A Polynomial Chaos Method for Dispersive Electromagnetics

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Outline

Acknowledgments

Collaborators

- H. T. Banks (NCSU)
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- Karen Barrese and Neel Chugh (REU 2008)
- Anne Marie Milne and Danielle Wedde (REU 2009)
- Erin Bela and Erik Hortsch (REU 2010)
- Megan Armentrout (MS 2011)
- Brian McKenzie (MS 2011)
- Duncan McGregor (MS 2013, PhD 2016?)

Outline

Maxwell's Equations

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Faraday)}$$

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} - \nabla \times \mathbf{H} = \mathbf{0}, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Ampere)}$$

$$\nabla \cdot \mathbf{D} = \nabla \cdot \mathbf{B} = 0, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Poisson/Gauss)}$$

$$\mathbf{E}(0, \mathbf{x}) = \mathbf{E_0}; \ \mathbf{H}(0, \mathbf{x}) = \mathbf{H_0}, \text{ in } \mathcal{D} \qquad \text{(Initial)}$$

$$\mathbf{E} \times \mathbf{n} = \mathbf{0}, \text{ on } (0, T) \times \partial\mathcal{D} \qquad \text{(Boundary)}$$

$\mathbf{E}$ = Electric field vector

$\mathbf{H}$ = Magnetic field vector

$\mathbf{J}$ = Current density

$\mathbf{D}$ = Electric flux density

$\mathbf{B}$ = Magnetic flux 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.

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

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

where $\epsilon = \epsilon_0\epsilon_\infty$ and $\mu = \mu_0\mu_r$.

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.

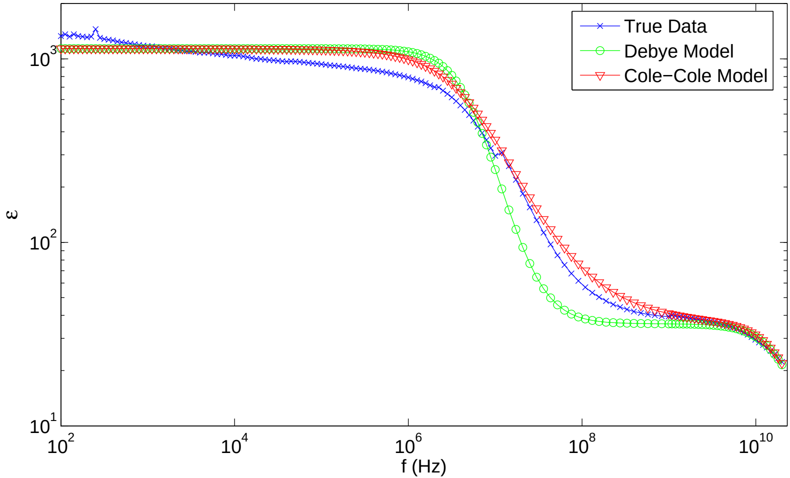


Figure : Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

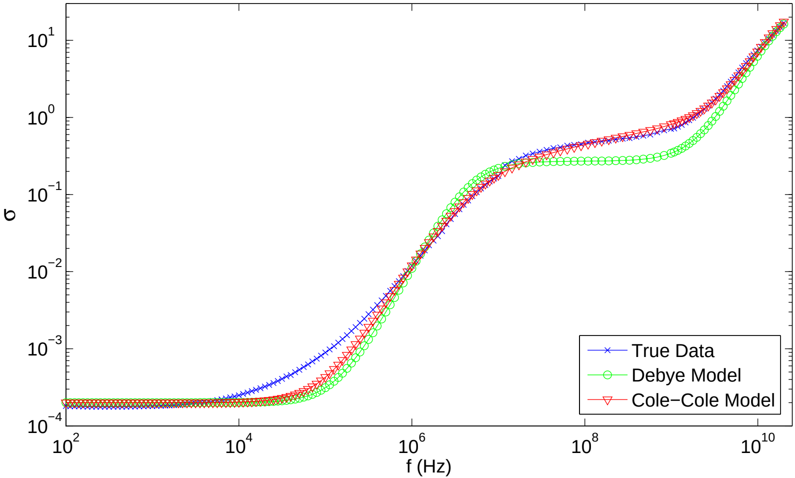


Figure : Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

Polarization Models

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

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

$$g(t,\mathbf{x}) = \epsilon_0\epsilon_d/\tau \quad e^{-t/\tau}$$

$$\text{or} \qquad \tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0\epsilon_d\mathbf{E}$$

$$\text{or} \qquad \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1+i\omega\tau}$$

  with $\epsilon_d := \epsilon_s - \epsilon_\infty$ and τ a relaxation time.
- Cole-Cole model [1936] (heuristic generalization) $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \alpha]$

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

Dispersive Media

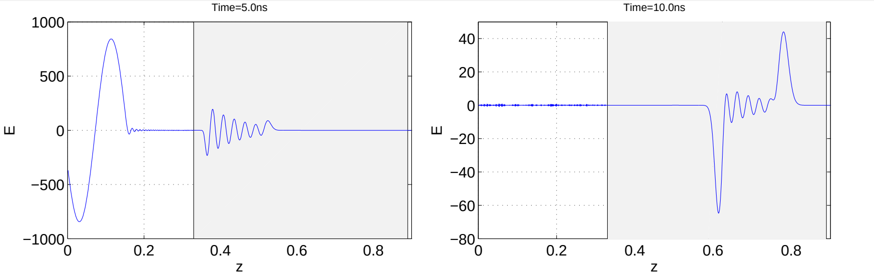


Figure : Debye model simulations.

