Computational Electromagnetics:
Finite Difference Time Domain Methods – Materials and Boundary Conditions

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Topics in this module

1. Dealing with dielectric materials
2. Absorbing boundary conditions
# Table of Contents

1. Dealing with dielectric materials

2. Absorbing boundary conditions
Dealing with dielectric materials – simplistic

\[ \frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H} \]

\[ \vec{D} = \varepsilon \vec{E} \]

\[ \varepsilon \vec{E} = \nabla \times \vec{H} \]

fixed appropriately in each Yee cell.

usual update equations.

\[ \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J} \]

Ohm's law: \[ \vec{J} = \sigma \vec{E} \]

\[ \nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t} + \sigma \vec{E} \]

FDTD

\[ \nabla \times H^{n-1/2} = \varepsilon \frac{\partial E^{n-1/2}}{\partial t} + \sigma \frac{E^{n-1/2}}{2} \]

as before \[ \left( \frac{E^n - E^{n-1}}{\Delta t} \right) \]

FD \[ \left( \frac{E^n + E^{n-1}}{2} \right) \]

Say want to update \( E^n \)

Need \( E^{n-1} \), \( H^{n-1/2} \).
Dealing with PECs

\[ E^n = \left[ \frac{1 - \sigma \Delta t/2\varepsilon}{1 + \sigma \Delta t/2\varepsilon} \right] E^{n-1} + \left[ \frac{1}{1 + \sigma \Delta t/2\varepsilon} \right] \frac{\Delta t}{\varepsilon} \left( \nabla \times H^{n-1/2} \right) \]

- dielectric materials: finite \( \sigma \).
- PEC \( \rightarrow \) \( \sigma \rightarrow \infty \)

Update Eqn: \( E^n = -E^{n-1} \)

If we initialize \( E \) to be zero on the PEC boundary, it stays zero.
Dealing with dispersive dielectric materials

\[
\tilde{D}(\omega) = \tilde{\varepsilon}_r(\omega) \varepsilon_0 \tilde{E}(\omega) \quad \text{(freq domain)}.
\]

Yee cell, time-space update.

Now, I need full time history of \( \vec{E} \) to get \( \vec{B} \).

\[
D(t) = \varepsilon_0 \int_{-\infty}^{t} E(t-r) \varepsilon_r(r) \, dr
\]

\[ D(t) = \varepsilon_0 \int E(t) \, dt \]

0 due to causality

\[ D(t) = \varepsilon_r \varepsilon_0 E(t) \quad \text{What is } \varepsilon_r(t) ? \]

\[ \varepsilon_r(t) = \varepsilon_r \delta(t) \]

\( \Rightarrow \) Instantaneous response

( Unrealistic)
Dispersive materials – Debye model

\[\tilde{\varepsilon}_r(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \frac{1}{1+j\omega \tau}\]

High freq. static

\[\varepsilon_r(t) = \{\varepsilon_\infty \delta(t) + \left[\frac{\varepsilon_s - \varepsilon_\infty}{\tau}\right] e^{-t/\tau} U(t)\}\]

relaxation time (approximation)

\[\beta(t) = \left(\frac{\varepsilon_s - \varepsilon_\infty}{\tau}\right) e^{-t/\tau} U(t)\]

Unit Step

\[D(t) = \varepsilon_0 \int_0^t E(t-\tau) \tilde{\varepsilon}_r(\tau) d\tau\]

Discrete

\[D = \varepsilon_0 \left[\varepsilon_\infty E^n + \sum_{m=0}^{n-1} E^{n-m} \int_{m \Delta t}^{(m+1) \Delta t} \beta(\tau) d\tau\right] \]

\[\bar{\beta}^m\]
Plugging the dispersive relation into FDTD

\[
D^n = \varepsilon_0 \left[ \varepsilon_\infty E^n + \frac{E^n - E^{n-1}}{\Delta t} + \sum_{m=0}^{n-2} \frac{E^{n-1}}{\bar{\beta}^m} \left( \frac{\bar{\beta}^{m+1} - \bar{\beta}^m}{\bar{\beta}^{m+1}} \right) \right] + \Delta t \left[ \nabla \times H^{n-1/2} \right]
\]

Update eqn:

\[
E^n = \left[ \frac{\varepsilon_\infty}{\varepsilon_\infty + \beta^0} \right] \left[ E^{n-1} - \frac{1}{\varepsilon_\infty} \frac{\nabla \times H^{n-1}}{\varepsilon_\infty} + \frac{\Delta t}{\varepsilon_0} \nabla \times H^{n-1/2} \right]
\]
Final simplifications

\[
\tilde{\psi} = \sum_{m=0}^{n-1} E_m \Delta \beta_m
\]

Still need: \( \tilde{\psi} = \sum_{m=0}^{n-1-m} E_m \Delta \beta_m \) \( \Delta \beta_m = \Delta \beta^{m+1} - \Delta \beta^m = \int_{m \Delta t}^{(m+1) \Delta t} \beta(t) \, dt - \int_{m \Delta t}^{(m+1) \Delta t} \beta(t) \, dt \)

