Modeling and Simulation of Electromagnetic Materials

Prof. Nathan L. Gibson

Department of Mathematics

Oregon State University OSU

Graduate Student Seminar
Feb 27, 2019

Projects

1. Electromagnetics
    - Dispersive Media
    - Numerical Analysis
    - Inverse Problems
    - Uncertainty Quantification
2. Hydropower Reservoir Networks
    - River system and modeling equations
    - Optimal Control
    - Robust Optimization
3. Magnetohydrodynamics
    - Modeling
    - Numerical Methods
    - Inverse Problems

Acknowledgments

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; PhD 2016)

Outline

1. **Electromagnetics**
   - Maxwell's Equations
   - Polarization Models
   - Distribution of Parameters
   - Polynomial Chaos
   - Results

Outline

1. **Electromagnetics**
   - Maxwell's Equations
   - Polarization Models
   - Distribution of Parameters
   - Polynomial Chaos
   - Results

2. **Conclusions**

Outline

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H} \qquad \text{(Ampere)}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \text{(Faraday)}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Poisson)}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss)}$$

$\mathbf{E} =$ Electric field vector

$\mathbf{H} =$ Magnetic field vector

$\rho =$ Electric charge density

$\mathbf{D} =$ Electric flux density

$\mathbf{B} =$ Magnetic flux density

$\mathbf{J} =$ Current density

With appropriate initial conditions and boundary conditions.

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

Complex permittivity

- We can usually define **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.

Dispersive Dielectrics

Debye Material

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

Dispersive Media

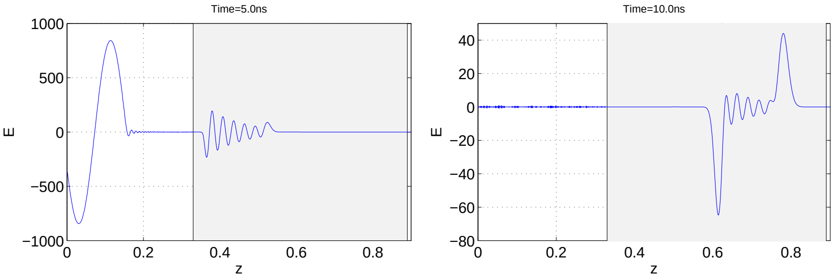


Figure: Debye model simulations.

Dry skin data

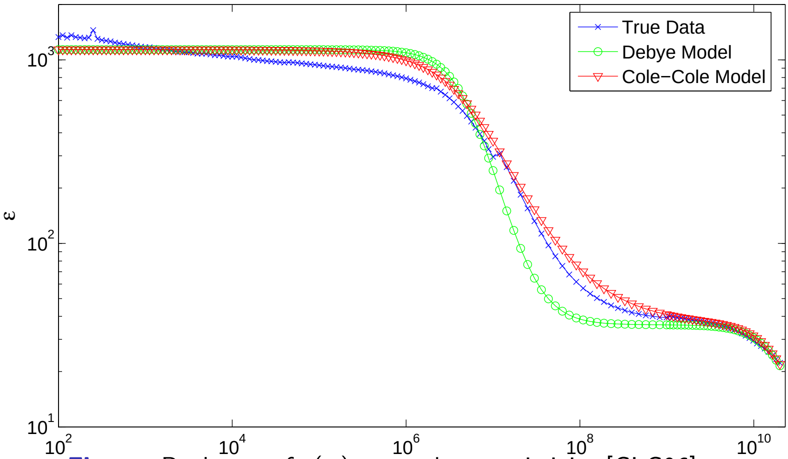


Figure: Real part of $\epsilon(\omega)$, ϵ, of the permittivity [GLG96].

Dry skin data

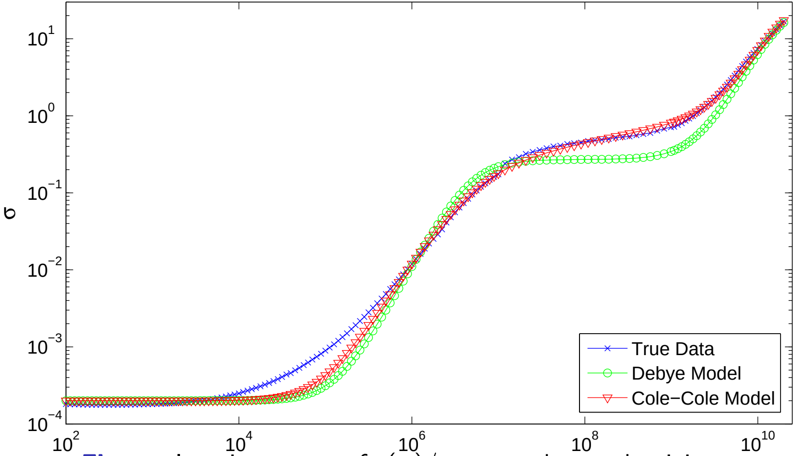


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Motivation

- The Cole-Cole model corresponds to a fractional order ODE in the time-domain and is difficult to simulate

