilon_0}\left(\frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k}+H_x\big|_{t-\frac{\Delta t}{2}}^{i,j,k}}{2}\right)+\frac{\left(\sigma_y^H\big|^{i,j,k}\right)\left(\sigma_z^H\big|^{i,j,k}\right)\Delta t}{\varepsilon_0^2}\left[\frac{1}{4}\left(H_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k}+H_x\big|_{t-\frac{\Delta t}{2}}^{i,j,k}\right)+\sum_{T=0}^{t-\frac{\Delta t}{2}}H_x\big|_T^{i,j,k}\right] = -\frac{c_0}{\mu_{xx}\big|^{i,j,k}}C_x^E\big|_t^{i,j,k}-\frac{c_0\Delta t\,\sigma_x^H\big|^{i,j,k}}{\varepsilon_0\,\mu_{xx}\big|^{i,j,k}}\sum_{T=0}^{t}C_x^E\big|_T^{i,j,k}$$

5. Derive the update equation by solving for H_x at the future time value.

$$H_x\big|_{t+\Delta t/2}^{i,j,k} = \left(m_{Hx1}\big|^{i,j,k}\right)H_x\big|_{t-\Delta t/2}^{i,j,k}+\left(m_{Hx2}\big|^{i,j,k}\right)C_x^E\big|_t^{i,j,k}+\left(m_{Hx3}\big|^{i,j,k}\right)I_{CEx}\big|_t^{i,j,k}+\left(m_{Hx4}\big|^{i,j,k}\right)I_{Hx}\big|_t^{i,j,k}$$

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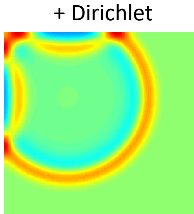
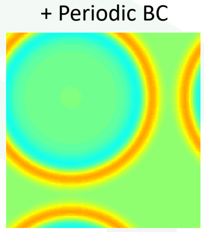
Code Development Sequence

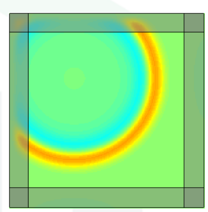
Step 1 – Basic Update + Dirichlet



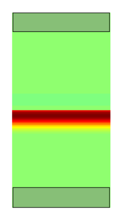
Step 2 – Basic Update + Periodic BC



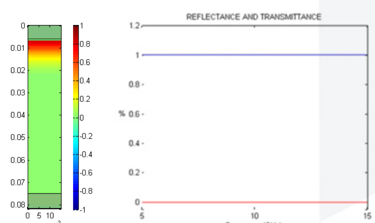
Step 3 – Add PML



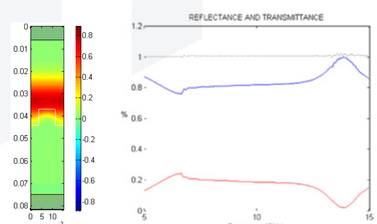
Step 4 – TF/SF



Step 5 – Calculate Response



Step 6 – Add a Device and Benchmark



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Numerical Boundary Conditions for 3D

Boundary Conditions

The update equations were formulated so that curl can be calculated separate from the update equation. Boundary condition problems occur only in the curl calculations.

$$\nabla \times \vec{\tilde{E}} \quad \downarrow$$

$$C_x^E\Big|_t^{i,j,k} = \frac{\tilde{E}_z\big|_t^{i,j+1,k} - \tilde{E}_z\big|_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y\big|_t^{i,j,k+1} - \tilde{E}_y\big|_t^{i,j,k}}{\Delta z}$$

$$C_y^E\Big|_t^{i,j,k} = \frac{\tilde{E}_x\big|_t^{i,j,k+1} - \tilde{E}_x\big|_t^{i,j,k}}{\Delta z} - \frac{\tilde{E}_z\big|_t^{i+1,j,k} - \tilde{E}_z\big|_t^{i,j,k}}{\Delta x}$$

$$C_z^E\Big|_t^{i,j,k} = \frac{\tilde{E}_y\big|_t^{i+1,j,k} - \tilde{E}_y\big|_t^{i,j,k}}{\Delta x} - \frac{\tilde{E}_x\big|_t^{i,j+1,k} - \tilde{E}_x\big|_t^{i,j,k}}{\Delta y}$$

Special boundary conditions are required at the high grid boundaries when computing the curl of $\vec{E}$.

$$\nabla \times \vec{H} \quad \downarrow$$

$$C_x^H\Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z\big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y\big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z}$$

$$C_y^H\Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z} - \frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z\big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x}$$

$$C_z^H\Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x} - \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x\big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y}$$

Special boundary conditions are required at the low grid boundaries when computing the curl of $\vec{H}$.

Handling the Boundary Conditions

A good way to handle the boundary conditions is to calculate the curl terms at the boundaries separate from the rest of the curl equation. This should be done explicitly without using 'if' statements.

For example,

$$C_x^E\Big|_t^{i,j,k} = \begin{cases} \dfrac{\tilde{E}_z\big|_t^{i,j+1,k} - \tilde{E}_z\big|_t^{i,j,k}}{\Delta y} - \dfrac{\tilde{E}_y\big|_t^{i,j,k+1} - \tilde{E}_y\big|_t^{i,j,k}}{\Delta z} & j < N_y \text{ and } k < N_z \\ \dfrac{\tilde{E}_z\big|_t^{i,1,k} - \tilde{E}_z\big|_t^{i,N_y,k}}{\Delta y} - \dfrac{\tilde{E}_y\big|_t^{i,N_y,k+1} - \tilde{E}_y\big|_t^{i,N_y,k}}{\Delta z} & j = N_y \text{ and } k < N_z \\ \dfrac{\tilde{E}_z\big|_t^{i,j+1,N_z} - \tilde{E}_z\big|_t^{i,j,N_z}}{\Delta y} - \dfrac{\tilde{E}_y\big|_t^{i,j,1} - \tilde{E}_y\big|_t^{i,j,N_z}}{\Delta z} & j < N_y \text{ and } k = N_z \\ \dfrac{\tilde{E}_z\big|_t^{i,1,N_z} - \tilde{E}_z\big|_t^{i,N_y,N_z}}{\Delta y} - \dfrac{\tilde{E}_y\big|_t^{i,N_y,1} - \tilde{E}_y\big|_t^{i,N_y,N_z}}{\Delta z} & j = N_y \text{ and } k = N_z \end{cases}$$

Calculating the curl terms separate from the update equations is an excellent way to isolate and modularize the boundary condition problem.

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MATLAB Code Implementation (1 of 3)

First, blindly try to calculate the curl.

```
% Compute CEx
for nx = 1 : Nx
    for ny = 1 : Ny
        for nz = 1 : Nz
            CEx(nx,ny,nz) = (Ez(nx,ny+1,nz) - Ez(nx,ny,nz))/dy ...
                          - (Ey(nx,ny,nz+1) - Ey(nx,ny,nz))/dz;
        end
    end
end
```

Two problems arise at the y-hi and z-hi sides of the grid.

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MATLAB Code Implementation (2 of 3)

Next, handle the z-hi problem explicitly outside of the `nz`-loop. Copy the code inside the `nz`-loop and paste it after the `nz`-loop.

```
% Compute CEx
for nx = 1 : Nx
    for ny = 1 : Ny
        for nz = 1 : Nz-1
            CEx(nx,ny,nz) = (Ez(nx,ny+1,nz) - Ez(nx,ny,nz))/dy ...
                          - (Ey(nx,ny,nz+1) - Ey(nx,ny,nz))/dz;
        end
        CEx(nx,ny,Nz) = (Ez(nx,ny+1,Nz) - Ez(nx,ny,Nz))/dy ...
                      - (Ey(nx,ny,1) - Ey(nx,ny,Nz))/dz;
    end
end
```

There is still a problem at the y-hi side of the grid, but now the problem occurs in two places.