Maxwell-Debye System

Combining Maxwell's Equations, Constitutive Laws, and the Debye model, we have

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

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\epsilon_0 \epsilon_d}{\tau} \mathbf{E} + \frac{1}{\tau} \mathbf{P} - \mathbf{J}, \tag{1b}$$

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

Assuming a solution to (1) of the form $\mathbf{E} = \mathbf{E_0} exp(i(\omega t - \mathbf{k} \cdot \mathbf{x}))$, the following relation must hold.

Debye Dispersion Relation

The dispersion relation for the Maxwell-Debye system is given by

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

where the complex permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + \epsilon_d \left(\frac{1}{1 + i\omega\tau}\right)$$

Here, $\mathbf{k}$ is the wave vector and $c = 1/\sqrt{\mu_0 \epsilon_0}$ is the speed of light.

2D Maxwell-Debye Transverse Electric (TE) curl equations

For simplicity in exposition and to facilitate analysis, we reduce the Maxwell-Debye model to two spatial dimensions (we make the assumption that fields do not exhibit variation in the z direction).

$$\mu_0 \frac{\partial H}{\partial t} = -\mathrm{curl}\ \mathbf{E}, \tag{2a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \mathbf{curl}\ H - \frac{\epsilon_0 \epsilon_d}{\tau} \mathbf{E} + \frac{1}{\tau} \mathbf{P} - \mathbf{J}, \tag{2b}$$

$$\tau \frac{\partial \mathbf{P}}{\partial t} = \epsilon_0 \epsilon_d \mathbf{E} - \mathbf{P}, \tag{2c}$$

where $\mathbf{E} = (E_x, E_y)^T, \mathbf{P} = (P_x, P_y)^T$ and $H_z = H$.

Note $\mathrm{curl}\ \mathbf{U} = \frac{\partial U_y}{\partial x} - \frac{\partial U_x}{\partial y}$ and $\mathbf{curl}\ V = \left(\frac{\partial V}{\partial y}, -\frac{\partial V}{\partial x}\right)^T$.

Stability Estimates for Maxwell-Debye

System is well-posed since solutions satisfy the following stability estimate.

Theorem (Li2010)

Let $\mathcal{D} \subset \mathbb{R}^2$, and let H, $\mathbf{E}$, and $\mathbf{P}$ be the solutions to (the weak form of) the 2D Maxwell-Debye TE system with PEC boundary conditions. Then the system exhibits energy decay

$$\mathcal{E}(t) \leq \mathcal{E}(0), \qquad \forall t \geq 0$$

where the energy is defined by

$$\mathcal{E}(t)^2 = \|\sqrt{\mu_0} H(t)\|_2^2 + \|\sqrt{\epsilon_0 \epsilon_\infty} \mathbf{E}(t)\|_2^2 + \left\| \frac{1}{\sqrt{\epsilon_0 \epsilon_d}} \mathbf{P}(t) \right\|_2^2$$

and $\|\cdot\|_2$ is the $L^2(\mathcal{D})$ norm.

