Inverse Problems for Distributions of Parameters in PDE Systems

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Outline

1. **Inverse Problems**
   - Preliminaries
   - Distributions

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2. **Maxwell's Equations**
   - Description
   - Simplifications
   - Discretization

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   - Random Polarization
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Acknowledgments

Collaborators

- H. T. Banks (NCSU)
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Students

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- Duncan McGregor (MS 2013, PhD 2016)

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$$\mathcal{A} = \begin{bmatrix} 0 & \frac{1}{\mu}\frac{\partial}{\partial x} \\ \frac{1}{\epsilon}\frac{\partial}{\partial x} & 0 \end{bmatrix}$$

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- $u = [H, E, P]^T$, $q = [\epsilon, \mu, \tau]$ with $c = \sqrt{(}1/\epsilon\mu)$

$$\mathcal{A} = \frac{1}{\tau}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1-\epsilon & c \\ 0 & \frac{\epsilon-1}{c} & -1 \end{bmatrix} + \begin{bmatrix} 0 & \frac{1}{\mu}\frac{\partial}{\partial x} & 0 \\ \frac{1}{\epsilon}\frac{\partial}{\partial x} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

  yields 1D Maxwell's equations with Debye polarization.

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An example of a numerical method is to replace $\frac{\partial u}{\partial x}$ at (t_j, x_i) with

$$\frac{U_{i,j} - U_{i-1,j}}{\Delta x}$$

for some fixed $\Delta x = x_i - x_{i-1}$. Called a finite difference.

Inverse Problems

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An inverse problem estimates quantities *indirectly* by using measurements of other quantities.

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For example, a parameter estimation inverse problem attempts to determine values of a parameter set given (discrete) observations of (some) state variables.

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- Mathematically, find

$$\min_{q \in Q_{ad}} \left\| error\left(E(q), \hat{E}\right) \right\|.$$

For example, with data measured at fixed x and discrete times t_j

$$\min_{q \in Q_{ad}} \frac{1}{N} \sum_{j=1}^{N} \left(E(t_j; q) - \hat{E}_j\right)^2$$

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  is called the nonlinear least squares method.
- Need a (fast) method for computing E.

Distributions of Parameters

In many systems, the dynamics are not completely described by a single parameter set. Often there are many different values of the parameters at work, and we only see the *average effect*.

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Expected value of solutions is given by

$$u(t,x;F) = \int_{\mathcal{Q}} \mathcal{U}(t,x;q)dF(q),$$

where $\mathcal{Q}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{Q})$.

Inverse Problem for F

- Given data $\{\hat{E}\}_j$ we seek to determine a probability distribution F^*, such that

$$F^* = \min_{F \in \mathfrak{P}(\mathcal{Q})} \mathcal{J}(F),$$

where, for example,

$$\mathcal{J}(F) = \sum_j \left(E(t_j; F) - \hat{E}_j \right)^2 .$$

- Given a trial distribution F_k we compute $E(t_j; F_k)$ and test $\mathcal{J}(F_k)$, then update F_{k+1} as necessary to find a minimum.
- Need either a parametrization or a discretization of F_k to have a finite dimensional problem.
- Need a (fast) method for computing $E(x, t; F)$.

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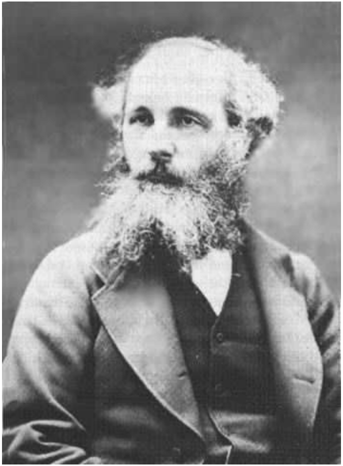
Maxwell's Equations



- Maxwell's Equations were formulated circa 1870.
- They represent a fundamental unification of electric and magnetic fields predicting electromagnetic wave phenomenon.

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	$\mathbf{D} =$	Electric displacement
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density
$\rho =$	Electric charge density	$\mathbf{J} =$	Current density

Note: Need 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.

