Computational Science:
Introduction to Finite-Difference Time-Domain

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...

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

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

It is desired to exceed the Courant limit by more than 10×.

How?
New Stability Condition

In an alternating-direction-implicit (ADI) algorithm, the grid resolution no longer needs to be considered. Only the cycle time of the highest frequency matters.

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

Simulations 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:

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

Up until now, this was solved using the Crank-Nicolson scheme

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

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

\[ n \rightarrow n+1/2: \quad \frac{u_{i,j}^{n+1/2} - u_{i,j}^{n-1/2}}{\Delta t/2} = \frac{\partial^2 u_{i,j}^{n+1/2}}{\partial x^2} + \frac{\partial^2 u_{i,j}^{n+1/2}}{\partial y^2} \]

\[ n+1/2 \rightarrow n+1: \quad \frac{u_{i,j}^{n+1} - u_{i,j}^{n+1/2}}{\Delta t/2} = \frac{\partial^2 u_{i,j}^{n+1}}{\partial x^2} + \frac{\partial^2 u_{i,j}^{n+1}}{\partial y^2} \]
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:

\[ \frac{E_{i+1/2,j,k} - E_{i-1/2,j,k}}{\Delta t} = \frac{1}{\varepsilon} \left( \frac{H_{i+1/2,j,k+1/2} - H_{i+1/2,j,k-1/2}}{\Delta y} - \frac{H_{i+1/2,j+1/2,k} - H_{i+1/2,j-1/2,k}}{\Delta z} \right) \]

ADI Finite-Difference Equations (now two steps):

\[ \frac{E_{i+1/2,j,k} - E_{i-1/2,j,k}}{\Delta t/2} = \frac{1}{\varepsilon} \left( \frac{H_{i+1/2,j,k+1/2} - H_{i+1/2,j,k-1/2}}{\Delta y} - \frac{H_{i+1/2,j+1/2,k} - H_{i+1/2,j-1/2,k}}{\Delta z} \right) \]

\[ \frac{E_{i+1/2,j,k} - E_{i+1/2,j,k}}{\Delta t/2} = \frac{1}{\varepsilon} \left( \frac{H_{i+1/2,j+1/2,k} - H_{i+1/2,j-1/2,k}}{\Delta y} - \frac{H_{i+1/2,j,k+1/2} - H_{i+1/2,j,k-1/2}}{\Delta z} \right) \]

Complete Set of Split Finite-Difference Equations
Derivation of ADI Update Equations (1 of 2)

Subiteration #1

Substitute Eq. (4.100) into Eq. (4.99) to eliminate the $H$ fields at the $n + 1/2$ time steps. Retain Eq. (4.100).

Derivation of ADI Update Equations (2 of 2)

Subiteration #2

Substitute Eq. (4.102) into Eq. (4.101) to eliminate the $H$ fields at the $n + 1$ time steps. Retain Eq. (4.102).
ADI Finite-Difference Equations

Subiteration #1

Note: the $\vec{H}$ field update equations remain unchanged.

Subiteration #2

Solution to ADI Finite-Difference Equations (1 of 2)

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.

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.
Solution to ADI Finite-Difference Equations (2 of 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
\[
\frac{df_i}{dx} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}
\]
Requires a minimum of 10 to 20 points per wavelength.

Fourier (Trigonometric) Approximation
\[
\frac{df}{dx} \approx \frac{2\pi}{N\Delta x} \text{FFT}^{-1}\left\{i\pi\text{FFT}\{f\}\right\}
\]
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.
S24 Update Equation (1 of 2)

Recall the S22 update equation for $E_{zz}$.

$$\frac{E_{zz}^{i,j} - \tilde{E}_{zz}^{i,j}}{\Delta t} = \left( \frac{c_0}{E_{zz}^{i,j}} \right)^2 \left( \frac{H_x^{i,j} - H_x^{i-1,j}}{\Delta x} - \frac{H_x^{i,j} - H_x^{i+1,j}}{\Delta x} \right)$$

A similar equation can be written, but with 4th-order accurate finite-differences.

$$\frac{E_{zz}^{i,j} - \tilde{E}_{zz}^{i,j}}{\Delta t} = \left( \frac{c_0}{E_{zz}^{i,j}} \right)^2 \left( \frac{-H_x^{i+1,j} + 27H_x^{i,j} - 27H_x^{i-1,j} + H_x^{i-2,j}}{24\Delta x} \right)$$

