Electromagnetic wave propagation in complex dispersive media

Associate Professor
Department of Mathematics
Oregon State University

Workshop on Quantification of Uncertainties in Material Science
January 15, 2016

A Polynomial Chaos Method for Microscale Modeling

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Outline

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Acknowledgments

Collaborators

- H. T. Banks (NCSU)
- V. A. Bokil (OSU)
- W. P. Winfree (NASA)

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)
- Duncan McGregor (MS 2013, PhD 2016?)

Preliminaries

Havriliak-Negami (H-N)

A general (phenomenological) material model that arises from considerations of the multi-scale nature of the spatial microstructure of a broad class of materials (e.g., glassy, soils, biological tissues, and amorphous polymers). [a]

[a] See "A complex plane representation of dielectric and mechanical relaxation processes in some polymers", J. Polym. Sci, 1967.

Corresponds to a fractional psuedo-differential equation model in the time domain, not suitable for efficient simulation.

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

- 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

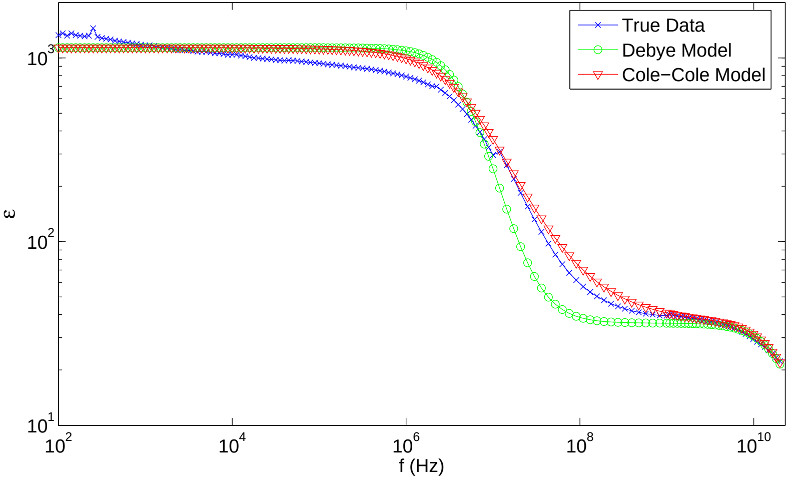

Figure : Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96]. Note: up to 10% spread in measurements was observed, but only averages were published.

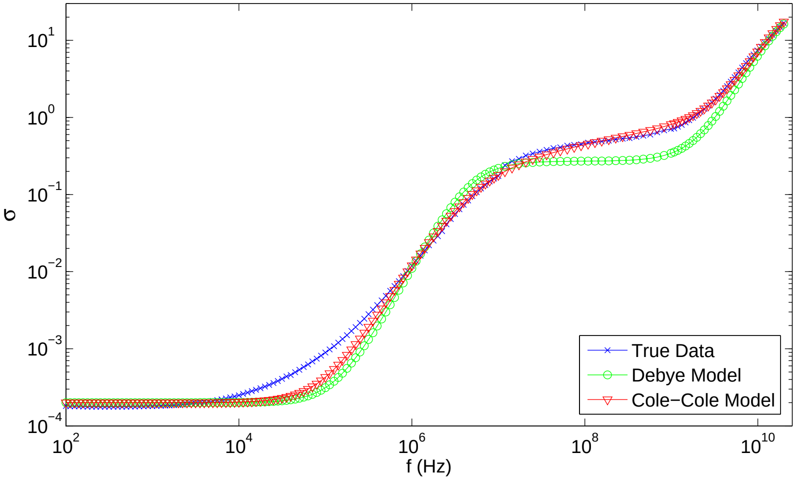

Figure : Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

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

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

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

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

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

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

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

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

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

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

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

- 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

- The macroscopic Debye polarization model can be derived from microscopic dipole formulations by passing to a limit over the molecular population [see, Elliot1993].

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- "Continuous spectrum relaxation functions" are also common in viscoelastic models.

