Polynomial Chaos Approach for Maxwell's Equations in Dispersive Media

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Outline

1. **Maxwell's Equations**
   - Dispersive Media
   - Polarization Models
   - Distribution of Parameters
2. **Dispersion Analysis**
   - Discrete Dispersion

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J} \text{ in } \mathbf{\Omega} \times (\mathbf{0}, \mathbf{T}]$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \text{ in } \mathbf{\Omega} \times (\mathbf{0}, \mathbf{T}]$$

$$\nabla \cdot \mathbf{D} = \nabla \cdot \mathbf{B} = \mathbf{0} \text{ in } \mathbf{\Omega} \times (\mathbf{0}, \mathbf{T}]$$

$$\mathbf{E}(\mathbf{0}, \mathbf{x}) = \mathbf{E_0}(\mathbf{x});\ \ \mathbf{H}(\mathbf{0}, \mathbf{x}) = \mathbf{H_0}(\mathbf{x}) \text{ in } \mathbf{\Omega}$$

$$\mathbf{E} \times \mathbf{n} = \mathbf{0} \text{ on } \partial\mathbf{\Omega},\ \ \mathbf{t} \in (\mathbf{0}, \mathbf{T}]$$

$\mathbf{E} =$	Electric field vector	$\mathbf{D} =$	Electric flux density
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density
$\mathbf{J} =$	Current density	$\mathbf{n} =$	Unit outward normal to $\partial\Omega$

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$
\begin{aligned}
\mathbf{D} &= \epsilon \mathbf{E} + \mathbf{P} \\
\mathbf{B} &= \mu \mathbf{H} + \mathbf{M} \\
\mathbf{J} &= \sigma \mathbf{E} + \mathbf{J}_s
\end{aligned}
$$

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Complex permittivity

- We can usually define $\mathbf{P}$ in terms of a convolution

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).
- In the frequency domain $\hat{\mathbf{D}} = \epsilon\hat{\mathbf{E}} + \hat{\mathbf{g}}\hat{\mathbf{E}} = \epsilon_0\epsilon(\omega)\hat{\mathbf{E}}$, 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.