Outline

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

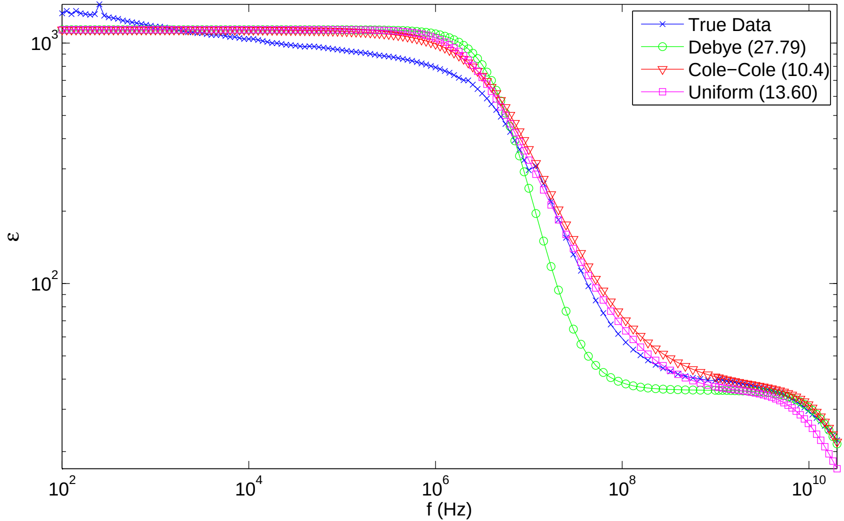


Figure : Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

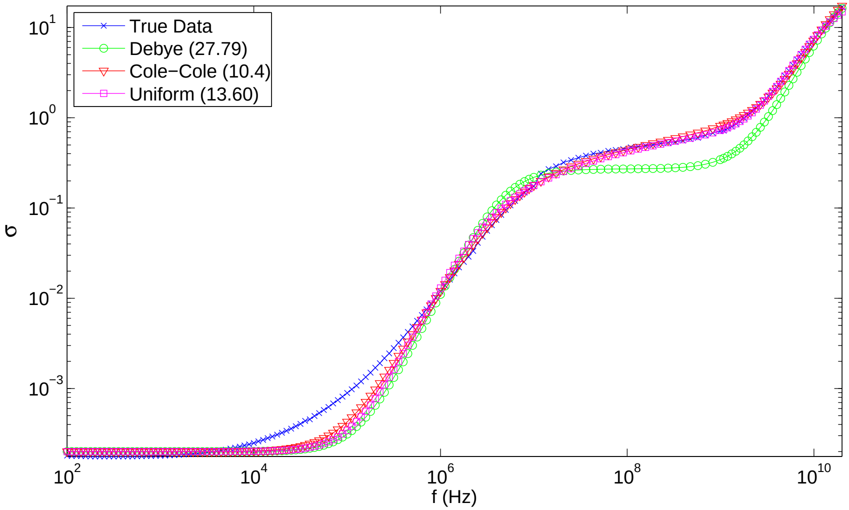


Figure : Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

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

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

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

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

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 $(t, \mathbf{x})$

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

Maxwell-Random Debye system

In a polydispersive Debye material, we have

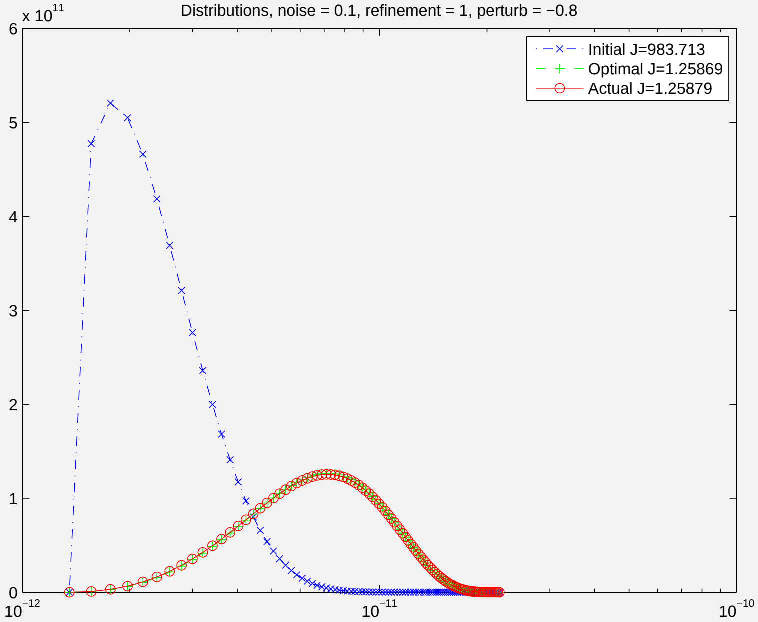
$$\mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}, \tag{3a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} - \mathbf{J} \tag{3b}$$

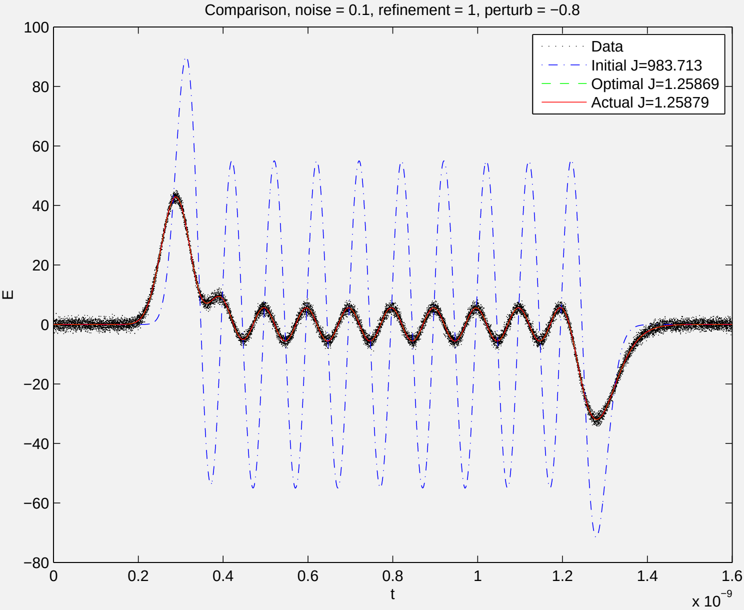
$$\tau \frac{\partial \mathcal{P}}{\partial t} + \mathcal{P} = \epsilon_0 \epsilon_d \mathbf{E} \tag{3c}$$

with

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



Comparison of initial to final distribution [Armentrout-G., 2011].



Comparison of simulations to data [Armentrout-G., 2011].

Theorem (G., 2015)

The dispersion relation for the system (3) is given by

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

where the expected complex permittivity is given by

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

Again, $\mathbf{k}$ is the wave vector and $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light.

Note: for a uniform distribution on $[\tau_a, \tau_b]$, this has an analytic form since

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

Proof: (for 2D)

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

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{4a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial P_x}{\partial t}, \tag{4b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial P_y}{\partial t}, \tag{4c}$$

$$\tau \frac{\partial \mathcal{P}_x}{\partial t} + \mathcal{P}_x = \epsilon_0 \epsilon_d E_x \tag{4d}$$

$$\tau \frac{\partial \mathcal{P}_y}{\partial t} + \mathcal{P}_y = \epsilon_0 \epsilon_d E_y. \tag{4e}$$

Proof: (cont.)

We assume plane wave solutions of the form

$$V = \tilde{V} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$$

where $\mathbf{x} = (x, y)^T$ and $\mathbf{k} = (k_x, k_y)^T$. We have, for example,

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

The rest is algebra. $\square$

- 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.