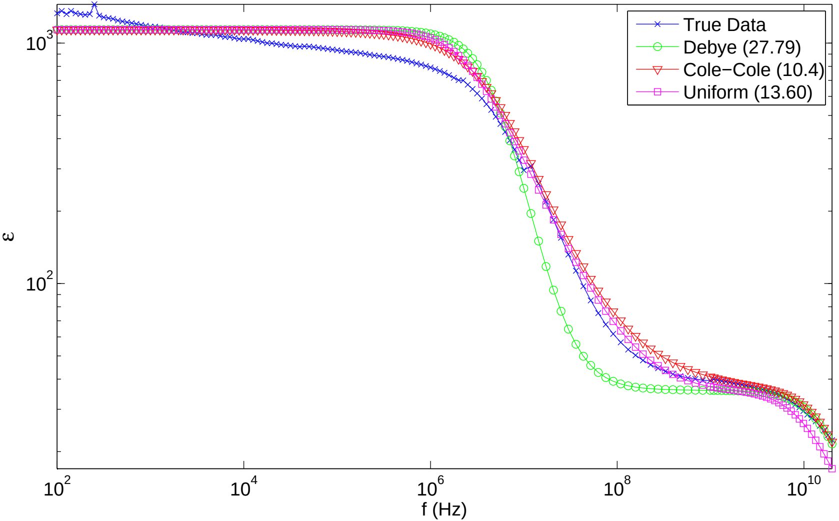

Figure : Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

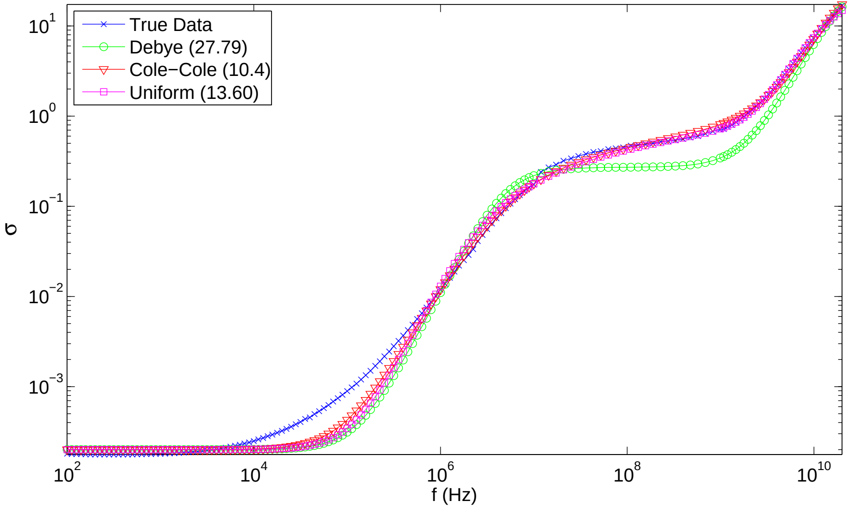

Figure : Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

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.

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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 to approximate each spatial component of the random polarization