Dry skin data

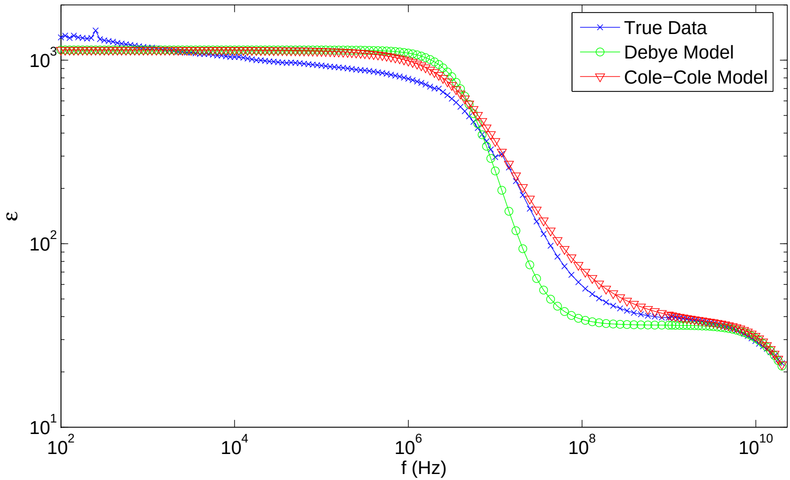


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

Dry skin data

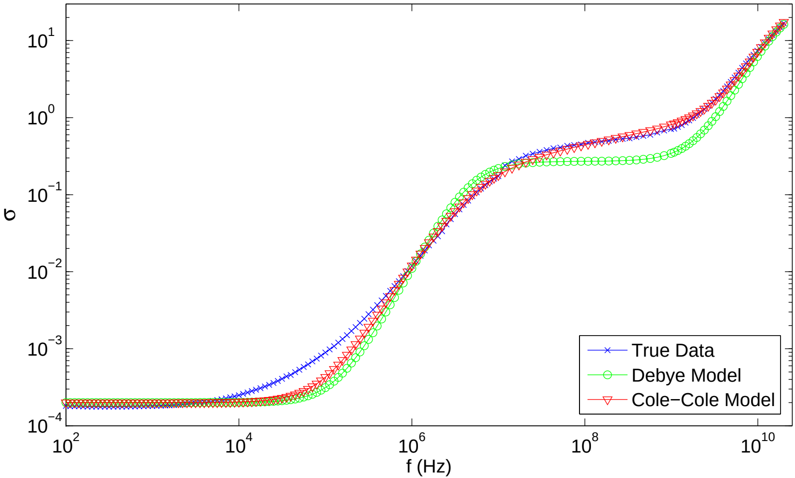


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

- Debye model [1929] $\mathbf{q} = [\epsilon_d, \tau]$

$$g(t,\mathbf{x}) = \epsilon_0\epsilon_d/\tau \quad e^{-t/\tau}$$
$$\text{or} \quad \tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0\epsilon_d\mathbf{E}$$
$$\text{or} \quad \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1-\omega\tau}$$

  with $\epsilon_d := \epsilon_s - \epsilon_\infty$ and τ a relaxation time.

- Cole-Cole model [1936] (heuristic generalization)
  $\mathbf{q} = [\epsilon_d, \tau, \alpha]$

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

Dispersive Dielectrics

Debye Material

Input is five cycles (periods) of a sine curve.

Dispersive Media

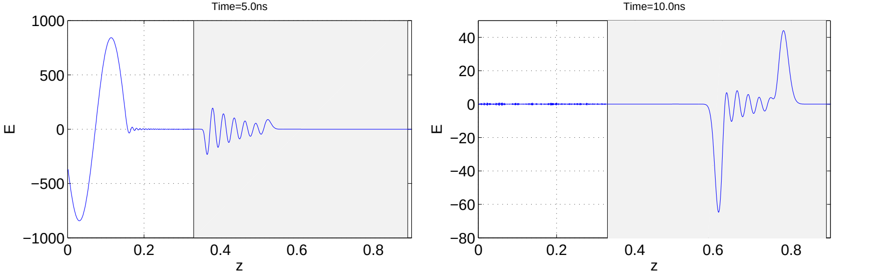


Figure: Debye model simulations.

Scalar Equations in Two Dimensions (cont)

Letting $H = H_z$, we have the 2D Maxwell-Debye TE scalar equations:

$$\begin{aligned}
\frac{\partial H}{\partial t} &= \frac{1}{\mu_0}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right),\\
\epsilon_0\epsilon_\infty \frac{\partial E_x}{\partial t} &= \frac{\partial H}{\partial y} - \frac{\partial P_x}{\partial t},\\
\epsilon_0\epsilon_\infty \frac{\partial E_y}{\partial t} &= -\frac{\partial H}{\partial x} - \frac{\partial P_y}{\partial t},\\
\frac{\partial P_x}{\partial t} &= \frac{\epsilon_0\epsilon_d}{\tau} E_x - \frac{1}{\tau} P_x,\\
\frac{\partial P_y}{\partial t} &= \frac{\epsilon_0\epsilon_d}{\tau} E_y - \frac{1}{\tau} P_y.
\end{aligned}$$

Stability Estimates for Maxwell-Debye

Theorem (Li2010)

For $\Omega \in \mathbb{R}^2$, let $\mathbf{E}$, $\mathbf{P}$, *and* H *be the solutions to the 2D Maxwell-Debye TE scalar equations with PEC boundary conditions. Then the Debye model satisfies the stability estimate*

$$\mathcal{E}(t) \leq \mathcal{E}(0)$$

where the energy is defined as

$$\mathcal{E}(t) = ||\sqrt{\mu_0}H(t)||_{L^2}^2 + ||\sqrt{\epsilon_0\epsilon_\infty}\mathbf{E}(t)||_{L^2}^2 + \left|\left|\frac{1}{\sqrt{\epsilon_0\epsilon_d}}\mathbf{P}(t)\right|\right|_{L^2}^2.$$

and the $L^2(\Omega)$ norm is defined as

$$\|\mathbf{U}(t)\|_2^2 = \int_\Omega |\mathbf{U}(z,t)|^2 dz.$$

Motivation for Distributions

- 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 (discrete distributions), idea comes from the known existence of multiple physical mechanisms: multi-pole debye (like stair-step approximation)
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times [von Schweidler1907]
- Empirical measurements suggest a log-normal or Beta distribution [Wagner1913] (but uniform is easier)
- Using Mellin transforms, can show Cole-Cole corresponds to a continuous distribution

