A Sequential Operator Splitting Method for Maxwell's Equations in Debye Dispersive Media

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Goals

- Develop a scheme that will allow improved computation times for Maxwell's Equations
- Application in mind: biomedical imaging
- The Debye media characterisation is suitable for human tissue

Maxwell's Equations

- Coupled system of partial differential equations relating electric and magnetic forces

Maxwell's Equations

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (1)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \quad (2)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (3)$$

$$\nabla \cdot \mathbf{D} = \rho, \quad (4)$$

- Terms of interest are **E** and **H**, the electric and magnetic field variables

Maxwell's Equations

- The field variables can be related to one another by the constitutive relations

Constitutive Relations

$$\begin{aligned} \mathbf{D} &= \varepsilon\mathbf{E} + \mathbf{P}, \\ \mathbf{B} &= \mu\mathbf{H}, \\ \mathbf{J} &= \sigma\mathbf{E}, \end{aligned}$$

ε	electric permittivity
μ	magnetic permittivity
σ	electric displacement

- These coefficients are determined by the material through which the wave propagates

Debye Media

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Debye Media Characterization

$$\hat{\varepsilon}(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau}, \quad (5)$$

$$\tau\frac{\partial \mathbf{P}}{\partial t} + \mathbf{P} = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\mathbf{E} \quad (6)$$

ε_s	static permittivity	ω	field frequency
ε_∞	infinite frequency permittivity	τ	relaxation time

- This provides us with a complex permittivity that indicates how the material affects the propagation of an electromagnetic wave

Reduction to One Dimension

- We let all wave movement be solely in the z-direction
- By combining the constitutive relations with Maxwell's curl equations (1) and (2), we get
- In the Debye medium with macroscopic polarization P we can therefore write the system as

One Dimensional System

$$\frac{\partial E}{\partial t} = \frac{1}{\varepsilon_\infty \varepsilon_0}\left(\frac{\partial H}{\partial z} - \frac{\partial P}{\partial t}\right) \quad (7)$$

$$\frac{\partial H}{\partial t} = \frac{1}{\mu_0}\frac{\partial E}{\partial z} \quad (8)$$

$$\frac{\partial P}{\partial t} = \left(\frac{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}{\tau}\right)E - \frac{1}{\tau}P \quad (9)$$

Yee Scheme

- Popular explicit method for solving Maxwell's Equations
- Staggers computational grid for field variables in space and time
- Conditionally stable if $c\dfrac{\Delta t}{\Delta z} \leq 1$ satisfied
- Second order accuracy in 1-D

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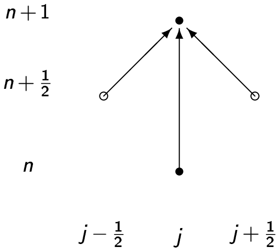
- We show the Yee Scheme in free space for illustration
- Note that in free space there is no polarization term, so $P = 0$ and $\varepsilon_\infty = 1$, thus $\dfrac{\partial P}{\partial t} = 0$ as well.

Yee Scheme

Yee Scheme in One Dimensional Free Space

$$E_k^{n+1} = E_k^n + \frac{1}{\varepsilon_0}\frac{\Delta t}{\Delta z}\left(H_{k+1/2}^{n+1/2} - H_{k-1/2}^{n+1/2}\right)$$

$$H_{k+1/2}^{n+1} = H_{k+1/2}^{n-1/2} + \frac{1}{\mu_0}\frac{\Delta t}{\Delta z}\left(E_{k+1}^n - E_k^n\right)$$



Open circle: H. Closed circle: E.

Motivations

Why operator splitting?

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- We want a numerical method that is unconditionally stable so that time and spatial steps may be chosen independently
- Higher dimensional problems can be broken down into multiple 1-D problems with operator splitting methods
- Implicit methods would allow a large one-off computation of a matrix inverse instead of many frequent computations

Notation

We will use the following notation to simplify frequently occurring terms, where V_j^n is a field variable at time step t_n and spatial node z_j.

$$
\begin{aligned}
\bar{V}_j^n &= \frac{1}{2}\left(V_j^{n+1/2} + V_j^{n-1/2}\right) \\
\delta_z V_{j+1/2}^n &= \frac{1}{\Delta z}\left(V_{j+1}^n - V_j^n\right) \\
\delta_t V_j^{n+1/2} &= \frac{1}{\Delta t}\left(V_j^{n+1} - V_j^n\right)
\end{aligned}
$$

PDE System

We scale the equations (7), (8), and (9) with:

