Numerical Methods for Maxwell’s Equations Involving Distributions of Polarization Relaxation Times

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Feb 5, 2010
Acknowledgements

- Karen Barrese and Neel Chugh (REU 2008)
- Anne Marie Milne and Danielle Wedde (REU 2009)
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Maxwell’s Equations in One Space Dimension

- Assume uniformity in the $x$-direction.
- Assume that the electric field is polarized to oscillate only in the $y$ direction.

Evolution equations involving $E$, $H$, $D$, $B$, $P$ and $J$:

\[
\frac{\partial D}{\partial t} + J = \frac{\partial H}{\partial z}
\]
\[
\frac{\partial B}{\partial t} = \frac{\partial E}{\partial z}
\]

Constitutive laws:

\[
B = \mu_0 H
\]
\[
D = \varepsilon_0 \varepsilon_\infty E + P
\]
\[
J = \sigma E + J_s
\]
Dispersive Media

- We can define $P$ in terms of a convolution

$$P(t, x) = g * E(t, x) = \int_{0}^{t} g(t - s, x; \vec{q})E(s, x)ds,$$

where $g$ is the dielectric response function (DRF).

- In the frequency domain $\hat{D} = \epsilon(\omega)\hat{E}$, where $\epsilon(\omega)$ is called the complex permittivity.

- $\epsilon(\omega)$ described by the polarization model.

- We are interested in ultra wide bandwidth electromagnetic pulse interrogation of dispersive dielectrics, therefore we want an accurate representation of $\epsilon(\omega)$ over a broad range of frequencies.
Dispersive Media

Figure: Debye model simulations from [BBL00]
Dry skin data

Figure: Real part of $\epsilon(\omega)$, $\epsilon$, or the permittivity.
Dry skin data

Figure: Imaginary part of $\epsilon(\omega)$, $\sigma$, or the conductivity.
Debye model $\vec{q} = [\epsilon_s, \epsilon_\infty, \tau]$

$$g(t, x) = \epsilon_0 (\epsilon_s - \epsilon_\infty) / \tau \ e^{-t/\tau}$$

or

$$\tau \dot{P} + P = \epsilon_0 (\epsilon_s - \epsilon_\infty) E$$

or

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + i \omega \tau}$$
Debye model $\tilde{q} = [\epsilon_s, \epsilon_\infty, \tau]$

$$g(t, x) = \epsilon_0 (\epsilon_s - \epsilon_\infty) / \tau \ e^{-t/\tau}$$

or

$$\tau \dot{P} + P = \epsilon_0 (\epsilon_s - \epsilon_\infty) E$$

or

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + i\omega\tau}$$

Cole-Cole model (heuristic generalization)

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + (i\omega\tau)^{1-\alpha}}$$

The DRF for the Cole-Cole is

$$g(t, x) = \frac{1}{2\pi i} \int_{\zeta-i\infty}^{\zeta+i\infty} \frac{\epsilon_0 (\epsilon_s - \epsilon_\infty)}{1 + (s\tau)^{1-\alpha}} e^{st} \ ds.$$
Motivation

- Broadband wave propagation suggests time-domain simulation.
- The Cole-Cole model corresponds to a fractional order ODE in the time-domain and is difficult to simulate.
- Debye is efficient to simulate, but does not represent permittivity well.
- Better fits to data are obtained by taking linear combinations of Debye models (multi-pole Debye), idea comes from the known existence of multiple physical mechanisms.
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times.
- Empirical measurements suggest a log-normal distribution [BB78], but uniform is easier.
Fit to dry skin data with uniform distribution

Figure: Real part of $\varepsilon(\omega)$, $\varepsilon$, or the permittivity.
Fit to Cole-Cole model with uniform distribution

Figure: Real part of $\epsilon(\omega)$, $\epsilon$, or the permittivity.
We define the stochastic polarization $\mathcal{P}(t, z; \tau)$ to be the solution to

$$\tau \dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E$$

where $\tau$ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.

The electric field depends on the macroscopic polarization, which we take to be the expected value of the stochastic polarization at each point $(t, z)$

$$P(t, z) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, z; \tau)f(\tau)d\tau.$$
Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear ODE

$$\dot{x} = -kx, \quad k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0, 1).$$

We apply a Polynomial Chaos expansion to the solution $x$:

$$x(t, \xi) = \sum_{j=0}^{p} \alpha_j(t) \phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi)$$

then the ODE becomes

$$\sum_{j=0}^{p} \dot{\alpha}_j(t) \phi_j(\xi) = -\sum_{j=0}^{p} \alpha_j(t) \xi \phi_j(\xi),$$
Triple recursion formula

\[
\sum_{j=0}^{p} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{p} \alpha_j(t)\xi\phi_j(\xi),
\]

