Modeling and Simulation of Electromagnetic Materials

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Projects

1. Electromagnetics
   - Maxwell's Equations
   - Dispersive Media
   - Numerical Analysis
   - Inverse Problems

2. Hydropower Reservoir Networks
   - River system and modeling equations
   - Optimal Control
   - Robust Optimization

3. Magnetohydrodynamics
   - Modeling
   - Numerical Methods
   - Inverse Problems
Acknowledgements

Collaborators

- H. T. Banks (NCSU)
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Students

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- Brian McKenzie (MS 2011)
- Duncan McGregor (PhD 2016)
Electromagnetics
- Maxwell’s Equations
- Polarization Models
- Distribution of Parameters
- Polynomial Chaos
- Results
Outline

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2 Conclusions
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Maxwell’s Equations

\[
\begin{align*}
\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} &= \nabla \times \mathbf{H} \quad \text{(Ampere)} \\
\frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} \quad \text{(Faraday)} \\
\nabla \cdot \mathbf{D} &= \rho \quad \text{(Poisson)} \\
\nabla \cdot \mathbf{B} &= 0 \quad \text{(Gauss)}
\end{align*}
\]

\[\mathbf{E} = \text{Electric field vector} \quad \mathbf{D} = \text{Electric flux density}\]
\[\mathbf{H} = \text{Magnetic field vector} \quad \mathbf{B} = \text{Magnetic flux density}\]
\[\rho = \text{Electric charge density} \quad \mathbf{J} = \text{Current density}\]

With appropriate initial conditions and boundary conditions.
Maxwell’s equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

\[
\begin{align*}
D &= \varepsilon E + P \\
B &= \mu H + M \\
J &= \sigma E + J_s
\end{align*}
\]

- **P** = Polarization  \( \varepsilon = \) Electric permittivity
- **M** = Magnetization  \( \mu = \) Magnetic permeability
- **J_s** = Source Current  \( \sigma = \) Electric Conductivity
Complex permittivity

- We can usually define $P$ in terms of a convolution

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

where $g$ is the dielectric response function (DRF).

- In the frequency domain $\hat{D} = \hat{\varepsilon} \hat{E} + \hat{g}\hat{E} = \varepsilon_0\varepsilon(\omega) \hat{E}$, where $\varepsilon(\omega)$ is called the complex permittivity.

- $\varepsilon(\omega)$ 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 $\varepsilon(\omega)$ over a broad range of frequencies.
Dispersive Dielectrics

Debye Material

Input is five cycles (periods) of a sine curve.
Figure: Debye model simulations.
Dry skin data

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{Real part of $\epsilon(\omega)$, $\epsilon$, or the permittivity [GLG96].}
\end{figure}
Dry skin data

Figure: Imaginary part of $\varepsilon(\omega)/\omega$, $\sigma$, or the conductivity.
\[ P(t, x) = g \ast E(t, x) = \int_0^t g(t - s, x; q)E(s, x)\, ds, \]

- Debye model [1929] \( q = [\epsilon_d, \tau] \)

\[ g(t, x) = \epsilon_0 \epsilon_d / \tau \ e^{-t/\tau} \]

or \( \tau \dot{P} + P = \epsilon_0 \epsilon_d E \)

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

with \( \epsilon_d := \epsilon_s - \epsilon_\infty \) and \( \tau \) a relaxation time.
\[ \mathbf{P}(t, \mathbf{x}) = g \ast \mathbf{E}(t, \mathbf{x}) = \int_0^t g(t - s, \mathbf{x}; \mathbf{q}) \mathbf{E}(s, \mathbf{x}) ds, \]

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with \( \epsilon_d := \epsilon_s - \epsilon_\infty \) and \( \tau \) 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.
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Empirical measurements suggest a log-normal or Beta distribution ([Wagner1913](#)) (but uniform is easier).
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- 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).

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- 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 $\epsilon(\omega)$, $\epsilon$, of the permittivity [REU2008].
Figure: Imaginary part of $\varepsilon(\omega)/\omega$, $\sigma$, or the conductivity [REU2008].
Distributions of Parameters

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

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

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

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

Alternatively we can swap the order of integration

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

and define the random polarization $\mathcal{P}(t, \mathbf{x}; F)$ to be the polarization corresponding to a random $\mathbf{q}$, 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 $\mathcal{P}(t, x; F)$ satisfies

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

where $\tau$ 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

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

Apply the Polynomial Chaos method to approximate the random polarization

\[ \tau \dot{\mathcal{P}} + \mathcal{P} = \varepsilon_0 \varepsilon_d E, \quad \tau = \tau(\xi) = r\xi + m, \quad \xi \in (-1, 1) \]

resulting in

\[ (rM + ml) \dot{\alpha} + \bar{\alpha} = \varepsilon_0 \varepsilon_d E \bar{e}_1. \]
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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

\[ A\dot{\alpha} + \alpha = \bar{g} \]

(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.
Distributions, noise = 0.1, refinement = 1, perturb = -0.8

Initial J=983.713
Optimal J=1.25869
Actual J=1.25879

Comparison of initial to final distribution [Armentrout-G., 2011].
**Figure:** Log plots of phase error versus $\theta$ 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.
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We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM, DG, etc.
Conclusions/Future Work

- We have presented a random ODE model for polydisperse Debye media, can be extended to many other important polarization models.
- We developed an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD), can be extended to FEM, DG, etc.
- We have shown (conditional) stability of the scheme via energy decay.
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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.
REFERENCES


