Finite-Difference Time-Domain Simulation of Electromagnetic waves

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May 17, 2007
Presented at “Mathematica Expository Workshop”
Physics Department, UPM
1D scalar wave
(Sourceless) Maxwell Equation
2D EM wave propagation from point source
Absorbing Boundary Condition in 1D
2D EM plane waves
Total field/scattered field method
Putting everything together
Further applications

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1D scalar wave

- One-dimension scalar wave equation: \( \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \).
- \( u = u(x, t) \) one-dimension scalar wave.
- Use finite difference method to discretize the scala wave equation

(Sourceless) Maxwell Equation

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1D scalar wave

- Taylor expand $u(x, t_n)$ about $x_i$, keeping time $t_n$ fixed,

$$
\begin{align*}
\left. u(x_i + \Delta x) \right|_{t_n} &= u\big|_{x_i,t_n} + \Delta x \cdot \frac{\partial u}{\partial x}\big|_{x_i,t_n} + \frac{(\Delta x)^2}{2} \cdot \frac{\partial^2 u}{\partial x^2}\big|_{x_i,t_n} + \frac{(\Delta x)^3}{6} \cdot \frac{\partial^3 u}{\partial x^3}\big|_{x_i,t_n} + \frac{(\Delta x)^4}{24} \cdot \frac{\partial^4 u}{\partial x^4}\big|_{\xi_1,t_n} \\
\left. u(x_i - \Delta x) \right|_{t_n} &= u\big|_{x_i,t_n} - \Delta x \cdot \frac{\partial u}{\partial x}\big|_{x_i,t_n} + \frac{(\Delta x)^2}{2} \cdot \frac{\partial^2 u}{\partial x^2}\big|_{x_i,t_n} + \frac{(\Delta x)^3}{6} \cdot \frac{\partial^3 u}{\partial x^3}\big|_{x_i,t_n} - \frac{(\Delta x)^4}{24} \cdot \frac{\partial^4 u}{\partial x^4}\big|_{\xi_2,t_n}
\end{align*}
$$
Combining both Eqs,

\[ u(x_i + \Delta x)|_{t_n} + u(x_i - \Delta x)|_{t_n} = 2u|x_i, t_n| + (\Delta x)^2 \cdot \frac{\partial^2 u}{\partial x^2}|_{x_i, t_n} + \]

\[ \frac{(\Delta x)^4}{12} \cdot \frac{\partial^4 u}{\partial x^4}|_{\xi_3, t_n} \]

where \( x_i - \Delta x \leq \xi_3 \leq x_i + \Delta x \).
1D scalar wave

- Short-hand notation:
  
  \[ u_i^n \equiv u(x_i, t_n) \equiv u(i\Delta x, n\Delta t) \]
  \[ u_{i\pm 1}^{n\pm 1} \equiv u(x_i \pm \Delta x, t_n \pm \Delta t) \equiv u[(i \pm 1)\Delta x, (n \pm 1)\Delta t] \]

Second-order accurate, central difference approximation to \( \frac{\partial^2 u}{\partial x^2} |_{x_i, t_n} \):

\[
\frac{\partial^2 u}{\partial^2 x} |_{x_i, t_n} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + O\left[(\Delta x)^2\right]
\]  

(3)

Likewise,

\[
\frac{\partial^2 u}{\partial^2 t} |_{x_i, t_n} = \frac{u_{i+1}^{n+1} - 2u_i^n + u_{i-1}^{n-1}}{(\Delta t)^2} + O\left[(\Delta t)^2\right]
\]  

(4)
1D scalar wave

Plug the difference approximation of \( \frac{\partial^2 u}{\partial x^2} |_{x_i, t_n} \) and \( \frac{\partial^2 u}{\partial t^2} |_{x_i, t_n} \) into the one-dimension scalar wave equation:

\[
\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2},
\]

we then obtain the iterative difference equation for the scalar wave

\[
u_i^{n+1} = (c\Delta t)^2\left[\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta x)^2}\right] + 2u_i^n - u_i^{n-1} + O[(\Delta x)^2 + (\Delta t)^2]
\]

Eq. (5) allows us to implement numerical iteration to simulate propagation of scalar wave.
1D scalar wave

- $\Delta x = x_i - x_{i-1} = x_{i+1} - x_i$ is the spatial interval (usually expressed in unit of wavelength, $\lambda$, e.g. $\Delta x = \frac{\lambda}{10}$.
- $\Delta t$ time step
- 1D grid points:

  $x_0 \bullet \bullet \bullet x_1 \bullet \bullet \bullet x_2 \bullet \bullet \bullet \ldots \bullet \bullet \bullet x_i - \Delta x \bullet \bullet \bullet x_i \bullet \bullet \bullet x_i + \Delta x \bullet \bullet \bullet \ldots \bullet \bullet \bullet x_{i_{\text{last}}}$

- Given $u_i^n$ is known, $u_i^{n+1}$ can be calculated by iteration
- Say $u_i^n = \sin(n\omega\Delta t)$

hyperlink to 1Dscalar.nb


Gauss’s Law for electric field \( \nabla \cdot \vec{D} = 0 \).