We introduce the random Hilbert space $V_F = (L^2(\Omega) \otimes L^2(\mathcal{D}))^2$ equipped with an inner product and norm as follows

$$(\mathbf{u}, \mathbf{v})_F = \mathbb{E}[(\mathbf{u}, \mathbf{v})_2],$$
$$\|\mathbf{u}\|_F^2 = \mathbb{E}[\|\mathbf{u}\|_2^2].$$

The weak formulation of the 2D Maxwell-Random Debye TE system is

$$\left(\frac{\partial H}{\partial t}, v\right)_2 = \left(-\frac{1}{\mu_0}\mathrm{curl}\ \mathbf{E}, v\right)_2, \tag{5}$$

$$\left(\epsilon_0\epsilon_\infty\frac{\partial \mathbf{E}}{\partial t}, \mathbf{u}\right)_2 = (H, \mathrm{curl}\ \mathbf{u})_2 - \left(\frac{\partial \mathbf{P}}{\partial t}, \mathbf{u}\right)_2, \tag{6}$$

$$\left(\frac{\partial \mathcal{P}}{\partial t}, \mathbf{w}\right)_F = \left(\frac{\epsilon_0\epsilon_d}{\tau}\mathbf{E}, \mathbf{w}\right)_F - \left(\frac{1}{\tau}\mathcal{P}, \mathbf{w}\right)_F, \tag{7}$$

for $v \in L^2(\mathcal{D})$, $\mathbf{u} \in H_0(\mathrm{curl}, \mathcal{D})^2$, and $\mathbf{w} \in V_F$.

Stability Estimates for Maxwell-Random Debye

System is well-posed since solutions satisfy the following stability estimate.

Theorem (G., 2015)

Let $\mathcal{D} \subset \mathbb{R}^2$, and let H, $\mathbf{E}$, and $\mathcal{P}$ be the solutions to the weak form of the 2D Maxwell-Random Debye TE system with PEC boundary conditions. Then the system exhibits energy decay

$$\mathcal{E}(t) \leq \mathcal{E}(0), \qquad \forall t \geq 0$$

where the energy is defined by

$$\mathcal{E}(t)^2 = \|\sqrt{\mu_0} H(t)\|_2^2 + \|\sqrt{\epsilon_0\epsilon_\infty}\mathbf{E}(t)\|_2^2 + \left\| \frac{1}{\sqrt{\epsilon_0\epsilon_d}} \mathcal{P}(t) \right\|_F^2 .$$

Proof: (for 2D)

By choosing $v = H$, $\mathbf{u} = \mathbf{E}$, and $\mathbf{w} = \mathcal{P}$ in the weak form, and adding all three equations into the time derivative of the definition of $\mathcal{E}^2$, we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d\mathcal{E}^2(t)}{dt} =& - \Big(\text{curl } \mathbf{E}, H\Big)_2 + \Big(H, \text{curl } \mathbf{E}\Big)_2 - \Big(\frac{\epsilon_0\epsilon_d}{\tau}\mathbf{E}, \mathbf{E}\Big)_F + \Big(\frac{1}{\tau}\mathcal{P}, \mathbf{E}\Big)_F \\
&+ \Big(\frac{1}{\tau}\mathbf{E}, \mathcal{P}\Big)_F - \Big(\frac{1}{\epsilon_0\epsilon_d\tau}\mathcal{P}, \mathcal{P}\Big)_F \\
=& - \epsilon_0\epsilon_d\Big(\frac{1}{\tau}\mathbf{E}, \mathbf{E}\Big)_F + 2\Big(\frac{1}{\tau}\mathcal{P}, \mathbf{E}\Big)_F - \frac{1}{\epsilon_0\epsilon_d}\Big(\frac{1}{\tau}\mathcal{P}, \mathcal{P}\Big)_F \\
=& \frac{-1}{\epsilon_0\epsilon_d}\left\|\frac{1}{\tau}(\mathcal{P} - \epsilon_0\epsilon_d\mathbf{E})\right\|_F^2.
\end{aligned}$$

$$\boxed{\frac{d\mathcal{E}(t)}{dt} = \frac{-1}{\epsilon_0\epsilon_d\mathcal{E}(t)}\left\|\frac{1}{\tau}(\mathcal{P} - \epsilon_0\epsilon_d\mathbf{E})\right\|_F^2 \leq 0.}$$

□

Outline

Polynomial Chaos

Apply Polynomial Chaos (PC) method to approximate each spatial component of 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 electric field depends on the macroscopic polarization, the expected value of the random polarization at each point $(t, \mathbf{x})$, which is

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

Note that A is positive definite if $\tau_r < \tau_m$ since $\lambda(M) \in (-1, 1)$.

Maxwell-PC Debye

Replace the Debye model with the PC approximation. In two dimensions we have the 2D Maxwell-PC Debye TE scalar equations

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{8a}$$

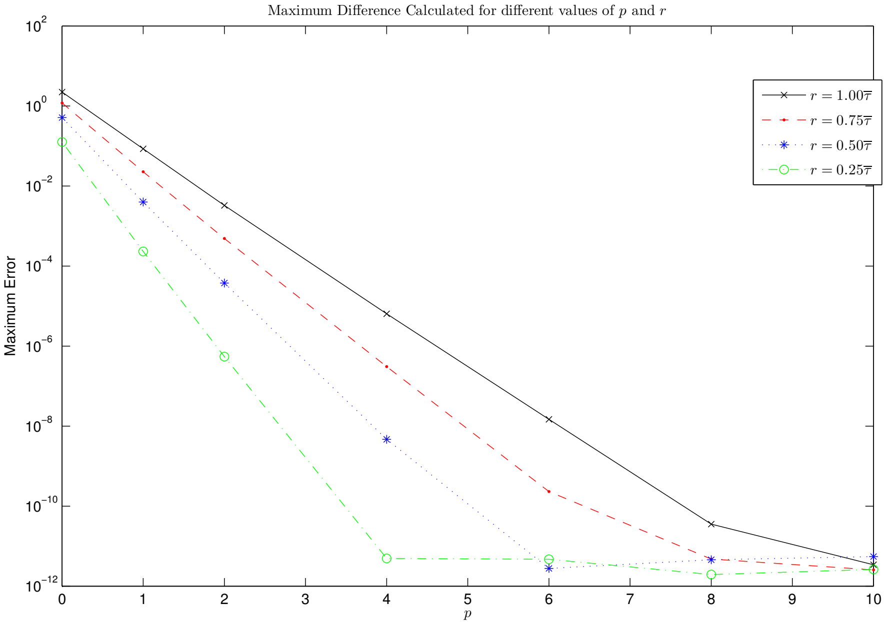
$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial \alpha_{0,x}}{\partial t}, \tag{8b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial \alpha_{0,y}}{\partial t}, \tag{8c}$$

