1 Inverse Problems
   - Preliminaries
   - Distributions
Outline

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2 Maxwell’s Equations
   - Description
   - Simplifications
   - Discretization
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   - Random Polarization
   - Polynomial Chaos
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4 Inverse Problem for Distribution
Acknowledgments

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4 Inverse Problem for Distribution
\[
\frac{\partial u}{\partial t} - Au = f
\]

where \( u \) is called a state variable, \( A \) is a linear operator depending on a set of parameters \( q \), and \( f \) is a source term.
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\frac{\partial u}{\partial t} - A u = f
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Examples

- \( A = c \frac{\partial}{\partial x}, \ q = c \) yields a one-way wave equation.
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\frac{\partial u}{\partial t} - \mathcal{A}u = f
\]
where \( u \) is called a state variable, \( \mathcal{A} \) is a linear operator depending on a set of parameters \( q \), and \( f \) is a source term.

Examples

- \( \mathcal{A} = c \frac{\partial}{\partial x}, \ q = c \) yields a one-way wave equation.
- \( u = [v, w]^T, \ q = [\epsilon, \mu] \) and

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

yields the 1D Maxwell’s equations (wave equation) with speed \( c = \sqrt{(1/\epsilon \mu)} \).
\[ \frac{\partial u}{\partial t} - Au = f \]

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\[ A = \begin{bmatrix} 0 & 1 \frac{\partial}{\partial x} \\ \frac{1}{\epsilon} \frac{\partial}{\partial x} & 0 \end{bmatrix} \]

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

\[ A = \frac{1}{\tau} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 - \epsilon & c \\ 0 & \frac{\epsilon - 1}{c} & -1 \end{bmatrix} + \begin{bmatrix} 0 & 1 \frac{\partial}{\partial x} & 0 \\ \frac{1}{\epsilon} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

yields 1D Maxwell’s equations with Debye polarization.
Forward Problem

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For all but a simple class of PDEs, this involves numerical approximations to discrete solutions

\[ U_{i,j} \approx u(x_i, t_j). \]

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.
Definition

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.
Parameter Identification

In the context of Maxwell’s equations:
- Estimate $q$ using $E(q)$ (not easily invertible)
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- Given *real-life* data $\hat{E}$, use several trial values of $q$ to compute (simulate) several $E(q)$ values

Mathematically, find $\min_{q \in Q} \| \text{error}(E(q), \hat{E}) \|$. For example, with data measured at fixed $x$ and discrete times $t_j$:

$$\min_{q \in Q} \sum_{j=1}^{N} (E(t_j; q) - \hat{E}_j)^2$$

is called the nonlinear least squares method.
Parameter Identification

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- The value of \( q \) that results in an \( E(q) \) which is a “best match” to \( \hat{E} \) is likely close to the *real-life* value of \( q \).
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- The value of $q$ that results in an $E(q)$ which is a “best match” to $\hat{E}$ is likely close to the *real-life* value of $q$.
- Mathematically, find

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

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 $E$. 
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*.

Example: population growth
\[
y' = -ry \quad \text{with} \quad r \sim N(0, 1).
\]

Expected value of solutions is given by
\[
u(t, x; F) = \int_{Q} U(t, x; q) \, dF(q),
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where $Q$ is some admissible set and $F \in P(Q)$. 

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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*. To account for the effect of possible multiple parameter sets \( q \), we define a probability distribution \( F(q) \).
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In these cases it not sufficient to use the average value of the parameters, rather one must compute all possible solutions and take the average of those.

Example: population growth \( y' = -ry \) with \( r \sim \mathcal{N}(0, 1) \).
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*. To account for the effect of possible multiple parameter sets $q$, we define a *probability distribution* $F(q)$. In these cases it not sufficient to use the average value of the parameters, rather one must compute all possible solutions and take the average of those.

