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 \( \mathbf{E} \) and \( \mathbf{H} \), the electric and magnetic field variables
Maxwell’s Equations

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

Constitutive Relations

\[ D = \varepsilon E + P, \]
\[ B = \mu H, \]
\[ J = \sigma E, \]

| \( \varepsilon \) | electric permittivity |
| \( \mu \) | magnetic permittivity |
| \( \sigma \) | electric displacement |

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

- We focus our attention on developing a scheme appropriate for Debye media
Debye Media

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Debye Media Characterization

\[ \hat{\varepsilon}(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau}, \]  
\[ \tau \frac{\partial P}{\partial t} + P = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) E \]  

<table>
<thead>
<tr>
<th>(\varepsilon_s)</th>
<th>static permittivity</th>
<th>(\omega)</th>
<th>field frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\varepsilon_\infty)</td>
<td>infinite frequency permittivity</td>
<td>(\tau)</td>
<td>relaxation time</td>
</tr>
</tbody>
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- 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

\[
\begin{align*}
\frac{\partial E}{\partial t} &= \frac{1}{\varepsilon_\infty \varepsilon_0} \left( \frac{\partial H}{\partial z} - \frac{\partial P}{\partial t} \right) \\
\frac{\partial H}{\partial t} &= \frac{1}{\mu_0} \frac{\partial E}{\partial z} \\
\frac{\partial P}{\partial t} &= \left( \frac{\varepsilon_0 (\varepsilon_s - \varepsilon_\infty)}{\tau} \right) E - \frac{1}{\tau} P
\end{align*}
\]
Yee Scheme

- Popular explicit method for solving Maxwell’s Equations
- Staggers computational grid for field variables in space and time
- Conditionally stable if \( \frac{\Delta t}{\Delta z} \leq 1 \) satisfied
- Second order accuracy in 1-D
Yee Scheme

- Popular explicit method for solving Maxwell’s Equations
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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 \( \frac{\partial P}{\partial t} = 0 \) as well.
Yee Scheme

Yee Scheme in One Dimensional Free Space

\[
\begin{align*}
E_{k}^{n+1} &= E_{k}^{n} + \frac{1}{\varepsilon_{0} \Delta z} \frac{\Delta t}{\Delta z} (H_{k+1/2}^{n+1/2} - H_{k-1/2}^{n+1/2}) \\
H_{k+1/2}^{n+1} &= H_{k+1/2}^{n-1/2} + \frac{1}{\mu_{0} \Delta z} \frac{\Delta t}{\Delta z} (E_{k+1}^{n} - E_{k}^{n})
\end{align*}
\]

Open circle: \( H \). Closed circle: \( E \).
Motivations

Why operator splitting?
Motivations

Why operator splitting?

- 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.
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 $z_j$.

\[
\bar{V}_j^n = \frac{1}{2} (V_{j+1/2}^{n+1} + V_{j-1/2}^{n-1/2})
\]

\[
\delta_z V_{j+1/2}^n = \frac{1}{\Delta z} (V_{j+1}^n - V_j^n)
\]

\[
\delta_t V_{j+1/2}^{n+1} = \frac{1}{\Delta t} (V_{j+1}^{n+1} - V_j^n)
\]
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

\[
\begin{align*}
\frac{\partial \tilde{E}}{\partial t} &= \frac{c_\infty}{\tau} \frac{\partial H}{\partial z} - \frac{\varepsilon_q - 1}{\tau} \tilde{E} + \frac{c_\infty}{\tau} P \\
\frac{\partial H}{\partial t} &= \frac{c_\infty}{\tau} \frac{\partial \tilde{E}}{\partial z} \\
\frac{\partial P}{\partial t} &= \frac{\varepsilon_q - 1}{c_\infty \tau} \tilde{E} - \frac{1}{\tau} P.
\end{align*}
\]

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

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

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

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

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

$$
\frac{\partial U}{\partial t} = \frac{1}{\tau} AU + BU + J. \quad (10)
$$
Split Scheme

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

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

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

\[
\frac{\partial \tilde{U}}{\partial t} = B\tilde{U} + J, \quad U(t_n) = \tilde{U}(t_{n+1})
\]

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

\[
\frac{\partial U}{\partial t} = \frac{1}{\tau}AU, \quad U(t_n) = \tilde{U}(t_{n+1})
\]
Split Scheme Step 1