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

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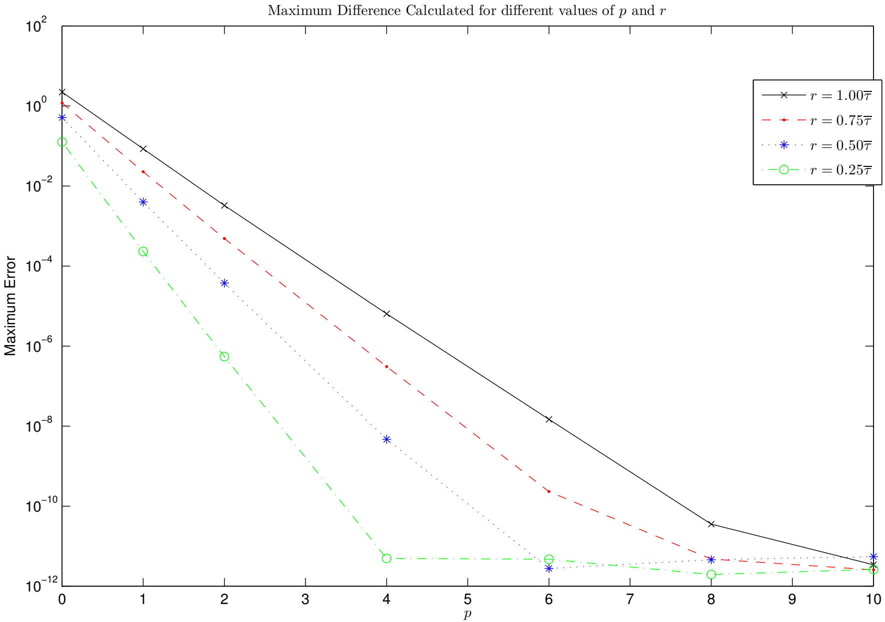
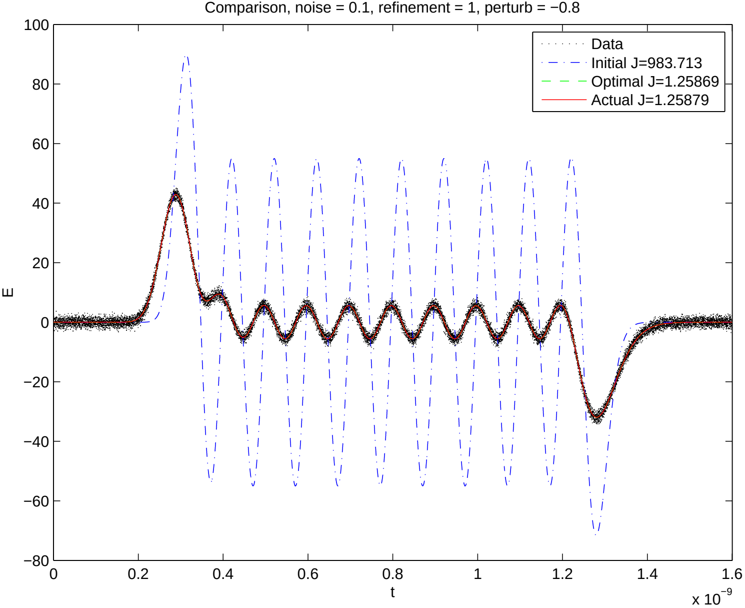
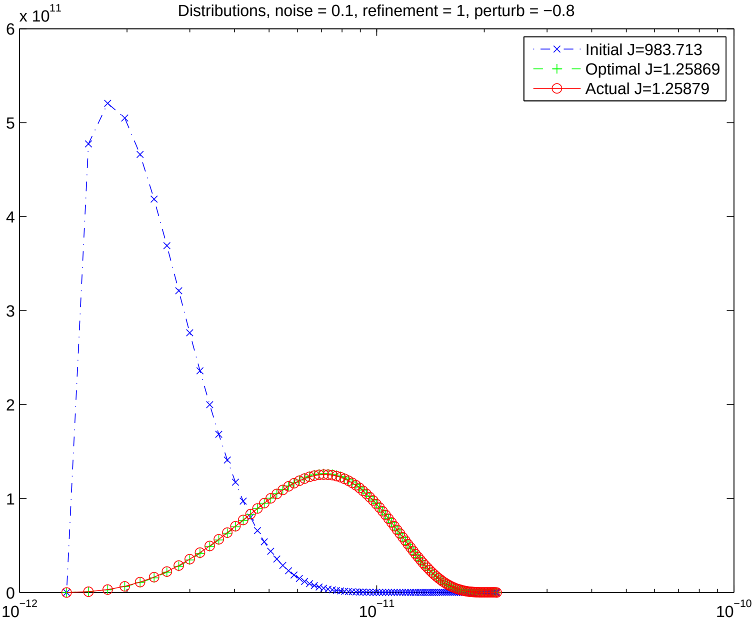
The electric field depends on the macroscopic polarization, the expected value of the random polarization at each point $(t, \mathbf{x})$, which is

