Uncertainty Quantification Techniques in PDE Systems

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OSU Math Colloquium
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Outline

1. Polynomial Chaos

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1. **Polynomial Chaos**
2. **Electromagnetics**
   - Maxwell-Debye
   - Maxwell-Random Debye
   - Maxwell-PC Debye
   - PC-Debye FDTD
   - PC-Debye FDTD
   - Conclusions

Outline

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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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where

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

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

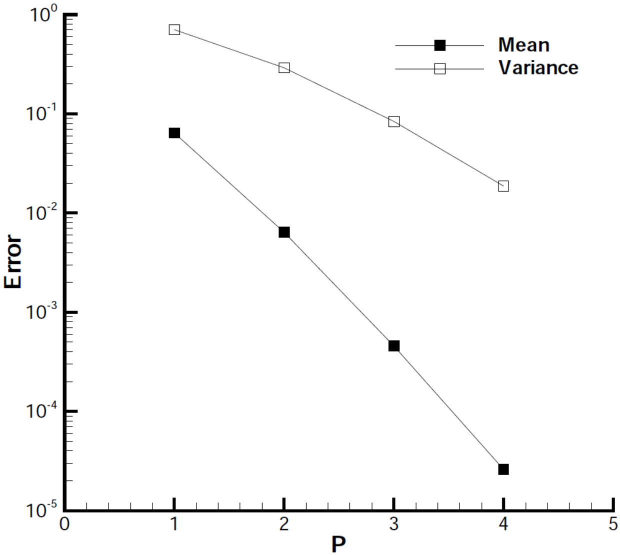

Figure: Convergence of error with Gaussian random variable by Hermitian-chaos.

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.

Outline

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- Brian McKenzie (MS 2011)
- Duncan McGregor (MS 2013, PhD 2016?)

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.

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

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

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
- 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.

Dry skin data

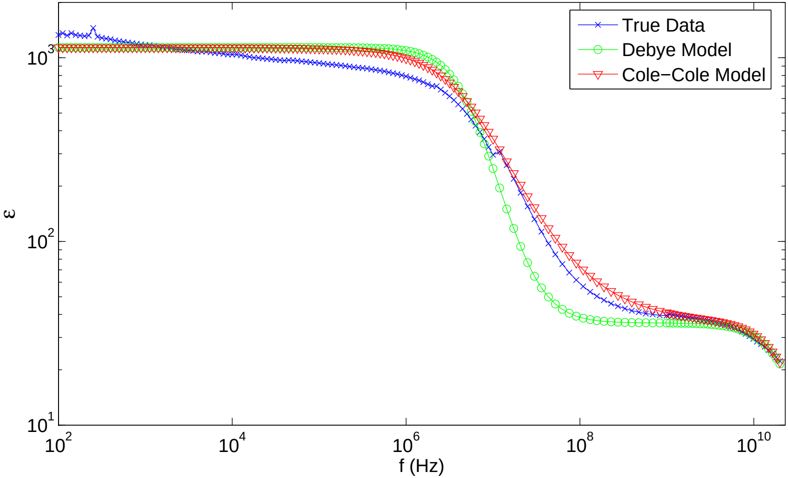

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

Dry skin data

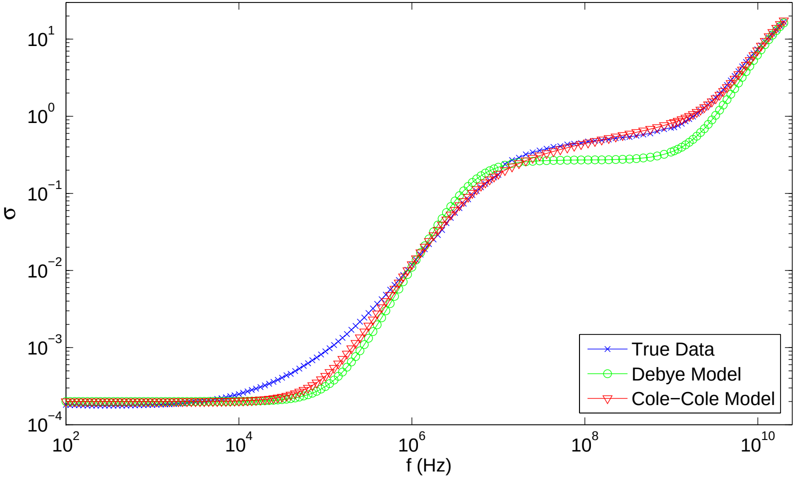

Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity.

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

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

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

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

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

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

Dispersive Media

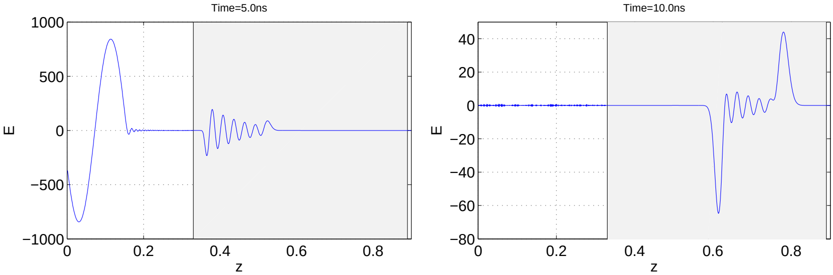


Figure: Debye model simulations.

Outline

Maxwell-Debye System

Combining Maxwell's Equations, Constitutive Laws, and the Debye model, we have

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

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

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

Assuming a solution to (1) of the form $\mathbf{E} = \mathbf{E_0} exp(i(\omega t - \mathbf{k} \cdot \mathbf{x}))$, the following relation must hold.

Debye Dispersion Relation

The dispersion relation for the Maxwell-Debye system is given by

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

where the complex permittivity is given by

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

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

2D Maxwell-Debye Transverse Electric (TE) curl equations

For simplicity in exposition and to facilitate analysis, we reduce the Maxwell-Debye model to two spatial dimensions (we make the assumption that fields do not exhibit variation in the z direction).

$$\mu_0 \frac{\partial H}{\partial t} = -\mathrm{curl}\ \mathbf{E}, \tag{2a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \mathbf{curl}\ H - \frac{\epsilon_0 \epsilon_d}{\tau}\mathbf{E} + \frac{1}{\tau}\mathbf{P} - \mathbf{J}, \tag{2b}$$

$$\tau \frac{\partial \mathbf{P}}{\partial t} = \epsilon_0 \epsilon_d \mathbf{E} - \mathbf{P}, \tag{2c}$$

where $\mathbf{E} = (E_x, E_y)^T, \mathbf{P} = (P_x, P_y)^T$ and $H_z = H$.

Note $\mathrm{curl}\ \mathbf{U} = \frac{\partial U_y}{\partial x} - \frac{\partial U_x}{\partial y}$ and $\mathbf{curl}\ V = \left(\frac{\partial V}{\partial y}, -\frac{\partial V}{\partial x}\right)^T$.

Stability Estimates for Maxwell-Debye

System is well-posed since solutions satisfy the following stability estimate.