- $\tilde{E} = \sqrt{\frac{\varepsilon_0 \varepsilon_\infty}{\mu_0}} E$
- $c_\infty = \frac{c}{\sqrt{\varepsilon_\infty}}$
- $\varepsilon_q = \frac{\varepsilon_s}{\varepsilon_\infty}$

Then the system becomes

$$\begin{aligned}
\frac{\partial \tilde{E}}{\partial t} &= c_\infty \frac{\partial H}{\partial z} - \frac{\varepsilon_q - 1}{\tau} \tilde{E} + \frac{c_\infty}{\tau} P \\
\frac{\partial H}{\partial t} &= c_\infty \frac{\partial \tilde{E}}{\partial z} \\
\frac{\partial P}{\partial t} &= \frac{\varepsilon_q - 1}{c_\infty \tau} \tilde{E} - \frac{1}{\tau} P.
\end{aligned}$$

We will now drop the tilde.

Original Formulation

- Using $U = (E, H, P)^T$, we can write the system in matrix form with a source term

$$\frac{\partial U}{\partial t} = \begin{pmatrix} \frac{-(\varepsilon_q - 1)}{\tau} & c_\infty \frac{\partial}{\partial z} & \frac{c_\infty}{\tau} \\ c_\infty \frac{\partial}{\partial z} & 0 & 0 \\ \frac{(\varepsilon_q - 1)}{c_\infty \tau} & 0 & -\frac{1}{\tau} \end{pmatrix} U + \begin{pmatrix} -c_\infty J_s \\ 0 \\ 0 \end{pmatrix}.$$

- It is convenient to write this system as a sum of operations, thus

$$\frac{\partial U}{\partial t} = \left[\begin{pmatrix} -\frac{\varepsilon_q - 1}{\tau} & 0 & \frac{c_\infty}{\tau} \\ 0 & 0 & 0 \\ \frac{\varepsilon_q - 1}{c_\infty \tau} & 0 & -\frac{1}{\tau} \end{pmatrix} + \begin{pmatrix} 0 & c_\infty \frac{\partial}{\partial z} & 0 \\ c_\infty \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] U + \begin{pmatrix} -c_\infty J_s \\ 0 \\ 0 \end{pmatrix}$$

- Thus with A, B, J matrices, we can write the split system as

$$\frac{\partial U}{\partial t} = \frac{1}{\tau} AU + BU + J. \tag{10}$$

Split Scheme

- We solve each iteration in two steps
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- Initial condition $U(t_n)$

1. Find intermediate solution $\tilde{U}(t_{n+1})$ on $[t_n, t_{n+1}]$:

$$\frac{\partial \tilde{U}}{\partial t} = B\tilde{U} + J,\ U(t_n) \tilde{=} U(t_n)$$

2. 'Final' solution for time step $U(t_{n+1})$ on $[t_n, t_{n+1}]$:

$$\frac{\partial U}{\partial t} = \frac{1}{\tau} AU,\ U(t_n) = \tilde{U}(t_{n+1})$$

Split Scheme Step 1

Updating $\frac{\partial \tilde{U}}{\partial t} = B\tilde{U} + J$:

$$\begin{aligned}
\frac{\tilde{E}_i^{n+1} - E_i^n}{\Delta t} &= \frac{c_\infty}{2}\delta_z\left(\tilde{H}_i^{n+1} + H_i^n\right) - c_\infty\left(J_s\right)_i^{n+\frac{1}{2}} \\
\frac{\tilde{H}_{i+\frac{1}{2}}^{n+1} - H_{i+\frac{1}{2}}^{n+1}}{\Delta t} &= \frac{c_\infty}{2}\delta_z\left(\tilde{E}_{i+\frac{1}{2}}^{n+1} + E_{i+\frac{1}{2}}^n\right) \\
\tilde{P}_i^{n+1} &= P_i^n
\end{aligned}$$

Split Scheme Step 2

Updating $\dfrac{\partial U}{\partial t} = \dfrac{1}{\tau} AU$:

$$
\begin{aligned}
\frac{E_i^{n+1} - \tilde{E}_i^{n+1}}{\Delta t} &= -\left(\frac{\varepsilon_q - 1}{2\tau}\right)\left(E_i^{n+1} + \tilde{E}_i^{n+1}\right) + \frac{c_\infty}{2\tau}\left(P_i^{n+1} + \tilde{P}_i^{n+1}\right) \\
\frac{P_i^{n+1} - \tilde{P}_i^{n+1}}{\Delta t} &= \left(\frac{\varepsilon_q - 1}{2c_\infty \tau}\right)\left(E_i^{n+1} + \tilde{E}_i^{n+1}\right) - \frac{1}{2\tau}\left(P_i^{n+1} + \tilde{P}_i^{n+1}\right) \\
H_i^{n+1} &= \tilde{H}_i^{n+1}
\end{aligned}
$$