Gauss’s Law for magnetic field \( \nabla \cdot \vec{B} = 0 \).

\( \vec{D} = \varepsilon \vec{E} \) \( \vec{D} \): electric flux density, \( \vec{E} \): electric field

\( \sigma \): electric conductivity, \( \sigma^* \): equivalent magnetic loss

\( \varepsilon \): electrical permittivity, \( \mu \): magnetic permeability

\( \vec{B} = \mu \vec{H} \) \( \vec{B} \): magnetic flux density, \( \vec{H} \): magnetic field

\[
\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \vec{E} - \frac{1}{\mu} \sigma^* \vec{H} \quad (6)
\]

\[
\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \vec{H} - \frac{1}{\varepsilon} \sigma \vec{H} \quad (7)
\]
The system of six coupled partial differential equations of the curl operator in Eq. (6) and Eq. (7) forms the basis of the FDTD numerical algorithm for electromagnetic wave interactions with general 3-D objects.

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma^* H_x \right] \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \sigma^* H_y \right] \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma^* H_z \right]
\end{align*}
\]
(Sourceless) Maxwell Equation

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial E_y}{\partial z} - \sigma E_x \right] \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial z} - \sigma E_y \right] \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right]
\end{align*}
\]  

(9)

- A general medium is characterized by \( \epsilon(i, j, k) \), \( \mu(i, j, k) \), \( \sigma(i, j, k) \), \( \sigma^*(i, j, k) \)
- A total of 6 fields present in the most general 3D case: \( E_x, E_y, E_z, H_x, H_y, H_z \)
The main purpose of FDTD:

- Given a set of fields $E_x, E_y, E_z, H_x, H_y, H_z$ are known for the entire domain of known spatial structure in terms of $\epsilon(i, j, k)$, $\mu(i, j, k)$, $\sigma(i, j, k)$ at time $t_n$
- times march the fields $E_x, E_y, E_z, H_x, H_y, H_z$ to the next time step, $t_{n+1}$
Assuming: $\frac{\partial u}{\partial z} = 0$, where $u = \{E_x, E_y, E_z, H_x, H_y, H_z\}$, the 6 partial equations, Eq.(8,9), reduces to

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu} - \frac{\partial E_z}{\partial y} - \sigma^* H_x \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \sigma^* H_y \right] \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right] \\
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_z}{\partial y} - \sigma E_x \right] \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_x}{\partial z} - \sigma E_y \right]
\end{align*}
\]
2D TMz and TEz modes

**TMz mode:**

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu} - \frac{\partial E_z}{\partial y} - \sigma^* H_x \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \sigma^* H_y \right] \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right]
\end{align*}
\]

\[ (12) \]

\{H_x, H_y, E_z\} propagating on the x-y plane \((\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \neq 0)\)

**TEz mode:**

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_z}{\partial y} - \sigma E_x \right] \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left[ \frac{\partial H_z}{\partial x} - \sigma E_y \right] \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma^* H_z \right]
\end{align*}
\]

\[ (13) \]

\{E_x, E_y, H_z\} propagating on the x-y plane \((\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \neq 0)\)
1D sourceless Maxwell Equations

$$\frac{\partial u}{\partial y} = 0, \quad \frac{\partial H_x}{\partial t} |_{t=0} = 0,$$
$$\Rightarrow x-\text{directed, } z-\text{polarised}$$

TEM mode:

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - \sigma E_z \right]$$
$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \sigma^* H_y \right]$$

$$\{ H_y, E_z \} \text{ propagating along the } x\text{-direction } (\frac{\partial u}{\partial x} \neq 0)$$

$$\frac{\partial u}{\partial y} = 0, \quad \frac{\partial E_x}{\partial t} |_{t=0} = 0,$$
$$\Rightarrow x-\text{directed, } y\text{-polarized}$$

TEM mode:

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_y}{\partial x} - \sigma^* H_z \right]$$
$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_z}{\partial x} - \sigma E_y \right]$$

$$\{ E_y, H_z \} \text{ propagating along the } x\text{-direction } (\frac{\partial u}{\partial x} \neq 0)$$
1D TEM mode

How to simulate the time marching of the $x$–directed $\{E_z, H_y\}$ fields in $z$-polarised TEM Mode?