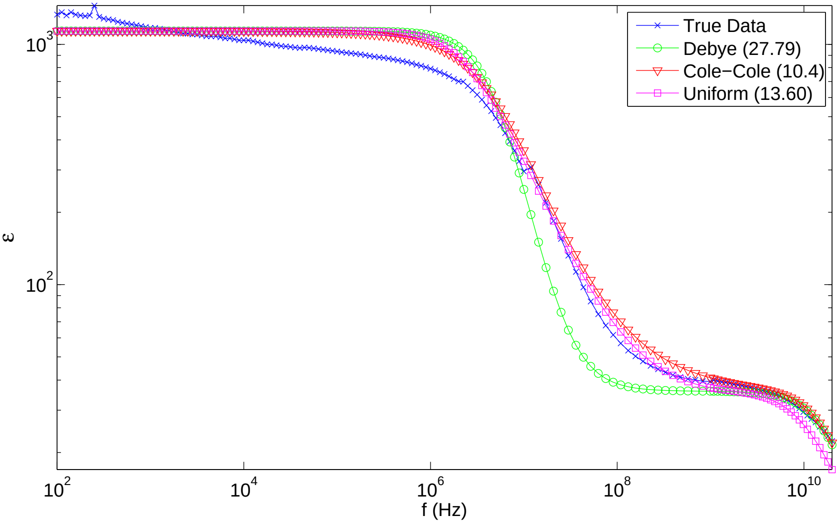


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

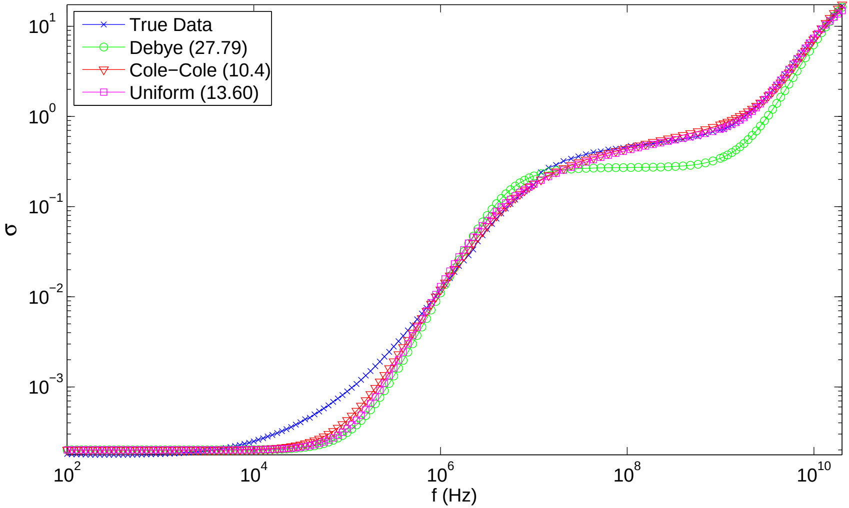


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

To account for the effect of possible multiple parameter sets $\mathbf{q}$, consider

$$h(t, \mathbf{x}; F) = \int_{\mathcal{Q}} g(t, \mathbf{x}; \mathbf{q}) dF(\mathbf{q}),$$

where $\mathcal{Q}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{Q})$.
Then the polarization becomes:

$$\mathbf{P}(t, \mathbf{x}) = \int_0^t h(t - s, \mathbf{x}; F) \mathbf{E}(s, \mathbf{x}) ds.$$

Random Polarization

Alternatively we can define the random polarization $\mathcal{P}(t, \mathbf{x}; \tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d\mathbf{E}$$

where τ 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 random polarization at each point $(t, \mathbf{x})$

$$\mathbf{P}(t, \mathbf{x}) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, \mathbf{x}; \tau) f(\tau) d\tau.$$