$$A\dot{\vec{\alpha}}_x + \vec{\alpha}_x = \vec{f}_x, \tag{8d}$$

$$A\dot{\vec{\alpha}}_y + \vec{\alpha}_y = \vec{f}_y. \tag{8e}$$

where $\vec{f}_x = \epsilon_0 \epsilon_d E_x \hat{e}_1$ and $\vec{f}_y = \epsilon_0 \epsilon_d E_y \hat{e}_1$. Denote $\vec{\boldsymbol{\alpha}} = [\vec{\alpha}_x, \vec{\alpha}_y]^T$.


Maximum Difference Calculated for different values of p and r
Maximum Error
p
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
0
1
2
3
4
5
6
7
8
9
10
$r = 1.00\overline{\tau}$
$r = 0.75\overline{\tau}$
$r = 0.50\overline{\tau}$
$r = 0.25\overline{\tau}$

Outline

Finite Difference Time Domain (FDTD)

We now define a discretization of the Maxwell-PC Debye model. Note that any scheme can be used independent of the spectral approach in random space employed here.

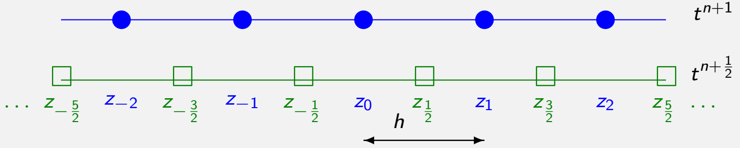
The Yee Scheme

- In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations in freespace.
- The finite difference time domain (FDTD) or Yee scheme 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

$$\boxed{\begin{aligned} \frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} &= -\frac{1}{\mu}\frac{E|_{\ell+1}^{n} - E|_{\ell}^{n}}{\Delta z} \\ \frac{E|_{\ell}^{n+1} - E|_{\ell}^{n}}{\Delta t} &= -\frac{1}{\epsilon}\frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} \end{aligned}}$$



- This gives an explicit second order accurate scheme in 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 d is the spatial dimension, and h is the (uniform) spatial step.
- 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 second order centered differences and an averaging of zero order terms.
- The resulting scheme remains second-order accurate in both time and space with the same CFL condition, $c_\infty \Delta t \leq h/\sqrt{d}$, except that $c_\infty = 1/\sqrt{\mu_0 \epsilon_0 \epsilon_\infty}$ is the fastest wave speed.
- 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)

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

become

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

Discrete Debye Dispersion Relation

(Petropolous1994) showed that for the Yee scheme applied to the 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 (mis-)representations of ω and τ given by

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

Discrete Debye Dispersion Relation (cont.)

The quantity K_Δ is given by

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

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-G,2012] or even higher spatial dimension [Bokil-G,2013].

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 at $\vec{\alpha}_j^n = \vec{\alpha}(t_n, z_j)$:

$$A\frac{\vec{\alpha}_j^{n+\frac{1}{2}} - \vec{\alpha}_j^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}_j^{n+\frac{1}{2}} + \vec{\alpha}_j^{n-\frac{1}{2}}}{2} = \frac{\vec{f}_j^{n+\frac{1}{2}} + \vec{f}_j^{n-\frac{1}{2}}}{2}. \tag{9}$$

Couple this with the equations from above:

$$\mu_0 \frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^{n}}{\Delta t} = -\frac{E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}}}{\Delta z} \tag{10a}$$

$$\epsilon_0\epsilon_\infty \frac{E_j^{n+\frac{1}{2}} - E_j^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^{n} - H_{j-\frac{1}{2}}^{n}}{\Delta z} - \frac{\alpha_{0,j}^{n+\frac{1}{2}} - \alpha_{0,j}^{n-\frac{1}{2}}}{\Delta t}. \tag{10b}$$

Let $\tau_h^{E_x}$, $\tau_h^{E_y}$, τ_h^{H} be the sets of spatial grid points on which the E_x, E_y, and H fields, respectively, will be discretized. The discrete L^2 grid norms are defined as

$$\|\mathbf{V}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|V_{x_{\ell+\frac{1}{2},j}}|^2 + |V_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \tag{11}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \tag{12}$$

with corresponding inner products. Each component $\boldsymbol{\alpha}_k$ is discretized on $\tau_h^{E_x} \times \tau_h^{E_y}$ with discrete L^2 grid norm

$$\|\vec{\boldsymbol{\alpha}}\|_\alpha^2 = \sum_{k=0}^{p} \|\boldsymbol{\alpha}_k\|_E^2,$$

with a corresponding inner product

$$(\vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\beta}})_\alpha = \sum_{k=0}^{p} \left(\boldsymbol{\alpha}_k, \boldsymbol{\beta}_k \right)_E.$$

Energy Decay and Stability

Energy decay implies that the method is stable and hence convergent.