- Yee’s algorithm
- Discretize the equation

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \sigma^* H_y \right]
\]
\[
\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left[ \frac{\partial H_y}{\partial x} - \sigma E_z \right]
\]  

(14)

using central difference method
1D Discretisation

Central difference method

\[
\frac{\partial u}{\partial t}\bigg|_{i,n} = \frac{u[i\Delta x, (n + 1/2)\Delta t] - u[i\Delta x, (n - 1/2)\Delta t]}{\Delta t} + O[(\Delta t)^2]
\]

\[
\frac{\partial u}{\partial x}\bigg|_{i,n} = \frac{u[(i - 1/2)\Delta x, n\Delta t] - u[(i + 1/2)\Delta x, n\Delta t]}{\Delta x} + O[(\Delta x)^2]
\]

Semi-implicit approximation

\[
u^n_i = \frac{u^{n+1/2}_i - u^{n-1/2}_i}{2}
\]
After some algebra, iterative expressions of the fields $E_z$ and $H_y$ are obtained from Eq. (14):

\[
E_z|_{i-1/2}^{n+1/2} = C_a|i-1/2 E_z|_{i-1/2}^{n-1/2} + C_b|i-1/2(H_y|_i^n - H_y|_{i-1}^n)
\]

\[
H_y|_i^{n+1} = D_a|i H_y|_i^n + D_b|i(E_z|_{i+1/2}^{n+1/2} - E_z|_{i-1}^{n+1/2})
\]
$C_a, C_b, D_a, D_b$ characterises the medium

$$
C_a|_{i-1/2} = \frac{(1 - \frac{\sigma_i}{2\epsilon_i})}{(1 + \frac{\sigma_i}{2\epsilon_i})}
$$

$$
C_b|_{i-1/2} = \frac{(\frac{\Delta t}{\epsilon_i})}{(1 + \frac{\sigma_i}{2\epsilon_i})}
$$

$$
D_a|_i = \frac{(1 - \frac{\sigma_i^*\Delta t}{2\mu_i})}{(1 + \frac{\sigma_i^*\Delta t}{2\mu_i})}
$$

$$
D_b|_i = \frac{(\frac{\Delta t}{\mu_i\Delta x})}{(1 + \frac{\sigma_i^*\Delta t}{2\mu_i})}
$$

- $C_a, C_b, D_a, D_d$ encode the physical characteristics of the medium through which the EM wave propagates
- Dispersive ones $\sigma = \sigma(\omega)$, Dissipative ones, $\sigma \neq 0$
- Non-vacuum medium, $\epsilon > \epsilon_0$ Magnetic medium, $\mu > \mu_0$. Usually, $\sigma^* = 0$
Leap-frog

Note that the fields $H_y|_{i}^{n+1}$, $E_z|_{i-1/2}^{n+1/2}$ are evaluated at different grid points and timestep (e.g. $i$ vs. $i \pm 1/2$, $n$ vs. $n \pm 1/2$)

- Begin with some given initial profile, e.g.
  
  $E_z|_{i-1/2}^{1/2}$, $i = \{i_{ini}, i_{ini+1}, \cdots, i_{ilast}\}$ →
  
  Do Loop $H_y|_{i}^{1}$ for $i = \{i_{ini}, i_{ini+1}, \cdots, i_{ilast}\}$ →
  
  Do Loop $E_z|_{i-1/2}^{3/2}$ for $i = \{i_{ini}, i_{ini+1}, \cdots, i_{ilast}\}$ → \cdots
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2D sourceless Maxwell Equations
1D sourceless Maxwell Equations
1D Discretization

Flow chart of Yee FDTD scheme
Fields leapfrog in time and space

Figure: Space-time chart of the Yee algorithm for a 1D wave propagation showing the use of central differences for the space derivatives and
Demo of 1D TEM z-polarized propagation

hyperlink to 1DTEMz.nb to see sinusoidal waveform generated by the hard source: $E_z[iini - 1/2, n] = \sin[2\pi fn\Delta t]$
Iterative difference equations for 2D TMz mode