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MATLAB Code Implementation (3 of 3)

Finally, the y-hi problem is handled explicitly outside of the `ny`-loop. Copy all of the code inside the `ny`-loop and paste it after the `ny`-loop.

```
% Compute CEx
for nx = 1 : Nx
    for ny = 1 : Ny-1
        for nz = 1 : Nz-1
            CEx(nx,ny,nz) = (Ez(nx,ny+1,nz) - Ez(nx,ny,nz))/dy ...
                          - (Ey(nx,ny,nz+1) - Ey(nx,ny,nz))/dz;
        end
        CEx(nx,ny,Nz) = (Ez(nx,ny+1,Nz) - Ez(nx,ny,Nz))/dy ...
                      - (Ey(nx,ny,1) - Ey(nx,ny,Nz))/dz;
    end
    for nz = 1 : Nz-1
        CEx(nx,Ny,nz) = (Ez(nx,1,nz) - Ez(nx,Ny,nz))/dy ...
                      - (Ey(nx,Ny,nz+1) - Ey(nx,Ny,nz))/dz;
    end
    CEx(nx,Ny,Nz) = (Ez(nx,1,Nz) - Ez(nx,Ny,Nz))/dy ...
                  - (Ey(nx,Ny,1) - Ey(nx,Ny,Nz))/dz;
end
```

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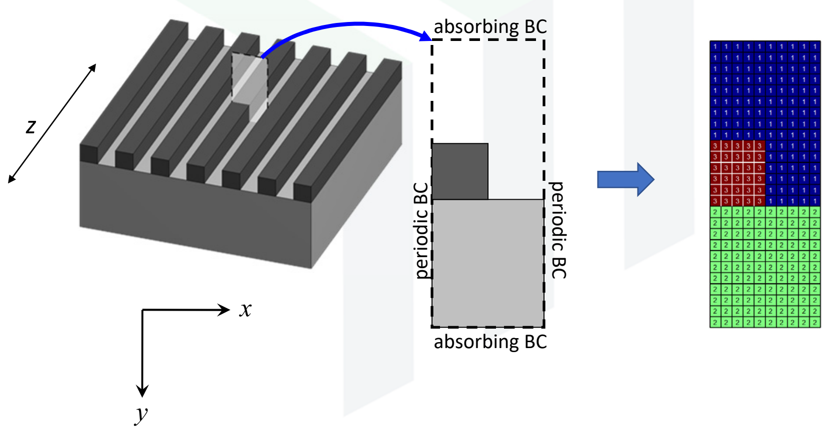
Reduction to Two Dimensions

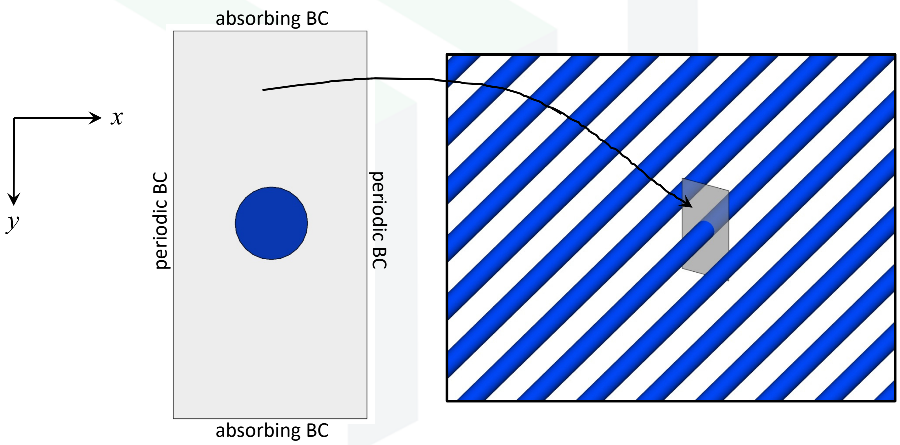
3D → 2D (Exact)

Sometimes it is possible to describe a physical device using just two dimensions. Doing so dramatically reduces the numerical complexity of the problem and is ALWAYS GOOD PRACTICE.



2D Grids are Infinite in the 3rd Dimension

Anything represented on a 2D grid, is actually a device that is of infinite extent along the 3rd dimension.



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What is Different in Two Dimensions?

- Assume it is the z direction that is uniform.
- All derivatives in the z direction are zero.

$$\frac{\partial}{\partial z} = 0$$

- There is no need for PML at the z axis boundaries.

$$\sigma'_z(z) = 0$$

$$s_z(z) = 1$$

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Revisions for Update Equation for H_x

The update coefficients are computed before the main FDTD loop.

$$m_{Hx0}\big|^{i,j,k} = \frac{1}{\Delta t} + \left(\frac{\sigma_y^H\big|^{i,j,k} + \cancel{\sigma_z^H\big|^{i,j,k}}}{2\varepsilon_0}\right) + \cancel{\frac{\left(\sigma_y^H\big|^{i,j,k}\right)\left(\sigma_z^H\big|^{i,j,k}\right)\Delta t}{4\varepsilon_0^2}}$$

$$m_{Hx1}\big|^{i,j,k} = \frac{1}{m_{Hx0}\big|^{i,j,k}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_y^H\big|^{i,j,k} + \cancel{\sigma_z^H\big|^{i,j,k}}}{2\varepsilon_0}\right) - \cancel{\frac{\left(\sigma_y^H\big|^{i,j,k}\right)\left(\sigma_z^H\big|^{i,j,k}\right)\Delta t}{4\varepsilon_0^2}}\right]$$

$$m_{Hx2}\big|^{i,j,k} = -\frac{1}{m_{Hx0}\big|^{i,j,k}}\frac{c_0}{\mu_{xx}\big|^{i,j,k}} \qquad m_{Hx3}\big|^{i,j,k} = -\frac{1}{m_{Hx0}\big|^{i,j,k}}\frac{c_0\Delta t}{\varepsilon_0}\frac{\sigma_x^H\big|^{i,j,k}}{\mu_{xx}\big|^{i,j,k}} \qquad \cancel{m_{Hx4}\big|^{i,j,k} = -\frac{1}{m_{Hx0}\big|^{i,j,k}}\frac{\Delta t}{\varepsilon_0^2}\left(\sigma_y^H\big|^{i,j,k}\right)\left(\sigma_z^H\big|^{i,j,k}\right)}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{CEx}\big|_t^{i,j,k} = \sum_{T=0}^{t} C_x^E\big|_t^{i,j,k} \qquad \cancel{I_{Hx}\big|_{t-\frac{\Delta t}{2}}^{i,j,k} = \sum_{T=\Delta t/2}^{t-\frac{\Delta t}{2}} H_x\big|_T^{i,j,k}} \qquad C_x^E\big|_t^{i,j,k} = \frac{\tilde{E}_z\big|_t^{i,j+1,k} - \tilde{E}_z\big|_t^{i,j,k}}{\Delta y} - \cancel{\frac{\tilde{E}_y\big|_t^{i,j,k+1} - \tilde{E}_y\big|_t^{i,j,k}}{\Delta z}}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$H_x\big|_{t+\Delta t/2}^{i,j,k} = \left(m_{Hx1}\big|^{i,j,k}\right) H_x\big|_{t-\Delta t/2}^{i,j,k} + \left(m_{Hx2}\big|^{i,j,k}\right) C_x^E\big|_t^{i,j,k} + \left(m_{Hx3}\big|^{i,j,k}\right) I_{CEx}\big|_t^{i,j,k} + \cancel{\left(m_{Hx4}\big|^{i,j,k}\right) I_{Hx}\big|_t^{i,j,k}}$$

