Lecture #25

Advanced FDTD Algorithms

Lecture Outline

• Alternating-Direction-Implicit (ADI) Algorithm
• Pseudospectral Time-Domain (PSTD)
• M24 Algorithm
  – Introduction
  – Formulation
  – Performance Improvement
Alternating-Direction-Implicit Algorithm

Some Limitations of Ordinary FDTD

Recall the Courant Stability Condition...

$$\Delta t \leq \frac{1}{c_0 \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}} \approx \frac{\Delta_{\text{min}}}{c_0 \sqrt{3}}$$

Problem – If the cell size is much less than the wavelength, then a prohibitively large number of iterations will be required due to the extremely small time step that ensures stability.

- Low-frequency bioelectromagnetics
- Simulation of VLSI circuits

We would like to exceed the Courant limit by more than 10×.

How?
New Stability Condition

In an alternating-direction-implicit (ADI) algorithm, we no longer have to consider the grid resolution. We need only look at the cycle time of the highest frequency.

\[
\Delta t \leq \frac{\tau_{\text{min}}}{N_x} \quad \text{with} \quad \tau_{\text{min}} = \frac{1}{f_{\text{max}}} \quad N_x \geq 20
\]

We can get away with extremely fine grid resolution without having to reduce \( \Delta t \) for stability! 😊

ADI-FDTD is unconditionally stable, but this does not mean unconditionally accurate.

Alternating Direction Implicit Method

Suppose we have the following PDE:

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}
\]

We have so far solved this using the Crank-Nicolson scheme

\[
\frac{u_n^{i,j} - u_n^{i,j}}{\Delta t} = \frac{\partial^2}{\partial x^2} \left( u_{n+1}^{i,j} + u_n^{i,j} \right) + \frac{\partial^2}{\partial y^2} \left( u_{n+1}^{i,j} + u_n^{i,j} \right)
\]

Instead, we can split this into two time-steps, each of duration \( \Delta t/2 \).

\[
\begin{align*}
& n \rightarrow n + 1/2 : \quad \frac{u_{n+1/2}^{i,j} - u_n^{i,j}}{\Delta t/2} = \frac{\partial^2}{\partial x^2} u_{n+1/2}^{i,j} + \frac{\partial^2}{\partial y^2} u_{n+1/2}^{i,j} \\
& n + 1/2 \rightarrow n + 1 : \quad \frac{u_n^{i,j} - u_{n+1/2}^{i,j}}{\Delta t/2} = \frac{\partial^2}{\partial x^2} u_{n+1}^{i,j} + \frac{\partial^2}{\partial y^2} u_{n+1}^{i,j}
\end{align*}
\]
Zheng/Chen/Zhang ADI Algorithm

**Spatial Derivatives:** Fields are staggered on an ordinary Yee grid.

**Time Derivatives:** Fields are collocated in time.

Original Finite-Difference Equation:

\[
\frac{E^{[1/2, j;k]}_{i+1/2} - E^{[1/2, j;k]}_{i}}{\Delta t} = \frac{1}{\epsilon} \left( \frac{H^{[1/2, 0,0;2,k]}_{i+1/2} - H^{[1/2, 0,0;2,k]}_{i}}{\Delta y} - \frac{H^{[1/2, 0,0;4,k]}_{i+1/2} - H^{[1/2, 0,0;4,k]}_{i}}{\Delta z} \right)
\]

ADI Finite-Difference Equations (now two steps):

\[
\frac{E^{[1/2, j;k]}_{i+1/2} - E^{[1/2, j;k]}_{i}}{\Delta t/2} = \frac{1}{\epsilon} \left( \frac{H^{[1/2, 0,0;2,k]}_{i+1/2} - H^{[1/2, 0,0;2,k]}_{i}}{\Delta y} - \frac{H^{[1/2, 0,0;4,k]}_{i+1/2} - H^{[1/2, 0,0;4,k]}_{i}}{\Delta z} \right)
\]

**Complete Set of Split Finite-Difference Equations**

Subiteration #1

\[
\begin{align*}
E^{[1/2, j;k]}_{i+1/2} &= E^{[1/2, j;k]}_{i} \\
H^{[1/2, 0,0;2,k]}_{i+1/2} &= H^{[1/2, 0,0;2,k]}_{i} \\
H^{[1/2, 0,0;4,k]}_{i+1/2} &= H^{[1/2, 0,0;4,k]}_{i}
\end{align*}
\]

Subiteration #2

\[
\begin{align*}
E^{[1/2, j;k]}_{i+1/2} &= E^{[1/2, j;k]}_{i} \\
H^{[1/2, 0,0;2,k]}_{i+1/2} &= H^{[1/2, 0,0;2,k]}_{i} \\
H^{[1/2, 0,0;4,k]}_{i+1/2} &= H^{[1/2, 0,0;4,k]}_{i}
\end{align*}
\]
Derivation of ADI Update Equations (1 of 2)

Subiteration #1

We substitute Eq. (4.100) into Eq. (4.99) to eliminate the H fields at the \( n+1/2 \) time steps.