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

\[
\frac{\tilde{E}_{i}^{n+1} - E_{i}^{n}}{\Delta t} = \frac{c_{\infty}}{2} \delta_z (\tilde{H}_{i+\frac{1}{2}}^{n+1} + H_{i}^{n}) - c_{\infty} (J_{s})_{i}^{n+\frac{1}{2}}
\]

\[
\frac{\tilde{H}_{i+\frac{1}{2}}^{n+1} - H_{i+\frac{1}{2}}^{n+1}}{\Delta t} = \frac{c_{\infty}}{2} \delta_z (\tilde{E}_{i+\frac{1}{2}}^{n+1} + E_{i+\frac{1}{2}}^{n})
\]

\[
\tilde{P}_{i}^{n+1} = P_{i}^{n}
\]
Split Scheme Step 2

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

$$\frac{E_{i}^{n+1} - \tilde{E}_{i}^{n+1}}{\Delta t} = -\left(\frac{\varepsilon_{q} - 1}{2\tau}\right)(E_{i}^{n+1} + \tilde{E}_{i}^{n+1}) + \frac{c_{\infty}}{2\tau}(P_{i}^{n+1} + \tilde{P}_{i}^{n+1})$$

$$\frac{P_{i}^{n+1} - \tilde{P}_{i}^{n+1}}{\Delta t} = \left(\frac{\varepsilon_{q} - 1}{2c_{\infty}\tau}\right)(E_{i}^{n+1} + \tilde{E}_{i}^{n+1}) - \frac{1}{2\tau}(P_{i}^{n+1} + \tilde{P}_{i}^{n+1})$$

$$H_{i}^{n+1} = \tilde{H}_{i}^{n+1}$$
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)**

$$
\begin{align*}
\delta_t(E_j^{n+1/2}) &= -\frac{2(\varepsilon_q - 1)}{2\tau - \gamma} E_j^{n+1} + c_\infty \delta_z(H_j^{n+1/2}) + \frac{2c_\infty}{2\tau - \gamma} (\bar{P}_j^{n+1/2}) \\
\delta_t(H_j^{n+1/2}) &= \frac{c_\infty}{4\tau - 2\gamma} \delta_z((2\tau + \gamma) E_j^{n+1} + (2\tau - \gamma) E_j^{n+1/2} - c_\infty \Delta t(\bar{P}_j^{n+1/2})) \\
\delta_t(P_j^{n+1/2}) &= \frac{2(\varepsilon_q - 1)}{c_\infty(2\tau - \gamma)} E_j^{n+1} - \left(\frac{1}{2\tau - \gamma}\right) (\bar{P}_j^{n+1/2}).
\end{align*}
$$
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.

\[
\delta_t(E_{j}^{n+1/2}) = -\frac{2(\varepsilon_q - 1)}{2\tau - \gamma} E_{j}^{n+1} + c_{\infty} \delta_z(\bar{H}_{j}^{n+1/2}) + \frac{2c_{\infty}}{2\tau - \gamma}(\bar{P}_{j}^{n+1/2})
\]

\[
\delta_t(E_{j}^{n+1/2}) = -\frac{\varepsilon_q - 1}{\tau}(\bar{E}_{j}^{n+1/2}) + c_{\infty} \delta_z(\bar{H}_{j}^{n+1/2}) + \frac{c_{\infty}}{\tau}(\bar{P}_{j}^{n+1/2}).
\]

Only the \( E \) and \( P \) terms differ. Taylor expansion on the differences yield \( O(\Delta t) \) 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

$$
\tilde{E}^{n+1} = \left(\frac{2\tau - \gamma}{2\tau + \gamma}\right)\tilde{E}^n + \theta \left(\frac{2\tau - \gamma}{2\tau + \gamma}\right)(\tilde{H}^{n+1} + \tilde{H}^n) + \frac{c_\infty \Delta t}{2\tau + \gamma}(\tilde{P}^{n+\frac{1}{2}})
$$

$$
\tilde{H}^{n+1} = \tilde{H}^n + \frac{\theta}{2\tau - \gamma} \left( (2\tau + \gamma)\tilde{E}^{n+1} + (2\tau - \gamma)\tilde{E}^n - c_\infty \Delta t \tilde{P}^{n+\frac{1}{2}} \right)
$$

$$
\tilde{P}^{n+1} = \frac{2\gamma}{c_\infty (2\tau - \gamma + \Delta t)} \tilde{E}^{n+1} + \frac{2\tau - \gamma - \Delta t}{2\tau - \gamma + \Delta t} \tilde{P}^n
$$

with $\gamma = \Delta t(\varepsilon_q - 1)$, $\eta_\infty = \frac{c_\infty \Delta t}{\Delta z}$, and $\theta = \eta_\infty i \sin\left(\frac{k\Delta z}{2}\right)$. 
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 $k$
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 $\omega$ and compare to the exact dispersion relation for Debye media,

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

- Phase error is defined to be

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

- 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 $k$
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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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.
Runetimes

- 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.
Conclusions

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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