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2D Update Equation for H_x

The update coefficients are computed before the main FDTD loop.

$$m_{Hx0}\big|^{i,j} = \frac{1}{\Delta t} + \left(\frac{\sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right) \qquad m_{Hx1}\big|^{i,j} = \frac{1}{m_{Hx0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right)\right]$$

$$m_{Hx2}\big|^{i,j} = -\frac{1}{m_{Hx0}\big|^{i,j}}\frac{c_0}{\mu_{xx}\big|^{i,j}} \qquad m_{Hx3}\big|^{i,j} = -\frac{1}{m_{Hx0}\big|^{i,j}}\frac{c_0\Delta t}{\varepsilon_0}\frac{\sigma_x^H\big|^{i,j}}{\mu_{xx}\big|^{i,j}}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{CEx}\big|_t^{i,j} = \sum_{T=0}^{t} C_x^E\big|_t^{i,j} \qquad C_x^E\big|_t^{i,j} = \frac{\tilde{E}_z\big|_t^{i,j+1} - \tilde{E}_z\big|_t^{i,j}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$H_x\big|_{t+\Delta t/2}^{i,j} = \left(m_{Hx1}\big|^{i,j}\right) H_x\big|_{t-\Delta t/2}^{i,j} + \left(m_{Hx2}\big|^{i,j}\right) C_x^E\big|_t^{i,j} + \left(m_{Hx3}\big|^{i,j}\right) I_{CEx}\big|_t^{i,j}$$

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2D Update Equation for H_y

The update coefficients are computed before the main FDTD loop.

$$m_{Hy0}\Big|^{i,j} = \frac{1}{\Delta t} + \left(\frac{\sigma_x^H\big|^{i,j}}{2\varepsilon_0}\right) \qquad m_{Hy1}\Big|^{i,j} = \frac{1}{m_{Hy0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_x^H\big|^{i,j}}{2\varepsilon_0}\right)\right]$$

$$m_{Hy2}\Big|^{i,j} = -\frac{1}{m_{Hy0}\big|^{i,j}}\frac{c_0}{\mu_{yy}\big|^{i,j}} \qquad m_{Hy3}\Big|^{i,j} = -\frac{1}{m_{Hy0}\big|^{i,j}}\frac{c_0\Delta t}{\varepsilon_0}\frac{\sigma_y^H\big|^{i,j}}{\mu_{yy}\big|^{i,j}}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{CEy}\Big|_t^{i,j} = \sum_{T=0}^{t} C_y^E\Big|_t^{i,j} \qquad C_y^E\Big|_t^{i,j} = -\frac{\tilde{E}_z\big|_t^{i+1,j} - \tilde{E}_z\big|_t^{i,j}}{\Delta x}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$H_y\Big|_{t+\frac{\Delta t}{2}}^{i,j} = \left(m_{Hy1}\big|^{i,j}\right)H_y\Big|_{t-\frac{\Delta t}{2}}^{i,j} + \left(m_{Hy2}\big|^{i,j}\right)C_y^E\Big|_t^{i,j} + \left(m_{Hy3}\big|^{i,j}\right)I_{CEy}\Big|_t^{i,j}$$

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2D Update Equation for H_z

The update coefficients are computed before the main FDTD loop.

$$m_{Hz0}\Big|^{i,j} = \frac{1}{\Delta t} + \left(\frac{\sigma_x^H\big|^{i,j} + \sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right) + \frac{\left(\sigma_x^H\big|^{i,j}\right)\left(\sigma_y^H\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2} \qquad m_{Hz1}\Big|^{i,j} = \frac{1}{m_{Hz0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_x^H\big|^{i,j} + \sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right) - \frac{\left(\sigma_x^H\big|^{i,j}\right)\left(\sigma_y^H\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2}\right]$$

$$m_{Hz2}\Big|^{i,j} = -\frac{1}{m_{Hz0}\big|^{i,j}}\frac{c_0}{\mu_{zz}\big|^{i,j}} \qquad m_{Hz4}\Big|^{i,j} = -\frac{1}{m_{Hz0}\big|^{i,j}}\frac{\Delta t}{\varepsilon_0^2}\left(\sigma_x^H\big|^{i,j}\right)\left(\sigma_y^H\big|^{i,j}\right)$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{Hz}\Big|_{t-\frac{\Delta t}{2}}^{i,j} = \sum_{T=\Delta t/2}^{t-\frac{\Delta t}{2}} H_z\Big|_T^{i,j} \qquad C_z^E\Big|_t^{i,j} = \frac{\tilde{E}_y\big|_t^{i+1,j} - \tilde{E}_y\big|_t^{i,j}}{\Delta x} - \frac{\tilde{E}_x\big|_t^{i,j+1} - \tilde{E}_x\big|_t^{i,j}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$H_z\Big|_{t+\frac{\Delta t}{2}}^{i,j} = \left(m_{Hz1}\big|^{i,j}\right)H_z\Big|_{t-\frac{\Delta t}{2}}^{i,j} + \left(m_{Hz2}\big|^{i,j}\right)C_z^E\Big|_t^{i,j} + \left(m_{Hz4}\big|^{i,j}\right)I_{Hz}\Big|_{t-\frac{\Delta t}{2}}^{i,j}$$

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2D Update Equation for D_x

The update coefficients are computed before the main FDTD loop.

$$m_{Dx0}\big|^{i,j} = \frac{1}{\Delta t} + \frac{\sigma_y^D\big|^{i,j}}{2\varepsilon_0} \qquad m_{Dx1}\big|^{i,j} = \frac{1}{m_{Dx0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \frac{\sigma_y^D\big|^{i,j}}{2\varepsilon_0}\right]$$

$$m_{Dx2}\big|^{i,j} = \frac{c_0}{m_{Dx0}\big|^{i,j}} \qquad m_{Dx3}\big|^{i,j} = \frac{1}{m_{Dx0}\big|^{i,j}}\frac{c_0 \Delta t\, \sigma_x^D\big|^{i,j}}{\varepsilon_0}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{CHx}\big|_{t-\frac{\Delta t}{2}}^{i,j} = \sum_{T=\Delta t/2}^{t-\frac{\Delta t}{2}} C_x^H\big|_T^{i,j} \qquad C_x^H\big|_{t+\frac{\Delta t}{2}}^{i,j} = \frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j} - H_z\big|_{t+\frac{\Delta t}{2}}^{i,j-1}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$\tilde{D}_x\big|_{t+\Delta t}^{i,j} = \left(m_{Dx1}\big|^{i,j}\right)\tilde{D}_x\big|_t^{i,j} + \left(m_{Dx2}\big|^{i,j}\right)C_x^H\big|_{t+\frac{\Delta t}{2}}^{i,j} + \left(m_{Dx3}\big|^{i,j}\right)I_{CHx}\big|_{t-\frac{\Delta t}{2}}^{i,j}$$

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2D Update Equation for D_y

The update coefficients are computed before the main FDTD loop.