We still retain Eq. (4.100).

Derivation of ADI Update Equations (2 of 2)

Subiteration #2

We substitute Eq. (4.102) into Eq. (4.101) to eliminate the H fields at the \( n+1 \) time steps.

We still retain Eq. (4.102).
ADI Finite-Difference Equations

Subiteration #1

This equation is written once for each occurrence of $E_x$ at a constant position $j$. This set of equations has the form of a tridiagonal matrix and is easily solved.

Subiteration #2

This equation is written once for each occurrence of $E_y$ at a constant position $k$. This set of equations has the form of a tridiagonal matrix and is easily solved.

This equation is written once for each occurrence of $E_z$ at a constant position $i$. This set of equations has the form of a tridiagonal matrix and is easily solved.

Note: H-field update equations remain unchanged.
Solution to ADI Finite-Difference Equations (2 of 2)

Subiteration #2

This equation is written once for each occurrence of $E_x$ at a constant position $k$. This set of equations has the form of a tridiagonal matrix and is easily solved.

This equation is written once for each occurrence of $E_y$ at a constant position $i$. This set of equations has the form of a tridiagonal matrix and is easily solved.

This equation is written once for each occurrence of $E_z$ at a constant position $j$. This set of equations has the form of a tridiagonal matrix and is easily solved.

Notes in ADI-FDTD

• ADI-FDTD is unconditionally stable for all $\Delta t$ so the Courant stability condition no longer applies.

• ADI-FDTD has accuracy issues.
  – Dispersion error increases steadily above the Courant stability condition.
  – Increasing error with increasing $\Delta t$.

• ADI-FDTD not well suited for electrically-large simulations.

• Best applied to electrically-small problems requiring very fine grids.
Pseudospectral Time-Domain

Purpose of PSTD

Numerical dispersion is a serious problem that is particularly severe in electrically large simulations.

It arises due to the numerical error arising from approximating the spatial derivatives in Maxwell’s equations.

Spectral accuracy is achieved when the fields are represented by trigonometric functions or Chebyshev polynomials. This means numerical dispersion decreases exponentially with sampling density.
Options for Approximating Spatial Derivatives

Finite-Difference Approximation

\[ \frac{df}{dx} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} \]

Requires a minimum of 10 to 20 points per wavelength.

Fourier (Trigonometric) Approximation

\[ \frac{df}{dx} \approx \frac{2\pi}{N\Delta x} \text{FFT}^{-1}\left\{ jn \text{FFT}\left\{ f \right\} \right\} \]

Requires a minimum of 2 points per wavelength.

Chebyshev Approximation

Requires a minimum of \( \pi \) points per wavelength.

Achieving Spectral Accuracy

Single-Domain PSTD

Internal medium must be continuously inhomogeneous.

Multidomain PSTD

When the internal medium is piecewise inhomogeneous, single-domain is applied to each subdomain and then matched at the boundaries.
Notes

Wraparound Effect
When trigonometric functions are used, the grid becomes inherently periodic. This can be mitigated by using a PML at the boundaries.

Gibb’s Phenomenon
When the field has discontinuities, like at a boundary of an object, a significant overshoot and ringing is introduced in the vicinity of the boundary.

M24 Algorithm

Data and diagrams in this section were borrowed from

Why M24?

- Problem – excessive phase error that accumulates during an FDTD simulation.
- Waves on a grid propagate differently than physical waves.
- Particularly severe for large structures.
- (2,4) scheme means 2\textsuperscript{nd}-order differences in time and 4\textsuperscript{th}-order differences in space.
- (4,4) scheme means 4\textsuperscript{th}-order differences in time and 4\textsuperscript{th}-order differences in space.
- These higher order schemes suffer from instability and more complicated boundary conditions.