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

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Linear, Isotropic, Non-dispersive and Non-conductive media

Assume no material dispersion, i.e., speed of propagation is not frequency dependent.

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} \\ \mathbf{B} &= \mu \mathbf{H} \end{aligned}}$$

$\epsilon = \epsilon_0 \epsilon_r$ $\epsilon_r =$ Relative Permittivity

$\mu = \mu_0 \mu_r$ $\mu_r =$ Relative Permeability

Maxwell's Equations in One Space Dimension

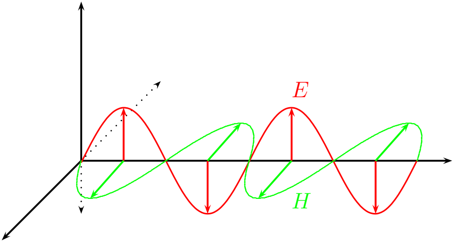
- The time evolution of the fields is thus completely specified by the curl equations

$$\epsilon \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H}$$
$$\mu \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}$$

- Assuming that the electric field is polarized to oscillate only in the y direction, propagate in the x direction, and there is uniformity in the z direction:

Equations involving E_y and H_z.

$$\epsilon \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x}$$
$$\mu \frac{\partial H_z}{\partial t} = -\frac{\partial E_y}{\partial x}$$



The Yee Scheme

In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations **(finite difference time domain or FDTD)**

- **Staggered Grids**: Choose E components on integer points in space and time, and H components on the half-grids in both variables.
- **Idea**:First order derivatives are much more accurately evaluated on staggered grids, such that if a variable is located on the integer grid, its first derivative is best evaluated on the half-grid and vice-versa.

Yee Scheme in One Space Dimension

$$\frac{H_z|_{r+\frac{1}{2}}^{n+\frac{1}{2}} - H_z|_{r+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\mu}\frac{E_y|_{r+1}^{n} - E_y|_{r}^{n}}{\Delta x}$$

$$\frac{E_y|_{r}^{n+1} - E_y|_{r}^{n}}{\Delta t} = -\frac{1}{\epsilon}\frac{H_z|_{r+\frac{1}{2}}^{n+\frac{1}{2}} - H_z|_{r-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x}$$

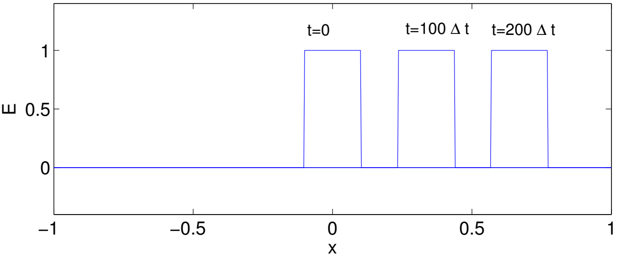
- This method is an explicit second order scheme in both space and time.
- It is conditionally stable with the CFL condition

$$\nu = \frac{c\Delta t}{\Delta x} \leq 1$$

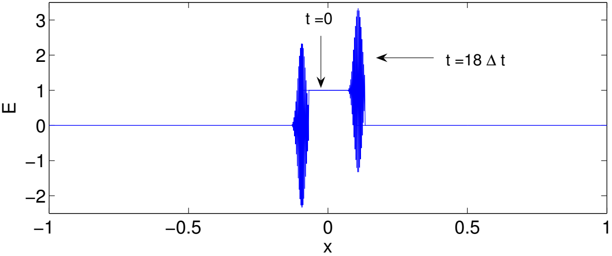
where ν is called the Courant number and $c = 1/\sqrt{\epsilon\mu}$.