$$m_{Dy0}\big|^{i,j} = \frac{1}{\Delta t} + \frac{\sigma_x^D\big|^{i,j}}{2\varepsilon_0} \qquad m_{Dy1}\big|^{i,j} = \frac{1}{m_{Dy0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \frac{\sigma_x^D\big|^{i,j}}{2\varepsilon_0}\right]$$

$$m_{Dy2}\big|^{i,j} = \frac{c_0}{m_{Dy0}\big|^{i,j}} \qquad m_{Dy3}\big|^{i,j} = \frac{1}{m_{Dy0}\big|^{i,j}}\frac{c_0 \Delta t\, \sigma_y^D\big|^{i,j}}{\varepsilon_0}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{CHy}\big|_{t-\frac{\Delta t}{2}}^{i,j} = \sum_{T=\Delta t/2}^{t-\frac{\Delta t}{2}} C_y^H\big|_T^{i,j} \qquad C_y^H\big|_{t+\frac{\Delta t}{2}}^{i,j} = -\frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j} - H_z\big|_{t+\frac{\Delta t}{2}}^{i-1,j}}{\Delta x}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$\tilde{D}_y\big|_{t+\Delta t}^{i,j} = \left(m_{Dy1}\big|^{i,j}\right)\tilde{D}_y\big|_t^{i,j} + \left(m_{Dy2}\big|^{i,j}\right)C_y^H\big|_{t+\frac{\Delta t}{2}}^{i,j} + \left(m_{Dy3}\big|^{i,j}\right)I_{CHy}\big|_{t-\frac{\Delta t}{2}}^{i,j}$$

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2D Update Equation for D_z

The update coefficients are computed before the main FDTD loop.

$$m_{Dz0}\big|^{i,j} = \frac{1}{\Delta t} + \frac{\sigma_x^D\big|^{i,j} + \sigma_y^D\big|^{i,j}}{2\varepsilon_0} + \frac{\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2} \qquad m_{Dz1}\big|^{i,j} = \frac{1}{m_{Dz0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \frac{\sigma_x^D\big|^{i,j} + \sigma_y^D\big|^{i,j}}{2\varepsilon_0} - \frac{\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2}\right]$$

$$m_{Dz2}\big|^{i,j} = \frac{c_0}{m_{Dz0}\big|^{i,j}} \qquad m_{Dz4}\big|^{i,j} = -\frac{1}{m_{Dz0}\big|^{i,j}}\frac{\Delta t}{\varepsilon_0^2}\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$I_{Dz}\big|_t^{i,j} = \sum_{T=0}^{t} \tilde{D}_z\big|_T^{i,j} \qquad C_z^H\big|_{t+\frac{\Delta t}{2}}^{i,j} = \frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j} - H_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j}}{\Delta x} - \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j} - H_x\big|_{t+\frac{\Delta t}{2}}^{i,j-1}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$\tilde{D}_z\big|_{t+\Delta t}^{i,j} = \left(m_{Dz1}\big|^{i,j}\right)\tilde{D}_z\big|_t^{i,j} + \left(m_{Dz2}\big|^{i,j}\right)C_z^H\big|_{t+\frac{\Delta t}{2}}^{i,j} + \left(m_{Dz4}\big|^{i,j}\right)I_{Dz}\big|_{t-\Delta t}^{i,j}$$

2D Update Equations for E_x, E_y, and E_z

The update coefficients are computed before the main FDTD loop.

$$m_{Ex1}\big|^{i,j} = \frac{1}{\varepsilon_{xx}\big|^{i,j}} \qquad m_{Ey1}\big|^{i,j} = \frac{1}{\varepsilon_{yy}\big|^{i,j}} \qquad m_{Ez1}\big|^{i,j} = \frac{1}{\varepsilon_{zz}\big|^{i,j}}$$

The update equations are computed inside the main FDTD loop.

$$\tilde{E}_x\big|_{t+\Delta t}^{i,j} = \left(m_{Ex1}\big|^{i,j}\right)\tilde{D}_x\big|_{t+\Delta t}^{i,j}$$

$$\tilde{E}_y\big|_{t+\Delta t}^{i,j} = \left(m_{Ey1}\big|^{i,j}\right)\tilde{D}_y\big|_{t+\Delta t}^{i,j}$$

$$\tilde{E}_z\big|_{t+\Delta t}^{i,j} = \left(m_{Ez1}\big|^{i,j}\right)\tilde{D}_z\big|_{t+\Delta t}^{i,j}$$

No changes here*!*

MATLAB Code for Update Equations

The update equation for H_x was

$$H_x\Big|_{t+\Delta t/2}^{i,j} = \left(m_{Hx1}\Big|^{i,j}\right) H_x\Big|_{t-\Delta t/2}^{i,j} + \left(m_{Hx2}\Big|^{i,j}\right) C_x^E\Big|_t^{i,j} + \left(m_{Hx3}\Big|^{i,j}\right) I_{CEx}\Big|_t^{i,j}$$

This could be implemented in MATLAB as follows

```
for ny = 1 : Ny
    for nx = 1 : Nx
        Hx(nx,ny) = mHx1(nx,ny)*Hx(nx,ny) + mHx2(nx,ny)*CEx(nx,ny) + mHx3(nx,ny)*ICEx(nx,ny);
    end
end
```

However, it is much simpler and faster to implement it using "vectorized" MATLAB commands.

```
Hx = mHx1.*Hx + mHx2.*CEx + mHx3.*ICEx;
```

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Calculating the PML Parameters

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MATLAB Code to Calculate PML Parameters

To calculate the PML parameters σ_x and σ_y we employ the 2× grid concept.

First, we calculate σ_x and σ_y on the 2× grid.

```
% COMPUTE PML PARAMETERS
Nx2 = 2*Nx;
Ny2 = 2*Ny;

sigx = zeros(Nx2,Ny2);
for nx = 1 : 2*NPML(1)
    nx1 = 2*NPML(1) - nx + 1;
    sigx(nx1,:) = (0.5*e0/dt)*(nx/2/NPML(1))^3;
end
for nx = 1 : 2*NPML(2)
    nx1 = Nx2 - 2*NPML(2) + nx;
    sigx(nx1,:) = (0.5*e0/dt)*(nx/2/NPML(2))^3;
end

sigy = zeros(Nx2,Ny2);
for ny = 1 : 2*NPML(3)
    ny1 = 2*NPML(3) - ny + 1;
    sigy(:,ny1) = (0.5*e0/dt)*(ny/2/NPML(3))^3;
end
for ny = 1 : 2*NPML(4)
    ny1 = Ny2 - 2*NPML(4) + ny;
    sigy(:,ny1) = (0.5*e0/dt)*(ny/2/NPML(4))^3;
end
```

This '2' is here because we are calculating the fictitious conductivity terms on the 2× grid, but NPML contains the size of the PML on the 1× grid.

$$\sigma'_x(x) = \frac{\varepsilon_0}{2\Delta t}\left(\frac{x}{L_x}\right)^3$$

$$\sigma'_y(y) = \frac{\varepsilon_0}{2\Delta t}\left(\frac{y}{L_y}\right)^3$$

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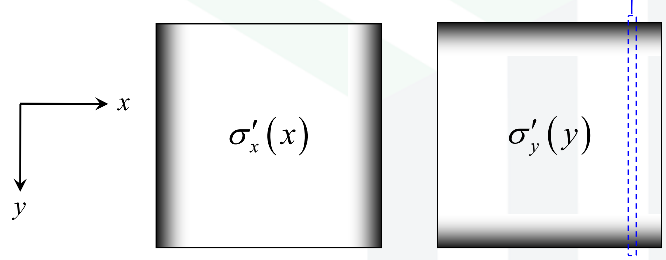
Visualizing the PML Parameters

If calculated correctly, the PML conductivity terms should look like:




```
e0 = 8.8542e-12
dt = 1.6678e-10
```

```
0.0265
0.0194
0.0136
0.0091
0.0057
0.0033
0.0017
0.0007
0.0002
0.0000
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
0.0000
0.0002
0.0007
0.0017
0.0033
0.0057
0.0091
0.0136
0.0194
0.0265
```

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MATLAB Code to Calculate Update Coefficients