Use \( \beta(t) = \frac{\varepsilon_s - \varepsilon_\infty}{\tau} e^{-t/\tau} U(t) \)

\[
\Delta \beta_m = -2 \left( \frac{\varepsilon_s - \varepsilon_\infty}{\varepsilon} \right) \left( 1 - 2 e^{-\Delta t/\tau} + e^{-2\Delta t/\tau} \right) e^{-m \Delta t/\tau}
\]

\( \Delta \beta_m \) 's resemble a geometric progression.

\[
\left( \frac{\Delta \beta_m^{m+1}}{\Delta \beta_m^m} = e^{-\Delta t/\tau} \right) \Rightarrow \tilde{\psi}^{n-1} = E^{n-1} \Delta \beta^0 + \sum_{m=1}^{n-2} E^{n-1-m} \Delta \beta_m
\]

\[
\frac{m-1 = p}{\sum_{p=0}^{n-3} E^{p+1} \Delta \beta_p} \quad \tilde{\psi}^{n-1} = E^{n-1} \Delta \beta^0 + (e^{-\Delta t/\tau}) \sum_{p=0}^{n-2} E^{n-2-p} \Delta \beta_p
\]
\[ \Psi^{n-1} = E^0 \Psi^{n-2} + e^{-\Delta t/c} \Psi \]

For \( \Psi \)

So far we were storing \( E, H \) at \( x, t \) grids
Now \( E, H, \Psi \) at \( x, t \) grids

+ No need to store entire history of \( E, H \)!
- Store one new Aux variable, \( \Psi \)

Reduced a convolution integral to a running summation.

→ Assumption: Debye model
Others: Lorentzian resonances

MEEP
→ Ab Initio group at MIT
Scheme, C++
Table of Contents

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ABC's come in 3 varieties (CEM in general)

1) Local ABC
2) Global ABC
3) Absorbing media (PML - perfectly matched layers)

Introduction and 1D situation

Engquist-Majda → 1st 2nd order

G. Mur → FDTD (1981)

Wave equation:
\[ \frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0 \]

\[ \frac{\partial E}{\partial x} = \frac{1}{c} \frac{\partial E}{\partial t} \]

\[ j(kx - wt) \]

Right hand side boundary

Impose:
\[ \frac{\partial E}{\partial x} + \frac{1}{c} \frac{\partial E}{\partial t} = 0 \]
What happens in 2D?

Numerical

What is \( R? \)

(Ref coefficient)

\[ j \left( \omega t - k_x x - k_y y \right) \]

Impose \( \frac{\partial^2 E}{\partial x^2} + \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0 \)

\[-jk_x + j\frac{\omega}{c} \neq 0 \]

\[ k_x^2 + k_y^2 = \left( \frac{\omega}{c} \right)^2 \]

Inc: \( e^{j(\omega t - k_x x - k_y y)} \)

Ref: \( Re^{j(\omega t + k_x x - k_y y)} \)

\[ \text{tot} = \text{inc} + \text{ref} \]

BC \( \rightarrow \)

\[ \left( \frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) (\text{tot}) = 0 \]

\[ (-k_x \cos \theta + R k \cos \theta) + \frac{1}{c} (\omega + R \omega) = 0 \]

\[ R = \frac{\cos \theta - 1}{\cos \theta + 1} \]
Implementing in FDTD

Want to impose \( \frac{\partial}{\partial z} \left( \frac{\partial E_y}{\partial t} \right) = 0 \) in FDTD.

Could do BKWD differences, but error is high.

Compromise: Use centre differences, but impose half a cell inside boundary.

**Adv:** accurate to 2\(^{nd}\) order
Substituting to get update eqn for \( E_y^{n+1}(i,j+\frac{1}{2}) \)

\[
E_y^{n+1}(i,j+\frac{1}{2}) = \gamma E_y^n(i,j+\frac{1}{2}) - \gamma E_y^{n+1}(i-1,j+\frac{1}{2}) + E_y^n(i-1,j+\frac{1}{2}), \quad \gamma = \frac{1-\alpha}{1+\alpha}, \quad \alpha = \frac{c\Delta t}{\Delta x}
\]

Implementing in FDTD from usual update eqns.

Set \( E_y^0 = 0 \) initial conditions.

reasonable in most cases.
Generalizing to higher order ABC? (Higdon)

\[
\left( \frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) E_x = 0 \quad \rightarrow \quad \text{1st order ABC}
\]

\[
\left( \frac{\partial}{\partial x} + \frac{\cos \theta_1}{c} \frac{\partial}{\partial t} \right) \left( \frac{\partial}{\partial x} + \frac{\cos \theta_2}{c} \frac{\partial}{\partial t} \right) E_x = 0 \quad \rightarrow \quad \text{2nd order ABC}
\]
Topics that were covered in this module

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References:
* Ch 12 of Computational Methods for Electromagnetics - Peterson, Ray, Mitra
* Computational Electrodynamics: The Finite-Difference Time-Domain Method – Allen Taflove (the ‘Bible’ for FDTD)