Polynomial Chaos for Dispersive Electromagnetics

Nathan L. Gibson

Associate Professor
Department of Mathematics

Oregon State University

Computational Aspects of Time Dependent Electromagnetic Wave Problems in Complex Materials
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Outline

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Acknowledgments

Collaborators

- H. T. Banks (NCSU)
- V. A. Bokil (OSU)

Students

- 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)
- Jacky Alvarez and Andrew Fisher (REU 2017)

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	$\mathbf{D} =$	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.

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

$\mathbf{P} =$	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

- For linear materials we can define **P** in terms of a convolution with **E**

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

where g is the dielectric response function (DRF).

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- 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.

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- 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.

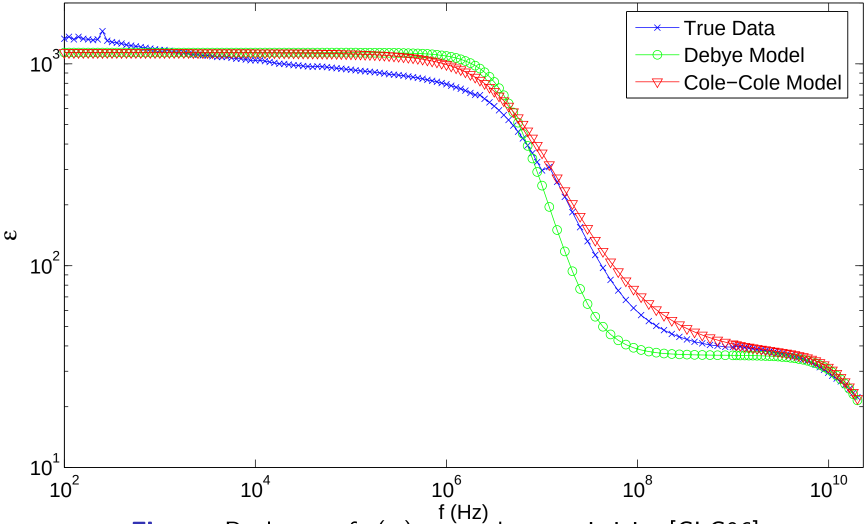

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

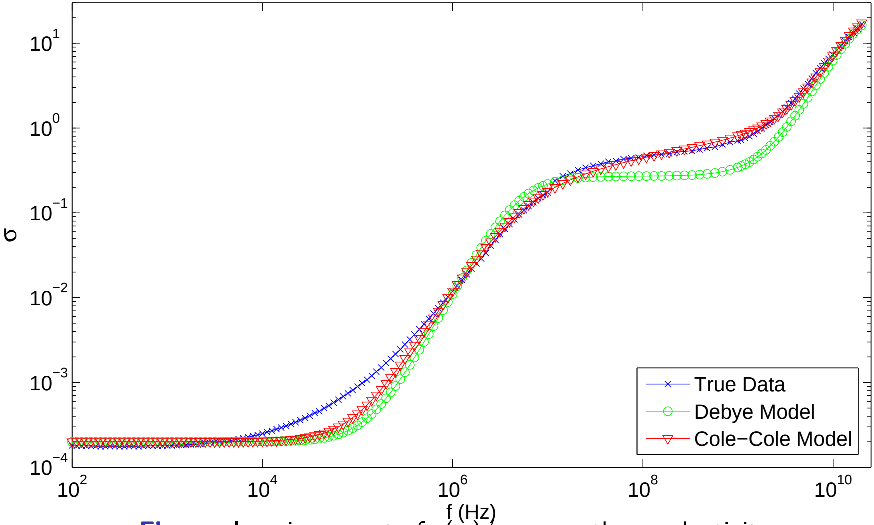

Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

Dispersive Media

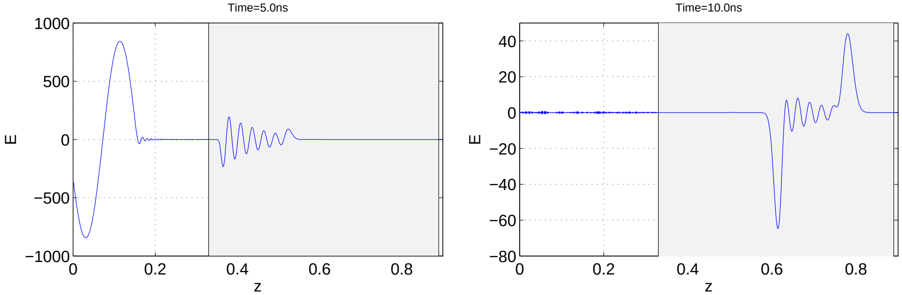

Figure: Debye model simulations [Banks2000].

Relaxation 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 [1913] $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau]$

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

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

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- Cole-Cole model [1941] (heuristic generalization)
  $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \alpha]$

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

Polarization Models

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- Cole-Cole model [1941] $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \alpha]$

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

- Davidson-Cole model [1951] $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \beta]$

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

- Havriliak-Negami model [1967] $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \alpha, \beta]$

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

Distributions of Relaxation Times

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$$F(y) = y^{\alpha\beta}\left(y^{2\alpha} + 2y^{\alpha}\cos(\pi\alpha) + 1\right)\sin(\beta\theta)/\pi - \beta/2,$$

where $y = \tau/\tau_0$ and θ is defined implictly by

$$(y^{\alpha} + cos(\pi\alpha))\, tan(\theta) = \sin(\pi\alpha).$$

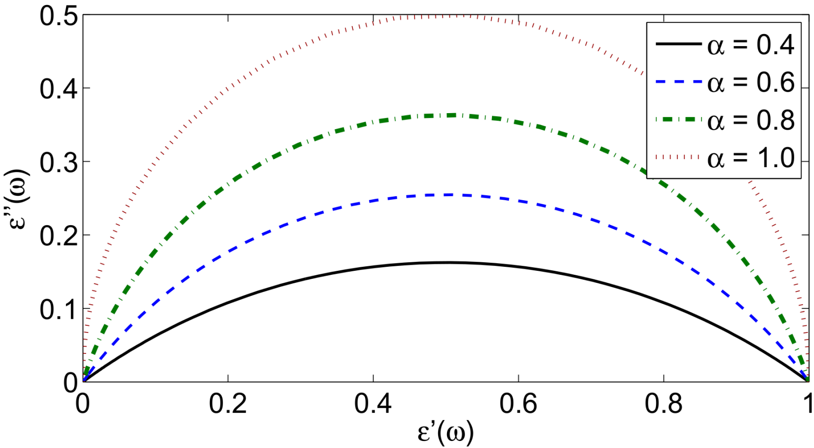

FIGURE 3. Cole-Cole plots for the CC model.