Next, overlay the PML functions onto the 1× grid to calculate the update coefficients containing PML terms.

```
% COMPUTE UPDATE COEFFICIENTS
sigHx = sigx(1:2:Nx2,2:2:Ny2);
sigHy = sigy(1:2:Nx2,2:2:Ny2);
mHx0  = (1/dt) + sigHy/(2*e0);
mHx1  = ((1/dt) - sigHy/(2*e0))./mHx0;
mHx2  = - c0./URxx./mHx0;
mHx3  = - (c0*dt/e0) * sigHx./URxx ./ mHx0;

sigHx = sigx(2:2:Nx2,1:2:Ny2);
sigHy = sigy(2:2:Nx2,1:2:Ny2);
mHy0  = (1/dt) + sigHx/(2*e0);
mHy1  = ((1/dt) - sigHx/(2*e0))./mHy0;
mHy2  = - c0./URyy./mHy0;
mHy3  = - (c0*dt/e0) * sigHy./URyy ./ mHy0;

sigDx = sigx(1:2:Nx2,1:2:Ny2);
sigDy = sigy(1:2:Nx2,1:2:Ny2);
mDz0  = (1/dt) + (sigDx + sigDy)/(2*e0) ...
        + sigDx.*sigDy*(dt/4/e0^2);
mDz1  = (1/dt) - (sigDx + sigDy)/(2*e0) ...
        - sigDx.*sigDy*(dt/4/e0^2);
mDz1  = mDz1 ./ mDz0;
mDz2  = c0./mDz0;
mDz4  = - (dt/e0^2)*sigDx.*sigDy./mDz0;
```

$$m_{Hx0}\big|^{i,j} = \frac{1}{\Delta t} + \left(\frac{\sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right) \qquad m_{Hx1}\big|^{i,j} = \frac{1}{m_{Hx0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_y^H\big|^{i,j}}{2\varepsilon_0}\right)\right]$$

$$m_{Hx2}\big|^{i,j} = -\frac{1}{m_{Hx0}\big|^{i,j}}\frac{c_0}{\mu_{xx}\big|^{i,j}} \qquad m_{Hx3}\big|^{i,j} = -\frac{1}{m_{Hx0}\big|^{i,j}}\frac{c_0\Delta t}{\varepsilon_0}\frac{\sigma_x^H\big|^{i,j}}{\mu_{xx}\big|^{i,j}}$$

$$m_{Hy0}\big|^{i,j} = \frac{1}{\Delta t} + \left(\frac{\sigma_x^H\big|^{i,j}}{2\varepsilon_0}\right) \qquad m_{Hy1}\big|^{i,j} = \frac{1}{m_{Hy0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \left(\frac{\sigma_x^H\big|^{i,j}}{2\varepsilon_0}\right)\right]$$

$$m_{Hy2}\big|^{i,j} = -\frac{1}{m_{Hy0}\big|^{i,j}}\frac{c_0}{\mu_{yy}\big|^{i,j}} \qquad m_{Hy3}\big|^{i,j} = -\frac{1}{m_{Hy0}\big|^{i,j}}\frac{c_0\Delta t}{\varepsilon_0}\frac{\sigma_y^H\big|^{i,j}}{\mu_{yy}\big|^{i,j}}$$

$$m_{Dz0}\big|^{i,j} = \frac{1}{\Delta t} + \frac{\sigma_x^D\big|^{i,j} + \sigma_y^D\big|^{i,j}}{2\varepsilon_0} + \frac{\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2}$$

$$m_{Dz1}\big|^{i,j} = \frac{1}{m_{Dz0}\big|^{i,j}}\left[\frac{1}{\Delta t} - \frac{\sigma_x^D\big|^{i,j} + \sigma_y^D\big|^{i,j}}{2\varepsilon_0} - \frac{\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)\Delta t}{4\varepsilon_0^2}\right]$$

$$m_{Dz2}\big|^{i,j} = \frac{c_0}{m_{Dz0}\big|^{i,j}}$$

$$m_{Dz4}\big|^{i,j} = -\frac{1}{m_{Dz0}\big|^{i,j}}\frac{\Delta t}{\varepsilon_0^2}\left(\sigma_x^D\big|^{i,j}\right)\left(\sigma_y^D\big|^{i,j}\right)$$

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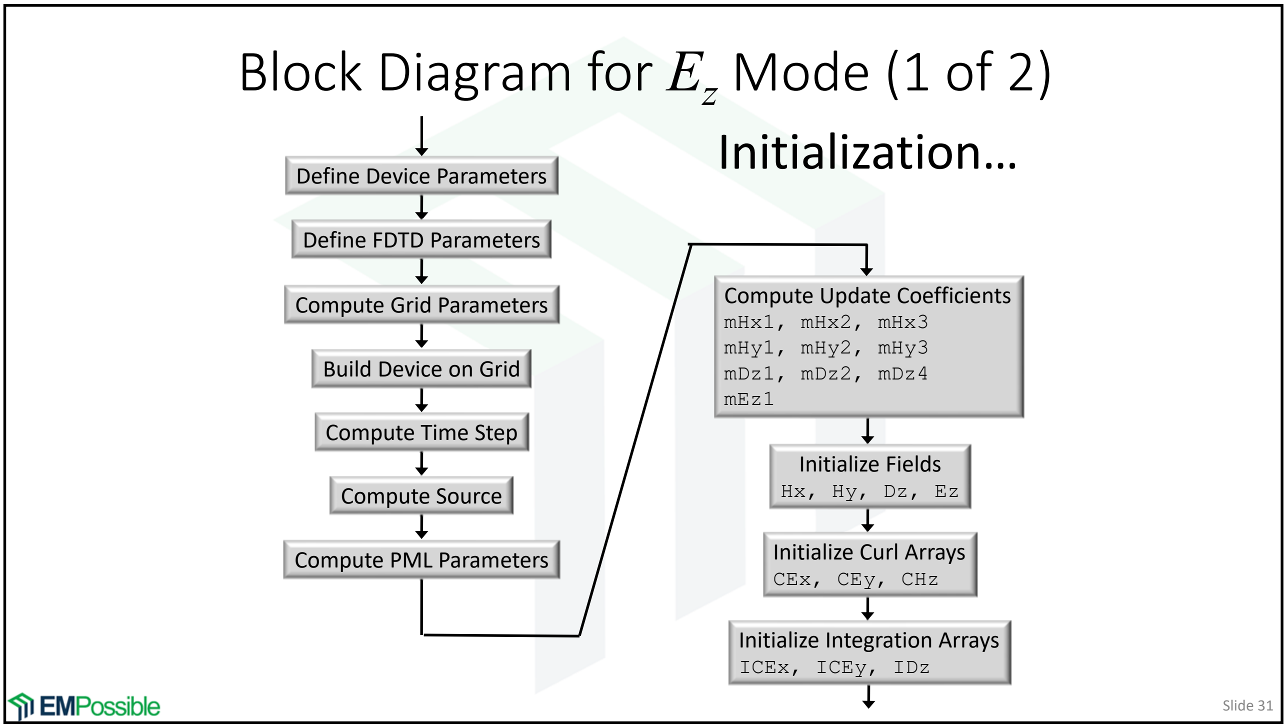
Slide 29