Notation

- \( L_{\#_1 \#_2} \)
  - \( L \) algorithm (S=standard, M=modified)
  - \( \#_1 \) order of accuracy in time
  - \( \#_2 \) order of accuracy in space
- S22 – Standard FDTD with 2\textsuperscript{nd}-order differences in time and 2\textsuperscript{nd}-order differences in space. This is what we learned this semester.
- S24, S44 – Improved formulations, but with some problems.
- M24 – Modified FDTD with 2\textsuperscript{nd}-order differences in time and 4\textsuperscript{th}-order differences in space. Currently state-of-the-art.
Recall our S22 update equation for $E_{z^*}$.

\[
\frac{\tilde{E}_{z^*}^{i,j}_{x+\Delta x,y} - \tilde{E}_{z^*}^{i,j}_{x,y}}{\Delta t} = \left( \frac{c_0}{\varepsilon_{z^*}} \right)^j \left( \frac{H_{x+\Delta x,y}^{i,j} - H_{x,y}^{i,j} - H_{x+\Delta x,y+\Delta y}^{i,j-1}}{\Delta x} - \frac{H_{x+\Delta x,y+\Delta y}^{i,j} - H_{x,y}^{i,j}}{\Delta y} \right)
\]

We can write a similar equation, but with 4th-order accurate finite-differences.

\[
\frac{\tilde{E}_{z^*}^{i,j}_{x+\Delta x,y} - \tilde{E}_{z^*}^{i,j}_{x,y}}{\Delta t} = \left( \frac{c_0}{\varepsilon_{z^*}} \right)^j \left( \frac{-H_{x+\Delta x,y}^{i,j} + 27 H_{x,y}^{i,j} - 27 H_{x+\Delta x,y+\Delta y}^{i,j-1} + H_{x,y+\Delta y}^{i,j-2}}{24 \Delta x} \right)
\]
S24 Contains Closed Contour Line Integrals

We recognize that the right hand side of our finite-difference equation has two expressions in the form of closed contour line integrals.

\[
\left(\frac{\varepsilon_0}{c_0}\right) \left[ \frac{\partial E}{\partial t} \right] \int_{\Gamma} \left( \frac{E - E'}{\Delta t} \right) + \frac{q}{8\kappa} \left( -hH^\text{in} \int_{\Gamma_j} + hH^\text{in} \int_{\Gamma_j} - hH^\text{in} \int_{\Gamma_j} + hH^\text{in} \int_{\Gamma_j} \right) \frac{1}{8(9\kappa)} \left( -3hH^\text{in} \int_{\Gamma_j} + 3hH^\text{in} \int_{\Gamma_j} + 3hH^\text{in} \int_{\Gamma_j} \right)
\]

\[
\left(\frac{\varepsilon_0}{c_0}\right) \left( \frac{\partial B}{\partial t} \right) - \frac{q}{8\kappa} \int_{\Gamma_j} \left( H \cdot d\ell \right) - \frac{1}{8(9\kappa)} \int_{\Gamma_j} \left( \vec{H} \cdot d\ell \right)
\]

Maxwell’s Equations in Integral Form

Recall Maxwell’s equations in integral form

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad \quad \int_{L} \vec{E} \cdot d\ell = -\frac{\partial}{\partial t} \int_{S} \vec{B} \cdot d\vec{s}
\]

\[
\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} \quad \quad \int_{L} \vec{H} \cdot d\ell = \frac{\partial}{\partial t} \int_{S} \vec{D} \cdot d\vec{s}
\]

These equations let us calculate the line integrals as surface integrals.
**Use Surface Integral Instead of Line Integral**

We calculate the line integrals by instead calculating the surface integrals over the area enclosed by each contour.

\[
\oint \vec{H} \cdot d\vec{l} = \frac{\partial}{\partial t} \int_{\Sigma} \vec{B} \cdot d\Sigma, \quad \oint \vec{H} \cdot d\vec{l} = \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \int_{\Sigma} ds
\]

\[
= \frac{\partial}{\partial t} \int_{\Sigma} \vec{E} \cdot d\vec{s}
\]

\[
= \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \int_{\Sigma} ds
\]

\[
= \varepsilon_0 \frac{\partial \vec{E}}{\partial t} h^2
\]

\[
= \varepsilon_0 \varepsilon_0 h^2 \frac{\partial E_z}{\partial t}
\]

---

**Compile New Equation**

We start with our S24 equation derived with line integrals.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \vec{E}}{\partial t} = \frac{9}{8h^2} \oint \vec{H} \cdot d\vec{l} - \frac{1}{8(9h^2)} \oint \vec{H} \cdot d\vec{l}
\]

We replace the line integrals with our new surface integrals.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \vec{E}}{\partial t} = \frac{9}{8h^2} \left[ \varepsilon_0 h^2 \frac{\partial E_z}{\partial t} \right]_{\Sigma} - \frac{1}{8(9h^2)} \left[ 9\varepsilon_0 h^2 \frac{\partial E_z}{\partial t} \right]_{\Sigma}
\]

Now we simplify.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \vec{E}}{\partial t} \bigg|_{\text{FDTD}} = \frac{9}{8} \left[ \varepsilon_0 \frac{\partial E_z}{\partial t} \right]_{\Sigma} - \frac{1}{8} \left[ \varepsilon_0 \frac{\partial E_z}{\partial t} \right]_{\Sigma}
\]

We see this is just a weighted sum of two applications of Ampere’s circuit law. The coefficients add up to unity (-1/8 + 9/8 = 1) so that the integrity of Maxwell’s equations is preserved.
Split The Outer Loop

Here, we split the outer loop into two distinct loops.