Equivalent Formulation

- For analysis we combine steps 1 and 2 into an equivalent scheme; allows computation of $U(t_{n+1})$ without $\tilde{U}(t_{n+1})$.
- Substitution: $\gamma = \Delta t(\varepsilon_q - 1)$

Equivalent Operator Splitting Scheme (E-OS)

$$
\begin{aligned}
\delta_t(E_j^{n+1/2}) &= -\frac{2(\varepsilon_q - 1)}{2\tau - \gamma} E_j^{n+1} + c_\infty \delta_z(\bar{H}_j^{n+1/2}) + \frac{2c_\infty}{2\tau - \gamma}(\bar{P}_j^{n+1/2}) \\
\delta_t(H_{j+1/2}^{n+1/2}) &= \frac{c_\infty}{4\tau - 2\gamma}\delta_z\big((2\tau + \gamma)E_{j+\frac{1}{2}}^{n+1} + (2\tau - \gamma)E_{j+\frac{1}{2}}^{n} - c_\infty \Delta t(\bar{P}_{j+1/2}^{n+1/2})\big) \\
\delta_t(P_j^{n+1/2}) &= \frac{2(\varepsilon_q - 1)}{c_\infty(2\tau - \gamma)} E_j^{n+1} - \big(\frac{1}{2\tau - \gamma}\big)(\bar{P}_j^{n+1/2}).
\end{aligned}
$$

Accuracy

Theorem

The E-OS scheme is a first-order perturbation of a Crank-Nicolson scheme, and thus first order accurate.

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Proof.

Crank-Nicolson (C-N) schemes are known to be second order accurate. We compare each equation with its respective C-N counterpart; here we present the first equation.

$$\begin{aligned}
\delta_t(E_j^{n+1/2}) &= -\frac{2(\varepsilon_q-1)}{2\tau-\gamma}E_j^{n+1} + c_\infty\delta_z(\bar{H}_j^{n+1/2}) + \frac{2c_\infty}{2\tau-\gamma}(\bar{P}_j^{n+1/2}) \\
\delta_t(E_j^{n+1/2}) &= -\frac{\varepsilon_q-1}{\tau}(\bar{E}_j^{n+1/2}) + c_\infty\delta_z(\bar{H}_j^{n+1/2}) + \frac{c_\infty}{\tau}(\bar{P}_j^{n+1/2}).
\end{aligned}$$

Only the E and P terms differ. Taylor expansion on the differences yield $\mathscr{O}(\Delta t)$ error. □

Von Neumann Stability Analysis

- We make the substitution $V_j^n = \tilde{V} e^{ikj\Delta z}$ for each equation of the E-OS scheme, in order to study the time evolution of the Fourier mode of the k^{th} wave.
- This yields the system

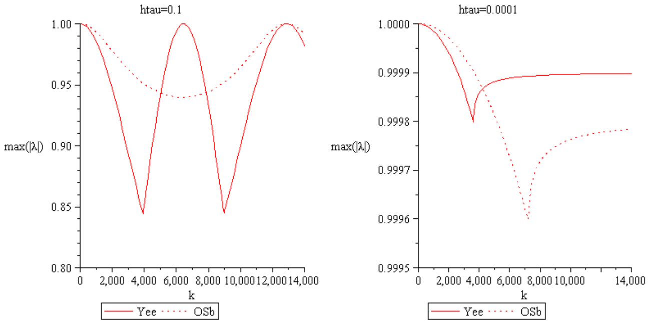
$$
\begin{aligned}
\tilde{E}^{n+1} &= \Big(\frac{2\tau-\gamma}{2\tau+\gamma}\Big)\tilde{E}^n + \theta\Big(\frac{2\tau-\gamma}{2\tau+\gamma}\Big)\big(\tilde{H}^{n+1}+\tilde{H}^n\big) + \frac{c_\infty \Delta t}{2\tau+\gamma}\big(\tilde{\bar{P}}^{n+\frac{1}{2}}\big) \\
\tilde{H}^{n+1} &= \tilde{H}^n + \frac{\theta}{2\tau-\gamma}\big((2\tau+\gamma)\tilde{E}^{n+1} + (2\tau-\gamma)\tilde{E}^n - c_\infty \Delta t \tilde{\bar{P}}^{n+\frac{1}{2}}\big) \\
\tilde{P}^{n+1} &= \frac{2\gamma}{c_\infty(2\tau-\gamma+\Delta t)}\tilde{E}^{n+1} + \frac{2\tau-\gamma-\Delta t}{2\tau-\gamma+\Delta t}\tilde{P}^n
\end{aligned}
$$

with $\gamma = \Delta t(\varepsilon_q - 1)$, $\eta_\infty = \frac{c_\infty \Delta t}{\Delta z}$, and $\theta = \eta_\infty i \sin(\frac{k\Delta z}{2})$.