We can eliminate the explicit dependence on \( \xi \) by using the triple recursion formula for Hermite polynomials

\[
\xi H_j = jH_{j-1} + H_{j+1}.
\]

Thus

\[
\sum_{j=0}^{p} \dot{\alpha}_j(t)\phi_j + \alpha_j(t)(j\phi_{j-1} + \phi_{j+1}) = 0.
\]
Galerkin Projection onto \( \text{span}(\{\phi_j\}_{j=0}^p) \)

Taking the weighted inner product with each basis gives

\[
\sum_{j=0}^{p} \dot{\alpha}_j(t) \langle \phi_j, \phi_i \rangle_W + \alpha_j(t) (j \langle \phi_{j-1}, \phi_i \rangle_W + \langle \phi_{j+1}, \phi_i \rangle_W) = 0,
\]

\[i = 0, \ldots, p.
\]

Where

\[
\langle f(\xi), g(\xi) \rangle_W = \int f(\xi)g(\xi)W(\xi)d\xi.
\]

Using orthogonality, \( \langle \phi_j, \phi_i \rangle_W = \langle \phi_i, \phi_i \rangle_W \delta_{ij} \), we have

\[
\dot{\alpha}_i \langle \phi_i, \phi_i \rangle_W + (i+1) \alpha_{i+1} \langle \phi_i, \phi_i \rangle_W + \alpha_{i-1} \langle \phi_i, \phi_i \rangle_W = 0, \quad i = 0, \ldots, p,
\]
Determistic ODE system

The system of ODEs can be written

\[ \dot{\vec{\alpha}} + M \vec{\alpha} = \vec{0}, \]

with

\[
M = \begin{bmatrix}
0 & 1 & 2 & \cdots & \cdots & \cdots \\
1 & 0 & 2 & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\
1 & 0 & \cdots & \cdots & \cdots & 0
\end{bmatrix}
\]
Generalizations

For any choice of family of orthogonal polynomials, there exists a triple recursion formula. For the arbitrary relation

\[ \xi \phi_j = a_j \phi_{j-1} + b_j \phi_j + c_j \phi_{j+1} \]

(with \( \phi_{-1} = 0 \)) then the matrix above becomes

\[
M = \begin{bmatrix}
    b_0 & a_1 \\
    c_0 & b_1 & 2 \\
    & \ddots & \ddots & \ddots \\
    &   & \ddots & \ddots & a_p \\
    &   &   & c_{p-1} & b_p
\end{bmatrix}
\]
Generalizations

Consider the non-homogeneous ODE

\[ \dot{x} + kx = g(t), \quad k = k(\xi) = \sigma \xi + \mu, \quad \xi \sim \mathcal{N}(0, 1). \]

then

\[ \dot{\alpha}_i + \sigma [(i + 1)\alpha_{i+1} + \alpha_{i-1}] + \mu \alpha_i = g(t)\delta_{0i}, \quad i = 0, \ldots, p, \]

or the deterministic ODE system

\[ \dot{\bar{\alpha}} + (\sigma M + \mu I)\bar{\alpha} = g(t)\bar{e}_1. \]
Exponential convergence

- Any set of orthogonal polynomials can be used in the truncated expansion, but there may be an optimal choice.
- If the polynomials are orthogonal with respect to weighting function $f(\xi)$, and $k$ has PDF $f(k)$, then it is known that the PC solution converges exponentially in terms of $p$.
- In practice, approximately 4 are generally sufficient.
**Figure:** Solution of each mode with Gaussian random coefficient by fourth-order Hermitian-chaos from [XK03].
Figure: Convergence of error with Gaussian random coefficient by fourth-order Hermitian-chaos from [XK03].
Generalized Polynomial Chaos

**Table:** Popular distributions and corresponding orthogonal polynomials.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Polynomial</th>
<th>Support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian</td>
<td>Hermite</td>
<td>$(−\infty, \infty)$</td>
</tr>
<tr>
<td>gamma</td>
<td>Laguerre</td>
<td>$[0, \infty)$</td>
</tr>
<tr>
<td>beta</td>
<td>Jacobi</td>
<td>$[a, b]$</td>
</tr>
<tr>
<td>uniform</td>
<td>Legendre</td>
<td>$[a, b]$</td>
</tr>
</tbody>
</table>

Note: Lognormal random variables may be handled as a non-linear function (e.g., Taylor expansion) of a normal random variable.
Stochastic Polarization

We wish to apply Polynomial Chaos method to

$$\tau \dot{P} + P = \epsilon_0 (\epsilon_s - \epsilon_\infty) E, \quad \tau = \tau(\xi) = \sigma \xi + \mu.$$