[Garrappa2016]

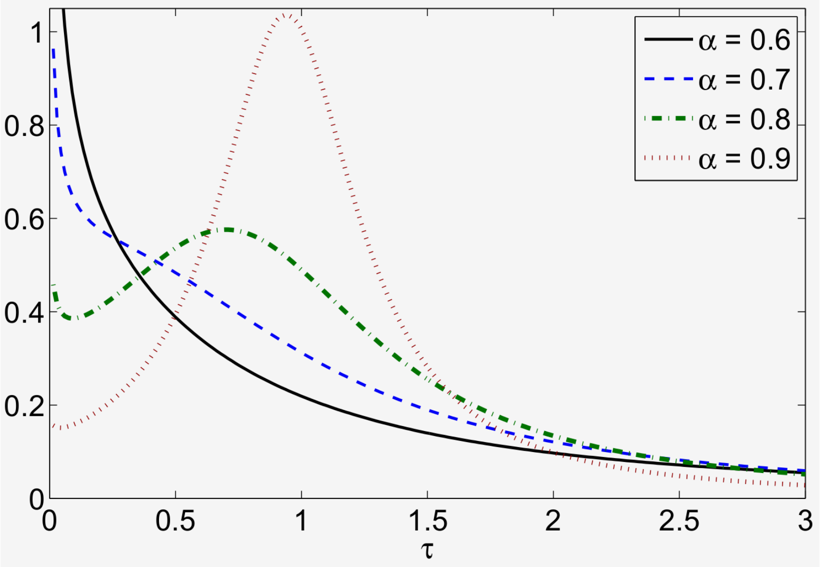

Figure: Relaxation Time Distribution for CC model [Garrappa2016].

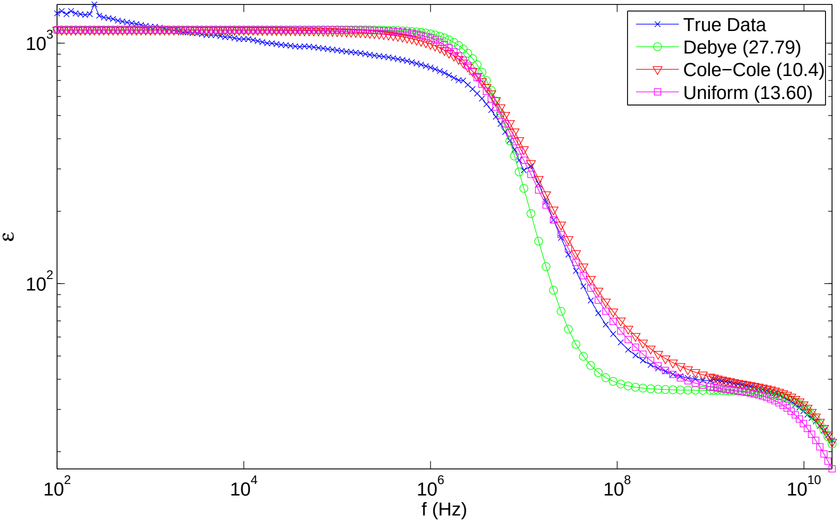

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

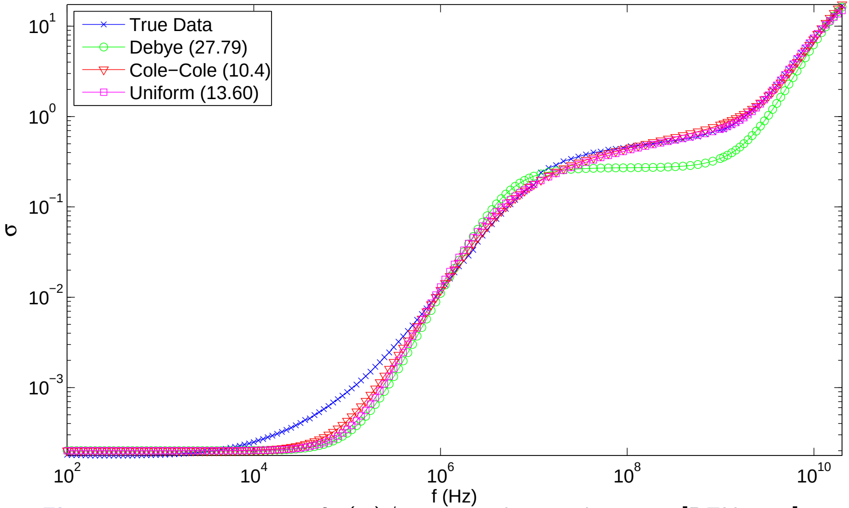

Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

To account for the effect of distributions of parameters $\mathbf{q}$, 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:

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

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

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

Random Polarization

In the case of relaxation polarization, the random polarization $\mathcal{P}(t, \mathbf{x}; \tau)$ solves

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

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

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

for a uniform distribution.

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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 $(t,\mathbf{x})$

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

Polynomial Chaos

Apply Polynomial Chaos (PC) method [Wiener 1938, Xiu 2004] to approximate each spatial component of the random polarization