Maxwell-Random Debye system

In a polydisperse Debye material, we have

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\mathbf{P}}{\partial t} \tag{1a}$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E} \tag{1b}$$

$$\tau \frac{\partial \mathcal{P}}{\partial t} + \mathcal{P} = \epsilon_0 \epsilon_d \mathbf{E} \tag{1c}$$

with

$$\mathbf{P}(t, \mathbf{x}) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, \mathbf{x}; \tau) f(\tau) d\tau.$$

Theorem (Gibson2013)

The dispersion relation for the system (1) *is given by*

$$\frac{\omega^2}{c^2}\epsilon(\omega) = |\vec{k}|^2$$

where the complex permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + \epsilon_d \mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right]$$

Here, $\vec{k}$ is the wave number and $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light in freespace.

Note: for a uniform distribution, this has an analytic form since

$$\mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right] = \frac{1}{2\tau_r\omega}\left[\arctan(\omega\tau) - i\frac{1}{2}\ln\left(1 + (\omega\tau)^2\right)\right]_{\tau=\tau_m-\tau_r}^{\tau=\tau_m+\tau_r}$$

Proof: (for 2D)

Letting $H = H_z$, we have the 2D Maxwell-Random Debye TE scalar equations:

$$\frac{\partial H}{\partial t} = \frac{1}{\mu_0}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right), \quad (2a)$$

$$\epsilon_0\epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial P_x}{\partial t}, \quad (2b)$$

$$\epsilon_0\epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial P_y}{\partial t}, \quad (2c)$$

$$\tau \frac{\mathcal{P}_x}{\partial t} + \mathcal{P}_x = \epsilon_0\epsilon_d E_x \quad (2d)$$

$$\tau \frac{\mathcal{P}_y}{\partial t} + \mathcal{P}_y = \epsilon_0\epsilon_d E_y. \quad (2e)$$

Proof: (cont.)

Assume plane wave solutions of the form

$$V = \tilde{V}\mathrm{e}^{(k_x x + k_y y - \omega t)}$$

and let $\vec{x} = (x, y)^T$ and $\vec{k} = (k_x, k_y)^T$. Then (2) becomes

$$-i\omega\tilde{H} = \frac{1}{\mu_0}\left(ik_y\tilde{E}_x - ik_x\tilde{E}_y\right), \tag{3a}$$

$$-\epsilon_0\epsilon_\infty i\omega\tilde{E}_x = ik_y\tilde{H} - (-i\omega\tilde{P}_x), \tag{3b}$$

$$-\epsilon_0\epsilon_\infty i\omega\tilde{E}_y = -ik_x\tilde{H} - (-i\omega\tilde{P}_y), \tag{3c}$$

$$-i\omega\tau\tilde{\mathcal{P}}_x + \tilde{\mathcal{P}}_x = \epsilon_0\epsilon_d\tilde{E}_x \tag{3d}$$

$$-i\omega\tau\tilde{\mathcal{P}}_y + \tilde{\mathcal{P}}_y = \epsilon_0\epsilon_d\tilde{E}_y. \tag{3e}$$

Proof: (cont.)

By (3d) we have

$$\tilde{P}_x = \mathbb{E}[\tilde{\mathcal{P}}_x] = \epsilon_0 \epsilon_d \tilde{E}_x \mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right] \tag{4}$$

Substituting into (3b) we have

$$\begin{aligned} -\epsilon_0 \epsilon_\infty i\omega \tilde{E}_x &= ik_y \tilde{H} + \left(i\omega\epsilon_0\epsilon_d \tilde{E}_x \mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right]\right), \\ -i\omega\epsilon_0 \left(\epsilon_\infty + \epsilon_d \mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right]\right) \tilde{E}_x &= ik_y \tilde{H}, \\ -i\omega\epsilon_0\epsilon(\omega)\tilde{E}_x &= ik_y \tilde{H}. \end{aligned} \tag{5}$$

Similarly for combining (3e) and (3c)

$$-i\omega\epsilon_0\epsilon(\omega)\tilde{E}_y = -ik_x \tilde{H}. \tag{6}$$

Proof: (cont.)