- It is straightforward to generalise the 1D case to 2D
- As an illustration, take the TMz mode of Eq.(12)
- The iterative difference for the 2D TMz mode are:
Iterative difference equations for 2D TMz mode

\[ E_z|_{i-1/2,j+1/2}^{n+1/2} = C_a(i - 1/2, j + 1/2)E_z|_{i-1/2,j+1/2}^{n-1/2} + \\
C_b(i - 1/2, j + 1/2)[H_y|_{i,j+1/2}^n - H_y|_{i-1,j+1/2}^n + \\
H_x|_{i-1/2,j}^n - H_x|_{i-1/2,j+1/2}^n] \]

\[ H_x|_{i-1/2,j+1}^{n+1} = D_a(i - 1/2, j + 1)H_x|_{i-1/2,j+1}^n + \\
D_b(i - 1/2, j + 1)[E_z|_{i-1/2,j+1/2}^{n+1/2} - E_z|_{i-1/2,j+3/2}^{n+1/2} \]

\[ H_y|_{i,j+1/2}^{n+1} = D_a(i, j + 1/2)H_y|_{i,j+1/2}^n + \\
D_b(i, j + 1/2)[E_z|_{i+1/2,j+1/2}^{n+1/2} - E_z|_{i-1/2,j+1/2}^{n+1/2} \]
Iterative difference equations for 2D TMz mode

The structure matrices, $C_a, C_b, D_a, D_b$ are similar to that of Eq. (15) except that now their values depend on $i, j$. 
Courant factor, $S$

- For the numerical model to converge, the time step $\Delta t$ has to obey the Courant-Freidrichs-Lewy (CFL) stability criterion:

$$\Delta t \leq \frac{1}{c \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}$$

- This translates into the choice of $\Delta t$ that is tied to $\Delta x$ via

$$\Delta t = \frac{\Delta x}{cS}$$

- In general, $S \geq \sqrt{N}$, where $N$ is the dimensionality of the problem
- For the 2D case, $S \geq \sqrt{2}$
Procedures

- Prepare the memory a 2D domain \( \{i_{ini}, \ldots i \ldots i_{last}\}, \{j_{ini}, \ldots j \ldots j_{last}\}\),
- Empty all initial values of the fields, \( u(i, j) \)
- Important: Generate the medium \( C_a(i, j), C_b(i, j), D_a(i, j), D_b(i, j) \) and store them in the memory
- Generate a point hardsource at the point \( i_0, j_0 \)
- the point hardsource can be sinusoidal, a Gaussian pulse or anything, e.g. \( E_z^n|_{i_0,j_0} = \sin(2\pi fn\Delta t) \) in the \( n \)-loop

hyperlink to 2DTMzdemo.nb
hyperlink to 2DTMzcontour.nb
Perfectly Matching Layers (PML) for 1D

- An EM wave crossing from Medium 1 to Medium 2 will suffer minimal reflection if
  \[
  \frac{\sigma_{M2}}{\epsilon_{M1}} = \frac{\sigma^*_{M2}}{\mu_{M1}}
  \]  \hspace{1cm} (16)

  is “perfectly matched” at the boundary.

- The relationship forces the wave impedance to match with that of the free space - causing reflectionless transmission

- We artificially place a PML around the outer boundary to absorb all wave fall upon the edges of the boundary
Reflectionless transmission of a plane wave at a PML/free-space interface

Free medium,
\[
\sigma_{PM} = \sigma^*_{RD} = 0,
\mu_{PM} = \mu_0; \varepsilon_{PD} = \varepsilon_0
\]
Perfectly Matching Layers (PML) for 1D

One possible piecewise graded PML is as followed:

<table>
<thead>
<tr>
<th>Layer 1</th>
<th>Layer 2</th>
<th>Layer 3</th>
<th>Layer 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{PML1} = \varepsilon_{PML1}$</td>
<td>$\sigma_{PML2}^* = \varepsilon_{PML2}$</td>
<td>$\sigma_{PML3}^* = \varepsilon_{PML3}$</td>
<td>$\sigma_{PML4}^* = \varepsilon_{PML4}$</td>
</tr>
<tr>
<td>$\sigma_{PML1} = \mu_{PML1}$</td>
<td>$\sigma_{PML2} = \mu_{PML2}$</td>
<td>$\sigma_{PML3} = \mu_{PML3}$</td>
<td>$\sigma_{PML4} = \mu_{PML4}$</td>
</tr>
<tr>
<td>$\varepsilon_{PML1} = 1\varepsilon_{FM}$</td>
<td>$\varepsilon_{PML2} = 2\varepsilon_{FM}$</td>
<td>$\varepsilon_{PML3} = 3\varepsilon_{FM}$</td>
<td>$\varepsilon_{PML4} = 4\varepsilon_{FM}$</td>
</tr>
<tr>
<td>$\mu_{PML1} = 1\mu_{FM}$</td>
<td>$\mu_{PML2} = 2\mu_{FM}$</td>
<td>$\mu_{PML3} = 3\mu_{FM}$</td>
<td>$\mu_{PML4} = 4\mu_{FM}$</td>
</tr>
</tbody>
</table>