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

(with ξ mean 0 and variance 1) resulting in

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

or

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

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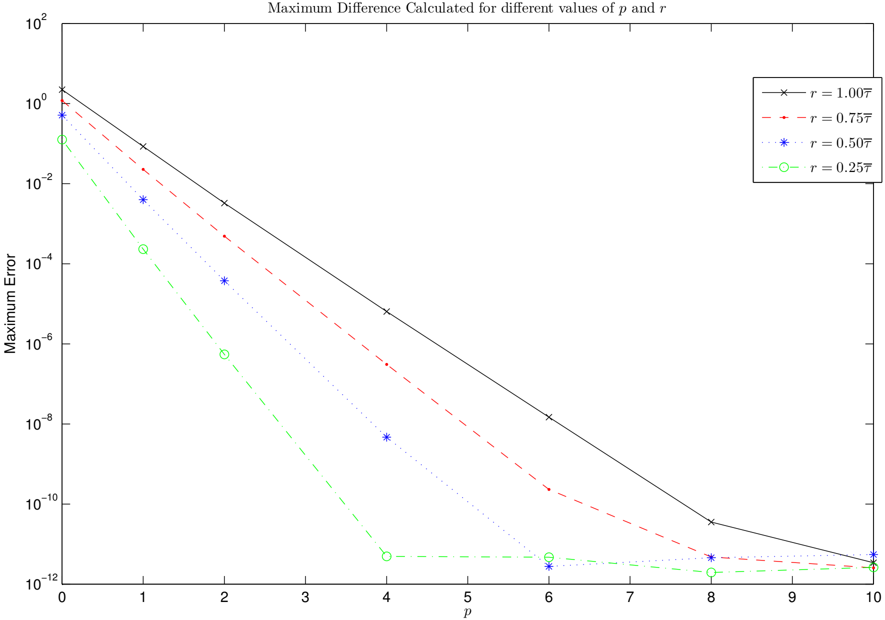
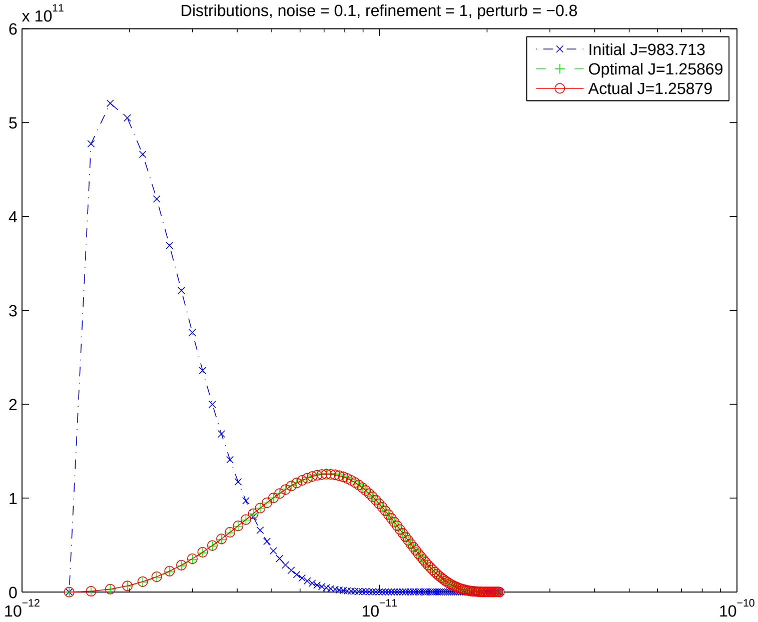
The electric field depends on the macroscopic polarization, the expected value of the random polarization at each point $(t, \mathbf{x})$, which is

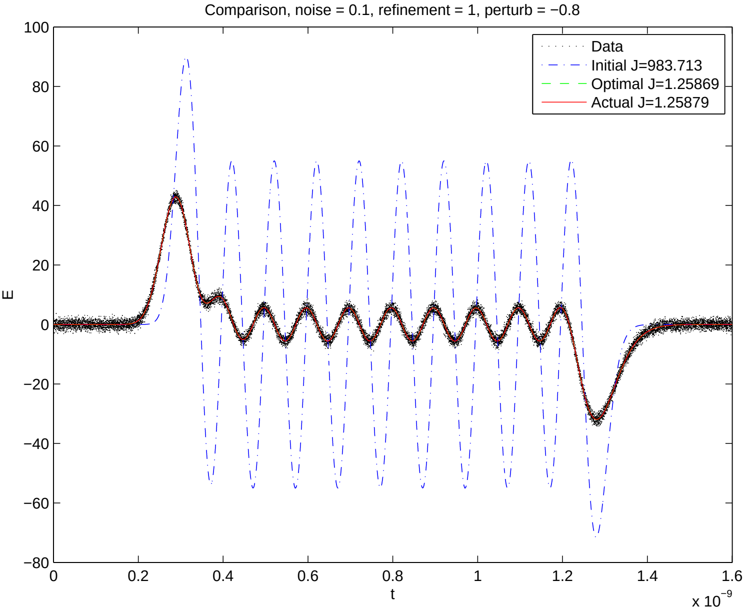
$$P(t, x; F) = \mathbb{E}[\mathcal{P}] \approx \alpha_0(t, \mathbf{x}).$$

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

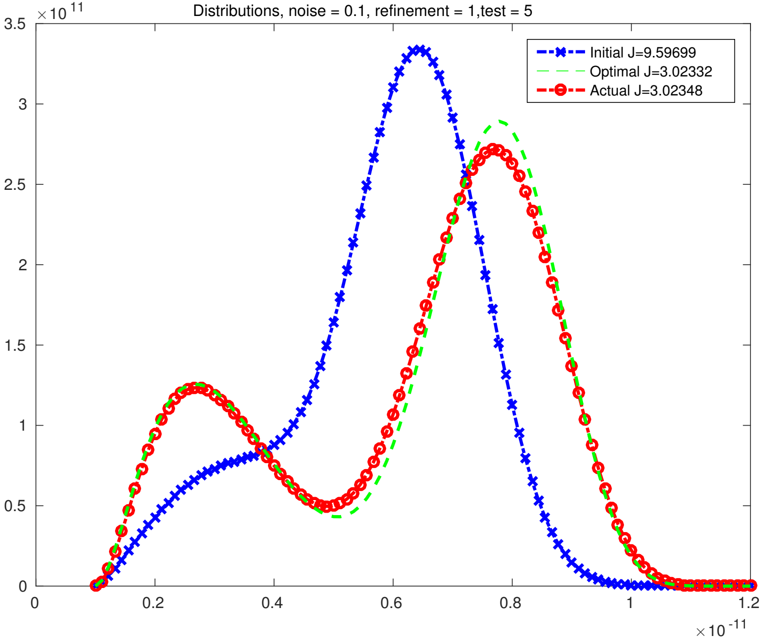

Maximum Difference Calculated for different values of p and r
Maximum Error
p
$r = 1.00\overline{\tau}$
$r = 0.75\overline{\tau}$
$r = 0.50\overline{\tau}$
$r = 0.25\overline{\tau}$
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
0 1 2 3 4 5 6 7 8 9 10



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



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


Distributions, noise = 0.1, refinement = 1,test = 5
×10 11
3.5
3
2.5
2
1.5
1
0.5
0
0
0.2
0.4
0.6
0.8
1
1.2
×10 -11
Initial J=9.59699
Optimal J=3.02332
Actual J=3.02348

(Deterministic) 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.

Maxwell-Random Debye system

In a polydispersive Debye material, we have

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

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} - \mathbf{J} \tag{2b}$$

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

with

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

Theorem (G., 2015)

The dispersion relation for the system (14) is given by

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

where the expected complex permittivity is given by

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

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Where $\mathbf{k}$ 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

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

The exact dispersion relation can be compared with a discrete dispersion relation to determine the amount of dispersion error.

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).

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

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \mathbf{curl}\ H - \frac{\epsilon_0 \epsilon_d}{\tau} \mathbf{E} + \frac{1}{\tau} \mathbf{P} - \mathbf{J}, \tag{3b}$$

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

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.