Substituting both (5) and (6) into (3a) yields

$$-i\omega\tilde{H} = \frac{1}{\mu_0}\left(\frac{(ik_y)^2}{-i\omega\epsilon_0\epsilon(\omega)} + \frac{(ik_x)^2}{-i\omega\epsilon_0\epsilon(\omega)}\right)\tilde{H},$$

$$-(i\omega)^2\mu_0\epsilon_0\epsilon(\omega) = k_y^2 + k_x^2$$

$$\frac{\omega^2}{c^2}\epsilon(\omega) = |\vec{k}|^2$$

□

- The proof is similar in 1 and 3 dimensions.
- The exact dispersion relation will be compared with a discrete dispersion relation to determine the amount of dispersion error.

Finite Difference Methods

The Yee Scheme

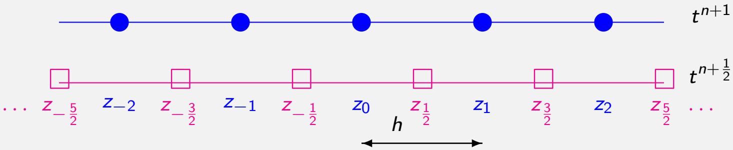
- In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations.
- The finite difference time domain (FDTD) or Yee algorithm solves for both the electric and magnetic fields in time and space using the coupled Maxwell's curl equations rather than solving for the electric field alone (or the magnetic field alone) with a wave equation.
- Approximates first order derivatives very accurately by evaluating on staggered grids.

Yee Scheme in One Space Dimension

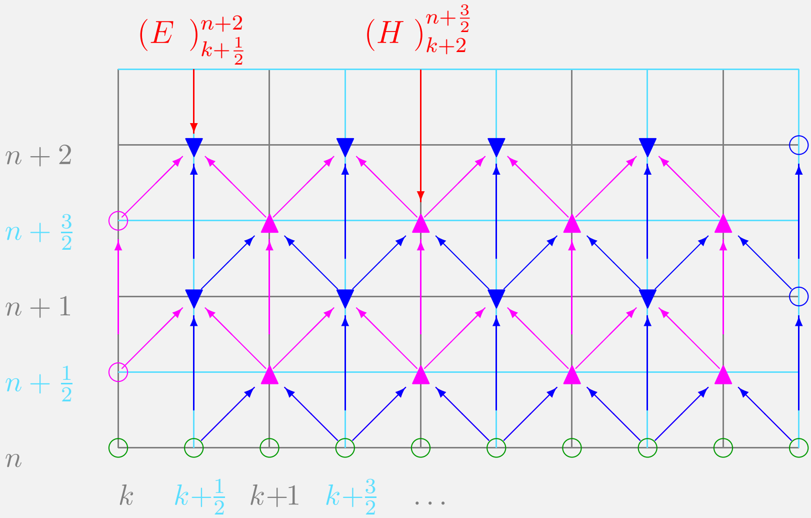
- **Staggered Grids**: The electric field/flux is evaluated on the primary grid in both space and time and the magnetic field/flux is evaluated on the dual grid in space and time.
- The Yee scheme is

$$\frac{H\big|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H\big|_{\ell+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\mu}\frac{E\big|_{\ell+1}^{n} - E\big|_{\ell}^{n}}{\Delta z}$$

$$\frac{E\big|_{\ell}^{n+1} - E\big|_{\ell}^{n}}{\Delta t} = -\frac{1}{\epsilon}\frac{H\big|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H\big|_{\ell-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z}$$



The FDTD or Yee grid in 1D



- This gives an explicit second order accurate scheme in both time and space.
- It is conditionally stable with the CFL condition

$$\nu = \frac{c\Delta t}{h} \leq \frac{1}{\sqrt{d}}$$

where ν is called the Courant number and $c = 1/\sqrt{\epsilon\mu}$ and d is the spatial dimension.
- The initial value problem is well-posed and the scheme is consistent and stable. The method is convergent by the Lax-Richtmyer Equivalence Theorem.
- The Yee scheme can exhibit numerical dispersion.
- Dispersion error can be reduced by decreasing the mesh size or resorting to higher order accurate finite difference approximations.

Extensions of the Yee Scheme to Dispersive Media

- The ordinary differential equation for the polarization is discretized using an averaging of zero order terms.
- The resulting scheme remains second-order accurate in both time and space with the same CFL condition.
- However, the Yee scheme for the Maxwell-Debye system is now dissipative in addition to being dispersive.

