Polynomial Chaos Approach for Maxwell's Equations in Dispersive Media

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Outline

Acknowledgments

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- Karen Barrese and Neel Chugh (REU 2008)
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- Megan Armentrout (MS 2011)
- Brian McKenzie (MS 2011)
- Duncan McGregor (MS 2013, PhD 2016?)

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.

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

$\mathbf{P} =$	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.
- 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

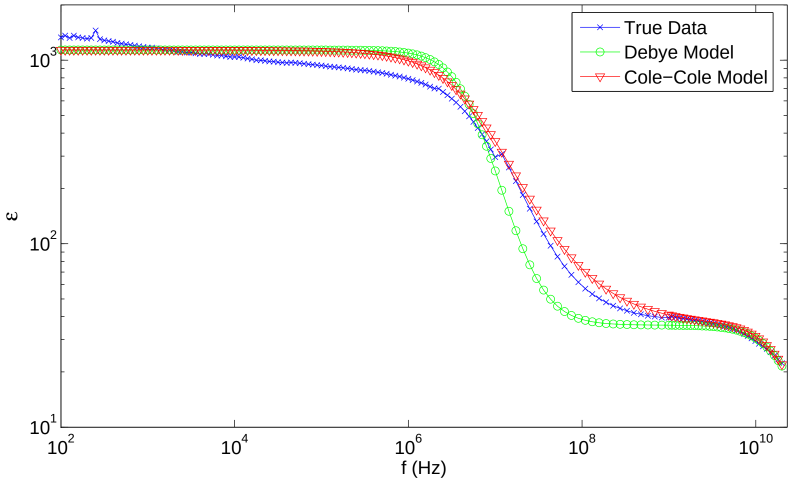


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

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) $\mathbf{q} = [\epsilon_\infty, \epsilon_d, \tau, \alpha]$

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

Outline

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.

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.

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
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times [von Schweidler1907]

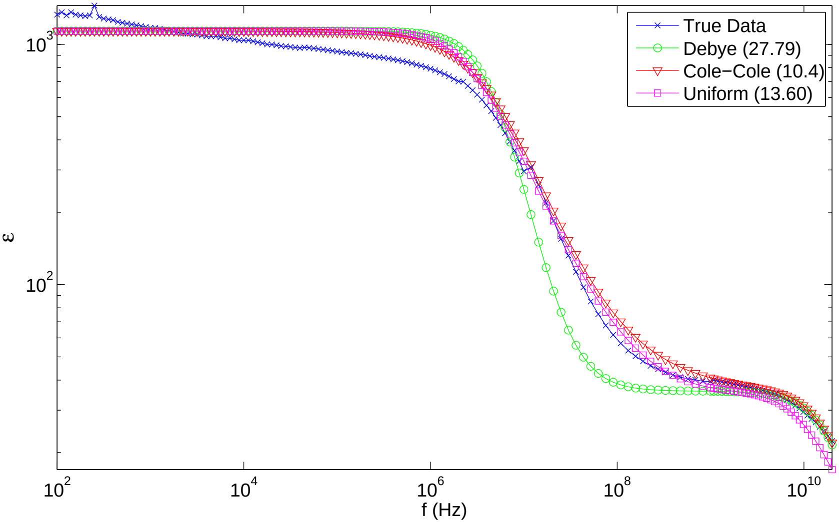


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

Random Polarization

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 $(t, \mathbf{x})$

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

Outline

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., 201X)

The dispersion relation for the system (2) *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

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

Stability Estimates for Maxwell-Random Debye

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

Theorem (G., 201X)

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

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

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

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{3a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial \alpha_{0,x}}{\partial t}, \tag{3b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial \alpha_{0,y}}{\partial t}, \tag{3c}$$

$$A\dot{\vec{\alpha}}_x + \vec{\alpha}_x = \vec{f}_x, \tag{3d}$$

$$A\dot{\vec{\alpha}}_y + \vec{\alpha}_y = \vec{f}_y. \tag{3e}$$

where $\vec{f}_x = \epsilon_0 \epsilon_d E_x \hat{e}_1$ and $\vec{f}_y = \epsilon_0 \epsilon_d E_y \hat{e}_1$.

Outline

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

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

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

Outline

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

$$A\frac{\vec{\alpha}_j^{n+\frac{1}{2}} - \vec{\alpha}_j^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}_j^{n+\frac{1}{2}} + \vec{\alpha}_j^{n-\frac{1}{2}}}{2} = \frac{\vec{f}_j^{n+\frac{1}{2}} + \vec{f}_j^{n-\frac{1}{2}}}{2}. \tag{4}$$

Couple this with the equations from above:

$$\epsilon_0\epsilon_\infty\frac{E_j^{n+\frac{1}{2}} - E_j^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n}{\Delta z} - \frac{\alpha_{0,j}^{n+\frac{1}{2}} - \alpha_{0,j}^{n-\frac{1}{2}}}{\Delta t} \tag{5a}$$

$$\mu_0\frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}}}{\Delta z}. \tag{5b}$$

Energy Decay and Stability

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

Theorem (G., 201X)