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

$$\left(\frac{\partial H}{\partial t}, v\right)_2 = \left(-\frac{1}{\mu_0}\mathrm{curl}\ \mathbf{E}, v\right)_2, \tag{4}$$

$$\left(\epsilon_0\epsilon_\infty \frac{\partial \mathbf{E}}{\partial t}, \mathbf{u}\right)_2 = (H, \mathrm{curl}\ \mathbf{u})_2 - \left(\frac{\partial \mathbf{P}}{\partial t}, \mathbf{u}\right)_2, \tag{5}$$

$$\left(\frac{\partial \mathcal{P}}{\partial t}, \mathbf{w}\right)_F = \left(\frac{\epsilon_0\epsilon_d}{\tau}\mathbf{E}, \mathbf{w}\right)_F - \left(\frac{1}{\tau}\mathcal{P}, \mathbf{w}\right)_F, \tag{6}$$

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

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

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

□

Maxwell-PC Debye

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

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{7a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial \alpha_{0,x}}{\partial t}, \tag{7b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial \alpha_{0,y}}{\partial t}, \tag{7c}$$

$$A\dot{\vec{\alpha}}_x + \vec{\alpha}_x = \vec{f}_x, \tag{7d}$$

$$A\dot{\vec{\alpha}}_y + \vec{\alpha}_y = \vec{f}_y. \tag{7e}$$

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 $\vec{\boldsymbol{\alpha}} = [\vec{\alpha}_x, \vec{\alpha}_y]^T$.

Finite Difference Time Domain (FDTD)

We now choose 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 [FEM: Yao 2018].

The Yee Scheme (FDTD)

- 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 $c_\infty = 1/\sqrt{\mu_0\epsilon_0\epsilon_\infty}$ is the fastest wave speed and d is the spatial dimension, and h is the (uniform) spatial step.
- The Yee scheme can exhibit numerical dispersion and dissipation.

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

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

Discrete Debye Dispersion Relation (cont.)

The quantity K_Δ is given by

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

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].

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

$$\|\mathbf{V}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|V_{x_{\ell+\frac{1}{2},j}}|^2 + |V_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \tag{8}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \tag{9}$$

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

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

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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 $\tau_m + \tau_r$).

Energy Decay and Stability (cont.)

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

$$\frac{\mathcal{E}_h^{n+1} - \mathcal{E}_h^n}{\Delta t} = -\left(\frac{2}{\mathcal{E}_h^{n+1} + \mathcal{E}_h^n}\right)\frac{1}{\epsilon_0\epsilon_d}\left\|\epsilon_0\epsilon_d \overline{\mathbf{E}}^{n+\frac{1}{2}}\hat{e}_1 - \overline{\vec{\alpha}}^{n+\frac{1}{2}}\right\|_{A^{-1}}^2 . \quad (10)$$

□

Theorem (G., 2015)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme 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

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

Dispersion Error

We define the phase error Φ for a scheme applied to a model to be

$$\Phi = \left| \frac{k_{\mathrm{EX}} - k_{\Delta}}{k_{\mathrm{EX}}} \right|, \tag{11}$$

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.

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- 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:

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

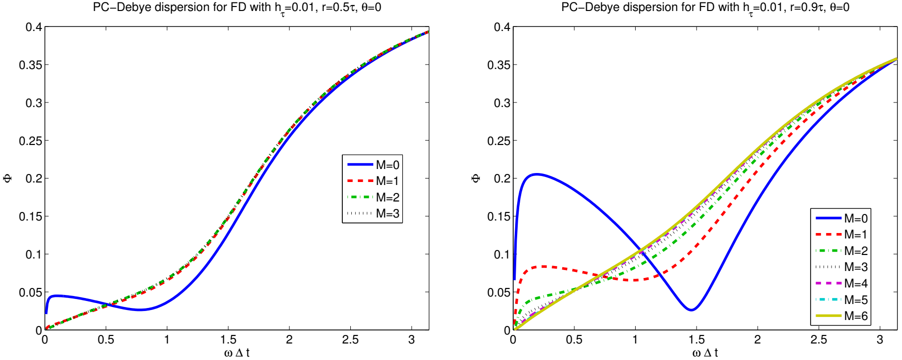
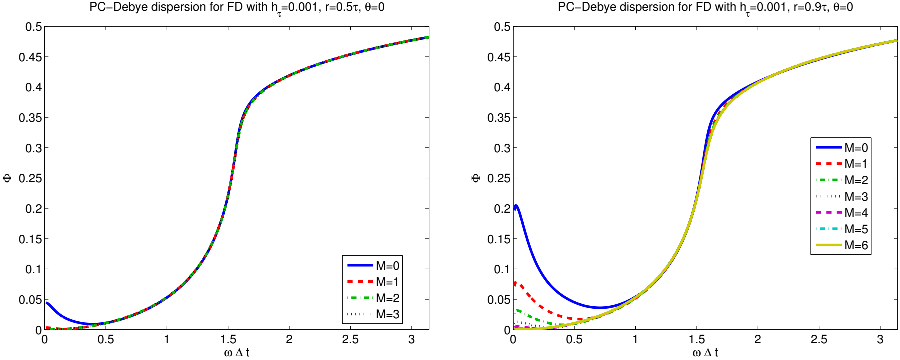


Figure: Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$.



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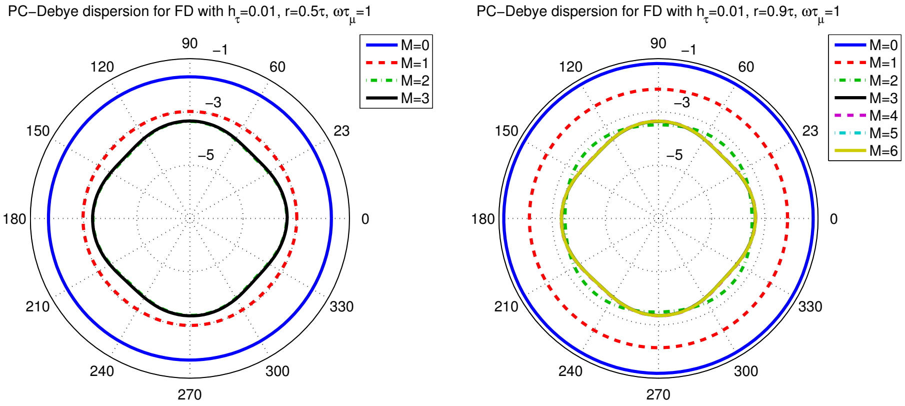
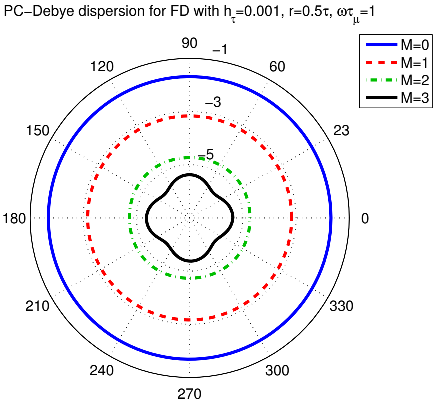
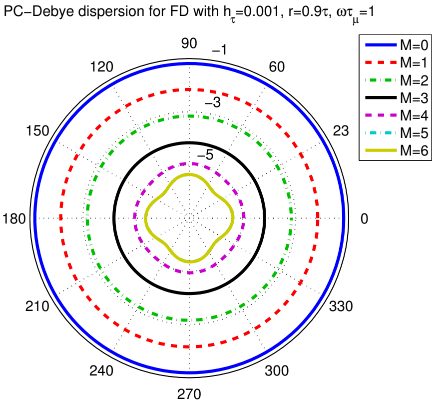


Figure: Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. Legend indicates degree M of the PC expansion.