Rearrange S24 Update Equation

For simplicity, let $h = \Delta x = \Delta y$

$$\left( \frac{c_0}{E_{zz}^{i,j}} \right) \frac{E_{zz}^{i,j} - \tilde{E}_{zz}^{i,j}}{\Delta t} = \frac{1}{24h} \left( -H_x^{i+1,j} + 27H_x^{i,j} - 27H_x^{i-1,j} + H_x^{i-2,j} \right)$$

The right hand side can be rearranged as follows

$$\left( \frac{c_0}{E_{zz}^{i,j}} \right) \frac{E_{zz}^{i,j} - \tilde{E}_{zz}^{i,j}}{\Delta t} = \frac{9}{8h} \left( -H_x^{i,j} + H_x^{i,j} + H_x^{i,j} + H_x^{i,j} - H_x^{i,j} - H_x^{i,j} + H_x^{i,j} \right)$$

$$\left( \frac{c_0}{E_{zz}^{i,j}} \right) \frac{E_{zz}^{i,j} - \tilde{E}_{zz}^{i,j}}{\Delta t} = \frac{1}{80h} \left( 38H_x^{i,j} - 38H_x^{i,j} + 38H_x^{i,j} + 38H_x^{i,j} - 38H_x^{i,j} - 38H_x^{i,j} + 38H_x^{i,j} \right)$$
S24 Contains Closed Contour Line Integrals

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

\[
\left( \frac{c_i}{\epsilon_i} \right) \left[ \frac{E_i - E_j}{\Delta z} \right] - \frac{g}{8\pi} \left[ \frac{\partial H_j}{\partial t} - \frac{\partial H_i}{\partial t} \right] - \frac{1}{8\pi \epsilon_0} \left[ 3H_j - 3H_i \right] - \frac{1}{8\pi \mu_0} \left[ 3E_j - 3E_i \right] - \frac{1}{4\pi} \left[ \frac{\partial E_j}{\partial t} - \frac{\partial E_i}{\partial t} \right]
\]

Maxwell’s Equations in Integral Form

Recall Maxwell’s equations in integral form

\[
\nabla \times \mathbf{E} = \frac{\partial \mathbf{B}}{\partial t} \quad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}
\]

These equations let the line integrals be calculated as surface integrals.
Use Surface Integral Instead of Line Integral

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

\[
\oint_{C_1} \mathbf{H} \cdot d\mathbf{l} = \frac{\partial}{\partial t} \int_S \mathbf{D} \cdot d\mathbf{s} = \frac{\partial}{\partial t} \int_S \mathbf{E} \cdot d\mathbf{s} = \varepsilon_0 \frac{\partial}{\partial t} \int_{C_1} \mathbf{H} \cdot d\mathbf{l} = \frac{\partial}{\partial t} \int_{C_1} \mathbf{E} \cdot d\mathbf{s} = \varepsilon_0 \frac{\partial}{\partial t} (3h)^2 = \varepsilon_0 \frac{\partial}{\partial t} \frac{\partial}{\partial t} \mathbf{E}.
\]

Compile New Equation

We start with the S24 equation derived with line integrals.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \mathbf{E}_i}{\partial t} = \frac{9}{8h^2} \oint_{C_i} \mathbf{H} \cdot d\mathbf{l} - \frac{1}{8(9h^2)} \oint_{C_j} \mathbf{H} \cdot d\mathbf{l}
\]

Replace the line integrals with the new surface integrals.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \mathbf{E}_i}{\partial t} = \left[ \varepsilon_0 \frac{\partial}{\partial t} \mathbf{H} \right]_{C_i} + \left[ \varepsilon_0 \frac{\partial}{\partial t} \mathbf{E}_j \right]_{C_i} = \left[ \varepsilon_0 \frac{\partial}{\partial t} \mathbf{H} \right]_{C_i} + \left[ \varepsilon_0 \frac{\partial}{\partial t} \mathbf{E}_j \right]_{C_i}
\]

Now simplify.

\[
\left( \frac{\varepsilon_0}{c_0} \right) \frac{\partial \mathbf{E}_i}{\partial t} = \left[ \frac{9}{8h^2} \varepsilon_0 \frac{\partial}{\partial t} \mathbf{H} \right]_{C_i} - \frac{1}{8(9h^2)} \left[ \varepsilon_0 \frac{\partial}{\partial t} \mathbf{E}_j \right]_{C_i}
\]

Observe that 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, the outer loop is split 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.

\[
\left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} = \frac{9}{8} \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} + \frac{1}{16} \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t}
\]

Assign Arbitrary Weights

More degrees of freedom are needed in order to reduce numerical error.