Numerical Stability: A Square Wave

- Case $c\Delta t = \Delta x$



- Case $c\Delta t > \Delta x$



Numerical Dispersion: A Square Wave

- Case $c\Delta t = \Delta x$
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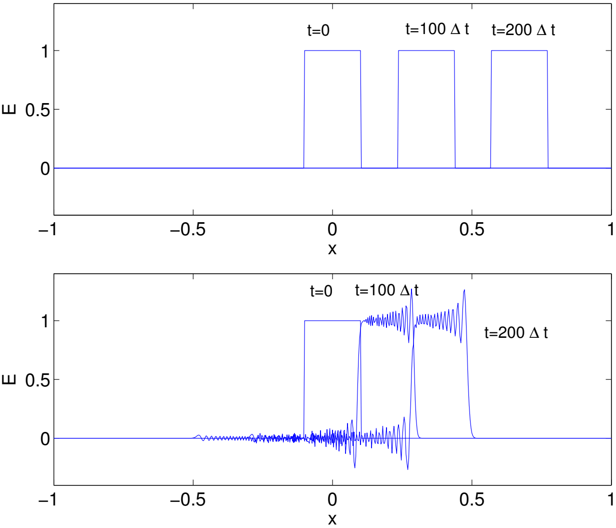

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Dispersive Dielectrics

- Recall

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

where **P** is the dielectric polarization.

- Debye model

$$g(t, \mathbf{x}) = \epsilon_0(\epsilon_s - \epsilon_\infty)/\tau \;\; e^{-t/\tau}$$

or

$$\tau \dot{\mathbf{P}} + \mathbf{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)\mathbf{E}$$

where $q = \{\epsilon_\infty, \epsilon_s, \tau\}$ and, in particular, τ is called the relaxation time.

Frequency Domain

- Converting to frequency domain via Fourier transforms

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

becomes

$$\hat{\mathbf{D}} = \epsilon(\omega)\hat{\mathbf{E}}$$

where $\epsilon(\omega)$ is called the complex permittivity.

- Debye model gives

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

- Cole-Cole model (heuristic generalization)

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

Unfortunately, the Cole-Cole model corresponds to a fractional order differential equation in the time domain, and simulation is not straight-forward.

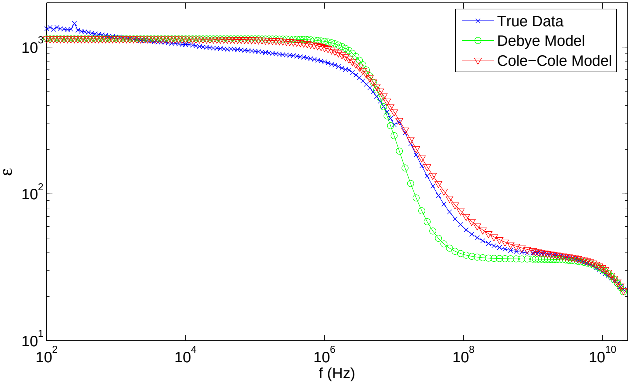

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity.

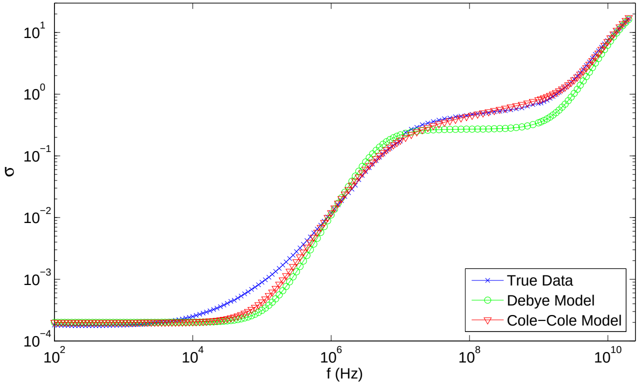

Figure: Imaginary part of $\epsilon(\omega)$, σ, or the conductivity.