Then

$$(\sigma M + \mu I) \dot{\tilde{\alpha}} + \tilde{\alpha} = \epsilon_0 (\epsilon_s - \epsilon_\infty) E \tilde{e}_1 =: \tilde{g}.$$  

The macroscopic polarization, the expected value of the stochastic polarization at each point \((t, z)\), is simply

$$P(t, z) = \alpha_0(t, z).$$
Kane Yee created an algorithm to solve for both the electric and magnetic fields in space and time using the coupled Maxwell’s curl equations in free space. The following grid shows how the electromagnetic field is updated throughout time and space using a staggered grid which allows the explicit method to achieve second order accuracy.
The FDTD or Yee grid in 1D

\[
(H_y)_{n+2}^{k+\frac{1}{2}} \quad (E_x)_{n+\frac{3}{2}}^{k+2}
\]
Applying the central difference approximation, based on the Yee scheme, our one dimensional equations

\[
\epsilon \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \sigma E - \frac{\partial P}{\partial t}
\]

and

\[
\mu \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z}
\]

become

\[
\frac{E_{k}^{n+\frac{1}{2}} - E_{k}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\epsilon} \frac{H_{k+\frac{1}{2}}^{n} - H_{k-\frac{1}{2}}^{n}}{\Delta z} - \frac{\sigma}{\epsilon} \frac{E_{k}^{n+\frac{1}{2}} + E_{k}^{n-\frac{1}{2}}}{2} - \frac{1}{\epsilon} \frac{P_{k}^{n+\frac{1}{2}} - P_{k}^{n-\frac{1}{2}}}{\Delta t}
\]

and

\[
\frac{H_{k+\frac{1}{2}}^{n+1} - H_{k+\frac{1}{2}}^{n}}{\Delta t} = -\frac{1}{\mu} \frac{E_{k+1}^{n+\frac{1}{2}} - E_{k}^{n+\frac{1}{2}}}{\Delta z}.
\]

Note that while the electric field and magnetic field are staggered in time, the electric field updates simultaneously with polarization.
For $\tau \dot{P} + P = \epsilon_d E$, once again using the central difference approximation (explicit trapezoidal), we have

$$
\frac{P_{k}^{n+\frac{1}{2}} - P_{k}^{n-\frac{1}{2}}}{\Delta t} + \frac{P_{k}^{n+\frac{1}{2}} + P_{k}^{n-\frac{1}{2}}}{2} = \epsilon_d \frac{E_{k}^{n+\frac{1}{2}} + E_{k}^{n-\frac{1}{2}}}{2}.
$$

Solving for $P_{k}^{n+\frac{1}{2}}$ in terms of $E_{k}^{n+\frac{1}{2}}$

$$
P_{k}^{n+\frac{1}{2}} = \frac{\Delta t \epsilon_d \left[ E_{k}^{n+\frac{1}{2}} + E_{k}^{n-\frac{1}{2}} \right] + (2\tau - \Delta t)P_{k}^{n-\frac{1}{2}}}{2\tau + \Delta t}
$$

we can eliminate $P_{k}^{n+\frac{1}{2}}$ from the $E_{k}^{n+\frac{1}{2}}$ update step to get

$$
E_{k}^{n+\frac{1}{2}} = \frac{\theta}{1 + \delta} \left[ H_{k+\frac{1}{2}}^{n} - H_{k-\frac{1}{2}}^{n} \right] + \frac{1 - \delta}{1 + \delta} E_{k}^{n-\frac{1}{2}} + \frac{2\Delta t}{\epsilon(2\tau + \Delta t)(1 + \delta)} P_{k}^{n-\frac{1}{2}}
$$

and

$$
H_{k+\frac{1}{2}}^{n+1} = -\frac{\Delta t}{\mu \Delta x} \left[ E_{k+1}^{n+\frac{1}{2}} - E_{k}^{n+\frac{1}{2}} \right] + H_{k+\frac{1}{2}}^{n}
$$

where $\theta = -\frac{\Delta t}{\epsilon \Delta x}$ and $\delta = \frac{\sigma \Delta t}{2\epsilon} + \frac{\Delta t \epsilon_d}{\epsilon(2\tau + \Delta t)}$. 