Theorem (Li2010)

Let $\mathcal{D} \subset \mathbb{R}^2$, and let H, $\mathbf{E}$, and $\mathbf{P}$ be the solutions to (the weak form of) the 2D Maxwell-Debye TE system with PEC boundary conditions. Then the system exhibits energy decay

$$\mathcal{E}(t) \leq \mathcal{E}(0), \qquad \forall t \geq 0$$

where the energy is defined by

$$\mathcal{E}(t)^2 = \|\sqrt{\mu_0} H(t)\|_2^2 + \|\sqrt{\epsilon_0 \epsilon_\infty} \mathbf{E}(t)\|_2^2 + \left\| \frac{1}{\sqrt{\epsilon_0 \epsilon_d}} \mathbf{P}(t) \right\|_2^2$$

and $\|\cdot\|_2$ is the $L^2(\mathcal{D})$ norm.

Motivation for Distributions

- 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)
- Using Mellin transforms, can show Cole-Cole corresponds to a continuous distribution

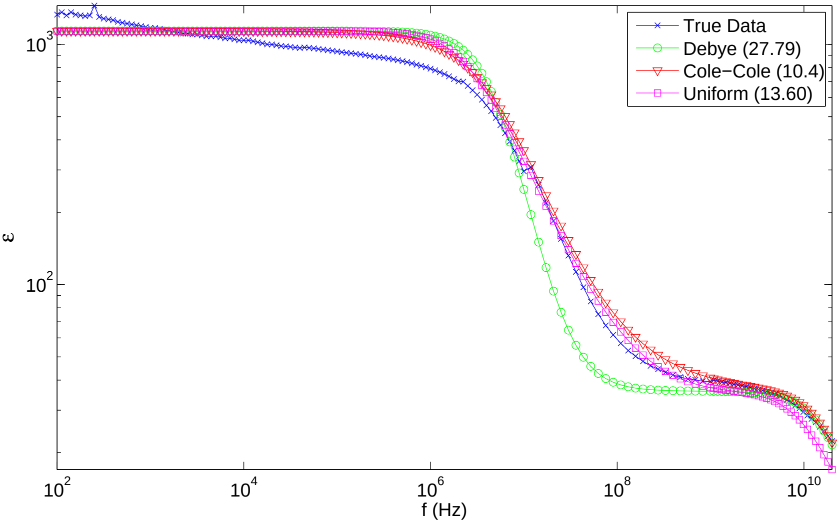


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

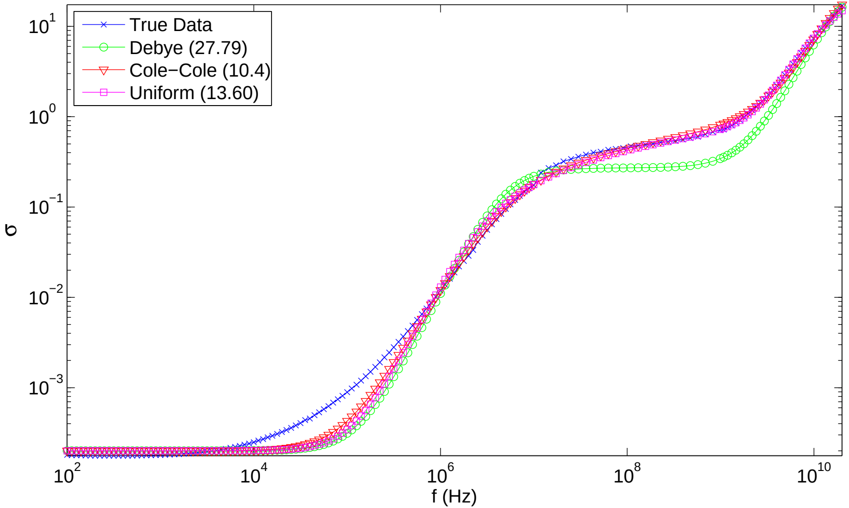


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

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.

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

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

Outline

Maxwell-Random Debye system

In a polydispersive Debye material, we have

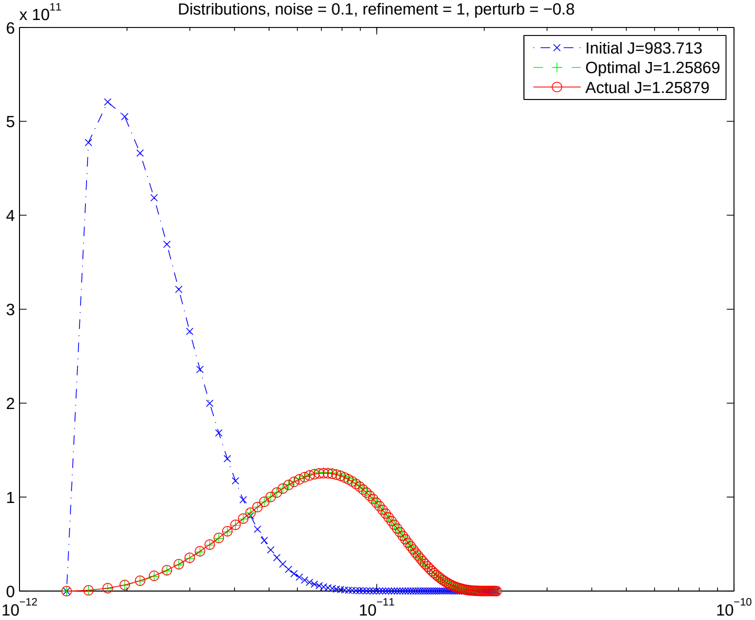
$$\mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}, \tag{3a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} - \mathbf{J} \tag{3b}$$

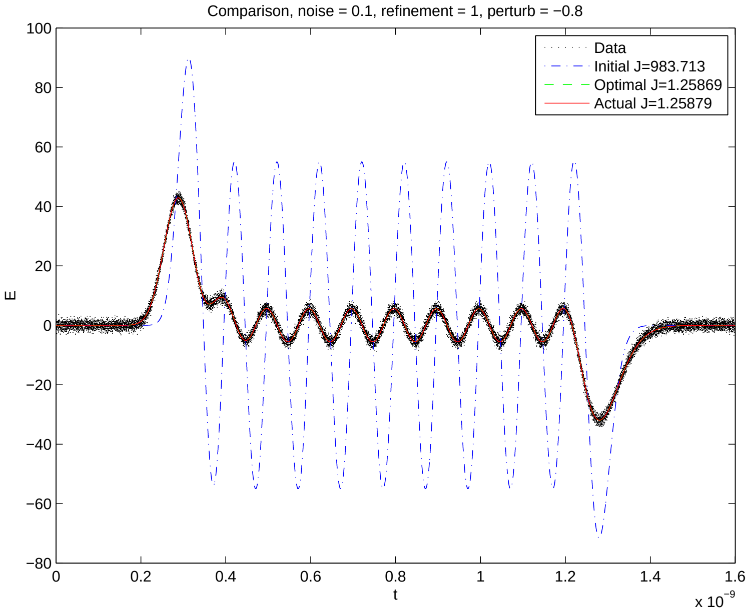
$$\tau \frac{\partial \mathcal{P}}{\partial t} + \mathcal{P} = \epsilon_0 \epsilon_d \mathbf{E} \tag{3c}$$

with

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



Comparison of initial to final distribution.



Comparison of simulations to data.