Free medium, $\sigma_{FM} = \sigma_{FM}^* = 0$, $\mu_{FM} = \mu_0$, $\varepsilon_{FM} = \varepsilon_0$
As an example, apply this to the x-directed, z-polarised 1D TEM mode, \( \{E_z, H_y\} \)

hyperlink: 1DTEMz.nb
(Graded) PML can also be implemented in a 2D domain albeit the generalisation is not straightforwardly trivial.

Oblique incident angles to the PML may not be fully attenuated.

The conductivity of the PML must have a certain anisotropy characteristic to ensure reflectionless transmission.
Perfectly Matching Layers (PML) for 2D

Figure: Structure of a 2D PML FDTD grid.

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Finite-Difference Time-Domain Simulation of Electromagnetic Waves
Perfectly Matching Layers (PML) for 2D

- Take the $x$-directed TEz mode $\{E_x, E_y, H_z\}$ as illustration
- To absorb obliquely incident waves, do the following
- TEz mode:

$$
\begin{align*}
\epsilon \frac{\partial E_x}{\partial t} + \sigma E_x &= \frac{\partial H_z}{\partial y} \\
\epsilon \frac{\partial E_y}{\partial t} + \sigma E_y &= -\frac{\partial H_z}{\partial x} \\
\mu \frac{\partial H_z}{\partial t} + \sigma^* H_z &= \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}
\end{align*}
$$
Perfectly Matching Layers (PML) for 2D

- Split $H_z = H_{zx} + H_{zy}$ and rewrite the TEz Maxwell equations

$$
\begin{align*}
\epsilon \frac{\partial E_x}{\partial t} + \sigma_y E_x &= \frac{\partial (H_{zx} + H_{zy})}{\partial y} \\
\epsilon \frac{\partial E_y}{\partial t} + \sigma_x E_y &= -\frac{\partial (H_{zx} + H_{zy})}{\partial x} \\
\mu \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} &= -\frac{\partial E_x}{\partial y} \\
\mu \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} &= -\frac{\partial E_x}{\partial y}
\end{align*}
$$

Note that we got 4 difference equations instead of 3
Perfectly Matching Layers (PML) for 2D

Descretisation yield \(^1\)

\[
E_{x}^{n+1}|_{i+1/2,j} = C_{ay}(i,j)E_{x}^{n}|_{i+1/2,j} + C_{by}(i,j)(H_{zx}^{n+1/2}|_{i+1/2,j+1/2} + H_{zy}^{n+1/2}|_{i+1/2,j+1/2} - H_{zx}^{n+1/2}|_{i+1/2,j-1/2} - H_{zy}^{n+1/2}|_{i+1/2,j-1/2})
\]

\[
E_{y}^{n+1}|_{i,j+1/2} = C_{ax}(i,j)E_{y}^{n}|_{i,j+1/2} + C_{bx}(i,j)(H_{zx}^{n+1/2}|_{i-1/2,j+1/2} + H_{zy}^{n+1/2}|_{i-1/2,j+1/2} - H_{zx}^{n+1/2}|_{i+1/2,j+1/2} - H_{zy}^{n+1/2}|_{i+1/2,j+1/2})
\]

Perfectly Matching Layers (PML) for 2D

\[ H_{zx}^{n+1/2}|_{i+1/2,j+1/2} = D_{ax}(i,j)H_{zx}^{n-1/2}|_{i+1/2,j+1/2} + D_{bx}(i,j)(E_{y}^{n}|_{i,j+1/2} - E_{y}^{n}|_{i+1,j+1/2}) \]  

(18)

\[ H_{zy}^{n+1/2}|_{i+1/2,j+1/2} = D_{ay}(i,j)H_{zy}^{n-1/2}|_{i+1/2,j+1/2} + D_{by}(i,j)(E_{x}^{n}|_{i+1/2,j+1} - E_{x}^{n}|_{i+1/2,j}) \]  