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- We described an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD)
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- We have proven (conditional) stability of the scheme via energy decay
- We have derived a discrete dispersion relation and computed phase errors

Lorentz Model

We employ the physical assumption that electrons behave as damped harmonic oscillators,

$$m\ddot{x} + 2m\nu\dot{x} + m\omega_0^2 x = F_{driving}.$$

The polarization is then defined as electron dipole moment density:

$$\ddot{P} + 2\nu\dot{P} + \omega_0^2 P = \epsilon_0\omega_p^2 E$$

where ω_0 is the resonant frequency, ν is a damping coefficient, and ω_p is referred to as a plasma frequency defined by $\omega_p^2 = (\epsilon_s - \epsilon_\infty)\omega_0^2$.

Complex Permittivity

Taking a Fourier transform of $D = \epsilon E + P$ and inserting the convolution form of the polarization model in for P, we get $\hat{D}(\omega) = \epsilon_0 \epsilon(\omega)\hat{E}(\omega)$ where

$$\epsilon(\omega) = \epsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i2\nu\omega}.$$

For multiple Lorentz poles, the complex permittivity includes a (weighted) sum of mechanisms:

$$\epsilon(\omega) = \epsilon_\infty + \sum_{i=1}^{N_p} \frac{\omega_{p,i}^2}{\omega_{0,i}^2 - \omega^2 - i2\nu_i\omega}.$$

Random Polarization

The multi-pole Lorentz model motivates a model with a continuum of Lorentz mechanisms, i.e., a distribution of dielectric parameters. We define a random polarization to be a function of a dielectric parameter treated as a random variable.

The random Lorentz model is

$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2 E$$

with parameter ω_0^2 treated as a random variable with probability distribution F on the interval (a, b). The macroscopic polarization is taken to be the expected value of the random polarization,

$$P(t, z) = \int_a^b \mathcal{P}(t, z; \omega_0^2)\, dF(\omega_0^2).$$

Random Polarization

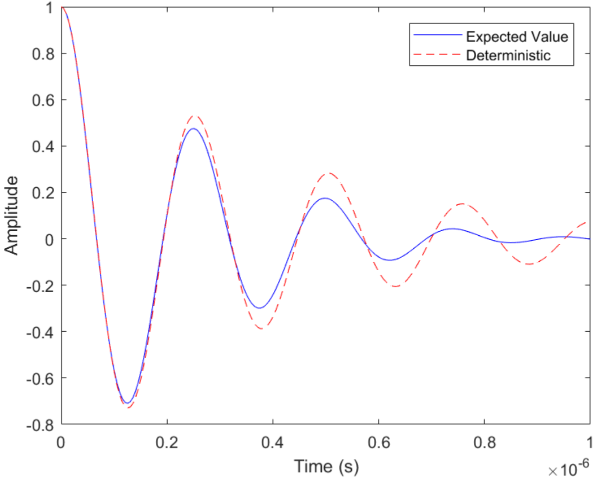

Figure: $\omega_0^2 \sim \mathcal{U}(0.75\overline{\omega}_0^2, 1.25\overline{\omega}_0^2)$

Complex Permittivity with random ω_0^2

Separate complex permittivity into real and imaginary parts ($\epsilon = \epsilon_r + i\epsilon_i$):

$$\epsilon_r = \epsilon_\infty + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2}$$

$$\epsilon_i = \frac{2\omega_p^2\nu\omega}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2}.$$

Analytic integration is possible for uniform distribution:

$$\mathbb{E}[\epsilon_r] = \frac{1}{b-a}\int_a^b \epsilon_r d\omega_0^2 = \epsilon_\infty + \frac{\omega_p^2}{2(b-a)}\left(\ln(\omega_0^2)^2 - 2\omega_0^2\omega^2 + \omega^4 + 4\nu^2\omega^2\right)\Big|_a^b$$

$$\mathbb{E}[\epsilon_i] = \frac{1}{b-a}\int_a^b \epsilon_i d\omega_0^2 = \frac{\omega_p^2}{(b-a)}\arctan\left(\frac{\omega^2 - \omega_0^2}{2\nu\omega}\right)\Big|_a^b$$

Saltwater Data

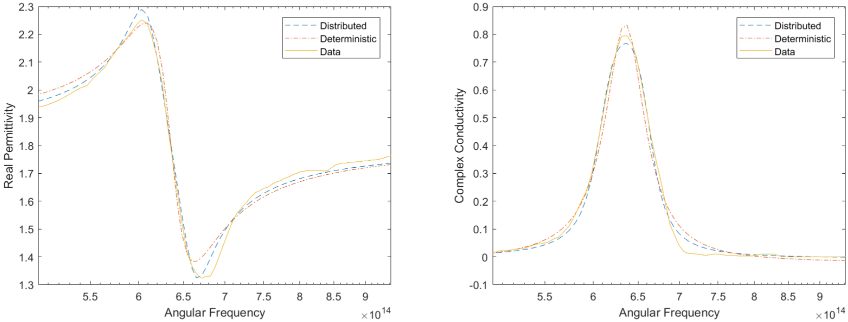

Figure: Fits for single-pole, saltwater data

Maxwell-Random Lorentz system

In a polydisperse Lorentz material, we have

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} \tag{14a}$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E} \tag{14b}$$

$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2 \mathcal{P} = \epsilon_0 \omega_p^2 \mathbf{E} \tag{14c}$$

with

$$\mathbf{P}(t, \mathbf{x}) = \int_a^b \mathcal{P}(t, \mathbf{x}; \omega_0^2) f(\omega_0^2) d\omega_0^2.$$

Theorem (Stability of Maxwell-Random Lorentz)

Let $\mathcal{D} \subset \mathbb{R}^2$ and suppose that $\mathbf{E} \in C(0,T;H_0(\mathrm{curl},\mathcal{D})) \cap C^1(0,T;(L^2(\mathcal{D}))^2)$, $\mathcal{P} \in C^1(0,T;\left(L^2(\Omega)\otimes L^2(\mathcal{D})\right)^2)$, *and* $H(t) \in C^1(0,T;L^2(\mathcal{D}))$ *are solutions of the weak formulation for the Maxwell-Random Lorentz system along with PEC boundary conditions. Then the system exhibits energy decay*

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

where the energy $\mathcal{E}(t)$ *is defined as*

$$\mathcal{E}(t)^2 = \left\|\sqrt{\mu_0}\, H(t)\right\|_2^2 + \left\|\sqrt{\epsilon_0\epsilon_\infty}\, \mathbf{E}(t)\right\|_2^2 + \left\|\frac{\omega_0}{\omega_p\sqrt{\epsilon_0}}\, \mathcal{P}(t)\right\|_F^2 + \left\|\frac{1}{\omega_p\sqrt{\epsilon_0}}\, \mathcal{J}(t)\right\|_F^2 \tag{15}$$

where $\|u\|_F^2 = \mathbb{E}[\|u\|_2^2]$ *and* $\mathcal{J} := \frac{\partial \mathcal{P}}{\partial t}$.