Yee Scheme for Maxwell-Debye System (in 1D)

$$\epsilon_0\epsilon_\infty \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \frac{\partial P}{\partial t}$$
$$\mu_0 \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z}$$
$$\tau \frac{\partial P}{\partial t} = \epsilon_0\epsilon_d E - P$$

become

$$\epsilon_0\epsilon_\infty \frac{E_j^{n+\frac{1}{2}} - E_j^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n}{\Delta z} - \frac{P_j^{n+\frac{1}{2}} - P_j^{n-\frac{1}{2}}}{\Delta t}$$
$$\mu_0 \frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}}}{\Delta z}$$
$$\tau \frac{P_j^{n+\frac{1}{2}} - P_j^{n-\frac{1}{2}}}{\Delta t} = \epsilon_0\epsilon_d \frac{E_j^{n+\frac{1}{2}} + E_j^{n-\frac{1}{2}}}{2} - \frac{P_j^{n+\frac{1}{2}} + P_j^{n-\frac{1}{2}}}{2}.$$

Discrete Debye Dispersion Relation

(Petropolous1994) showed that for the Yee scheme applied to the (deterministic) Maxwell-Debye, the discrete dispersion relation can be written

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

where the discrete complex permittivity is given by

$$\epsilon_\Delta(\omega) = \epsilon_\infty + \epsilon_d \left(\frac{1}{1 - i\omega_\Delta \tau_\Delta}\right)$$

with discrete representations of ω and τ given by

$$\omega_\Delta = \frac{\sin\left(\omega \Delta t/2\right)}{\Delta t/2}, \qquad \tau_\Delta = \sec(\omega \Delta t/2)\tau$$

Discrete Debye Dispersion Relation (cont.)

The quantity K_Δ is given by

$$K_\Delta = \frac{\sin(k\Delta z/2)}{\Delta z/2}$$

in 1D and is related to the symbol of the discrete first order spatial difference operator by

$$iK_\Delta = \mathcal{F}(\mathcal{D}_{1,\Delta z}).$$

In this way, we see that the left hand side of the discrete dispersion relation

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

is unchanged when one moves to higher order spatial derivative approximations (Bokil-Gibson2011) or even higher spatial dimension.

Polynomial Chaos

Apply Polynomial Chaos (PC) method to approximate the random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d E, \quad \tau = \tau(\xi) = \tau_r\xi + \tau_m$$

resulting in

$$(\tau_r M + \tau_m I)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\hat{e}_1$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{f}.$$

The macroscopic polarization, the expected value of the random polarization at each point (t, x), is simply

$$P(t, x; F) = \mathbb{E}[\mathcal{P}] \approx \alpha_0(t, x).$$

The discretization of the PC system

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{f}$$

is performed similarly to the deterministic system in order to preserve second order accuracy. Applying second order central differences to $\vec{\alpha}_j^{n+\frac{1}{2}} = \vec{\alpha}(t_n, z_j)$:

$$A\frac{\vec{\alpha}_j^{n+\frac{1}{2}} - \vec{\alpha}_j^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}_j^{n+\frac{1}{2}} + \vec{\alpha}_j^{n-\frac{1}{2}}}{2} = \frac{\vec{f}_j^{n+\frac{1}{2}} + \vec{f}_j^{n-\frac{1}{2}}}{2}. \tag{7}$$

Couple this with the equations from above:

$$\epsilon_0\epsilon_\infty\frac{E_j^{n+\frac{1}{2}} - E_j^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n}{\Delta z} - \frac{\alpha_{0,j}^{n+\frac{1}{2}} - \alpha_{0,j}^{n-\frac{1}{2}}}{\Delta t} \tag{8a}$$

$$\mu_0\frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}}}{\Delta z}. \tag{8b}$$

Energy Decay and Stability

Theorem (Gibson2013)