Von Neumann Stability Analysis

- We rewrite the system in the form $\tilde{U}^{n+1} = S\tilde{U}^n$.
- Eigenvalue analysis on the stability matrix S prohibitively convoluted, so we conduct numerical experiments to show stability over a broad range of k.
- Stability experiments and numerical simulations indicate the scheme is stable

Von Neumann Stability Analysis



Largest eigenvalue as a function of k

Dispersion

- To conduct dispersion analysis we make the substitution into the von Neumann analysis of
$$\tilde{V}^n = V_0 e^{-i\omega n\Delta t},$$
yielding in terms of the stability matrix S
$$\begin{bmatrix} E_0 e^{-i\omega(n+1)\Delta t} \\ H_0 e^{-i\omega(n+1)\Delta t} \\ P_0 e^{-i\omega(n+1)\Delta t} \end{bmatrix} = S \begin{bmatrix} E_0 \\ H_0 \\ P_0 \end{bmatrix} e^{-i\omega n\Delta t}.$$
- This leads us to conclude that $(S - e^{-i\omega\Delta t} I)U_0 = 0$, so the dispersion relation is
$$\det(S - e^{-i\omega\Delta t} I) = 0.$$

Numerical Dispersion Experiments

- We solve for the wave number k as a function of ω and compare to the exact dispersion relation for Debye media,

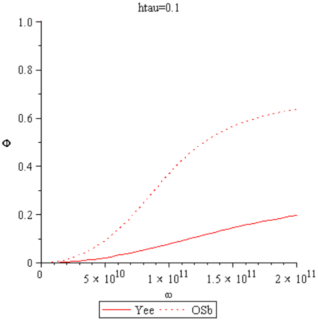
$$k_{ex}(\omega) = \frac{\omega}{c}\sqrt{\frac{\varepsilon_s - i\omega\tau\varepsilon_\infty}{1 - i\omega\tau}}.$$

- Phase error is defined to be

$$\Phi(\omega) = \frac{|k(\omega) - k_{ex}(\omega)|}{|k_{ex}(\omega)|}.$$

- The operator splitting scheme is more dispersive than the Yee scheme, but by less than an order of magnitude.

Numerical Dispersion Experiments

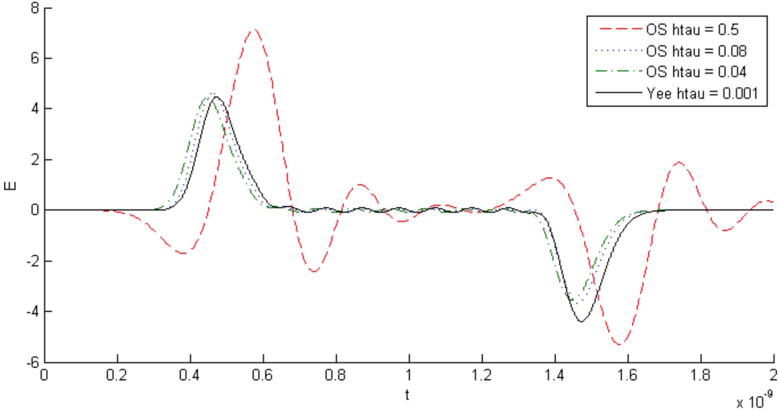


Phase error as a function of k

Setup

- A numerical experiment was run simulating an energy source travelling in one dimension through free space, a Debye medium, and then free space again.
- Simulates real-world interrogation applications
- Used Yee scheme with high accuracy ($h_\tau = 0.001$) as a reference
    - $\Delta t = \tau h_\tau$
    - $\Delta z = c\Delta t/\eta$

Pulse Amplitude During Experiment



Comparison of Yee and Operator Splitting Schemes

Runtimes

- As expected, Yee scheme had faster run times in one dimensional case

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Runtimes

- As expected, Yee scheme had faster run times in one dimensional case
- Bottleneck of the operator splitting scheme is computation of a large matrix inverse
- The inverse matrix needed to solve the operator splitting scheme needs only to be computed once
- The Yee scheme cannot take advantage of a single-cost computation
- It is strongly expected that in higher dimensions the operator splitting scheme can take advantage of single-cost computations and reduction to multiple 1-D problems

Summary

- This operator splitting scheme is numerically convergent and unconditionally stable.
- Improvements in computation time are expected in higher-dimensional settings to be built upon the one-dimensional scheme.

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