Proof involves showing that

$$\frac{d\mathcal{E}(t)}{dt} = \frac{-1}{\mathcal{E}(t)}\left\|\sqrt{\frac{2\nu}{\epsilon_0\omega_p^2}}\mathcal{J}\right\|_F^2 \leq 0.$$

Polynomial Chaos

We wish to approximate the random polarization with orthogonal polynomials of the standard random variable ξ. Let $\omega_0^2 = r\xi + m$ and $\xi \in [-1, 1]$. Suppressing the dimension of $\mathcal{P}$ and the spatial dependence, we have

$$\mathcal{P}(\xi, t) = \sum_{i=0}^{\infty} \alpha_i(t)\phi_i(\xi) \to \ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2 E.$$

Utilizing the Triple Recursion Relation for orthogonal polynomials:

$$\xi\phi_n(\xi) = a_n\phi_{n+1}(\xi) + b_n\phi_n(\xi) + c_n\phi_{n-1}(\xi).$$

the differential equation becomes

$$\sum_{i=0}^{\infty} \left[\ddot{\alpha}_i(t) + 2\nu\dot{\alpha}_i(t) + m\alpha_i(t)\right]\phi_i(\xi)$$

$$+ r\sum_{i=0}^{\infty} \alpha_i(t)\left[a_i\phi_{i+1}(\xi) + b_i\phi_i(\xi) + c_i\phi_{i-1}(\xi)\right] = \epsilon_0\omega_p^2 E\phi_0(\xi).$$

Galerkin Projection

We apply a Galerkin Projection onto the space of polynomials of degree at most p:

$$\ddot{\vec{\alpha}} + 2\nu\dot{\vec{\alpha}} + A\vec{\alpha} = \vec{f}$$

$$A = rM + mI, \quad M = \begin{pmatrix} b_0 & c_1 & 0 & \cdots & 0 \\ a_0 & b_1 & c_2 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & a_{p-2} & b_{b-1} & c_p \\ 0 & \cdots & 0 & a_{p-1} & b_p \end{pmatrix}.$$

Or we can write as a first order system:

$$\dot{\vec{\alpha}} = \vec{\beta}$$
$$\dot{\vec{\beta}} = -A\vec{\alpha} - 2\nu I\vec{\beta} + \vec{f},$$

where $\vec{f} = \hat{e}_1\epsilon_0\overline{\omega}_p^2 E$ with $\overline{\omega}_p$ meaning expected value.

Maxwell-PC Lorentz

The polynomial chaos system coupled with 1D Maxwell's equations becomes

$$\begin{aligned}
\epsilon_\infty \epsilon_0 \frac{\partial E}{\partial t} &= -\frac{\partial H}{\partial z} - \beta_0 \\
\frac{\partial H}{\partial t} &= -\frac{1}{\mu_0}\frac{\partial E}{\partial z} \\
\dot{\vec{\alpha}} &= \vec{\beta} \\
\dot{\vec{\beta}} &= -A\vec{\alpha} - 2\nu I\vec{\beta} + \vec{f}
\end{aligned}$$

Initial Conditions:

$$E(0,z) = H(0,z) = \vec{\alpha}(0,z) = \vec{\beta}(0,z) = 0$$

Boundary Conditions:

$$E(t,0) = E_L(t) \text{ and } E(t,z_R) = 0$$

We stagger three discrete meshes in the x and y directions and two discrete meshes in time:

$$\tau_h^{E_x} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_j \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J \right\}$$

$$\tau_h^{E_y} := \left\{ \left(x_{\ell}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L, 0 \leq j \leq J-1 \right\}$$

$$\tau_h^{H} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J-1 \right\}$$

$$\tau_t^{E} := \left\{ \left(t^n \right) | 0 \leq n \leq N \right\}$$

$$\tau_t^{H} := \left\{ \left(t^{n+\frac{1}{2}} \right) | 0 \leq n \leq N-1 \right\}.$$

Staggered L^2 normed spaces

Next, we define the L^2 normed spaces

$$\mathbb{V}_E := \left\{ \mathbf{F} : \tau_h^{E_x} \times \tau_h^{E_y} \longrightarrow \mathbb{R}^2 \mid \mathbf{F} = (F_{x_{l+\frac{1}{2},j}}, F_{y_{l,j+\frac{1}{2}}})^T, \|\mathbf{F}\|_E < \infty \right\} \tag{18}$$

$$\mathbb{V}_H := \left\{ U : \tau_h^{H} \longrightarrow \mathbb{R} \mid U = (U_{l+\frac{1}{2},j+\frac{1}{2}}), \|U\|_H < \infty \right\} \tag{19}$$

with the following discrete norms and inner products

$$\|\mathbf{F}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|F_{x_{\ell+\frac{1}{2},j}}|^2 + |F_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \forall\ \mathbf{F} \in \mathbb{V}_E \tag{20}$$

$$(\mathbf{F}, \mathbf{G})_E = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(F_{x_{\ell+\frac{1}{2},j}} G_{x_{\ell+\frac{1}{2},j}} + F_{y_{\ell,j+\frac{1}{2}}} G_{y_{\ell,j+\frac{1}{2}}} \right), \forall\ \mathbf{F}, \mathbf{G} \in \mathbb{V}_E \tag{21}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \forall\ U \in \mathbb{V}_H \tag{22}$$

$$(U, V)_H = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} U_{\ell+\frac{1}{2},j+\frac{1}{2}} V_{\ell+\frac{1}{2},j+\frac{1}{2}}, \forall\ U, V \in \mathbb{V}_H. \tag{23}$$