Theorem (G., 201X)

The dispersion relation for the system (3) *is given by*

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

where the expected complex permittivity is given by

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

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

Theorem (G., 201X)

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Again, $\mathbf{k}$ 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

$$\mathbb{E}\left[\frac{1}{1+i\omega\tau}\right] = \frac{1}{\omega(\tau_b - \tau_a)}\left[\arctan(\omega\tau) + i\frac{1}{2}\ln\left(1+(\omega\tau)^2\right)\right]_{\tau=\tau_b}^{\tau=\tau_a}.$$

Proof: (for 2D)

Letting $H = H_z$, we have the 2D Maxwell-Random Debye TE scalar equations:

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{4a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial P_x}{\partial t}, \tag{4b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial P_y}{\partial t}, \tag{4c}$$

$$\tau \frac{\partial \mathcal{P}_x}{\partial t} + \mathcal{P}_x = \epsilon_0 \epsilon_d E_x \tag{4d}$$

$$\tau \frac{\partial \mathcal{P}_y}{\partial t} + \mathcal{P}_y = \epsilon_0 \epsilon_d E_y. \tag{4e}$$

Proof: (cont.)

We assume plane wave solutions of the form

$$V = \tilde{V} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$$

where $\mathbf{x} = (x, y)^T$ and $\mathbf{k} = (k_x, k_y)^T$. We have, for example,

$$\tilde{P}_x = \mathbb{E}[\tilde{\mathcal{P}}_x] = \epsilon_0 \epsilon_d \tilde{E}_x \mathbb{E}\left[\frac{1}{1 + i\omega\tau}\right].$$

The rest is algebra. □

Proof: (cont.)

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$$V = \tilde{V}\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$$

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The rest is algebra. □

- The proof is similar in 1 and 3 dimensions.
- The exact dispersion relation will be compared with a discrete dispersion relation to determine the amount of dispersion error.

We introduce the Hilbert space $V_F = (L^2(\Omega) \otimes L^2(\mathcal{D}))^2$ equipped with an inner product and norm as follows

$$(\mathbf{u}, \mathbf{v})_F = \mathbb{E}[(\mathbf{u}, \mathbf{v})_2],$$
$$\|\mathbf{u}\|_F^2 = \mathbb{E}[\|\mathbf{u}\|_2^2].$$

The weak formulation of the 2D Maxwell-Random Debye TE system is

$$\left(\frac{\partial H}{\partial t}, v\right)_2 = \left(-\frac{1}{\mu_0}\mathrm{curl}\ \mathbf{E}, v\right)_2, \tag{5}$$

$$\left(\epsilon_0\epsilon_\infty \frac{\partial \mathbf{E}}{\partial t}, \mathbf{u}\right)_2 = (H, \mathrm{curl}\ \mathbf{u})_2 - \left(\frac{\partial \mathbf{P}}{\partial t}, \mathbf{u}\right)_2, \tag{6}$$

$$\left(\frac{\partial \mathcal{P}}{\partial t}, \mathbf{w}\right)_F = \left(\frac{\epsilon_0\epsilon_d}{\tau}\mathbf{E}, \mathbf{w}\right)_F - \left(\frac{1}{\tau}\mathcal{P}, \mathbf{w}\right)_F, \tag{7}$$

for $v \in L^2(\mathcal{D})$, $\mathbf{u} \in H_0(\mathrm{curl}, \mathcal{D})^2$, and $\mathbf{w} \in V_F$.

Stability Estimates for Maxwell-Random Debye

System is well-posed since solutions satisfy the following stability estimate.

Theorem (G., 201X)

Let $\mathcal{D} \subset \mathbb{R}^2$, and let H, $\mathbf{E}$, and $\mathcal{P}$ be the solutions to the weak form of the 2D Maxwell-Random Debye TE system with PEC boundary conditions. Then the system exhibits energy decay

$$\mathcal{E}(t) \leq \mathcal{E}(0), \qquad \forall t \geq 0$$

where the energy is defined by

$$\mathcal{E}(t)^2 = \|\sqrt{\mu_0} H(t)\|_2^2 + \|\sqrt{\epsilon_0 \epsilon_\infty} \mathbf{E}(t)\|_2^2 + \left\| \frac{1}{\sqrt{\epsilon_0 \epsilon_d}} \mathcal{P}(t) \right\|_F^2 .$$

Proof: (for 2D)

By choosing $v = H$, $\mathbf{u} = \mathbf{E}$, and $\mathbf{w} = \mathcal{P}$ in the weak form, and adding all three equations into the time derivative of the definition of $\mathcal{E}^2$, we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d\mathcal{E}^2(t)}{dt} =& -\Big(\mathrm{curl}\ \mathbf{E}, H\Big)_2 + \Big(H, \mathrm{curl}\ \mathbf{E}\Big)_2 - \Big(\frac{\epsilon_0\epsilon_d}{\tau}\mathbf{E}, \mathbf{E}\Big)_F + \Big(\frac{1}{\tau}\mathcal{P}, \mathbf{E}\Big)_F \\
& + \Big(\frac{1}{\tau}\mathbf{E}, \mathcal{P}\Big)_F - \Big(\frac{1}{\epsilon_0\epsilon_d\tau}\mathcal{P}, \mathcal{P}\Big)_F \\
=& -\epsilon_0\epsilon_d\Big(\frac{1}{\tau}\mathbf{E}, \mathbf{E}\Big)_F + 2\Big(\frac{1}{\tau}\mathcal{P}, \mathbf{E}\Big)_F - \frac{1}{\epsilon_0\epsilon_d}\Big(\frac{1}{\tau}\mathcal{P}, \mathcal{P}\Big)_F \\
=& \frac{-1}{\epsilon_0\epsilon_d}\left\|\frac{1}{\tau}(\mathcal{P} - \epsilon_0\epsilon_d\mathbf{E})\right\|_F^2.
\end{aligned}$$

$$\boxed{\frac{d\mathcal{E}(t)}{dt} = \frac{-1}{\epsilon_0\epsilon_d\mathcal{E}(t)}\left\|\frac{1}{\tau}(\mathcal{P} - \epsilon_0\epsilon_d\mathbf{E})\right\|_F^2 \le 0.}$$

□

Outline

Polynomial Chaos

Apply Polynomial Chaos (PC) method to approximate each spatial component of the random polarization

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

resulting in

$$(\tau_r M + \tau_m I)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\hat{e}_1$$

or

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

Polynomial Chaos

Apply Polynomial Chaos (PC) method to approximate each spatial component of the random polarization

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

resulting in

$$(\tau_r M + \tau_m I)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\hat{e}_1$$

or

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

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

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

Note that A is positive definite if $\tau_r < \tau_m$ since $\lambda(M) \in (-1, 1)$.

Maxwell-PC Debye

Replace the Debye model with the PC approximation. In two dimensions we have the 2D Maxwell-PC Debye TE scalar equations

$$\mu_0 \frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}, \tag{8a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - \frac{\partial \alpha_{0,x}}{\partial t}, \tag{8b}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \frac{\partial \alpha_{0,y}}{\partial t}, \tag{8c}$$

$$A\dot{\vec{\alpha}}_x + \vec{\alpha}_x = \vec{f}_x, \tag{8d}$$

$$A\dot{\vec{\alpha}}_y + \vec{\alpha}_y = \vec{f}_y. \tag{8e}$$

where $\vec{f}_x = \epsilon_0 \epsilon_d E_x \hat{e}_1$ and $\vec{f}_y = \epsilon_0 \epsilon_d E_y \hat{e}_1$.

Outline

Finite Difference Time Domain (FDTD)

We now define 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.