(19)
Perfectly Matching Layers (PML) for 2D

\[
\begin{align*}
C_{ay}(i,j) &= e^{-\sigma_y(j)\Delta t/\epsilon(i,j)} \\
C_{by}(i,j) &= \frac{1 - e^{\sigma_y(j)\Delta t/\epsilon(i,j)}}{\sigma_y(j)\Delta x} \\
C_{ax}(i,j) &= e^{-\sigma_x(i)\Delta t/\epsilon(i,j)} \\
C_{bx}(i,j) &= \frac{1 - e^{\sigma_x(i)\Delta t/\epsilon(i,j)}}{\sigma_x(i)\Delta x}
\end{align*}
\]

\[
\begin{align*}
D_{ay}(i,j) &= e^{-\sigma_y^*(j+1/2)\Delta t/\mu(i,j)} \\
D_{by}(i,j) &= \frac{1 - e^{\sigma_y^*(j+1/2)\Delta t/\mu(i,j)}}{\sigma_y^*(j + 1/2)\Delta x} \\
D_{ax}(i,j) &= e^{-\sigma_x^*(i+1/2)\Delta t/\mu(i,j)} \\
D_{bx}(i,j) &= \frac{1 - e^{\sigma_x^*(i+1/2)\Delta t/\mu(i,j)}}{\sigma_x^*(i + 1/2)\Delta x}
\end{align*}
\]

(20)
Note that in order to implement the 4 iterative difference equations, we first need to generate 8 matrices for the medium.

- \( C_{ax}(i,j) \), \( C_{bx}(i,j) \), \( D_{ax}(i,j) \), \( D_{bx}(i,j) \),
- \( C_{ay}(i,j) \), \( C_{by}(i,j) \), \( D_{ay}(i,j) \), \( D_{by}(i,j) \)

For \( C \)'s, \( D \)'s in the active domain,
- \( \sigma_{x,y}(i,j) \), \( \sigma_{x,y}^{*}(i,j) \), \( \epsilon(i,j) \), \( \mu(i,j) \) assume vacuum values

For \( C \)'s, \( D \)'s in the surrounding graded PML,
- \( \sigma_{x,y}(i,j) \), \( \sigma_{x,y}^{*}(i,j) \), \( \epsilon(i,j) \), \( \mu(i,j) \) fulfil the perfectly matched condition of Eq.(16)

hyperlink to 2DPML.nb
With the active domain surrounded by the graded PML, the EM waves propagating outwards will be almost perfectly attenuated (thus never reflected back into the active domain) when they hit the edges.

This simulates an “artificial infinity” as in most realistic scenario.
2D TEz mode from point (hard) source in PML-surrounded domain

- Model the propagation of TEz mode EM waves generated by a sinusoidal point (hard) source based on the 4 iterative equations in a PML-surrounded medium
- Note that now there is no visible reflection from the boundary, thanks to the layered PML

hyperlink to 2DPoint3DPML.nb
hyperlink to 2DPointCountourPML.nb
Illustration: 2D TEz mode from point source interacting with a square block of PEC

- Place a square of Perfect Electric Conductor (PEC) at the center of the active domain to interact with the cylindrical wave

hyperlink to 2DPointCountour_PECbloc_PML.nb
Look-up method to generate 2D EM plane waves

Look-up table method:

- Our purpose: to generate a 2D plane EM waves (TMz mode for illustration) that move in an arbitrary direction $\hat{m}$ at an angle $\phi$ with respect to $\hat{x}$.
- Look-up table method save us from evaluating the EM fields at each grid points using the iterative difference equations.
- First, generate a 1D EM waves along a reference straight line at an adjustable angle $\phi$ across the domain.
- The grid points along the 1D reference straight line is indexed by integer $m$, starting from $m_0 - 2$ to some $m_{max}$. The origin $m_0$ coincide with the origin of the 2D grid.
1D scalar wave
(Sourceless) Maxwell Equation
2D EM wave propagation from point source
Absorbing Boundary Condition in 1D
2D EM plane waves
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Further applications

Figure: The look-up table

Yoon Tiem Leong School of Physics, USM, Penang
Finite-Difference Time-Domain Simulation of Electromagnetic waves
The point source is located at $m = m_0 - 2$, $E_{inc}^{n}_{m_0-2} = E_0 \sin(2\pi fn\Delta t)$.

From $m = m_0 - 2$, a 1D $E_{inc}^{n}_m$ field will propagate along the $\hat{m}$ direction at every $m$, whereas a 1D $H_{inc}^{n}_{m+1/2}$ field will propagate in the $\hat{m}$ direction at every $m + 1/2$.

The 1D fields along $\hat{m}$ is equivalent to a 1D TEM $m$–directed EM waves, with component $H_{inc}^{n}_{m+1/2}$ and $E_{inc}^{n}_m$.