We define a space and inner product for the random polarization in vector notation, since $\vec{\alpha}$ and $\vec{\beta}$ are now $2 \times p + 1$ matrices:

$$\mathbb{V}_\alpha := \left\{ \vec{\boldsymbol{\alpha}} : \tau_h^{E_x} \times \tau_h^{E_y} \longrightarrow \mathbb{R}^2 \times \mathbb{R}^{p+1} \;\middle|\; \vec{\boldsymbol{\alpha}} = [\boldsymbol{\alpha}_0, \ldots, \boldsymbol{\alpha}_p], \boldsymbol{\alpha}_k \in \mathbb{V}_E, \|\vec{\boldsymbol{\alpha}}$$

where the discrete L^2 grid norm and inner product are defined as

$$\|\vec{\boldsymbol{\alpha}}\|_\alpha^2 = \sum_{k=0}^{p} \|\boldsymbol{\alpha}_k\|_E^2, \quad \forall\, \vec{\boldsymbol{\alpha}} \in \mathbb{V}_\alpha$$

$$(\vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\beta}})_\alpha = \sum_{k=0}^{p} \Big(\boldsymbol{\alpha}_k, \boldsymbol{\beta}_k\Big)_E, \quad \forall\, \vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\beta}} \in \mathbb{V}_\alpha.$$

We choose both spatial steps to be uniform and equal $(\Delta x = \Delta y = h)$, and require that the usual CFL condition for two dimensions holds:

$$\sqrt{2} c_\infty \Delta t \leq h. \tag{24}$$

Theorem (Energy Decay for Maxwell-PC Lorentz-FDTD)

If the stability condition (24) is satisfied, then the Yee scheme for the 2D TE mode Maxwell-PC Lorentz system satisfies the discrete identity

$$\delta_t \mathcal{E}_h^{n+\frac{1}{2}} = \frac{-1}{\overline{\mathcal{E}}_h^{n+\frac{1}{2}}} \left\| \sqrt{\frac{2\nu}{\epsilon_0 \omega_p^2}} \overline{\vec{\beta}}_h^{n+\frac{1}{2}} \right\|_A^2 \tag{25}$$

for all n where

$$\mathcal{E}_h^n = \left(\mu_0 (H^{n+\frac{1}{2}}, H^{n-\frac{1}{2}})_H + \| \sqrt{\epsilon_0 \epsilon_\infty}\ \mathbf{E}^n \|_E^2 + \left\| \sqrt{\frac{\omega_0^2}{\epsilon_0 \omega_p^2}} \vec{\alpha}^n \right\|_\alpha^2 + \left\| \sqrt{\frac{1}{\epsilon_0 \omega_p^2}} \vec{\beta}^n \right\|_\alpha^2 \right)^{1/2} \tag{26}$$

defines a discrete energy.

In the above $\|\vec{\alpha}\|_A^2 := (A\vec{\alpha}, \vec{\alpha})_\alpha$ given A positive definite, which is true iff $r < m$. Note that $\|\vec{\alpha}\|_\alpha^2 \approx \|\mathbb{E}[\mathcal{P}]\|_2^2 + \|\text{StdDev}(\mathcal{P})\|_2^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathcal{P}\|_F^2$ so that this is a natural extension of the Maxwell-Random Lorentz energy (15).

Theorem

The dispersion relation for the Maxwell-Random Lorentz system is given by

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

where the expected complex permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + (\epsilon_s - \epsilon_\infty)\mathbb{E}\left[\frac{\omega_0^2}{\omega_0^2 - \omega^2 - i2\nu\omega}\right].$$

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

The exact dispersion relation can be compared with a discrete dispersion relation to determine the amount of dispersion error.

Dispersion Error

We define the phase error Φ for a scheme applied to a model to be

$$\Phi = \left| \frac{k_{EX} - k_{\Delta}}{k_{EX}} \right|, \tag{27}$$

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

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- We wish to examine the phase error as a function of ω in the range around $\overline{\omega}_0$. Δt is determined by $h := \overline{\omega}_0 \Delta t/(2\pi)$, while $\Delta x = \Delta y$ are determined by the CFL condition.
- We assume a uniform distribution and the following parameters Lorentz material:

$$\epsilon_{\infty} = 1, \quad \epsilon_s = 2.25, \quad \nu = 2.8 \times 10^{15} \text{ 1/sec}, \quad \overline{\omega}_0 = 4 \times 10^{16} \text{ rad/sec}.$$

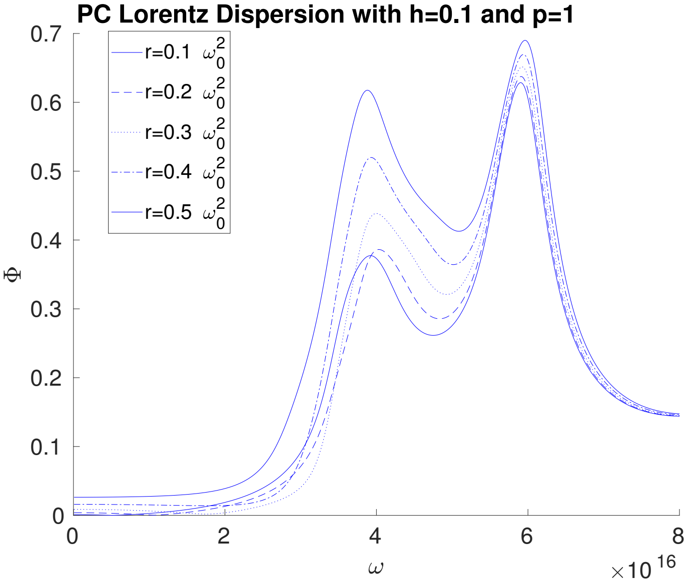
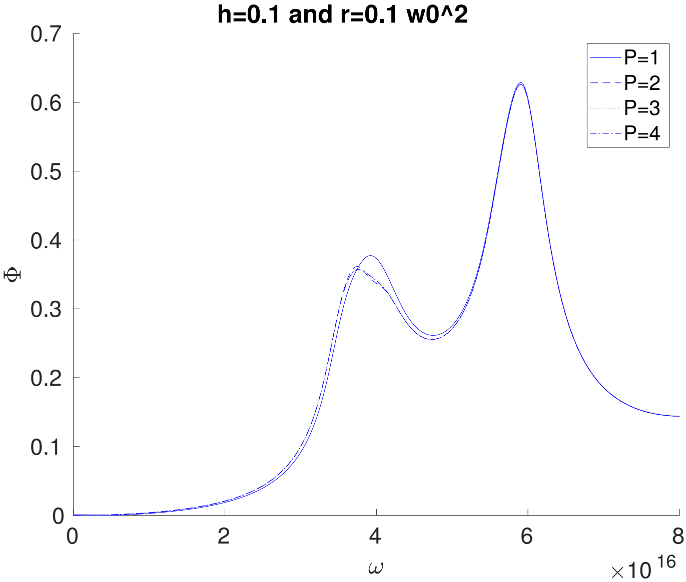


Figure: Plots of phase error at $\theta = 0$.