Example: population growth $y' = -ry$ with $r \sim \mathcal{N}(0, 1)$. 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 $F \in \mathcal{P}(\mathcal{Q})$. 
Inverse Problem for $F$

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

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

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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2. Maxwell’s Equations
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   - Discretization

3. Polarization
   - Description
   - Random Polarization
   - Polynomial Chaos

4. Inverse Problem for Distribution
Maxwell’s Equations were formulated circa 1870. They represent a fundamental unification of electric and magnetic fields predicting electromagnetic wave phenomenon.
Maxwell’s Equations

\[
\frac{\partial D}{\partial t} + J = \nabla \times H \quad \text{(Ampere)}
\]

\[
\frac{\partial B}{\partial t} = -\nabla \times E \quad \text{(Faraday)}
\]

\[
\nabla \cdot D = \rho \quad \text{(Poisson)}
\]

\[
\nabla \cdot B = 0 \quad \text{(Gauss)}
\]

**E** = Electric field vector  \hspace{1cm} **D** = Electric displacement

**H** = Magnetic field vector  \hspace{1cm} **B** = Magnetic flux density

**\rho** = Electric charge density  \hspace{1cm} **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.

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

- **P** = Polarization
- **M** = Magnetization
- **J_s** = Source Current

\( \epsilon = \) Electric permittivity
\( \mu = \) Magnetic permeability
\( \sigma = \) Electric Conductivity
Linear, Isotropic, Non-dispersive and Non-conductive media

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

\[
\begin{align*}
D &= \varepsilon E \\
B &= \mu H
\end{align*}
\]

\[
\begin{align*}
\varepsilon &= \varepsilon_0 \varepsilon_r \\
\varepsilon_r &= \text{Relative Permittivity} \\
\mu &= \mu_0 \mu_r \\
\mu_r &= \text{Relative Permeability}
\end{align*}
\]
Maxwell’s Equations in One Space Dimension

- The time evolution of the fields is thus completely specified by the curl equations
  \[
  \varepsilon \frac{\partial E}{\partial t} = \nabla \times H \\
  \mu \frac{\partial H}{\partial t} = -\nabla \times E
  \]

- 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 \( H_z \).

\[
\varepsilon \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} \\
\mu \frac{\partial H_z}{\partial t} = -\frac{\partial E_y}{\partial x}
\]
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.
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 \( \nu \) is called the Courant number and \( c = 1/\sqrt{\epsilon \mu} \).
Maxwell’s Equations

Discretization

Numerical Stability: A Square Wave

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

- Case $c\Delta t > \Delta x$
Numerical Dispersion: A Square Wave

- Case $c\Delta t = \Delta x$
- Case $c\Delta t < \Delta x$
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4 Inverse Problem for Distribution
Dispersive Dielectrics

- Recall
  \[ D = \varepsilon E + P \]
  where \( P \) is the dielectric polarization.

- Debye model
  \[ g(t, x) = \frac{\varepsilon_0 (\varepsilon_s - \varepsilon_\infty)}{\tau} e^{-t/\tau} \]
  or
  \[ \tau \dot{P} + P = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) E \]
  where \( q = \{ \varepsilon_\infty, \varepsilon_s, \tau \} \) and, in particular, \( \tau \) 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 $\epsilon(\omega)$, $\epsilon$, or the permittivity.
Figure: Imaginary part of $\epsilon(\omega)$, $\sigma$, or the conductivity.
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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[In 1913, Wagner proposed a (continuous) distribution of relaxation times. Empirical measurements suggest a log-normal or Beta distribution [Bottcher-Bordewijk1978]. One can show that the Cole-Cole model corresponds to a continuous distribution. It is possible to calculate the necessary distribution function by the method of Fuoss and Kirkwood.
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- “Continuous spectrum relaxation functions” are also common in viscoelastic models.
Figure: Real part of $\epsilon(\omega)$, called simply $\epsilon$, or the permittivity. Model A refers to the Debye model with a uniform distribution on $\tau$. 
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 $\tau$ 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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The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point $(x, t)$

$$P(x, t; F) = \int_{\tau_a}^{\tau_b} \mathcal{P}(x, t; \tau) f(\tau) d\tau.$$
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.
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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 \( \xi \) by using the triple recursion formula for Hermite polynomials

\[ \xi H_j = jH_{j-1} + H_{j+1}. \]