Theorem (G., 2015)

For $n \geq 0$, let $\mathbf{U}^n = [H^{n-\frac{1}{2}}, E_x^n, E_y^n, \alpha_{0,x}^n, \ldots, \alpha_{0,y}^n, \ldots]^T$ be the solutions of the 2D Maxwell-PC Debye TE FDTD scheme with PEC boundary conditions. If the usual CFL condition for Yee scheme is satisfied $c_\infty \Delta t \leq h/\sqrt{2}$, then there exists the energy decay property

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

where the discrete energy is given by

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

Note: $\|\mathcal{P}\|_F^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathbb{E}[\mathcal{P}]^2 + Var(\mathcal{P})\|_2^2 \approx \|\vec{\boldsymbol{\alpha}}\|_\alpha^2$.

Energy Decay and Stability (cont.)

Proof.

First, showing that this is a discrete energy, i.e., a positive definite function of the solution, involves recognizing that

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

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 $\tau_m + \tau_r$).

The rest follows the proof for the deterministic case [Bokil-G, 2014] to show

$$\frac{\mathcal{E}_h^{n+1} - \mathcal{E}_h^n}{\Delta t} = -\left(\frac{2}{\mathcal{E}_h^{n+1} + \mathcal{E}_h^n}\right) \frac{1}{\epsilon_0\epsilon_d} \left\| \epsilon_0\epsilon_d \overline{\mathbf{E}}^{n+\frac{1}{2}} \hat{e}_1 - \overline{\vec{\alpha}}^{n+\frac{1}{2}} \right\|_{A^{-1}}^2 . \qquad (13)$$

$\square$

Theorem (G., 2015)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme in (9) and (10) is given by

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

where the discrete expected 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

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

and

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

Substituting into (9) yields

$$A\tilde{\alpha}\left(\frac{2i}{\Delta t}\sin(\omega\Delta t/2)\right) + \cos(\omega\Delta t/2)\tilde{\alpha} = \epsilon_0\epsilon_d \cos(\omega\Delta t/2)\tilde{E}\hat{e}_1 \qquad (14)$$

which implies

$$\tilde{\alpha}_0 = \hat{e}_1^T \left(I + i\omega_\Delta A_\Delta\right)^{-1} \hat{e}_1 \epsilon_0\epsilon_d \tilde{E}. \qquad (15)$$

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 a scheme applied to a model to be

$$\Phi = \left| \frac{k_{\mathrm{EX}} - k_{\Delta}}{k_{\mathrm{EX}}} \right|, \tag{16}$$

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 $[0, \pi]$. Δt is determined by $h_\tau \tau_m$, while $\Delta x = \Delta y$ determined by CFL condition.
- We note that $\omega\Delta t = 2\pi/N_{\mathrm{ppp}}$, where N_{ppp} is the number of points per period, and is related to the number of points per wavelength as, $N_{\mathrm{ppw}} = \sqrt{\epsilon_\infty}\nu N_{\mathrm{ppp}}$.
- We assume a uniform distribution and the following parameters which are appropriate constants for modeling aqueous Debye type materials:

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

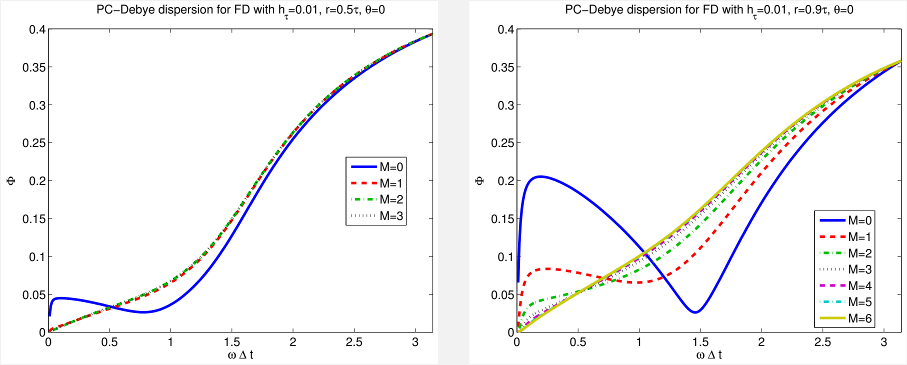


Figure : Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$.

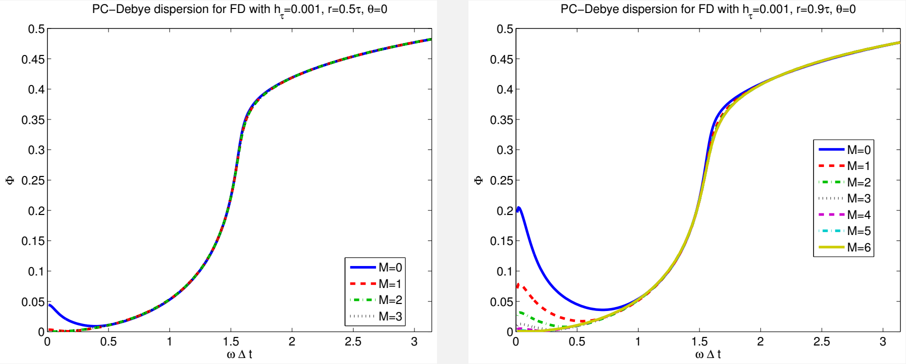
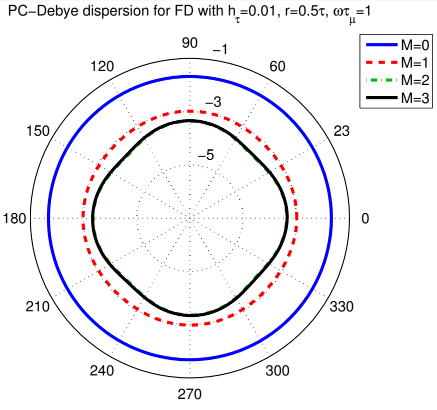


Figure : Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.001$.