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

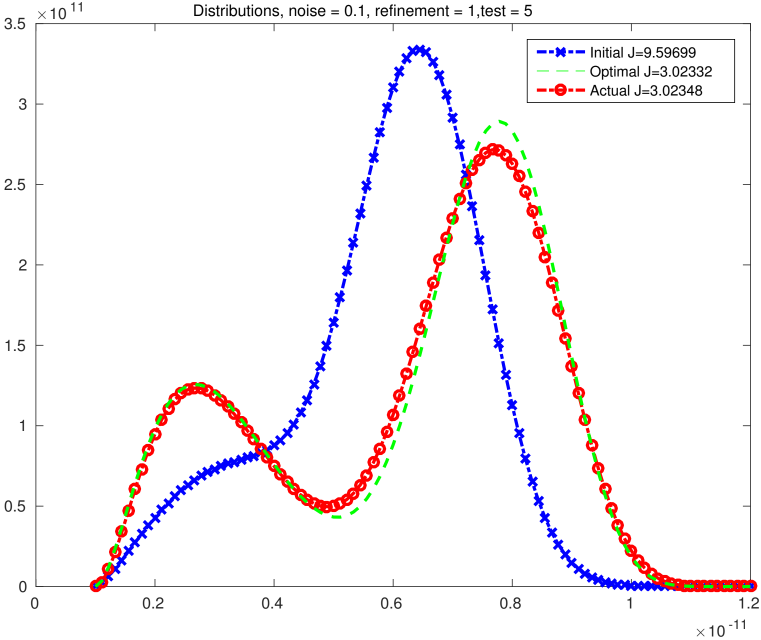

Maximum Difference Calculated for different values of p and r
Maximum Error
p
r = 1.00τ̄
r = 0.75τ̄
r = 0.50τ̄
r = 0.25τ̄
10^2
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
0
1
2
3
4
5
6
7
8
9
10



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



Comparison of initial to final distribution [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

Maxwell-Random Debye system

In a polydispersive Debye material, we have

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

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

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

with

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

Theorem (G., 2015)

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

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

where the expected complex permittivity is given by

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

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

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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.

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.

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.

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

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

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].

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

$$\Phi = \left| \frac{k_{\mathrm{EX}} - k_{\Delta}}{k_{\mathrm{EX}}} \right|, \tag{2}$$

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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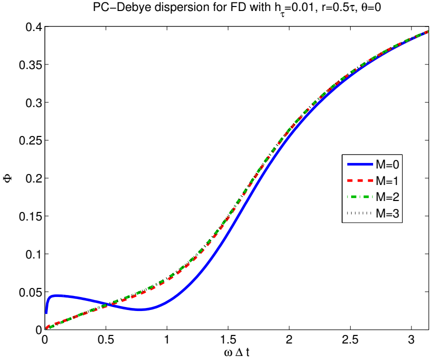
- We wish to examine the phase error as a function of $\omega\Delta t$ in the range $[0, \pi]$. Δt is determined by $h_\tau \tau_m$, while $\Delta x = \Delta y$ determined by CFL condition.
- We note that $\omega\Delta t = 2\pi/N_{\mathrm{ppp}}$, where N_{ppp} is the number of points per period, and 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:

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



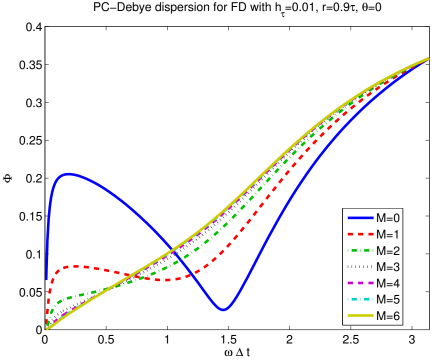
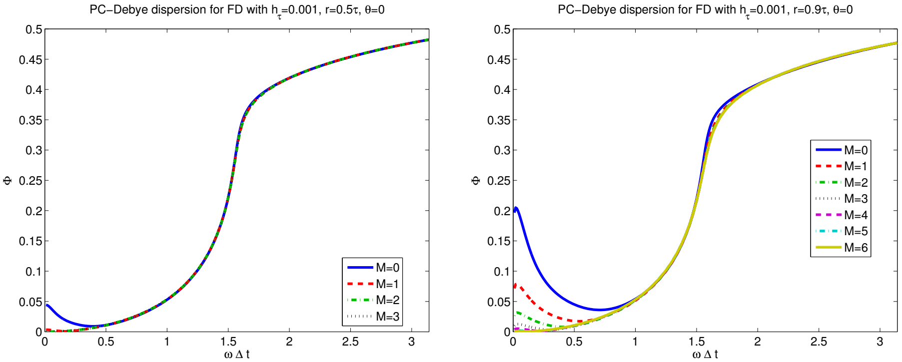


Figure : Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$.