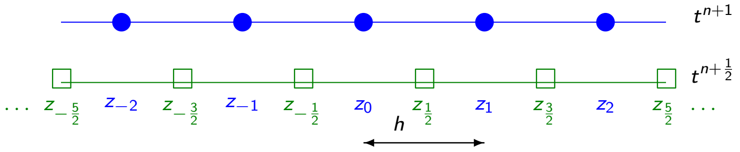
The Yee Scheme

- In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations in freespace.
- The finite difference time domain (FDTD) or Yee scheme solves for both the electric and magnetic fields in time and space using the coupled Maxwell's curl equations rather than solving for the electric field alone (or the magnetic field alone) with a wave equation.
- Approximates first order derivatives very accurately by evaluating on staggered grids.

Yee Scheme in One Space Dimension

- **Staggered Grids**: The electric field/flux is evaluated on the primary grid in both space and time and the magnetic field/flux is evaluated on the dual grid in space and time.
- The Yee scheme is

$$\boxed{\begin{aligned} \frac{H|^{n+\frac{1}{2}}_{\ell+\frac{1}{2}} - H|^{n-\frac{1}{2}}_{\ell+\frac{1}{2}}}{\Delta t} &= -\frac{1}{\mu}\frac{E|^{n}_{\ell+1} - E|^{n}_{\ell}}{\Delta z} \\ \frac{E|^{n+1}_{\ell} - E|^{n}_{\ell}}{\Delta t} &= -\frac{1}{\epsilon}\frac{H|^{n+\frac{1}{2}}_{\ell+\frac{1}{2}} - H|^{n+\frac{1}{2}}_{\ell-\frac{1}{2}}}{\Delta z} \end{aligned}}$$



- 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 d is the spatial dimension, and h is the (uniform) spatial step.
- The initial value problem is well-posed and the scheme is consistent and stable. The method is convergent by the Lax-Richtmyer Equivalence Theorem.
- The Yee scheme can exhibit numerical dispersion.
- Dispersion error can be reduced by decreasing the mesh size or resorting to higher order accurate finite difference approximations.

Extensions of the Yee Scheme to Dispersive Media

- The ordinary differential equation for the polarization is discretized using second order centered differences and an averaging of zero order terms.
- The resulting scheme remains second-order accurate in both time and space with the same CFL condition, $c_\infty \Delta t \leq h/\sqrt{d}$, except that $c_\infty = 1/\sqrt{\mu_0 \epsilon_0 \epsilon_\infty}$ is the fastest wave speed.
- However, the Yee scheme for the Maxwell-Debye system is now dissipative in addition to being dispersive.

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

$$\mu_0 \frac{H^{n+1}_{j+\frac{1}{2}} - H^{n}_{j+\frac{1}{2}}}{\Delta t} = -\frac{E^{n+\frac{1}{2}}_{j+1} - E^{n+\frac{1}{2}}_{j}}{\Delta z}$$
$$\epsilon_0 \epsilon_\infty \frac{E^{n+\frac{1}{2}}_{j} - E^{n-\frac{1}{2}}_{j}}{\Delta t} = -\frac{H^{n}_{j+\frac{1}{2}} - H^{n}_{j-\frac{1}{2}}}{\Delta z} - \frac{P^{n+\frac{1}{2}}_{j} - P^{n-\frac{1}{2}}_{j}}{\Delta t}$$
$$\tau \frac{P^{n+\frac{1}{2}}_{j} - P^{n-\frac{1}{2}}_{j}}{\Delta t} = \epsilon_0 \epsilon_d \frac{E^{n+\frac{1}{2}}_{j} + E^{n-\frac{1}{2}}_{j}}{2} - \frac{P^{n+\frac{1}{2}}_{j} + P^{n-\frac{1}{2}}_{j}}{2}.$$

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

$$\omega_\Delta = \frac{\sin\left(\omega\Delta t/2\right)}{\Delta t/2}, \qquad \tau_\Delta = \sec(\omega\Delta t/2)\tau.$$

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].

Outline

The discretization of the PC system

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

is performed similarly to the deterministic system in order to preserve second order accuracy. Applying second order central differences at $\vec{\alpha}_j^n = \vec{\alpha}(t_n, z_j)$:

$$A\frac{\vec{\alpha}_j^{n+\frac{1}{2}} - \vec{\alpha}_j^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}_j^{n+\frac{1}{2}} + \vec{\alpha}_j^{n-\frac{1}{2}}}{2} = \frac{\vec{f}_j^{n+\frac{1}{2}} + \vec{f}_j^{n-\frac{1}{2}}}{2}. \tag{9}$$

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Couple this with the equations from above:

$$\epsilon_0\epsilon_\infty\frac{E_j^{n+\frac{1}{2}} - E_j^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n}{\Delta z} - \frac{\alpha_{0,j}^{n+\frac{1}{2}} - \alpha_{0,j}^{n-\frac{1}{2}}}{\Delta t} \tag{10a}$$

$$\mu_0\frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}}}{\Delta z}. \tag{10b}$$

Let $\tau_h^{E_x}$, $\tau_h^{E_y}$, τ_h^H be the sets of spatial grid points on which the E_x, E_y, and H fields, respectively, will be discretized. The discrete L^2 grid norms are defined as

$$\|\mathbf{V}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|V_{x_{\ell+\frac{1}{2},j}}|^2 + |V_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \tag{11}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \tag{12}$$

with corresponding inner products. Each component of α_k is discretized on $\tau_h^{E_x} \times \tau_h^{E_y}$ with discrete L^2 grid norm

$$\|\vec{\alpha}\|_\alpha^2 = \sum_{k=0}^{p} \|\alpha_k\|_E^2,$$

with a corresponding inner product

$$(\vec{\alpha}, \vec{\beta})_\alpha = \sum_{k=0}^{p} \left(\alpha_k, \beta_k \right)_E.$$

Energy Decay and Stability

Energy decay implies that the method is stable and hence convergent.

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Theorem (G., 201X)

For $n \geq 0$, let $\mathbf{U}^n = [H^{n-\frac{1}{2}}, E_x^n, E_y^n, \alpha_{0,x}^n, \ldots, \alpha_{0,y}^n, \ldots]^T$ be the solutions of the 2D Maxwell-PC Debye TE FDTD scheme with PEC boundary conditions. If the usual CFL condition for Yee scheme is satisfied $c_\infty \Delta t \leq h/\sqrt{2}$, then there exists the energy decay property

$$\mathcal{E}_h^{n+1} \leq \mathcal{E}_h^n$$

where the discrete energy is given by

$$(\mathcal{E}_h^n)^2 = \left|\left|\sqrt{\mu_0}\overline{H}^n\right|\right|_H^2 + ||\sqrt{\epsilon_0\epsilon_\infty}\mathbf{E}^n||_E^2 + \left|\left|\frac{1}{\sqrt{\epsilon_0\epsilon_d}}\vec{\alpha}^n\right|\right|_\alpha^2.$$

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Note: $\|\mathcal{P}\|_F^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathbb{E}[\mathcal{P}]^2 + Var(\mathcal{P})\|_2^2 \approx \|\vec{\alpha}\|_\alpha^2$.

Energy Decay and Stability (cont.)

Proof.

First, showing that this is a discrete energy, i.e., a positive definite function of the solution, involves recognizing that

$$(\mathcal{E}_h^n)^2 = \mu_0 \|\overline{H}^n\|_H^2 + \epsilon_0 \epsilon_\infty (E^n, \mathcal{A}_h E^n)_E + \frac{1}{\epsilon_0 \epsilon_d} (\vec{\alpha}^n - E\hat{e}_1, A^{-1}(\vec{\alpha}^n - E\hat{e}_1))_\alpha$$

with $\mathcal{A}_h$ positive definite when the CFL condition is satisfied, and A^{-1} is always positive definite (eigenvalues between $\tau_m - \tau_r$ and $\tau_m + \tau_r$).