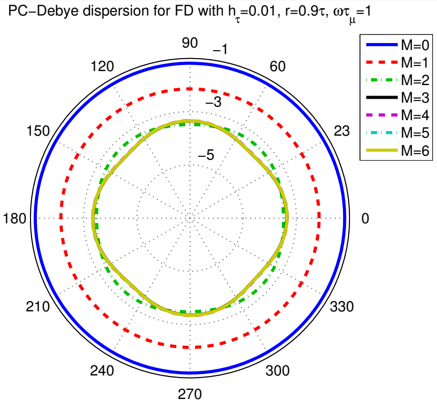
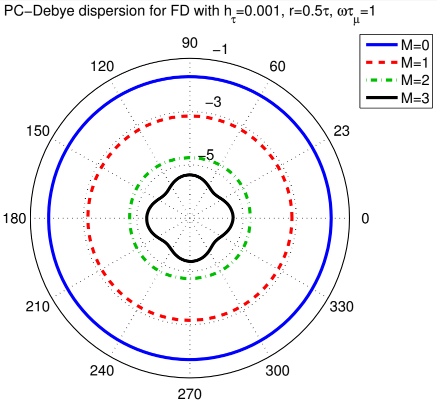


Figure : Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. Legend indicates degree M of the PC expansion.



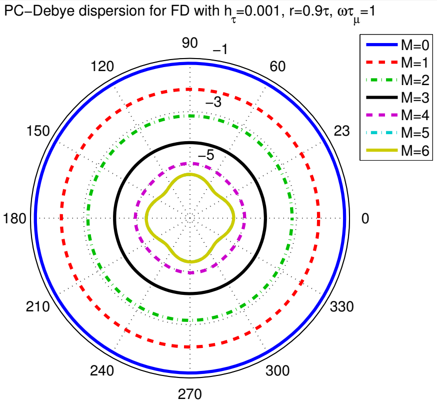


Figure : Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.001$. Legend indicates degree M of the PC expansion.

Outline

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media
- We described an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD)
- We have shown (conditional) stability of the scheme via energy decay
- We have used a discrete dispersion relation to compute phase errors
- Exponential convergence in the number of PC terms was demonstrated

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- BOKIL, V. A. & GIBSON, N. L. (2013), Stability and Dispersion Analysis of High Order FDTD Methods for Maxwell's Equations in Dispersive Media, *Contemporary Mathematics*, Vol. 586.
- BOKIL, V. A. & GIBSON, N. L. (2014), Convergence Analysis of Yee Schemes for Maxwell's Equations in Debye and Lorentz Dispersive Media, *IJNAM*.
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Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear IVP

$$\dot{y} + ky = g, \quad y(0) = y_0$$

with

$$k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0,1), \quad g(t) = 0.$$

We can represent the solution y as a Polynomial Chaos (PC) expansion in terms of (normalized) orthogonal Hermite polynomials H_j:

$$y(t,\xi) = \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi).$$

Substituting into the ODE we get

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi) = 0.$$

Triple recursion formula

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi) = 0.$$

We can eliminate the explicit dependence on ξ by using the triple recursion formula for Hermite polynomials

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

Thus

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)(j\phi_{j-1}(\xi) + \phi_{j+1}(\xi)) = 0.$$

Galerkin Projection onto span($\{\phi_i\}_{i=0}^p$)

In order to approximate y we wish to find a finite system for at least the first few α_i.
We take the weighted inner product with the ith basis, $i = 0, \dots, p$,

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

where

$$\langle f(\xi), g(\xi) \rangle_W := \int f(\xi) g(\xi) W(\xi) d\xi.$$

By orthogonality, $\langle \phi_j, \phi_i \rangle_W = \langle \phi_i, \phi_i \rangle_W \delta_{ij}$, we have

$$\dot{\alpha}_i \langle \phi_i, \phi_i \rangle_W + (i+1)\alpha_{i+1}\langle \phi_i, \phi_i \rangle_W + \alpha_{i-1}\langle \phi_i, \phi_i \rangle_W = 0, \quad i = 0, \dots, p.$$

Deterministic ODE system

Let $\vec{\alpha}$ represent the vector containing $\alpha_0(t), \ldots, \alpha_p(t)$.
Assuming $\alpha_{-1}(t)$, $\alpha_{p+1}(t)$, etc., are identically zero, the system of ODEs can be written

$$\dot{\vec{\alpha}} + M\vec{\alpha} = \vec{0},$$

with

$$M = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & p \\ & & & 1 & 0 \end{bmatrix}$$

The degree p PC approximation is $y(t,\xi) \approx y^p(t,\xi) = \sum_{j=0}^{p} \alpha_j(t)\phi_j(\xi)$.
The mean value $\mathbb{E}[y(t,\xi)] \approx \mathbb{E}[y^p(t,\xi)] = \alpha_0(t)$.
The variance $Var(y(t,\xi)) \approx \sum_{j=1}^{p} \alpha_j(t)^2$.