To obtain these degrees of freedom, assign arbitrary weights to the terms in our equation.

\[
\left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} = K_1 \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} + K_2 \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} + K_3 \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t}
\]

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

\[
\left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} = (1 - K_1 - K_2) \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} + K_1 \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t} + K_2 \left[ \frac{\varepsilon_{\text{eff}}}{c_0} \right] \frac{\partial \vec{E}_z}{\partial t}
\]
M24 Update Equation for Ez (1 of 2)

Starting with

\[
\left[ \frac{\varepsilon_{\infty}}{c_0} \frac{\partial \vec{E}}{\partial t} \right]_{\text{FDTD}} = (1 - K_1 - K_2) \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \right]_{C_1} + K_1 \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_x}{\partial t} \right]_{C_1} + K_2 \left[ \varepsilon_{\infty} \frac{\partial \vec{E}_y}{\partial t} \right]_{C_1}
\]

Each term on the right is calculated as...

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_z}{\partial t} \right]_{C_1} = \frac{1}{h} \left( -H_x \big|_{i,\frac{j}{2}}^{|i+\frac{1}{2}} + H_y \big|_{i,\frac{j}{2}}^{|i+1/2} + H_z \big|_{i,\frac{j}{2}}^{|i+1/2} - H_x \big|_{i,\frac{j}{2}}^{|i-1/2} \right)
\]

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_x}{\partial t} \right]_{C_1} = \frac{1}{3h} \left( H_y \big|_{i,\frac{j}{2}}^{|i+1/2} - H_y \big|_{i,\frac{j}{2}}^{|i-1/2} - H_x \big|_{i,\frac{j}{2}}^{|i+1/2} + H_x \big|_{i,\frac{j}{2}}^{|i-1/2} \right)
\]

\[
\left[ \varepsilon_{\infty} \frac{\partial \vec{E}_y}{\partial t} \right]_{C_1} = \frac{1}{6h} \left( H_y \big|_{i,\frac{j}{2}}^{|i+1/2} + H_y \big|_{i,\frac{j}{2}}^{|i-1/2} - H_x \big|_{i,\frac{j}{2}}^{|i+1/2} - H_x \big|_{i,\frac{j}{2}}^{|i-1/2} \right)
\]

So the overall update equation is now

\[
\left( \frac{\varepsilon_{\infty}^{|j-1/r^1|}}{c_0} \right) \frac{\vec{E}_z |_{i,j}^{r-1}}{\Delta t} = \left( \frac{1 - K_1 - K_2}{h} \right) \left( -H_x |_{i+\frac{1}{2}}^{j-1} + H_x |_{i+\frac{1}{2}}^{j+1/2} + H_y |_{i+\frac{1}{2}}^{j+1/2} - H_y |_{i+\frac{1}{2}}^{j-1/2} \right)
\]

\[
+ \frac{K_1}{3h} \left( H_x |_{i+\frac{1}{2}}^{j-1/2} - H_x |_{i+\frac{1}{2}}^{j+1/2} + H_y |_{i+\frac{1}{2}}^{j+1/2} - H_y |_{i+\frac{1}{2}}^{j-1/2} \right)
\]

\[
+ \frac{K_2}{6h} \left( H_x |_{i+\frac{1}{2}}^{j+1/2} + H_x |_{i+\frac{1}{2}}^{j-1/2} - H_x |_{i+\frac{1}{2}}^{j+1/2} - H_x |_{i+\frac{1}{2}}^{j-1/2} \right)
\]
Optimum Values for $K_1$ and $K_2$

<table>
<thead>
<tr>
<th>NRES</th>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$\Phi_n$</th>
</tr>
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<td>0.0967169433</td>
<td>$1.283 \times 10^{-20}$</td>
</tr>
</tbody>
</table>

Global Phase Error

$$\Phi_n = \frac{1}{2\pi} \int_0^{2\pi} \left[ \frac{k_i - \hat{k}_i(\theta)}{\hat{k}_i} \right] d\theta$$

$k_i$ = physical wave number

$\hat{k}_i$ = numerical wave number

$\theta$ = angle of wave through grid

Global Phase Error Vs. Frequency

Fig. 3. Frequency bandwidth for the different schemes ($R = 20, f_e = 900$ MHz). For $f \leq f_e$, the M24 scheme has the least upper bound on the global dispersion error.
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 M24 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.