Distributions of Relaxation Times

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

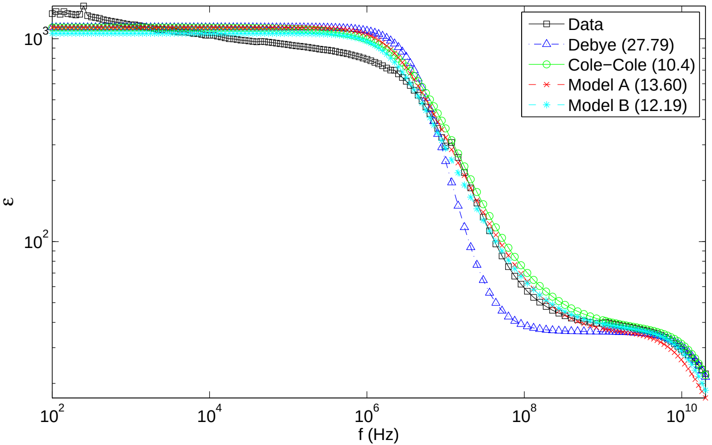

Figure: Real part of $\epsilon(\omega)$, called simply ϵ, or the permittivity. Model A refers to the Debye model with a uniform distribution on τ.

Random Polarization

We define the random polarization $\mathcal{P}(x,t;\tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E$$

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

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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 (x, t)

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

Numerical Approximation of Random Polarization

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Numerical Approximation of Random Polarization

Recall, to solve the inverse problem for the distribution of relaxation times, we need a method of accurately and efficiently simulating $P(x, t; F)$.

- Could apply a quadrature rule to the integral in the expected value. Results in a linear combination of individual Debye solves.
- Alternatively, we can use a method which separates the time derivative from the randomness and applies a truncated expansion in random space, called Polynomial Chaos. Results in a linear system.

Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear ODE

$$\dot{y} = -ky, \quad k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0, 1).$$

We apply a Polynomial Chaos expansion in terms of orthogonal Hermite polynomials H_j to the solution y:

$$y(t, \xi) = \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi)$$

then the ODE becomes

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi),$$

Triple recursion formula

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi),$$

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

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

Galerkin Projection onto span($\{\phi_i\}_{i=0}^{p}$)

Taking the weighted inner product with each basis gives

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

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

Where

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

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Where

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

Using 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

Letting $\vec{\alpha}$ represent the vector containing $\alpha_0(t), \ldots, \alpha_p(t)$ (and assuming $\alpha_{p+1}(t)$, 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 mean value of $y(t, \xi)$ is $\alpha_0(t)$.

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

$$M = \begin{bmatrix} b_0 & a_1 & & & \\ c_0 & b_1 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_p \\ & & & c_{p-1} & b_p \end{bmatrix}$$

Generalizations

Consider the non-homogeneous ODE

$$\dot{y} + ky = g(t), \quad k = k(\xi) = \sigma\xi + \mu, \quad \xi \sim \mathcal{N}(0, 1).$$

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

$$\dot{\vec{\alpha}} + (\sigma M + \mu I)\vec{\alpha} = g(t)\vec{e_1}.$$

Exponential convergence

- Any set of orthogonal polynomials can be used in the truncated expansion, but there may be an optimal choice.
- If the polynomials are orthogonal with respect to weighting function $f(\xi)$, and k has PDF $f(k)$, then it is known that the PC solution converges exponentially in terms of p.
- In practice, approximately 4 are generally sufficient.

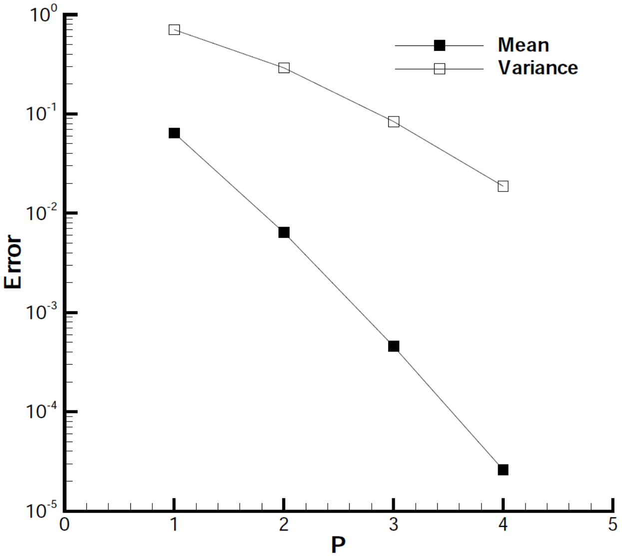

Figure: Convergence of error with Gaussian random coefficient by fourth-order Hermitian-chaos.