Need a similar approach for discretizing the PC system

\[ A \ddot{\alpha} + \dot{\alpha} = \vec{g}. \]

First consider applying central differences (explicit trapezoidal) to \( \vec{\alpha} = \vec{\alpha}(z_k) \):

\[
A \frac{\vec{\alpha}^{n+\frac{1}{2}} - \vec{\alpha}^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}^{n+\frac{1}{2}} + \vec{\alpha}^{n-\frac{1}{2}}}{2} = \frac{\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}}{2}.
\]

Combining like terms gives

\[(2A + \Delta tl)\vec{\alpha}^{n+\frac{1}{2}} = (2A - \Delta tl)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t \left( \vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}} \right) \]

Note that now it is simpler to solve the discrete electric field equation for \( E_k^{n+\frac{1}{2}} \) and plug in here (in \( \vec{g}^{n+\frac{1}{2}} \)), than it would be to solve this system explicitly for \( \vec{\alpha}_0^{n+\frac{1}{2}} \).
Solving for $E_{k}^{n+\frac{1}{2}}$ in

$$
\frac{E_{k}^{n+\frac{1}{2}} - E_{k}^{n-\frac{1}{2}}}{\Delta t} = - \frac{1}{\epsilon} \frac{H_{k+\frac{1}{2}}^{n} - H_{k-\frac{1}{2}}^{n}}{\Delta z} - \frac{\sigma}{\epsilon} \frac{E_{k}^{n+\frac{1}{2}} + E_{k}^{n-\frac{1}{2}}}{2} - \frac{1}{\epsilon} \frac{\alpha_{0,k}^{n+\frac{1}{2}} - \alpha_{0,k}^{n-\frac{1}{2}}}{\Delta t}
$$

we get

$$
E_{k}^{n+\frac{1}{2}} = \frac{\theta}{1 + \delta} \left[ H_{k+\frac{1}{2}}^{n} - H_{k-\frac{1}{2}}^{n} \right] + \frac{1 - \delta}{1 + \delta} E_{k}^{n-\frac{1}{2}} - \frac{1}{\epsilon(1 + \delta)} \left[ \alpha_{0,k}^{n+\frac{1}{2}} - \alpha_{0,k}^{n-\frac{1}{2}} \right]
$$

where now $\theta = - \frac{\Delta t}{\epsilon \Delta x}$ and $\delta = \frac{\sigma \Delta t}{2 \epsilon}$.

We substitute this expression into the first element of $\mathbf{g}^{n+\frac{1}{2}}$. Since $\alpha_{0,k}^{n+\frac{1}{2}}$ now appears on the right hand side of the first row, we must move this term to the left hand side.
Explicit Update Step

All other rows of our system stay the same, thus

$$(2\tilde{A} + \Delta t I)\tilde{\alpha}^{n+\frac{1}{2}} = (2\tilde{A} - \Delta t I)\tilde{\alpha}^{n-\frac{1}{2}} + \Delta t \left(\tilde{g}^{n-\frac{1}{2}} + \tilde{h}^n\right)$$

where $\tilde{A} = A$ except for $\epsilon_d \Delta t / (1 + \delta)$ added to the $(1, 1)$ element. We let

$$\tilde{g}^{n-\frac{1}{2}} = \frac{2\epsilon_d \Delta t}{1 + \delta} E_k^{n-\frac{1}{2}}$$

and

$$\tilde{h}^n = \frac{\epsilon_d \Delta t \theta}{1 + \delta} \left[ H_k^{n+\frac{1}{2}} - H_k^{n-\frac{1}{2}} \right]$$
Updinating Scheme

Thus given $E^{n-\frac{1}{2}}$, $\vec{\alpha}^{n-\frac{1}{2}}$, and $H^n$ for all $k$, we may compute the updated variables by solving the following

$$(2\tilde{A} + \Delta tI)\vec{\alpha}^{n+\frac{1}{2}} = (2\tilde{A} - \Delta tI)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t \left(\tilde{g}^{n-\frac{1}{2}} + \tilde{h}^n\right)$$

$$E_k^{n+\frac{1}{2}} = \frac{\theta}{1 + \delta} \left[H_k^{n+\frac{1}{2}} - H_k^{n-\frac{1}{2}}\right] + \frac{1 - \delta}{1 + \delta} E_k^{n-\frac{1}{2}}$$

$$- \frac{1}{\epsilon(1 + \delta)} \left[\alpha_{0,k}^{n+\frac{1}{2}} - \alpha_{0,k}^{n-\frac{1}{2}}\right]$$

$$H_k^{n+1} = -\frac{\Delta t}{\mu\Delta x} \left[E_k^{n+\frac{1}{2}} - E_k^{n+\frac{1}{2}}\right] + H_k^{n+\frac{1}{2}}$$

Note that $(2\tilde{A} + \Delta tI)$ is tridiagonal and small.
Broadband pulse propagation in a Debye dielectric. Note the frequency dependent attenuation.

**Figure:** Top: pulse in freespace and pulse in .015 m inside a Debye dielectric. Bottom: FFT of signals.
Broadband pulse propagation in a Stochastic Debye dielectric. (This simulation was performed using simple quadrature [BG06].)

Figure:Broadband pulse .015 m inside a Debye dielectric, computed with a deterministic model and two uniform distribution models.
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