Motivation

- 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

Motivation

- 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)

Motivation

- 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]

Motivation

- 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)

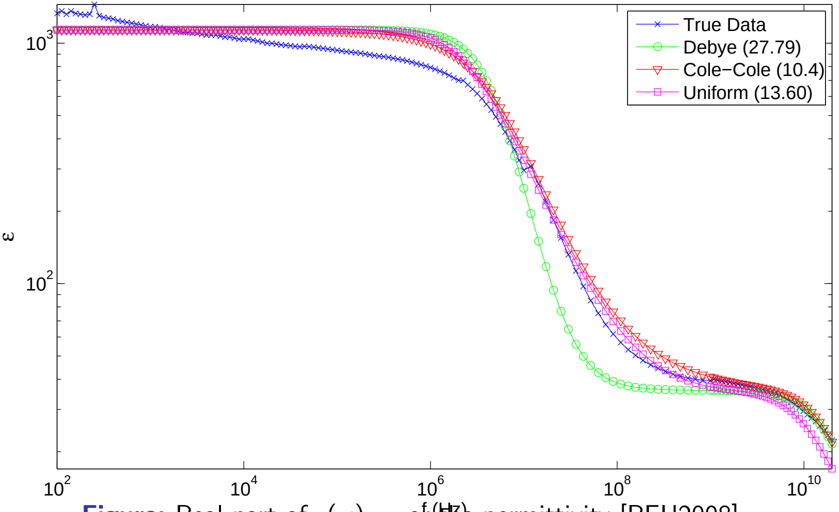


Figure: Real part of $\epsilon(\omega)$, ϵ, of the permittivity [REU2008].

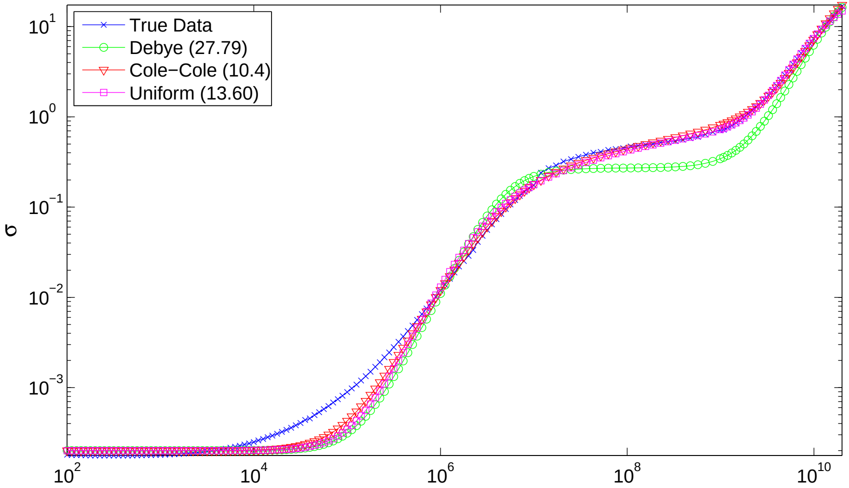


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

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

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

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

$$\mathbf{P}(t, \mathbf{x}) = \int_0^t \int_{\mathcal{Q}} g(t - s, \mathbf{x}; \mathbf{q}) dF(\mathbf{q}) \, \mathbf{E}(s, \mathbf{x}) ds.$$

Alternatively we can swap the order of integration

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

and define the random polarization $\mathcal{P}(t, \mathbf{x}; F)$ to be the polarization corresponding to a random q, thus the macroscopic polarization $\mathbf{P}$ is understood to be the expected value of $\mathcal{P}$.