For $n \geq 0$, *let* $\mathbf{U}^n = [H^n, E_x^n, E_y^n, \alpha_{0,x}^n, \ldots, \alpha_{0,y}^n, \ldots]^T$ *be the solutions of the 2D TE mode Maxwell-PC Debye FDTD scheme with PEC boundary conditions. If the usual CFL condition for Yee scheme is satisfied* $c\Delta t \leq \Delta z/\sqrt{2}$, *then there exists the energy decay property*

$$\mathcal{E}_h^{n+1} \leq \mathcal{E}_h^n$$

where

$$\mathcal{E}_h^n = \left|\left|\sqrt{\mu_0}\overline{H}^n\right|\right|_H^2 + ||\sqrt{\epsilon_0\epsilon_\infty}\mathbf{E}^n||_E^2 + \left|\left|\frac{1}{\sqrt{\epsilon_0\epsilon_d}}\vec{\alpha}^n\right|\right|_\alpha^2.$$

Note: $\mathbb{E}[\|\mathcal{P}\|^2] = \|\mathbb{E}[\mathcal{P}]^2 + Var(\mathcal{P})\|^2 \approx \|\vec{\alpha}\|_\alpha^2$
Energy decay implies that the method is (conditionally) stable and hence convergenent.

Energy Decay and Stability (cont.)

Proof.

Involves recognizing that

$$(\mathcal{E}_h^n)^2 = \mu_0 \|\overline{H}^n\|_H^2 + \epsilon_0\epsilon_\infty (E^n, \mathcal{A}_h E^n)_E + \frac{1}{\epsilon_0\epsilon_d}(\vec{\alpha}^n - E\hat{e}_1, A^{-1}(\vec{\alpha}^n - E\hat{e}_1))_\alpha^2$$

with $\mathcal{A}_h$ positive definite when the CFL condition is satisfied, and A^{-1} is always positive definite (eigenvalues between $\tau_m - \tau_r$ and $\tau_m + \tau_r$). □

Theorem (Gibson2013)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme in (8) and (7) is given by

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

where the discrete complex permittivity is given by

$$\epsilon_\Delta(\omega) := \epsilon_\infty + \epsilon_d \hat{e}_1^T \left(I - i\omega_\Delta A_\Delta\right)^{-1} \hat{e}_1$$

and the discrete PC matrix is given by

$$A_\Delta := \sec(\omega\Delta t/2)A.$$

The definitions of the parameters ω_Δ and K_Δ are the same as before. Recall the exact complex permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + \epsilon_d \mathbb{E}\left[\frac{1}{1 - i\omega\tau}\right]$$

Proof: (for 1D)

Assume plane wave solutions of the form

$$V_j^n = \tilde{V} \mathrm{e}^{i(kj\Delta z - \omega n \Delta t)}$$

and

$$\alpha_{\ell,j}^n = \tilde{\alpha}_\ell \mathrm{e}^{i(kj\Delta z - \omega n \Delta t)}$$

Substitute into (8b)

$$\mu_0 \tilde{H} \mathrm{e}^{i\left(k(j+\frac{1}{2})\Delta z - \omega(n+\frac{1}{2})\Delta t\right)} \left(\mathrm{e}^{\frac{-i\omega\Delta t}{2}} - \mathrm{e}^{\frac{i\omega\Delta t}{2}}\right) / \Delta t$$

$$= \tilde{E} \mathrm{e}^{i\left(k(j+\frac{1}{2})\Delta z - \omega(n+\frac{1}{2})\Delta t\right)} \left(\mathrm{e}^{\frac{ik\Delta z}{2}} - \mathrm{e}^{\frac{-ik\Delta z}{2}}\right) / \Delta z$$

$$\mu_0 \tilde{H} \left(\frac{-2i}{\Delta t} \sin(\omega \Delta t/2)\right) = -\tilde{E} \left(\frac{2i}{\Delta z} \sin(k\Delta z/2)\right)$$

$$\left(\frac{\mu_0 \Delta z}{\Delta t}\right) \tilde{H} \sin(\omega \Delta t/2) = \tilde{E} \sin(k \Delta z/2) \tag{9}$$

Proof: (cont.)