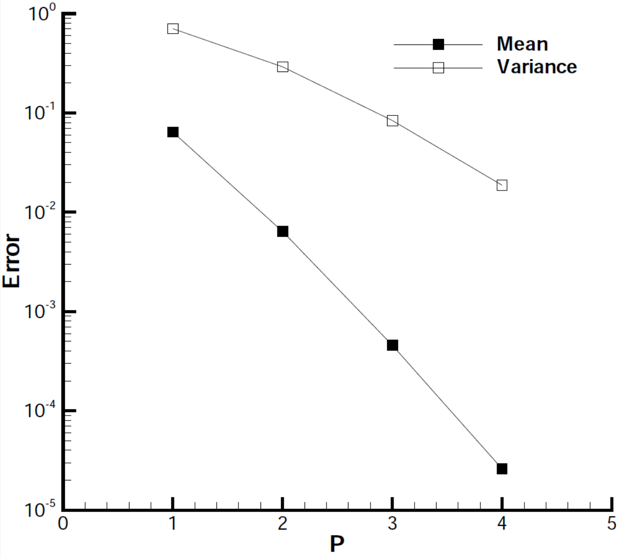

Figure : Convergence of error with Gaussian random variable by Hermitian-chaos.

Generalizations

Consider the non-homogeneous IVP

$$\dot{y} + ky = g(t), \quad y(0) = y_0$$

with

$$k = k(\xi) = \sigma\xi + \mu, \quad \xi \sim \mathcal{N}(0,1),$$

then

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

or the deterministic ODE system is

$$\dot{\vec{\alpha}} + (\sigma M + \mu I)\vec{\alpha} = g(t)\vec{e_1}.$$

Note that the initial condition for the PC system is $\vec{\alpha}(0) = y_0\vec{e_1}$.

Generalizations

For any choice of family of orthogonal polynomials, there exists a triple recursion formula. Given 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

$$M = \begin{bmatrix} b_0 & a_1 & & & \\ c_0 & b_1 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_p \\ & & & c_{p-1} & b_p \end{bmatrix}$$

Generalized Polynomial Chaos

Table : Popular distributions and corresponding orthogonal polynomials.

Distribution	Polynomial	Support
Gaussian	Hermite	$(-\infty, \infty)$
gamma	Laguerre	$[0, \infty)$
beta	Jacobi	$[a, b]$
uniform	Legendre	$[a, b]$

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

Numerical Approximation of Random Polarization

- Could apply a quadrature rule to the integral in the expected value. Results in a linear combination of individual Debye solves.
- Alternatively, we can use a method which separates the time derivative from the randomness and applies a truncated expansion in random space, called Polynomial Chaos. Results in a linear system.

Random Polarization

We can apply Polynomial Chaos method to our random polarization

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

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1} =: \vec{g}$$

or

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

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

$$P(t, x; F) = \alpha_0(t, x).$$

Applying the central difference approximation, based on the Yee scheme, Maxwell's equations with conductivity and polarization included

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

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 polarization updates simultaneously with the electric field.

For $\tau\dot{P} + P = \epsilon_d E$, once again using the central difference approximation (explicit trapezoidal), we have

$$\tau\frac{P_k^{n+\frac{1}{2}} - P_k^{n-\frac{1}{2}}}{\Delta t} + \frac{P_k^{n+\frac{1}{2}} + P_k^{n-\frac{1}{2}}}{2} = \epsilon_d \frac{E_k^{n+\frac{1}{2}} + E_k^{n-\frac{1}{2}}}{2}.$$

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

$$E_k^{n+\frac{1}{2}} = \frac{\theta}{1+\delta}\left[H^n_{k+\frac{1}{2}} - H^n_{k-\frac{1}{2}}\right] + \frac{1-\delta}{1+\delta}E_k^{n-\frac{1}{2}} + \frac{2\Delta t}{\epsilon(2\tau+\Delta t)(1+\delta)}P_k^{n-\frac{1}{2}}$$

and

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

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

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

Applying second order central differences, as before, 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

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

Note that we first solve the discrete electric field equation for $E_k^{n+\frac{1}{2}}$ and plug in here (in $\vec{g}^{n+\frac{1}{2}}$) to update $\vec{\alpha}$.

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 $\vec{g}^{n+\frac{1}{2}}$. 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

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

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

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

and

$$\tilde{\vec{h}}^{n} = \frac{\epsilon_d \Delta t \theta}{1+\delta} \left[H^n_{k+\frac{1}{2}} - H^n_{k-\frac{1}{2}} \right]$$

Updating 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

$$
\begin{aligned}
(2\tilde{A} + \Delta t I)\vec{\alpha}^{n+\frac{1}{2}} &= (2\tilde{A} - \Delta t I)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t \left(\tilde{\vec{g}}^{n-\frac{1}{2}} + \tilde{\vec{h}}^{n} \right) \\
E_k^{n+\frac{1}{2}} &= \frac{\theta}{1+\delta} \left[H^n_{k+\frac{1}{2}} - H^n_{k-\frac{1}{2}} \right] + \frac{1-\delta}{1+\delta} E_k^{n-\frac{1}{2}} \\
&\quad - \frac{1}{\epsilon(1+\delta)} \left[\alpha_{0,k}^{n+\frac{1}{2}} - \alpha_{0,k}^{n-\frac{1}{2}} \right] \\
H^{n+1}_{k+\frac{1}{2}} &= -\frac{\Delta t}{\mu \Delta x} \left[E_{k+1}^{n+\frac{1}{2}} - E_k^{n+\frac{1}{2}} \right] + H^n_{k+\frac{1}{2}}
\end{aligned}
$$

Note that $(2\tilde{A} + \Delta t I)$ is tridiagonal and small.

Comments on Polynomial Chaos

- Gives a simple and efficient method to simulate systems involving distributions of parameters.
- Works equally well in three spatial dimensions.
- Limitation: choice of polynomials depends on type of distribution.
- Need error estimates to be sure that a sufficient number of polynomials is used in the expansion.