Note, half of the terms are included in the first outer loop and the remaining are included in the second outer loop.

\[
\left[ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right]_{\text{FDTD}} = \frac{9}{8} \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_1 - \frac{1}{16} \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_2 - \frac{1}{16} \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_3
\]

Assign Arbitrary Weights

We need more degrees of freedom in order to reduce numerical error. To do this, we assign arbitrary weights to the terms in our equation.

\[
\left[ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right]_{\text{FDTD}} = K_1 \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_1 + K_2 \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_2 + K_3 \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_3
\]

Note that in order to preserve the integrity of Maxwell’s equations, we require that \( K_1 + K_2 + K_3 = 1 \). To enforce this, our equation is written as

\[
\left[ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right]_{\text{FDTD}} = (1 - K_1 - K_2) \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_1 + K_1 \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_2 + K_2 \left\{ \frac{\varepsilon_r}{c_0} \frac{\partial \vec{E}}{\partial t} \right\}_3
\]
### M24 Update Equation for Ez (1 of 2)

Starting with

\[
\left(\frac{\varepsilon_{\infty}}{c_0}\right) \frac{\partial \vec{E}_z}{\partial t} \bigg|_{\text{FDTD}} = (1 - K_1 - K_2) \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_1} \right] + K_1 \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_2} \right] + K_2 \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_3} \right]
\]

Each term on the right is calculated as...

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_1} \right] = \frac{1}{\Delta t} \left( H_z^{i,j+1} + H_z^{i,j-1} + H_x^{i+1,j} - H_x^{i,j} \right)
\]

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_2} \right] = \frac{1}{3\Delta t} \left( H_z^{i,j+1} - H_z^{i,j-2} - H_z^{i+2,j} + 2H_z^{i,j} \right)
\]

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \bigg|_{c_3} \right] = -\frac{1}{6\Delta t} \left( H_z^{i+1,j} + H_z^{i+2,j} - H_z^{i,j+1} + H_z^{i,j+2} + H_y^{i,j+1} - H_y^{i+1,j} \right)
\]

### M24 Update Equation for Ez (2 of 2)

So the overall update equation is now

\[
\left(\frac{\varepsilon_{\infty}}{c_0}\right) \frac{\Delta \vec{E}_z}{\Delta t} = \left(1 - K_1 - K_2\right) \left(-\frac{1}{\Delta t} H_z^{i,j+1} + H_z^{i,j-1} + H_y^{i+1,j} - H_y^{i,j} \right)
\]

\[
+ \frac{K_1}{3\Delta t} \left(H_z^{i+1,j+2} - H_z^{i-1,j+2} - H_z^{i,j} + H_y^{i+1,j+2}ight)
\]

\[
+ \frac{K_2}{6\Delta t} \left(H_z^{i+1,j} + H_y^{i+1,j+1} - H_y^{i+1,j} - H_y^{i+1,j+1} \right)
\]
Optimum Values for $K_1$ and $K_2$

<table>
<thead>
<tr>
<th>NRES</th>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$\Phi_{n,1}$</th>
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<td>35</td>
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<td>0.0667144748</td>
<td>$1.263 \times 10^{-30}$</td>
</tr>
</tbody>
</table>

**Global Phase Error**

$$\Phi_n = \frac{1}{2\pi} \int_{0}^{2\pi} \left( \frac{\bar{k}_i - \bar{k}_i(\theta)}{\bar{k}_i} \right)^2 d\theta$$

- $k_i$ = physical wave number
- $\bar{k}_i$ = numerical wave number
- $\theta$ = angle of wave through grid
Global Phase Error Vs. NRES

Fig. 4. Global error comparison of the S22, S44, and M24 schemes versus \( R \). The M24-WB is the wideband version of the MN scheme.

Memory Requirements

Fig. 5. Minimum resolution factors and computer memory requirements for the S22, S44, and M24 schemes that will keep the total phase error under 5°. Computer memory values are based on 4 bytes per real number and square computational domains that are \( D_{\text{max}} \times D_{\text{max}} \) large.