Don’t forget to apply PML at the $m_{max}$ end to avoid the 1D reference wave from bouncing back.
Look-up method to generate 2D EM plane waves

- At a general grid coordinates \( \{i', j'\} \), \( d \) can be calculated for that point via 
  \[ d = (i' - i_{ini}) \cos \phi + (j' - j_{ini}) \sin \phi. \]
- The TEM electric field at that point is denoted 
  \[ E_{inc} |_{d}^{n}(\equiv E_{inc} |_{i', j'}^{n}) \]
- \( E_{inc} |_{d}^{n} \) can be calculated by taking weighted average of \( E_{inc} |_{m'}^{n} \) and \( E_{inc} |_{m'+1}^{n} \), where \( m' \leq d \leq m' + 1 \).
- Likewise for \( H_{inc} |_{d}^{n}(\equiv H_{inc} |_{i', j'}^{n}) \)
- From \( E_{inc} |_{d}^{n}, H_{inc} |_{d}^{n} \), we then can work out the three incident fields in \( TMz \) mode via 
  - \( E_{z,inc} |_{d}^{n} = E_{inc} |_{d}^{n} \),
  - \( H_{x,inc} |_{d}^{n} = -H_{inc} |_{d}^{n} \sin \phi \),
  - \( H_{x,inc} |_{d}^{n} = H_{inc} |_{d}^{n} \cos \phi \)
Look-up method to generate 2D EM plane waves

hyperlink to incidentplane.nb
The 2D plane waves are called incident waves.  
Their evolution is based on the \( \hat{m} \)-directed 1D reference wave.  
They are running in the background and are independent from the iterative difference equations of Eqs. (17), (18), (19).  
In other words, the incident fields can’t be used to interact with the medium.  
Then what good are they for?
Ideas

- The physical (measurable) total electric and magnetic fields

\[
\vec{E}_{\text{total}} = \vec{E}_{\text{inc}} + \vec{E}_{\text{scat}}
\]

\[
\vec{H}_{\text{total}} = \vec{H}_{\text{inc}} + \vec{H}_{\text{scat}}
\]

- \(\vec{E}_{\text{inc}}, \vec{H}_{\text{inc}}\) are the incident plane waves that are generated using look-up table as discussed earlier

- They are assumed to be present at every grid point (actually only the \(\vec{E}_{\text{inc}}, \vec{H}_{\text{inc}}\) field near the TF/SF boundary will be required) in the computer memory when simulation of the EM wave propagation through the FDFT grid
Ideas

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Figure: Zoning of total-field/scattered field of the FDTD grid

Yoon Tiem Leong  School of Physics, USM, Penang
Finite-Difference Time-Domain Simulation of Electromagnetic
Ideas

- Divide the FDTD grid into (1) region of total field, (2) region of scattered field

- Take

\[
E_{x}^{n+1}|_{i+1/2,j} = C_{ay}(i,j)E_{x}|_{i+1/2,j} + C_{by}(i,j)(H_{zx}^{n+1/2}|_{i+1/2,j+1/2} + H_{zy}^{n+1/2}|_{i+1/2,j+1/2} - H_{zx}^{n+1/2}|_{i+1/2,j-1/2} - H_{zy}^{n+1/2}|_{i+1/2,j-1/2})
\]

as example
For\[i = iiniprime, i <= ilastprime, i++,
    For\[j = jiniprime, j <= jlastprime, j++,
        Ex[i + 1/2, j] = 
        Ex[i + 1/2, j]*Cay[i + 1/2, j] + 
        (Hzx[i + 1/2, j + 1/2]+Hzy[i + 1/2, j+1/2]- 
        Hzx[i + 1/2, j - 1/2]-Hzy[i+1/2,j-1/2])* 
        Cby[i + 1/2, j];
    ];
];(*end for i, j*)
Illustration

- $E_x[i + 1/2, j]$ is understood as scattered field for $\{i + 1/2, j\}$ in the scattered field region but as total field for $\{i + 1/2, j\}$ in the total field region (the TF/SF boundary belongs to the TF region).

- Note that to update the LHS $E_x[i + 1/2, j]$, we need $H_z[i + 1/2, j - 1/2]$ and $H_z[i + 1/2, j + 1/2]$ on the RHS.
Boundary condition for consistency

- For $i_{ini} + 1/2 \leq i'+1/2 \leq ilast-1/2$, no problem when j run from jiniprime till $jini-1$ since all the fields in the RHS are scattered field.