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

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

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

Theorem (G., 2013)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme in (4) and (5) 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

$$\Phi = \left| \frac{k_{\mathrm{EX}} - k_{\Delta}}{k_{\mathrm{EX}}} \right|, \tag{6}$$

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 assume a uniform distribution and the following parameters which are appropriate constants for modeling aqueous Debye type materials:

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

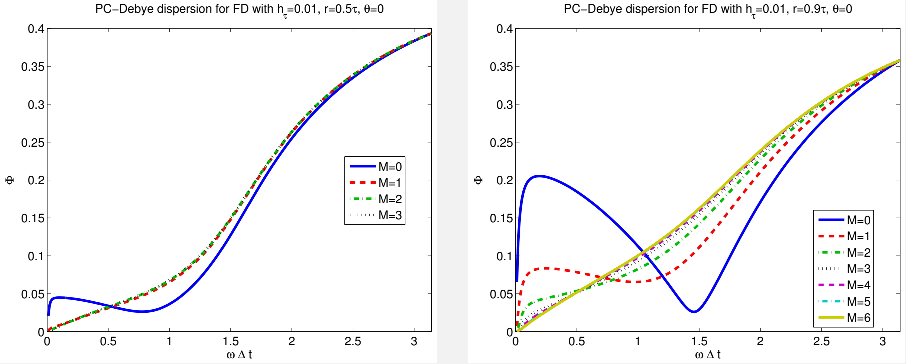
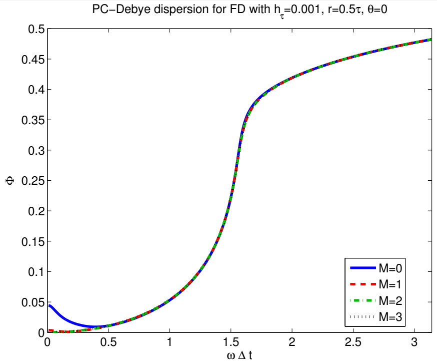
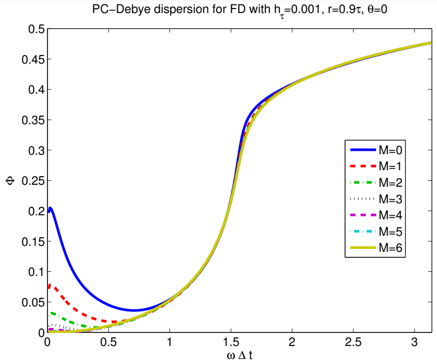


Figure: Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$.





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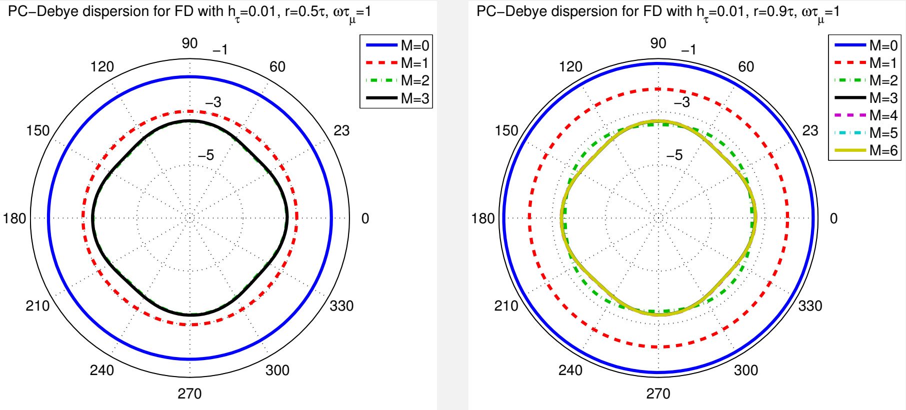
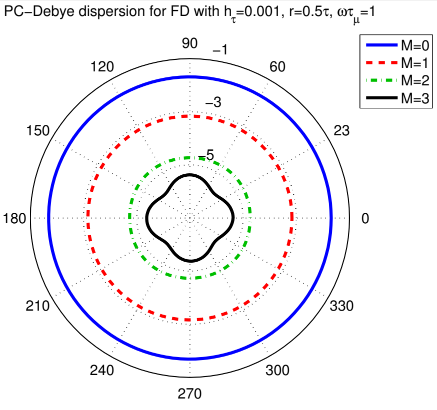
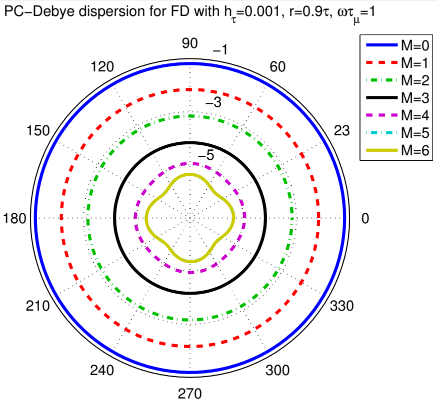


Figure: Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. Legend indicates degree M of the PC expansion.





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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

References

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