Thus

\[ \sum_{j=0}^{\infty} \dot{\alpha}_j(t) \phi_j + \alpha_j(t)(j \phi_{j-1} + \phi_{j+1}) = 0. \]
Taking the weighted inner product with each basis gives

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

\(i = 0, \ldots, p.\)

Where

\[
\langle f(\xi), g(\xi) \rangle_W = \int f(\xi)g(\xi)W(\xi)d\xi.
\]
Galerkin Projection onto \( \text{span}(\{\phi_i\}_{i=0}^{p}) \)

Taking the weighted inner product with each basis gives

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

\( i = 0, \ldots, p. \)

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

\[
\dot{\alpha}_i \langle \phi_i, \phi_i \rangle_W + (i + 1) \alpha_{i+1} \langle \phi_i, \phi_i \rangle_W + \alpha_{i-1} \langle \phi_i, \phi_i \rangle_W = 0, \quad i = 0, \ldots, p,
\]
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

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

\[ \dot{\alpha}_i + \sigma [(i + 1)\alpha_{i+1} + \alpha_{i-1}] + \mu \alpha_i = g(t)\delta_{0i}, \quad i = 0, \ldots, p, \]

or the deterministic ODE system

\[ \ddot{\alpha} + (\sigma M + \mu I)\dot{\alpha} = g(t)\hat{e}_1. \]
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.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Polynomial</th>
<th>Support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian</td>
<td>Hermite</td>
<td>$(-\infty, \infty)$</td>
</tr>
<tr>
<td>gamma</td>
<td>Laguerre</td>
<td>$[0, \infty)$</td>
</tr>
<tr>
<td>beta</td>
<td>Jacobi</td>
<td>$[a, b]$</td>
</tr>
<tr>
<td>uniform</td>
<td>Legendre</td>
<td>$[a, b]$</td>
</tr>
</tbody>
</table>

Note: lognormal random variables may be handled as a non-linear function (e.g., Taylor expansion) of a normal random variable.
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

\[ (rM + ml) \dot{\alpha} + \alpha = \epsilon_0 (\epsilon_s - \epsilon_{\infty}) E \mathbf{e}_1 =: \vec{g} \]

or

\[ A \dot{\alpha} + \alpha = \vec{g}. \]
Random Polarization

We can apply Polynomial Chaos method to our random polarization

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

resulting in

\[ (rM + ml)\dot{\alpha} + \alpha = \epsilon_0 (\epsilon_s - \epsilon_\infty) E \hat{e}_1 =: \tilde{g} \]

or

\[ A\dot{\alpha} + \alpha = \tilde{g}. \]

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

\[
\frac{E_{k+\frac{1}{2}}^{n+\frac{1}{2}} - E_{k-\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\epsilon} \frac{H_{k+\frac{1}{2}}^{n+\frac{1}{2}} - H_{k-\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta z} - \frac{\sigma}{\epsilon} \frac{E_{k+\frac{1}{2}}^{n+\frac{1}{2}} + E_{k-\frac{1}{2}}^{n-\frac{1}{2}}}{2} - \frac{1}{\epsilon} \frac{P_{k+\frac{1}{2}}^{n+\frac{1}{2}} - P_{k-\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t}
\]

and

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

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

\[ A \ddot{\alpha} + \dot{\alpha} = \vec{g}. \]

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

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

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

\[ F^* = \min_{F \in \mathbb{P}(Q)} J(F), \]

where

\[ J(F) = \sum_j k \left( E(t_j; F) - \hat{E}_j \right)^2. \]
Comparison of simulations to data [Armentrout-G., 2011].
Comparison of initial to final distribution [Armentrout-G., 2011].