Energy Decay and Stability (cont.)

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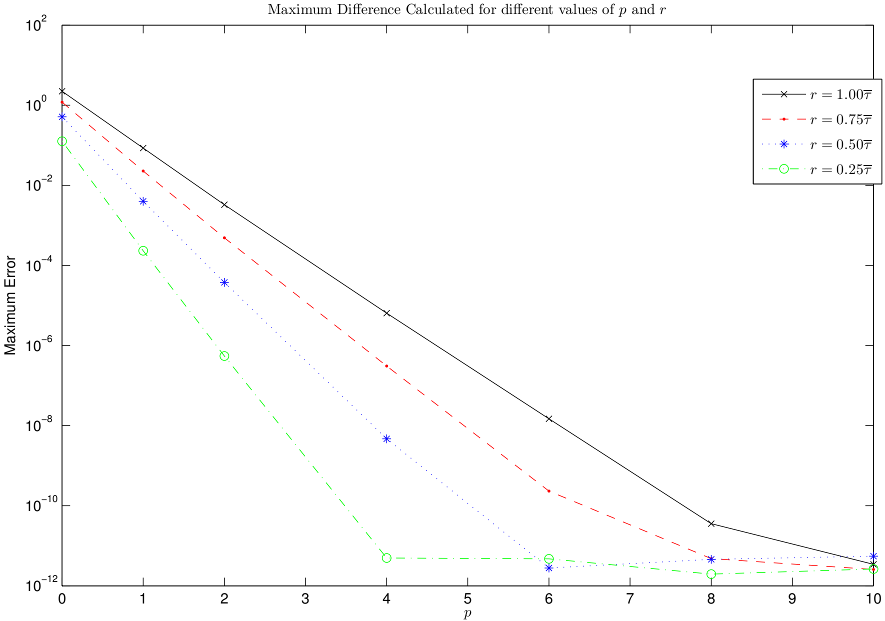
with $\mathcal{A}_h$ positive definite when the CFL condition is satisfied, and A^{-1} is always positive definite (eigenvalues between $\tau_m - \tau_r$ and $\tau_m + \tau_r$).

The rest follows the proof for the deterministic case [Bokil-G, 201X] to show

$$\frac{\mathcal{E}_h^{n+1} - \mathcal{E}_h^n}{\Delta t} = -\left(\frac{2}{\mathcal{E}_h^{n+1} + \mathcal{E}_h^n}\right)\frac{1}{\epsilon_0\epsilon_d}\left\|\epsilon_0\epsilon_d \overline{\mathbf{E}}^{n+\frac{1}{2}}\hat{\mathrm{e}}_1 - \overline{\vec{\alpha}}^{n+\frac{1}{2}}\right\|_{A^{-1}}^2. \qquad (13)$$

□


Maximum Difference Calculated for different values of p and r
Maximum Error
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
p
$r = 1.00\overline{\tau}$
$r = 0.75\overline{\tau}$
$r = 0.50\overline{\tau}$
$r = 0.25\overline{\tau}$

Theorem (G., 2013)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme in (9) and (10) 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

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

Proof: (for 1D)

Assume plane wave solutions of the form

$$V_j^n = \tilde{V}\mathrm{e}^{i(\omega n\Delta t - kj\Delta z)}$$

and

$$\alpha_{\ell,j}^n = \tilde{\alpha}_\ell \mathrm{e}^{i(\omega n\Delta t - kj\Delta z)}$$

Substituting into (9) yields

$$A\tilde{\alpha}\left(\frac{2i}{\Delta t}\sin(\omega\Delta t/2)\right) + \cos(\omega\Delta t/2)\tilde{\alpha} = \epsilon_0\epsilon_d\cos(\omega\Delta t/2)\tilde{E}\hat{e}_1 \tag{14}$$

which implies

$$\tilde{\alpha}_0 = \hat{e}_1^T\left(I + i\omega_\Delta A_\Delta\right)^{-1}\hat{e}_1\epsilon_0\epsilon_d\tilde{E}. \tag{15}$$

The rest of the proof follows as before. □

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The rest of the proof follows as before. □

Note that the same relation holds in 2 and 3D as well as with higher order accurate spatial difference operators.

Dispersion Error

We define the phase error Φ for a scheme applied to a model to be

$$\Phi = \left| \frac{k_{\mathrm{EX}} - k_{\Delta}}{k_{\mathrm{EX}}} \right|, \tag{16}$$

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:

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

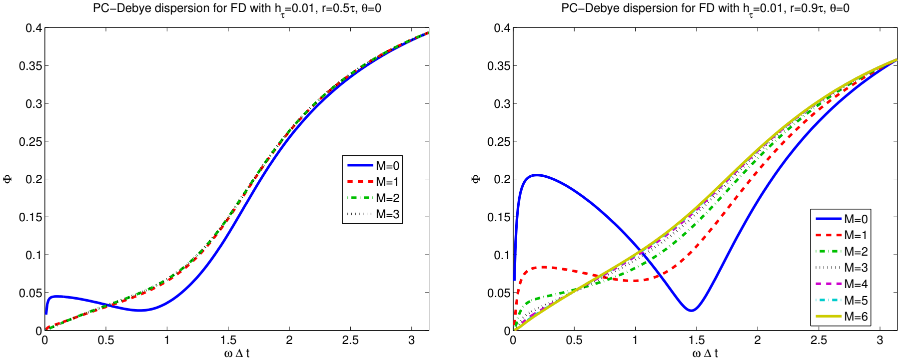
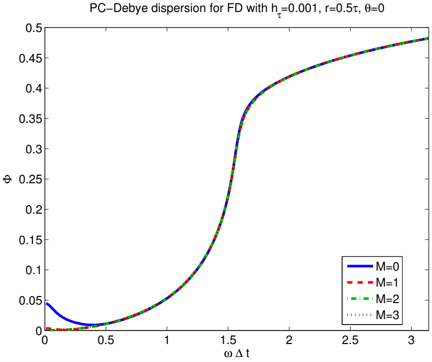
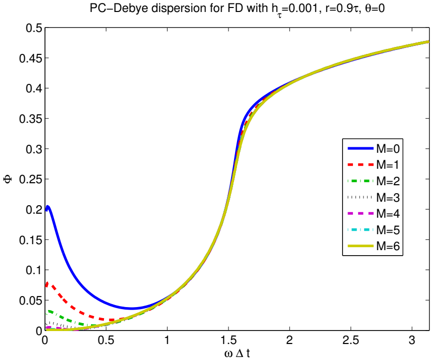


Figure: Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$.