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.

Random Polarization

We can apply Polynomial Chaos method to our random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E, \quad \tau = \tau(\xi) = r\xi + r$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1} =: \vec{g}$$

or

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

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

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

Applying the central difference approximation, based on the Yee scheme, Maxwell's equations with conductivity and polarization included

$$\epsilon \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \sigma E - \frac{\partial P}{\partial t}$$

and

$$\mu \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z}$$

become

$$\frac{E_k^{n+\frac{1}{2}} - E_k^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\epsilon}\frac{H_{k+\frac{1}{2}}^{n} - H_{k-\frac{1}{2}}^{n}}{\Delta z} - \frac{\sigma}{\epsilon}\frac{E_k^{n+\frac{1}{2}} + E_k^{n-\frac{1}{2}}}{2} - \frac{1}{\epsilon}\frac{P_k^{n+\frac{1}{2}} - P_k^{n-\frac{1}{2}}}{\Delta t}$$

and

$$\frac{H_{k+\frac{1}{2}}^{n+1} - H_{k+\frac{1}{2}}^{n}}{\Delta t} = -\frac{1}{\mu}\frac{E_{k+1}^{n+\frac{1}{2}} - E_k^{n+\frac{1}{2}}}{\Delta z}.$$

Note that while the electric field and magnetic field are staggered in time, the polarization updates simultaneously with the electric field.

Need a similar approach for discretizing the PC system

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

Applying second order central differences, as before, to $\vec{\alpha} = \vec{\alpha}(z_k)$:

$$A\frac{\vec{\alpha}^{n+\frac{1}{2}} - \vec{\alpha}^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}^{n+\frac{1}{2}} + \vec{\alpha}^{n-\frac{1}{2}}}{2} = \frac{\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}}{2}.$$

Combining like terms gives

$$(2A + \Delta t I)\vec{\alpha}^{n+\frac{1}{2}} = (2A - \Delta t I)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t \left(\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}\right)$$

Note that we first solve the discrete electric field equation for $E_k^{n+\frac{1}{2}}$ and plug in here (in $\vec{g}^{n+\frac{1}{2}}$) to update $\vec{\alpha}$.

Comments on Polynomial Chaos

- Gives a simple and efficient method to simulate systems involving distributions of parameters.
- Works equally well in three spatial dimensions.
- Limitation: choice of polynomials depends on type of distribution.
- Need error estimates to be sure that a sufficient number of polynomials is used in the expansion.

Outline

1. Inverse Problems
   - Preliminaries
   - Distributions
2. Maxwell's Equations
   - Description
   - Simplifications
   - Discretization
3. Polarization
   - Description
   - Random Polarization
   - Polynomial Chaos
4. **Inverse Problem for Distribution**

Inverse Problem for RTD

Now that we have a numerical method for simulating Maxwell's equations with random polarization

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

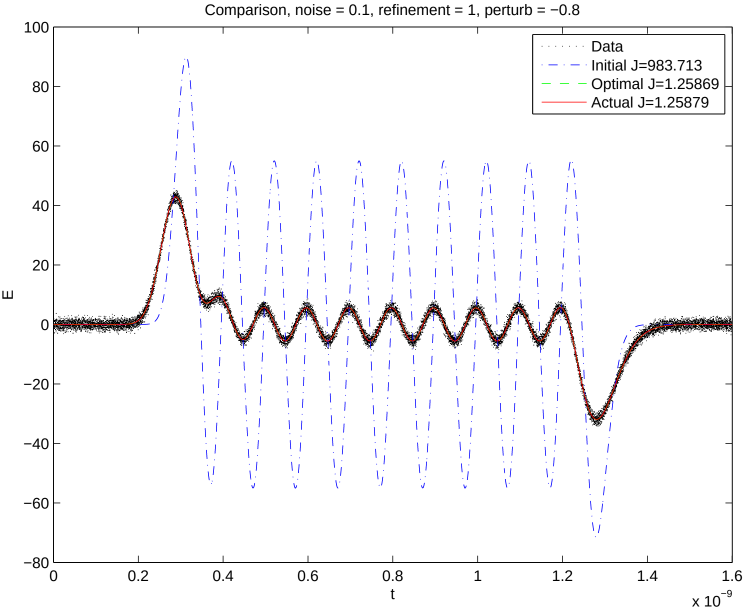
we address the inverse problem for the relaxation time distribution F.