Implementation

E_z Mode

Slide 30


Block Diagram for Ez Mode (1 of 2)
Initialization…
Define Device Parameters
Define FDTD Parameters
Compute Grid Parameters
Build Device on Grid
Compute Time Step
Compute Source
Compute PML Parameters
Compute Update Coefficients
mHx1, mHx2, mHx3
mHy1, mHy2, mHy3
mDz1, mDz2, mDz4
mEz1
Initialize Fields
Hx, Hy, Dz, Ez
Initialize Curl Arrays
CEx, CEy, CHz
Initialize Integration Arrays
ICEx, ICEy, IDz
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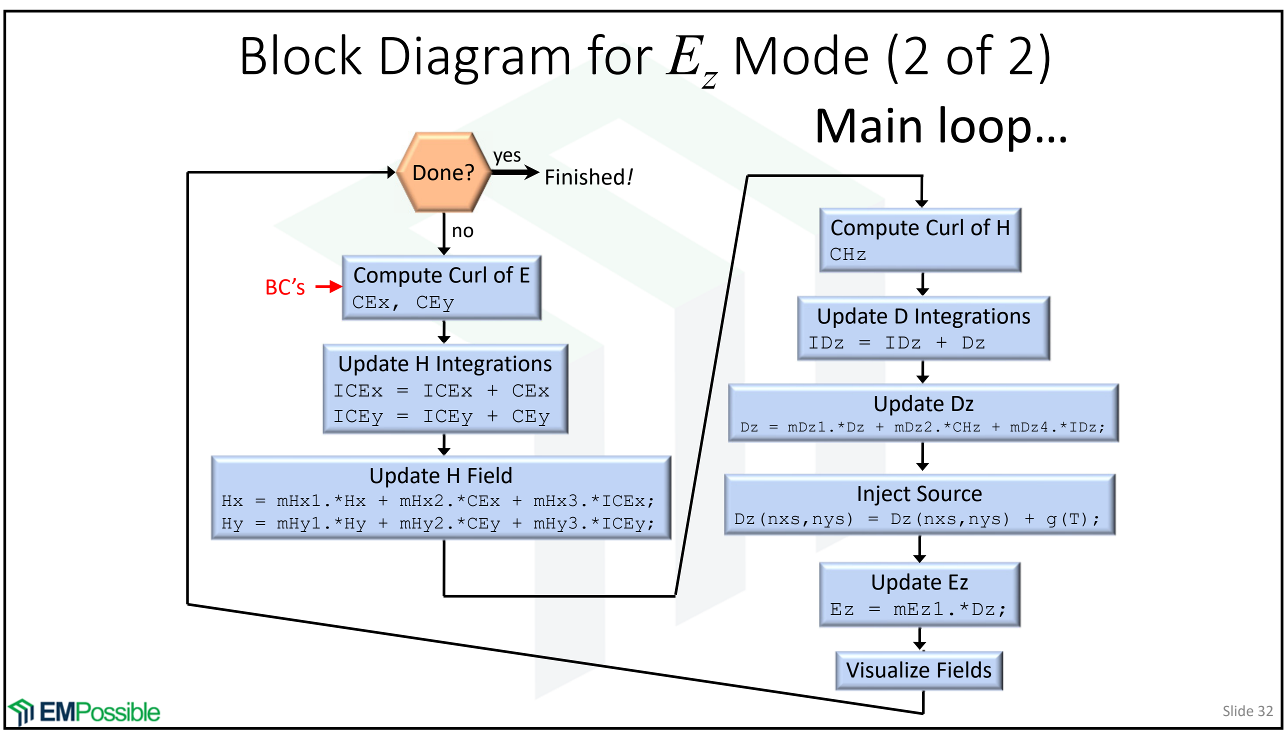
Block Diagram for Ez Mode (2 of 2)
Main loop…
Done?
yes
Finished!
no
BC's
Compute Curl of E
CEx, CEy
Update H Integrations
ICEx = ICEx + CEx
ICEy = ICEy + CEy
Update H Field
Hx = mHx1.*Hx + mHx2.*CEx + mHx3.*ICEx;
Hy = mHy1.*Hy + mHy2.*CEy + mHy3.*ICEy;
Compute Curl of H
CHz
Update D Integrations
IDz = IDz + Dz
Update Dz
Dz = mDz1.*Dz + mDz2.*CHz + mDz4.*IDz;
Inject Source
Dz(nxs,nys) = Dz(nxs,nys) + g(T);
Update Ez
Ez = mEz1.*Dz;
Visualize Fields
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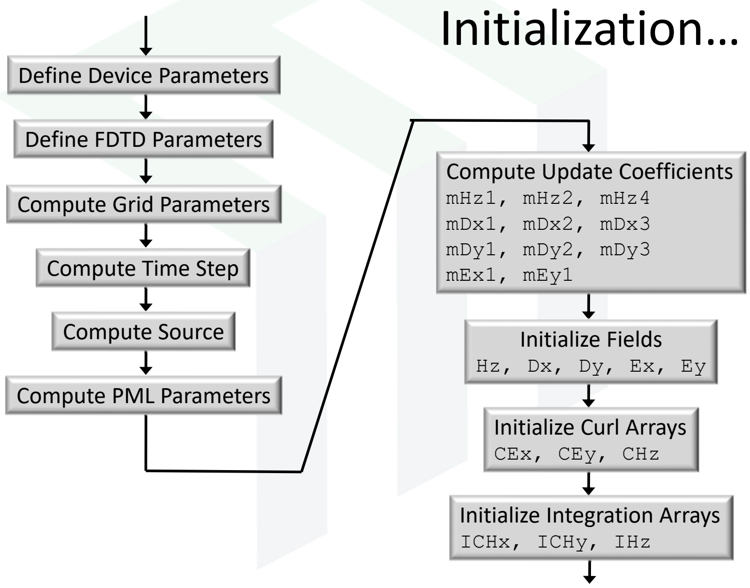
Slide 32

Implementation
H_z Mode

Block Diagram for H_z Mode (1 of 2)

Initialization…



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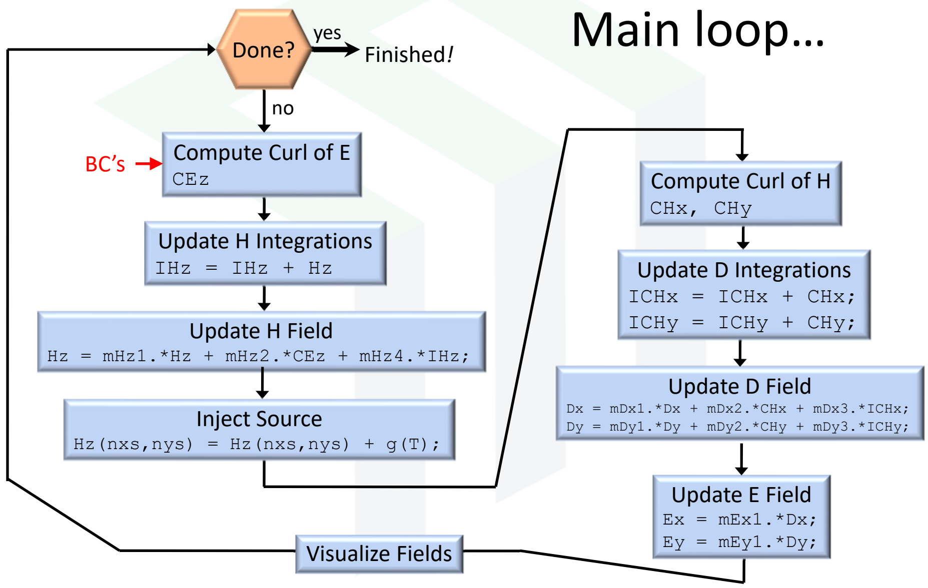
Block Diagram for H_z Mode (2 of 2)

Main loop…



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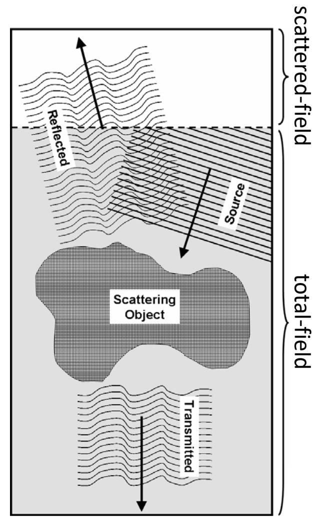
Slide 35