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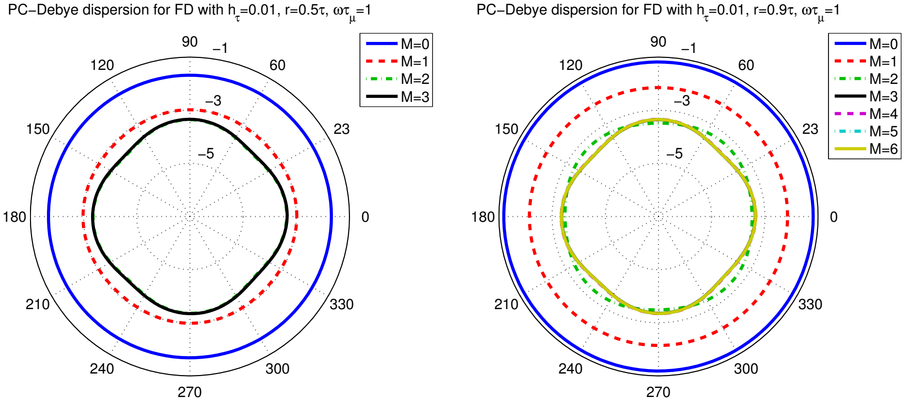

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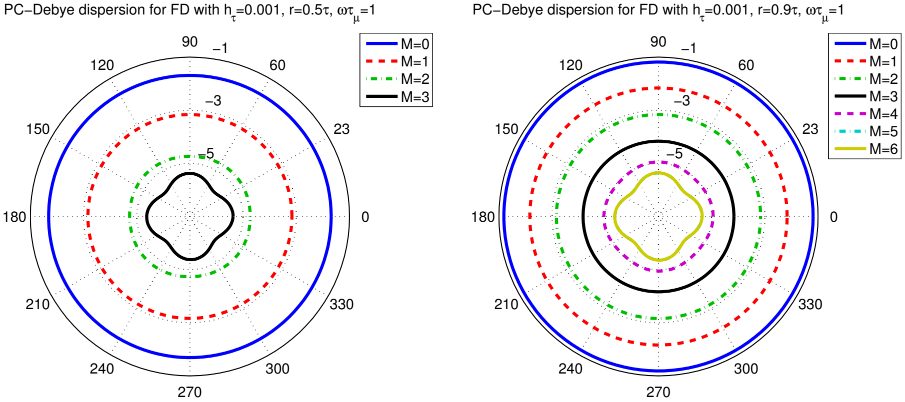

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Conclusions/Future Work

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- We described an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD)
- 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 demonstrated

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. (201X), Convergence Analysis of Yee Schemes for Maxwell's Equations in Debye and Lorentz Dispersive Media, *Submitted.*

GIBSON, N. L. (201X), Polynomial Chaos for Dispersive Electromagnetics, *Submitted.*

Outline

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  - Luis Gomez-Cunya (Ph.D. student)
  - Parnian Hosseini (Ph.D. student)
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Outline

Reservoir Operations

The broad context of the problem of interest is a PDE-constrained optimal control problem with uncertainty. In particular, one must

- meet electrical demand with hydro-power production
- mitigate flooding
- preserve ecological conditions
- possibly maximize revenue
- etc.

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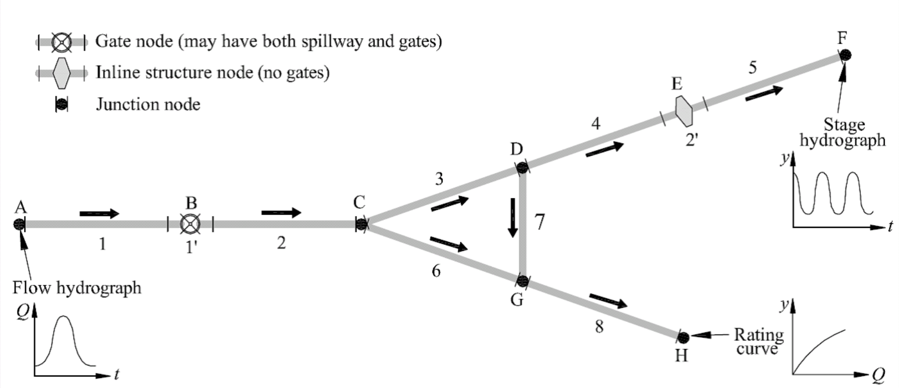
all without perfect knowledge of the system, the inflows, the demand, or prices.

Simple River System

Consider this simple network system



Unknowns: flow discharge upstream Q_u and downstream Q_d, water depth downstream y_d for each reach $i = 1, \ldots, 8$.

Simulation of Unsteady Flows

- Most free surface flows are unsteady and nonuniform.
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Saint-Venant equations: PDEs representing conservation of mass and momentum for a control volume:

$$B\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = 0, \tag{17}$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + gA\left(\frac{\partial y}{\partial x} + S_f - S_0\right) = 0, \tag{18}$$

where x is a distance along the channel in the longitudinal direction, t is time, y is a water depth, Q is a flow discharge,
B is a width of the channel, g is an acceleration due to gravity,
A is a cross-sectional area of the flow, S_f is a friction slope, S_0 is a river bed slope.

Initial and boundary conditions are required to close the system.

System of Equations to Solve

At each time step we need to guarantee

- Continuity at each **node**

$$\sum Q_{in} = \sum Q_{out}$$

- Compatibility at each **node**

$$\mathrm{WSE}_{\text{upstream reach}} = \mathrm{WSE}_{\text{downstream reach}}$$

- Conservation of mass at each **reach**

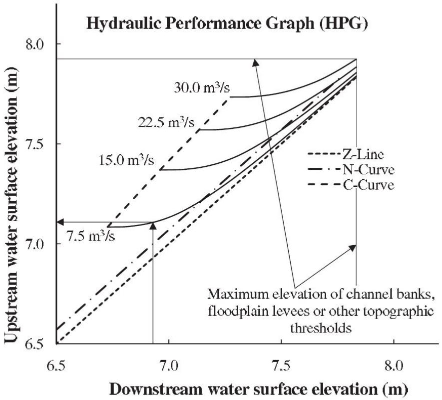
$$(\text{Total Inflow} - \text{Total Outflow})_{\Delta t} = \text{Change in Storage}_{\Delta t}$$

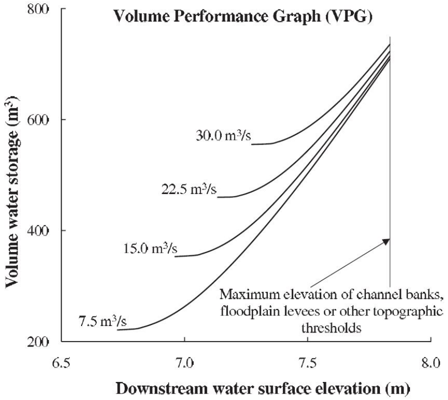
Hydraulic and Volume Performance Graphs

- The Hydraulic Performance Graph (HPG) of a channel reach summarizes the dynamic relation between the flow through and the depth at the ends of the reach under gradually varied flow conditions.
- The Volume Performance Graph (VPG) of a channel reach summarizes the corresponding storage.
- The HPG and VPG are unique to a channel reach with a given geometry and roughness.
- They can be pre-computed, in high resolution, decoupled from unsteady reach boundary conditions by solving the PDE system for all feasible conditions in the reach.
- The performance graphs can be interpolated for use with different reach boundary conditions.
- The performance graphs approach is built into the OSU-Rivers software, and greatly reduces computational time.

Hydraulic and Volume Performance Graphs. Examples

Example of the HPG and the VPG for a mild-sloped channel.





Outline

Sources of Uncertainty

Hydrological conditions (particularly inflows) and power demand (and price) are the main sources of uncertainties.