- Given data $\{\hat{E}\}_j$ we seek to determine a probability distribution F^*, such that

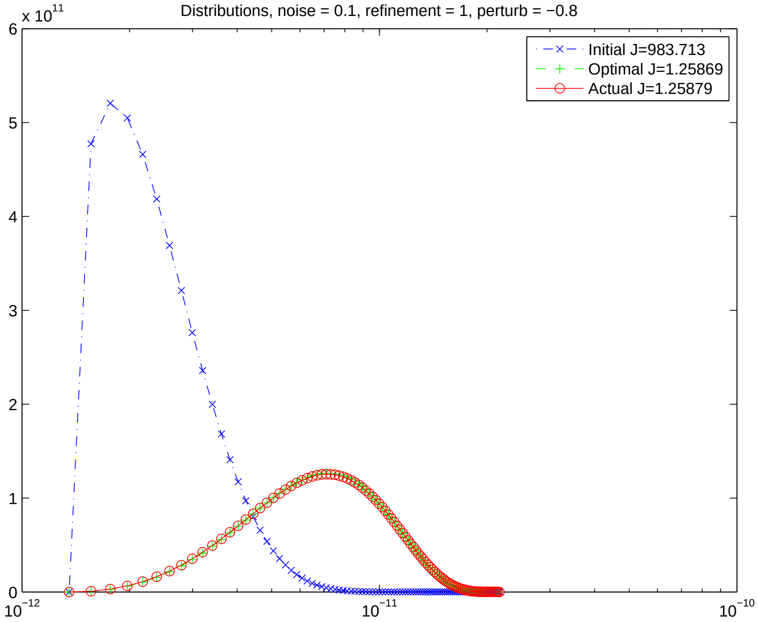
$$F^* = \min_{F\in\mathfrak{P}(\mathcal{Q})} \mathcal{J}(F),$$

where

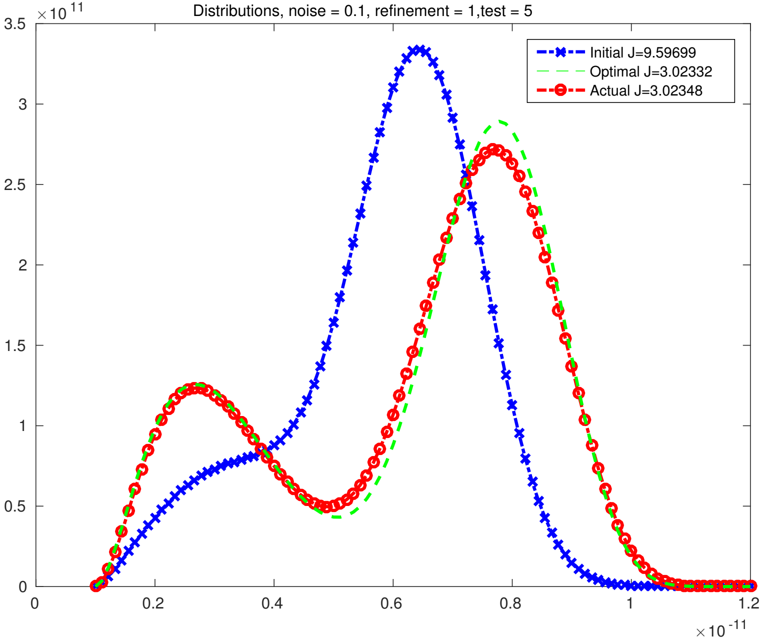
$$\mathcal{J}(F) = \sum_j k\left(E(t_j;F) - \hat{E}_j\right)^2.$$



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