Similarly (8a) yields

$$\left(\epsilon_0\epsilon_\infty \frac{\Delta z}{\Delta t}\tilde{E} + \frac{\Delta z}{\Delta t}\tilde{\alpha}_0\right)\sin(\omega\Delta t/2) = \tilde{H}\sin(k\Delta z/2) \tag{10}$$

and (7) yields

$$A\tilde{\alpha}\left(\frac{-2i}{\Delta t}\sin(\omega\Delta t/2)\right) + \cos(\omega\Delta t/2)\tilde{\alpha} = \epsilon_0\epsilon_d\cos(\omega\Delta t/2)\tilde{E}\hat{e}_1 \tag{11}$$

which implies

$$\tilde{\alpha}_0 = \hat{e}_1^T\left(I - i\omega_\Delta A_\Delta\right)^{-1}\hat{e}_1\epsilon_o\epsilon_d\tilde{E}. \tag{12}$$

The rest of the proof follows as before. □

Note that the same relation holds in 2 and 3D as well as with higher order accurate spatial difference operators.

Dispersion Error

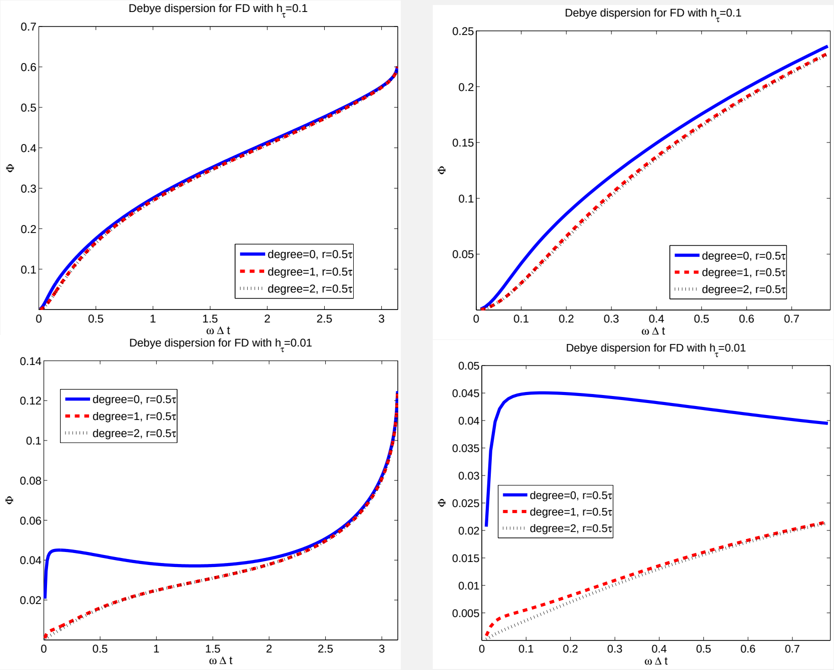
We define the phase error Φ for any method applied to a particular model to be

$$\Phi = \left| \frac{k_{\text{EX}} - k_{\Delta}}{k_{\text{EX}}} \right|, \tag{13}$$

where the numerical wave number k_{Δ} is implicitly determined by the corresponding dispersion relation and k_{EX} is the exact wave number for the given model.

- We wish to examine the phase error as a function of $\omega\Delta t$ in the range $[0, \pi]$.
- We note that $\omega\Delta t = 2\pi / N_{\text{ppp}}$, where N_{ppp} is the number of points per period, and is related to the number of points per wavelength as, $N_{\text{ppw}} = \sqrt{\epsilon_\infty}\nu N_{\text{ppp}}$.
- We assume the following parameters which are appropriate constants for modeling water Debye type materials:

$$\epsilon_\infty = 1, \quad \epsilon_s = 78.2, \quad \tau_m = 8.1 \times 10^{-12} \text{ sec}, \quad \tau_r = 0.5\tau_m.$$


Debye dispersion for FD with h_τ=0.1
Φ
ω Δ t
degree=0, r=0.5τ
degree=1, r=0.5τ
degree=2, r=0.5τ
Debye dispersion for FD with h_τ=0.1
Φ
ω Δ t
degree=0, r=0.5τ
degree=1, r=0.5τ
degree=2, r=0.5τ
Debye dispersion for FD with h_τ=0.01
Φ
ω Δ t
degree=0, r=0.5τ
degree=1, r=0.5τ
degree=2, r=0.5τ
Debye dispersion for FD with h_τ=0.01
Φ
ω Δ t
degree=0, r=0.5τ
degree=1, r=0.5τ
degree=2, r=0.5τ