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Chosen approach

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- Stochastic representation of the solutions - discharge and water depth
- Robust optimization

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Assumptions on the uncertain inputs

- We have M predictions, $M > 1$, of the inflow function Q_{u_1}, forecast for the same points in time $\{t_j\}_{j=1}^{n}$.
- The logarithm of the inflow function Q_{u_1} can be represented as a Gaussian process.

Parametrization of the Stream Inflow

- $L_i(t_j) = \ln Q_{u_1,i}(t_j)$ is the value of the logarithm of the ith inflow at t_j.
- Expectation of the log stream inflow $\bar{L}$ and its covariance $C(t_j, t_k)$,

$$\begin{aligned}
\bar{L}(t_j) &= \frac{1}{M}\sum_{i=1}^{M} L_i(t_j), \quad j = 1, \ldots, n, \\
C(t_j, t_k) &= \frac{1}{M-1}\sum_{i=1}^{M}(L(t_j) - \bar{L}(t_j))(L_{u_1,i}(t_k) - \bar{L}(t_k)).
\end{aligned}$$

- $Q_{u_1}(t)$ can be represented as

$$Q_{u_1}(t) = exp\left(\bar{L}(t) + \sum_{k=1}^{\infty}\sqrt{\lambda_k}\psi_k(t)\xi_k\right).$$

- (λ_k, ψ_k): $\lambda\psi(t) = \int C(s,t)\psi(s)ds$.
- $\{\xi\}_{k=1}^{\infty}$ is a sequence of standard normal random variables.

Parametrization of the Stream Inflow

Truncation of infinite series representation

We use

$$Q_{u_1}^N(t) = \exp\left(\bar{L}(t) + \sum_{k=1}^{N} \sqrt{\lambda_k}\psi_k(t)\xi_k\right).$$

Number of terms N can be chosen in different ways:

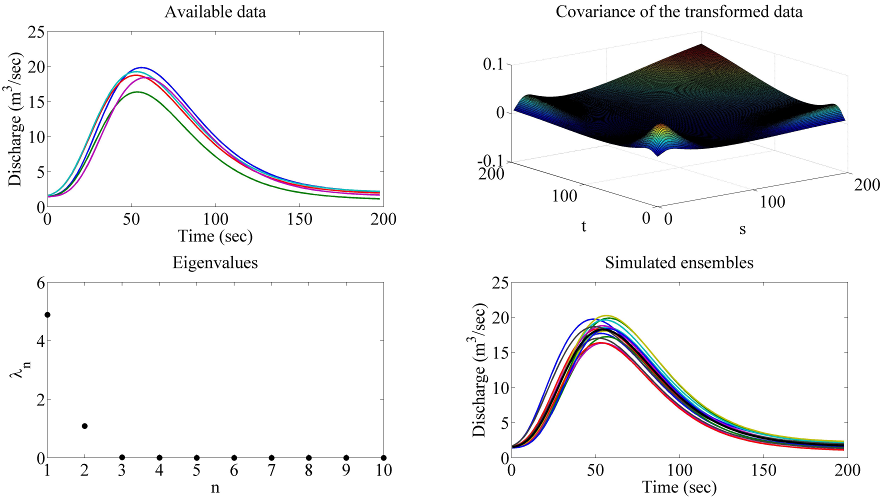
- Use $\sum_{k=1}^{\infty} \lambda_k = \int C(t,t)dt = 1$ to choose N such that $\sum_{k=1}^{N} \lambda_k > c$, $0 < c < 1$.
- Assume $\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots$ and choose N such that $\lambda_k > c\lambda_1$, $k = 1, \ldots, N$, $0 < c < 1$.
- Sensitivity of the solution, e.g., Q_d, to the distribution of the random variables $\{\xi_k\}_{k=1}^N$

$$\mathrm{DS}_{\mathcal{E}}[\rho, \rho_2](Q_d) = \frac{\|\mathcal{E}_\rho(Q_d) - \mathcal{E}_{\rho_2}(Q_d)\|}{d(\rho, \rho_2)},$$

where $\mathcal{E}_\rho(Q_d)$ is a quantity of interest associated with Q_d (mean or variance) with respect to the probability density ρ; ρ_2 is a perturbation of the density

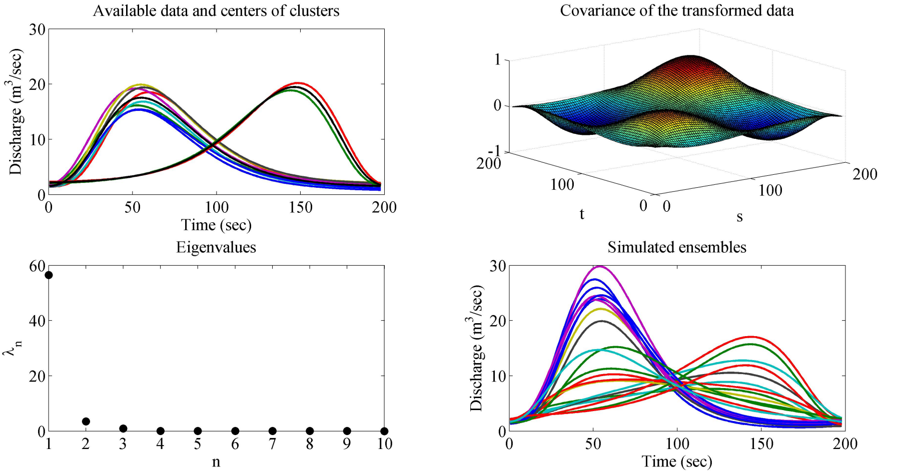
Numerical Experiments. Stochastic Parametrizations

Experiment 1: 5 predictions



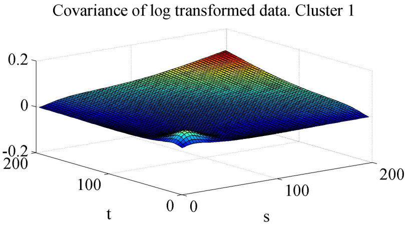
Numerical Experiments. Stochastic Parametrizations

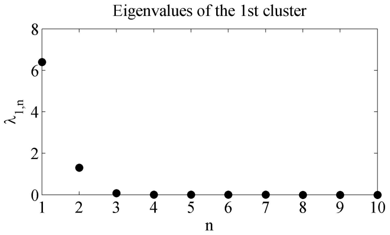
Experiment 2 (mixture distribution): 10 predictions, $p = 0.8$

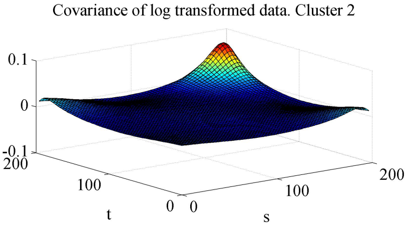


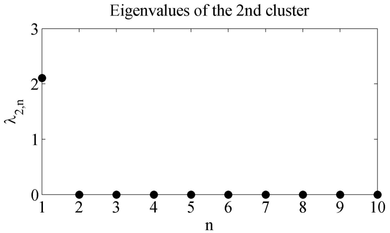
Numerical Experiments. Stochastic Parametrizations

Experiment 2 continued (k-means clustering)



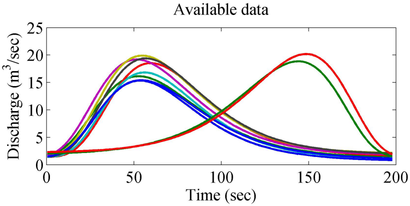


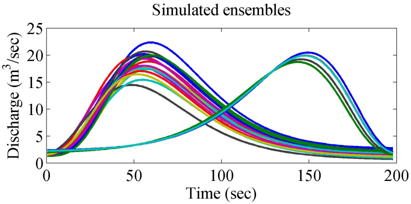




Numerical Experiments. Stochastic Parametrizations

Experiment 2 continued (k-means clustering)





Outline

1. Polynomial Chaos
2. Electromagnetics
   - Maxwell-Debye
   - Maxwell-Random Debye
   - Maxwell-PC Debye
   - PC-Debye FDTD
   - PC-Debye FDTD
   - Conclusions
3. **Reservoir Operations**
   - Problem formulation
   - Sources of uncertainty and assumptions
   - **Stochastic representation of the solutions**
   - Robust optimization
   - Future work

Polynomial Chaos Representation of the Solutions

Goal: Given the parametrization of the uncertain inputs, provide the stochastic representation of the solutions.