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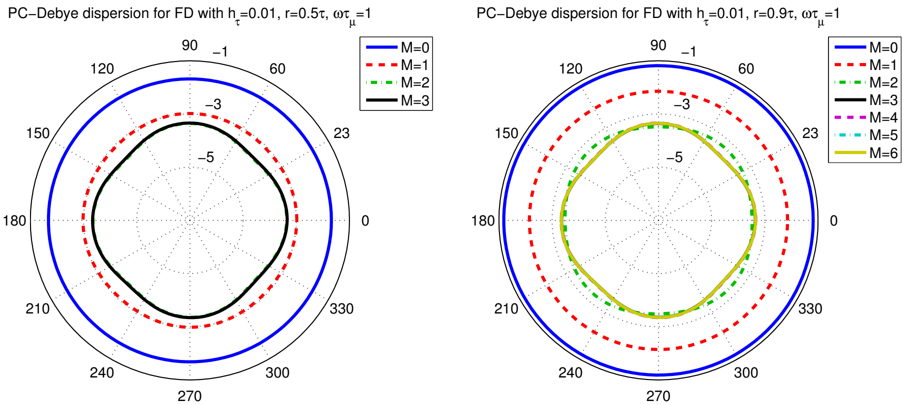
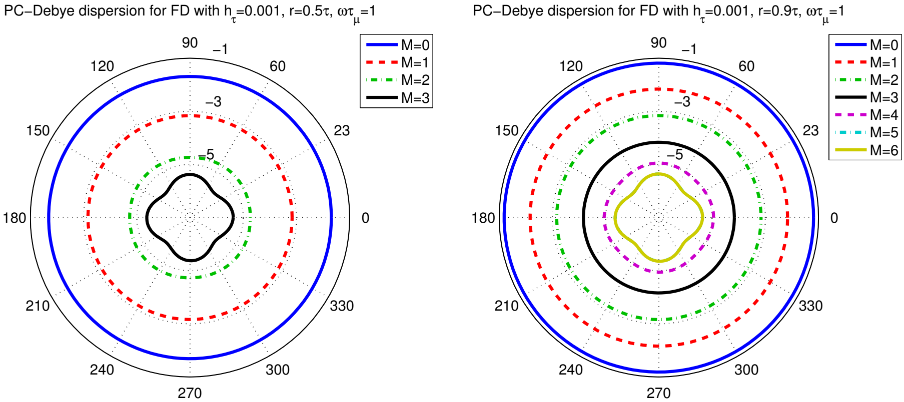


Figure : Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. Legend indicates degree M of the PC expansion.



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- Exponential convergence in the number of PC terms was demonstrated
- We have proven (conditional) stability of the scheme via energy decay (not shown)[1]
- We have derived a discrete dispersion relation and computed phase errors

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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

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

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

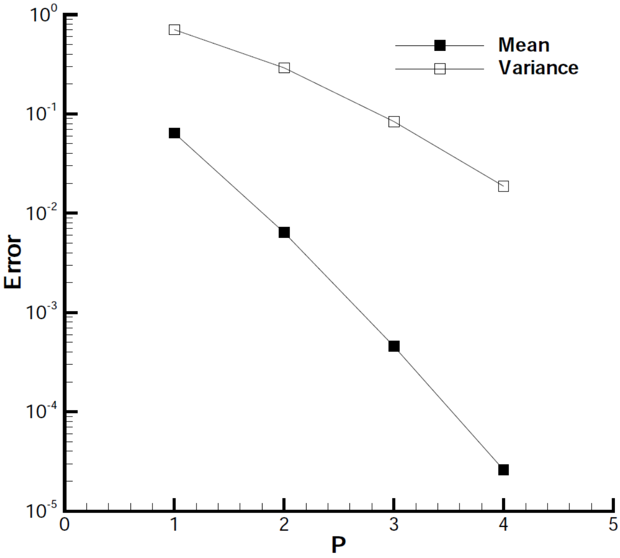

Figure : Convergence of error with Gaussian random variable by Hermitian-chaos.

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.