Random Polarization

For the Debye model the random polarization $\mathcal{P}(t, \mathbf{x}; F)$ satisfies

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

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

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

for a uniform distribution $\mathcal{U}[\tau_a, \tau_b]$.
The electric field depends on the macroscopic polarization, which in this example becomes

$$\mathbf{P}(t, \mathbf{x}) = \frac{1}{\tau_b - \tau_a} \int_{\tau_a}^{\tau_b} \mathcal{P}(t, \mathbf{x}; \tau) d\tau.$$

Polynomial Chaos

Apply the Polynomial Chaos method to approximate the random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d E, \quad \tau = \tau(\xi) = r\xi + m, \quad \xi \in (-1, 1)$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\vec{e_1}.$$

Polynomial Chaos

Apply the Polynomial Chaos method to approximate the random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d E, \quad \tau = \tau(\xi) = r\xi + m, \quad \xi \in (-1, 1)$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\vec{e_1}.$$

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

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

Existence of PC Solutions

Theorem (REU2010)

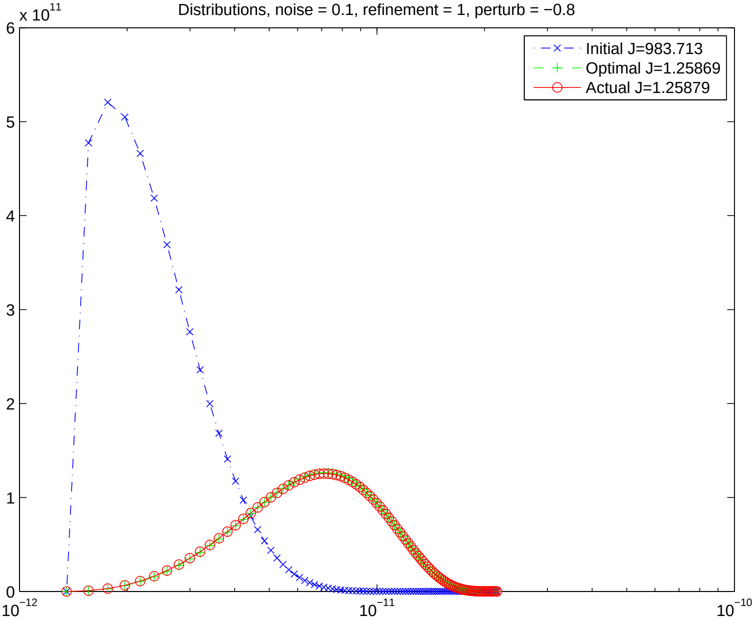
For the beta-Jacobi chaos (including uniform-Legendre), there exists a unique solution to the system

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

(with initial conditions) for any p.

Proof.

Relies on the fact that the invertibility of A follows from $\rho(M) < 1$ and the assumption that $\tau_\mu > \tau_\sigma$. This is physically reasonable as to disallow negative relaxation times. □



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

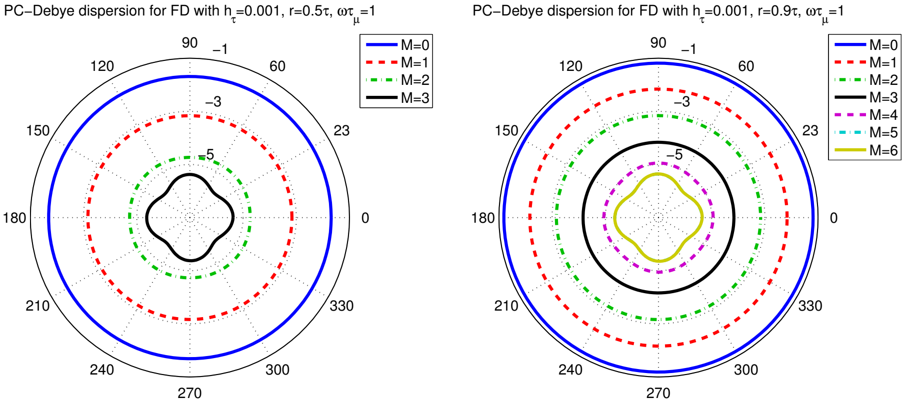


Figure: Log plots of phase error versus θ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.001$. Legend indicates degree M of the PC expansion.

Outline

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM (Done by others), DG, etc.

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM (Done by others), DG, etc.
- We have shown (conditional) stability of the scheme via energy decay

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM (Done by others), DG, etc.
- We have shown (conditional) stability of the scheme via energy decay
- We have used a discrete dispersion relation to compute phase errors

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM (Done by others), DG, etc.
- 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 confirmed

Conclusions/Future Work

- We have presented a random ODE model for polydispersive Debye media, can be extended to many other important polarization models (Lorentz: Done; Non-linear: ?; Viscoelastic: In progress)
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM (Done by others), DG, etc.
- 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 confirmed
- Questions remaining: Random Maxwell? Random media vs effective distribution?

References

- Bokil, V. A. & Gibson, N. L. (2012), Analysis of Spatial High Order Finite Difference Methods for Maxwell's equations in dispersive media, *IMA J. Numer. Anal.* 32 (3): 926-956.
- 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*, 11(4).
- Gibson, N. L. (2015), A Polynomial Chaos Method for Dispersive Electromagnetics, *Comm. in Comp. Phys.*, 18(5).