Total-Field/Scattered-Field Plane Wave Source

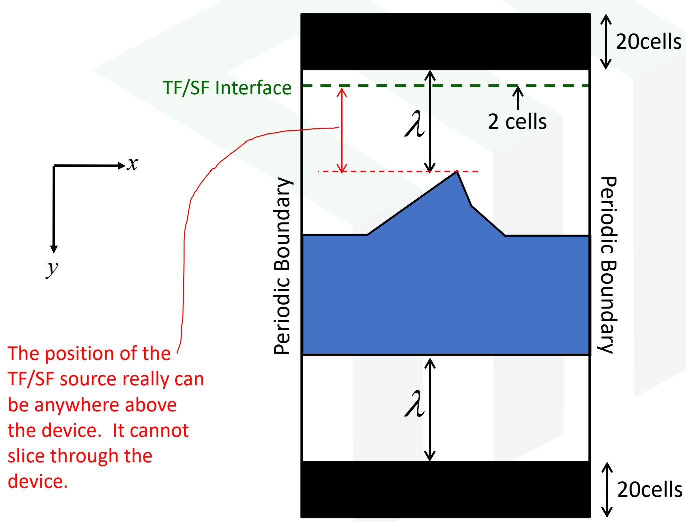
Slide 36

Total-Field / Scattered-Field

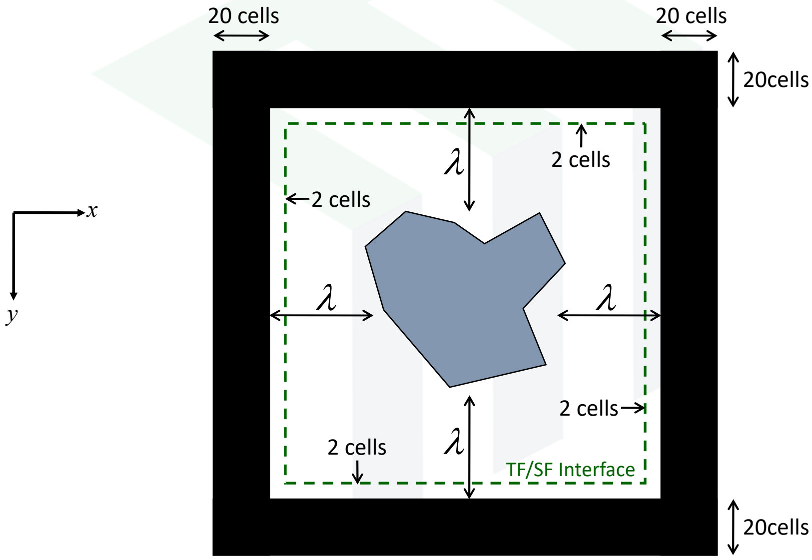
- The total-field/scattered-field (TF/SF) condition is a technique to inject a "one-way" source.
- Benefits
  - Eliminates backward propagating power
    - Needed for calculation of reflection
    - Minimizes power incident on PML
  - Ensures waves at the boundaries are only travelling outward
  - 100% of power injected by the source is incident on the device being simulated.



Typical 2D FDTD Grid Layout For Modeling Periodic Structures



Typical 2D FDTD Grid Layout For Modeling General Scatterers



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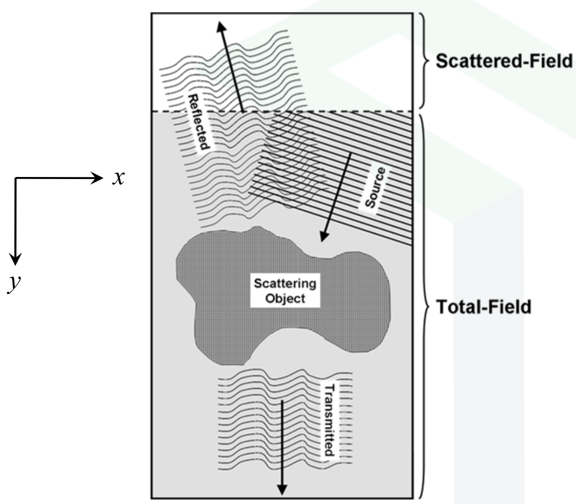
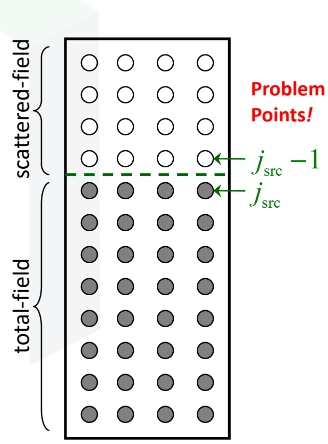
The Total-Field/Scattered-Field Framework



2D FDTD Grid



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Slide 40

Correction to Finite-Difference Equations at the Problem Cells (1 of 2)

On the scattered-field side of the TF/SF interface, the finite-difference equation contains a term from the total-field side. Due to the staggered nature of the Yee grid, this only occurs in the update equation for a magnetic field. In fact, this only occurs in the computation of the curl of $\vec{E}$ used in the update equations for $\vec{H}$.

$$C_x^E\Big|_t^{i,j_{\text{src}}-1} = \frac{\tilde{E}_z\big|_t^{i,j_{\text{src}}} - \tilde{E}_z\big|_t^{i,j_{\text{src}}-1}}{\Delta y}$$

This is an equation in the scattered-field, but $E_z^{j\text{src}}$ is a total-field quantity.

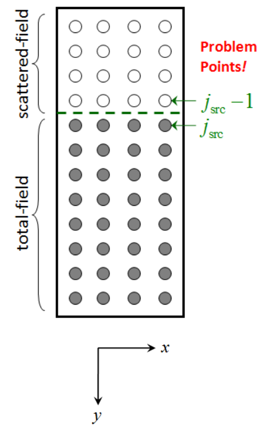
It is necessary to subtract the source from $E_z^{j\text{src}}$ to make it look like a scattered-field quantity.

$$C_x^E\Big|_t^{i,j_{\text{src}}-1} = \frac{\left(\tilde{E}_z\big|_t^{i,j_{\text{src}}} - E_z^{\text{src}}\big|_t^{i,j_{\text{src}}}\right) - \tilde{E}_z\big|_t^{i,j_{\text{src}}-1}}{\Delta y}$$

$$C_x^E\Big|_t^{i,j_{\text{src}}-1} = \underbrace{\frac{\tilde{E}_z\big|_t^{i,j_{\text{src}}} - \tilde{E}_z\big|_t^{i,j_{\text{src}}-1}}{\Delta y}}_{\text{standard curl equation}} - \frac{1}{\Delta y} E_z^{\text{src}}\Big|_t^{i,j_{\text{src}}}$$

Across entire row (all values of i)

This is a correction term that can be implemented after calculating the curl to inject a source.



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Slide 41

Correction to Finite-Difference Equations at the Problem Cells (2 of 2)

On the total-field side of the TF/SF interface, the finite-difference equation contains a term from the scattered-field side. Due to the staggered nature of the Yee grid, this only occurs in the update equation for $\vec{D}$. In fact, this only occurs in the computation of the curl of $\vec{H}$ used in the update equations for $\vec{D}$.

$$C_z^H\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} = \frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j_{\text{src}}}}{\Delta x} - \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}}{\Delta y}$$

This is an equation in the scattered-field, but $\tilde{H}_x^{j\text{src}-1}$ is a total-field quantity.