- However, right at $j = jini$, a consistency problem arises.

- Right at $j = jini$, $E_x[i'+1/2,jini]$ becomes a total field but $H_z[i'+1/2,jini-1/2]$ is a scattered field.
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Figure: Detail of field component locations in a 2D FDTD grid
Boundary condition for consistency

- Re-express $H_{z,s}[i' + 1/2, jini - 1/2] = H_{z,t}[i' + 1/2, jini - 1/2] - H_{z,inc}[i' + 1/2, jini - 1/2]$

- Practically, this means that in the FDTD code we add a boundary condition such that whenever $j = jini$, we have to replace $H_{z}[i' + 1/2, j - 1/2]$ by $H_{z}[i' + 1/2, j - 1/2] - H_{z,inc}[i' + 1/2, j - 1/2]$ after exiting the loop.
Boundary conditions for consistency

For\[i = i_{iniprime}, i \leq ilastprime, i++,
\]
For\[j = j_{iniprime}, j \leq j_{lastprime}, j++,
\]
\[Ex[i + 1/2, j] = Ex[i + 1/2, j]*Cay[i + 1/2, j] + (Hzx[i + 1/2, j + 1/2]+Hzy[i + 1/2, j+1/2]-Hzx[i + 1/2, j - 1/2]-Hzy[i+1/2,j-1/2])*Cby[i + 1/2, j];
\]

\[Ex[i + 1/2, j_{ini}] = Ex[i + 1/2, j_{ini}] - Hzinc[i + 1/2, j_{ini} - 1/2]*Cby[i + 1/2, j_{ini}]\]
Boundary conditions for consistency

- There are a total of 8 such boundary conditions for consistency at the TF/SF boundary, i.e. \( i = i_{ini}, i_{last}, j = j_{ini}, j_{last} \)

- Now you see why we need \( H_{inc} \) and \( E_{inc} \) near or on the TF/SF boundary

- These incident plane waves will excite total fields that will interact with the structure within the total field region
Fields evolution in the absence of structure

- In the absence of any structure in the total field region, i.e. the total field region is a vacuum, we should see only a 2D plane waves $E_x, E_y, H_z$ that are exactly as that of incident plane waves $E_{inc,x}, E_{inc,y}, H_{inc,z}$.
- The scattered fields in the SF region should void of any perturbations (approximately).
- However, due to numerical artifact effect, we still see some leakage especially at the sharp corners of the TF/SF.
- In the program that I will show, the leakage is too serious, and this may be caused by some programming mistake when I implemented the 8 boundary conditions (apology).

hyperlink to TFSFvacuum.nb
Revision

1. Prepare PML to surround the FDTD grid
2. Generate a 2D background incident fields $E_{inc}, H_{inc}$
3. Use TF/SF method to excite 2D total fields that will interact with the medium via the interactive difference equations of Eqs. (17, 18, Sadiku4). In particular, implementation of the boundary conditions at the TF/SF surface is essential (but the programming could be cumbersome)

Once you have programmed the Mathematica for procedures as mentioned above, the task left to do is to construct any medium of your interest (by programming the $C$’s and $D$’s matrices of Eq. (20)) to investigate how a 2D EM waves interact with the medium constructed.
EM waves interacting with a square PEC block

A simple example of a structure located within the total field region that will interact with the incident EM plane waves is a square PEC block that will reflect the incident EM waves that fall upon its surface.

hyperlink to TFSFPECblock.nb
Further simulation results

hyperlink to TFSFPECwall.nb
hyperlink to TFSFsingleslit.nb hyperlink to tangyong.nb
1D scalar wave
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Generalisation to 3D

- Generalisation to 3D is possible but probably would be too texting for Mathematica
- Illustrate with an example of a triple loop storing values to a matrix $M[i,j,k]$ for $i=[1,200], i=[j,200], k=[1,200]$ compare.nb c.f. compare.f95
- My opinion (may be wrong): Mathematica may be good for graphical illustration but not optimised for numerical intensive programe such as FDTD (esp. for large grid or for 3D cases) - too slow and get ‘saturated’ easily
Sub-wavelength diffractive optical element with binary profile

Application: Use FDTD to simulate 3D EM waves when interacting with a sub-wavelength diffractive optical element (SWDOE) with binary profile (2D or 3D)
Sub-wavelength diffractive optical element with binary profile

Subwavelength diffraction optical elements (SWDOEs) with binary features are artificially structured on a suitable optical substrate. Controlling the dimensions of a SWDOE determine whether it will form a polarizer, waveplate or polarisation dependent filter.