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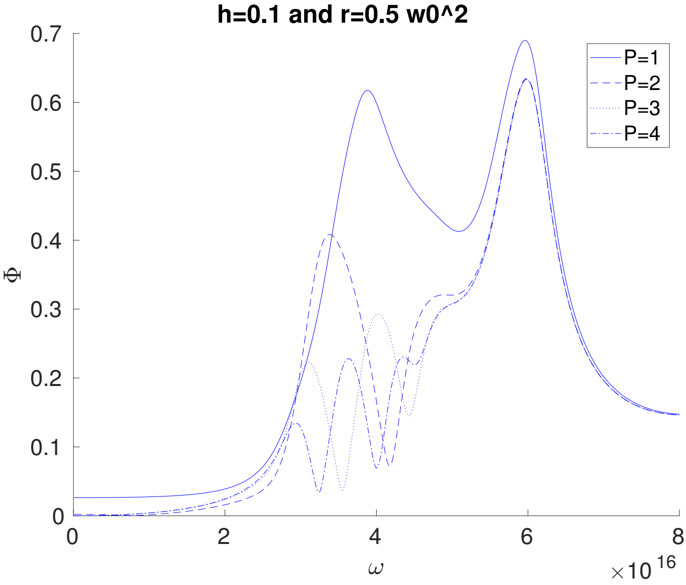

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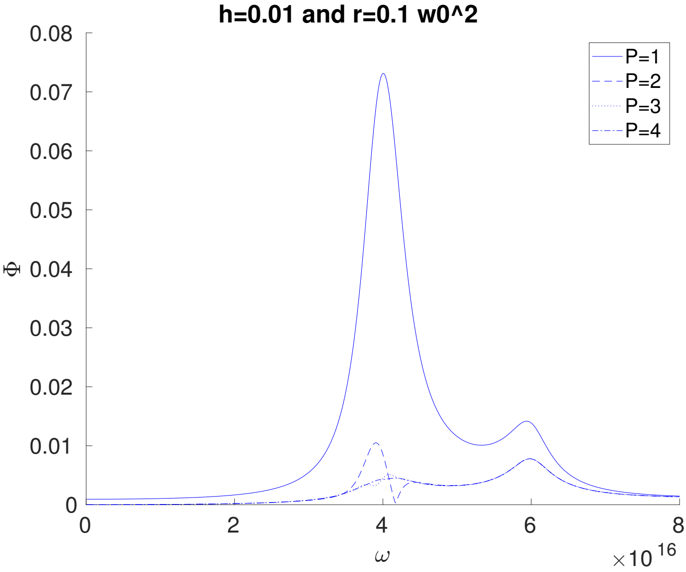

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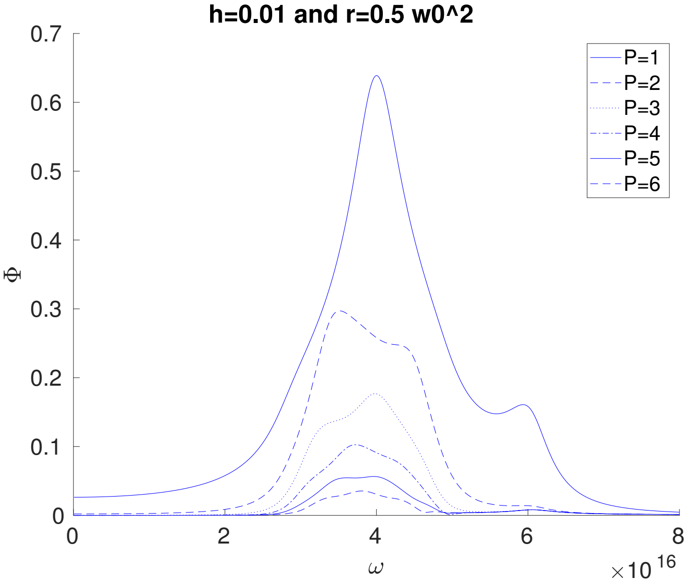

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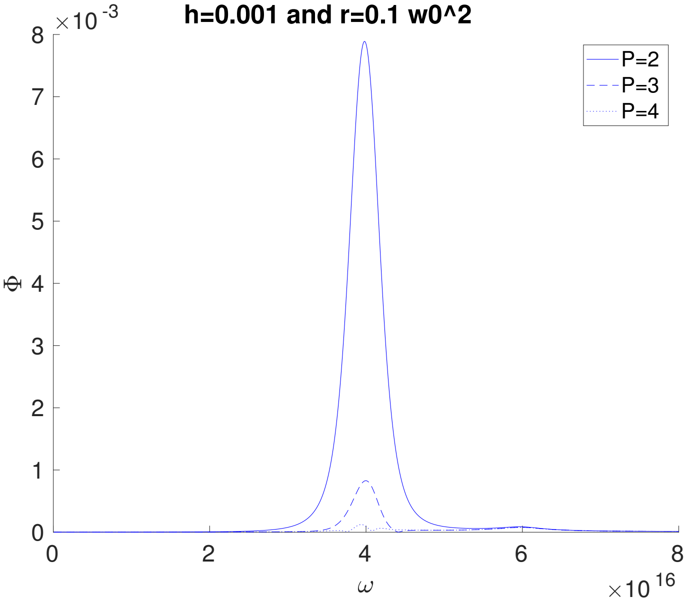

Figure: Plots of phase error at $\theta = 0$.

Future Directions

- Extend to
  - Drude
  - meta-material models
  - nonlinear polarization models
  - viscoelastic system (partially done)
- Inverse problems from (actual) time-domain data

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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, $i = 0, \ldots, p$,

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

where

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

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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 $Var(y(t,\xi)) \approx \sum_{j=1}^{p} \alpha_j(t)^2$.

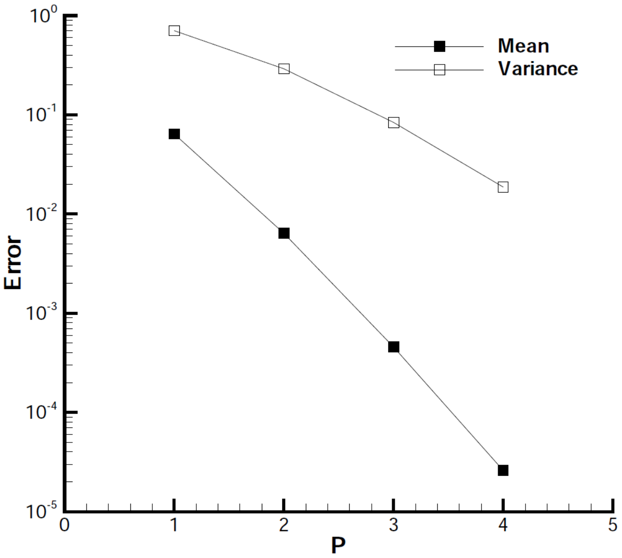

Figure: Convergence of error with Gaussian random variable by Hermitian-chaos.

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

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

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.