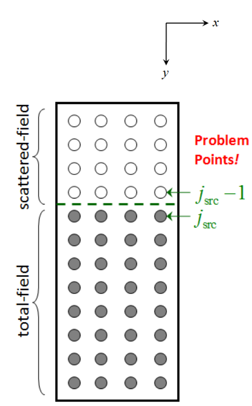
We must add the source to $\tilde{H}_x^{j\text{src}-1}$ to make it look like a total-field quantity.

$$C_z^H\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} = \frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j_{\text{src}}}}{\Delta x} - \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - \left(H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1} + \tilde{H}_x^{\text{src}}\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}\right)}{\Delta y}$$

$$C_z^H\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} = \underbrace{\frac{H_y\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j_{\text{src}}}}{\Delta x} - \frac{H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_x\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}}{\Delta y}}_{\text{standard update equation}} + \frac{1}{\Delta y}\tilde{H}_x^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}$$

entire row

This is a correction term that can be implemented after calculating the curl to inject a source.



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Slide 42

The Two Source Terms

From the previous slides, two source functions must be calculated before the main FDTD loop. These are:

$$\tilde{H}_x^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1} \qquad E_z^{\text{src}}\Big|_t^{i,j_{\text{src}}}$$

Across entire row (all values of i)

A few observations must be accounted for before these source functions can be calculated correctly.

1. The amplitude of these functions can be different because $\vec{E}$ and $\vec{H}$ are related through the material impedance.
2. These functions are a half grid cell apart and have a small time delay between them.
3. These functions exist at different time steps.

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Calculation of the Source Functions (E_z Mode)

Calculate the electric field as

$$E_z^{\text{src}}\Big|_t^{i,j_{\text{src}}} = g(t)$$

Calculate the magnetic field as

$$\tilde{H}_x^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1} = \sqrt{\frac{\varepsilon_{\text{r,src}}}{\mu_{\text{r,src}}}}\, g\left(t + \frac{n_{\text{src}}\Delta y}{2c_0} + \frac{\Delta t}{2}\right)$$

Amplitude due to Maxwell's equations

Delay through one half of a grid cell

Half time step difference

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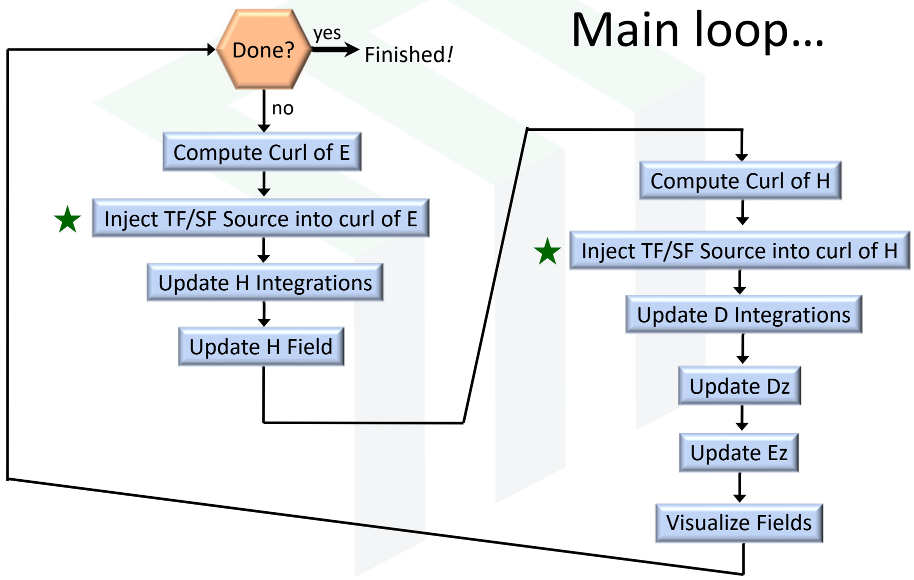
TF/SF Block Diagram for E_z Mode

Main loop…



H Mode Curl Calculations

The curl calculations requiring modifications are

$$C_z^E\Big|_t^{i,j} = \frac{\tilde{E}_y\big|_t^{i+1,j} - \tilde{E}_y\big|_t^{i,j}}{\Delta x} - \frac{\tilde{E}_x\big|_t^{i,j+1} - \tilde{E}_x\big|_t^{i,j}}{\Delta y}$$

$$C_x^H\Big|_{t+\frac{\Delta t}{2}}^{i,j} = \frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j} - H_z\big|_{t+\frac{\Delta t}{2}}^{i,j-1}}{\Delta y}$$

After correcting for TF/SF, these are

$$C_z^E\Big|_t^{i,j_{\text{src}}-1} = \frac{\tilde{E}_y\big|_t^{i+1,j_{\text{src}}-1} - \tilde{E}_y\big|_t^{i,j_{\text{src}}-1}}{\Delta x} - \frac{\tilde{E}_x\big|_t^{i,j_{\text{src}}} - \tilde{E}_x\big|_t^{i,j_{\text{src}}-1}}{\Delta y} + \frac{\tilde{E}_{x,\text{src}}\big|_t^{i,j_{\text{src}}}}{\Delta y}$$

$$C_x^H\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} = \frac{H_z\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}} - H_z\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}}{\Delta y} - \frac{H_{z,\text{src}}\big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1}}{\Delta y}$$

H Mode Source Functions

Calculate the electric field as

$$\tilde{E}_{x,\text{src}}\Big|_{t}^{i,j_{\text{src}}} = g(t)$$

Calculate the magnetic field as

$$H_{z,\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1} = -\sqrt{\frac{\varepsilon_{\text{r,src}}}{\mu_{\text{r,src}}}}\, g\left(t + \frac{n_{\text{src}}\Delta y}{2c_0} + \frac{\Delta t}{2}\right)$$

Amplitude due to Maxwell's equations

Delay through one half of a grid cell

Half time step difference

EMPossible

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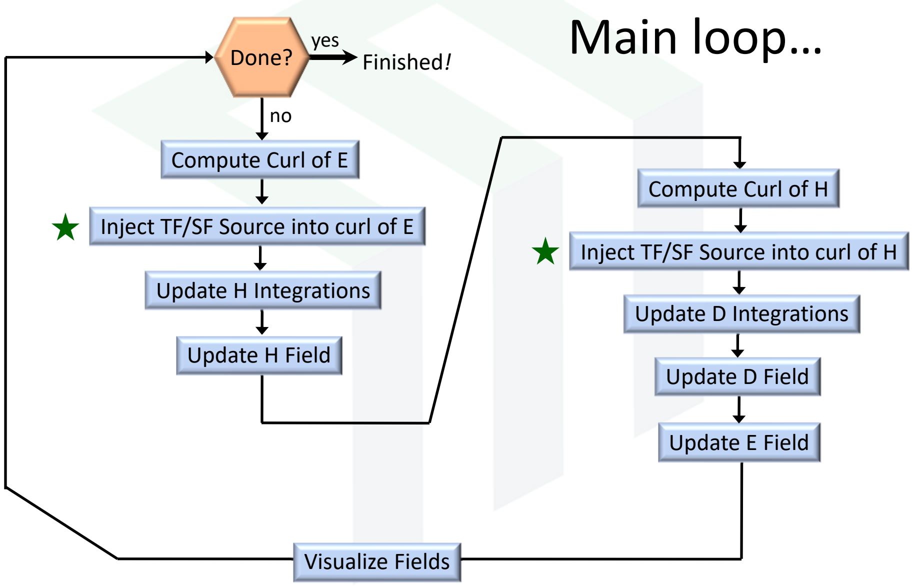
TF/SF Block Diagram for H_z Mode



EMPossible

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