Approach: Generalized Polynomial Chaos (gPC) Expansion.

Consider a flow discharge at the most downstream reach, Q_{d_8}. Its representation in terms of a degree p polynomial expansion

$$Q_{d_8}^{p}(t,\vec{\xi}) = \sum_{i=0}^{M_p} v_i(t)\phi_i(\vec{\xi}), \tag{19}$$

- $\vec{\xi} = (\xi_1, \xi_2, \ldots, \xi_N)$ are r.v. in the representation of Q_{u_1}
- $\{\phi_i\}_{i=0}^{M_p}$ are the N-variate orth. polynomial functions of degree up to p
- if $\{\xi_k\}$ are i.i.d. $N(0,1)$, $\{\phi_i\}_{i=0}^{M_p}$ are chosen as tensor products of univariate Hermite polynomials.
- $M_p < (N+p)!/(N!p!)$ (max number of polynomial basis functions)

Polynomial Chaos Representation of the Solutions

Each gPC expansion coefficient can be represented via a projection

$$v_i(t) = \mathbb{E}[Q_{d_8}(t, \vec{\xi})\phi_i(\vec{\xi})] = \int_\Gamma Q_{d_8}(t, \mathbf{z})\phi_i(\mathbf{z})\rho(\mathbf{z})d\mathbf{z}. \tag{20}$$

- $\Gamma = \prod_{k=1}^N \Gamma_k$, $\Gamma_k = \xi_k(\Omega)$, where $(\Omega, \mathcal{F}, P)$ is a probability space
- $\rho(\mathbf{z})$ is a joint probability density of the random vector $\vec{\xi}$

One could derive the coupled PDE system for these coefficients, but this would be *intrusive* as it changes the system we would like to solve (not good, especially since we have pre-computed solutions).

Instead, the computation of the coefficients v_i, $i = 0, \ldots, M_p$ can be done *non-intrusively* with the use of the stochastic collocation method.

Combined with the performance graphs approach, the stochastic solutions are computed very efficiently.

Stochastic Collocation and gPC

- Choose a set of collocation points $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,N}) \in \Gamma$ and weights w_j, $j = 1, \ldots, N_{cp}$.
- For each $j = 1, \ldots, N_{cp}$ evaluate the inflow function $Q_{u_1,j}(t) = Q_{u_1}(t, \mathbf{z}_j)$.
- Simulate deterministically the corresponding downstream flow $Q_{d_8,j}(t)$.
- Approximate the gPC expansion coefficients using Gaussian Quadrature

$$v_i(t) = \mathbb{E}[Q_{d_8}(t, \vec{\xi})\phi_i(\vec{\xi})] \approx \sum_{j=1}^{N_{cp}} w_j Q_{d_8}(t, \mathbf{z}_j)\phi_i(\mathbf{z}_j). \tag{21}$$

- Construct the N-variate, pth-order gPC approximation, if necessary

$$Q_{d_8}^{p}(t, \vec{\xi}) = \sum_{i=0}^{M_p} v_i(t)\phi_i(\vec{\xi}). \tag{22}$$

- Or just use $\mathbb{E}[Q_{d_8}(t, \vec{\xi})] \approx v_0(t), \quad \mathrm{Var}[Q_{d_8}(t, \vec{\xi})] \approx \sum_{i=1}^{M_p} v_i(t)^2.$

Outline

Objective and Constraints

Let Q_t denote a turbine flow of a dam and y a depth of reservoir.

Let P be a price, and E be a produced (surplus) hydro-power energy, then $R = P \cdot E$ is a revenue.

Objective:

$$\max_{Q_t} R,$$

Subject to constraints:

$$0 < Q_t < Q_{crit},$$
$$0 < \left| \frac{dQ_t}{dt} \right| < \dot{Q}_{\max},$$
$$y_{\min} < y < y_{\max}.$$

Robust Optimization Under Uncertainty

Robust optimization captures two design concepts:

- **Robustness** of an engineered system is the insensitiveness of the system performance to noises from all possible sources, including both external noises and control variable variations.

- **Reliability** of an engineered system is the ability to fulfill its design purpose for some specified time. In a narrow sense, reliability is the probability that a system will not exceed a specified limit state (ultimate or serviceability) within the specified operating time frame.

With respect to optimization under uncertainty,

- **robustness** is achieved by considering both the mean and variance of the original objective function.
- **reliability** is achieved by considering the constraints to be probabilistic.

Mathematical Formulation

The deterministic constrained optimization problem can be formulated as

$$\text{find} \qquad \max_q R(q), \tag{23}$$

$$\text{subject to} \qquad y(x,t;q) \leq y_{crit}(x), \tag{24}$$

where q is a control.

We assume the inflows are random and reformulate our problem as follows

$$\text{find} \qquad \max_q \Big(E[R(q)] - r\mathrm{Var}[R(q)] \Big), \tag{25}$$

$$\text{subject to} \qquad P(y(x,t;q) > y_{crit}(x)) \leq \alpha, \tag{26}$$

where r is a risk tolerance coefficient, α is a reliability level the decision maker wishes to achieve.

The mean and variance can be computed directly from the PC expansion of R.

Algorithm for the Estimation of the Probability of Failure

Probabilistic constraints

- Associated probability can be quite small (MC method would require many samples).
- Sampling of the system is expensive.

Given x fixed, let $y(x,t) = y(t)$.

1. Assume we have computed values of $y(t)$ at the chosen collocation points $\mathbf{z}_j \in \Gamma$, $j = 1, \ldots, N_{cp}$. Obtain $y^p(t, \vec{\xi})$, the gPC representation of $y(t)$ in terms of r.v. $\{\xi_k\}_{k=1}^N$.
2. For the purpose of comparison sample the gPC representation $y^p(t)$ by MC method for the first estimate of the failure probability.
3. Find $\vec{\xi}_{MPP}$, the most probable point (MPP), the point closest to the origin such that $y^p(t, \vec{\xi}_{MPP}) = y_{crit}$ (constrained optimization subproblem).
4. Sample the system to get $y(t, \vec{\xi}_{MPP})$. Update the surrogate model.
5. Find the next approximation of the failure probability by MC sampling the updated surrogate model.
6. Repeat steps (3)-(5) N more times, where N is $dim(\Gamma)$.

Algorithm for the Estimation of the Probability of Failure

Now we have the system values $y(t)$ evaluated at $(N+1)$ candidate MPP points.

7. Using only the last $(N+1)$ data points construct a linear approximation $y_{lin}(t,\vec{\xi})$ of the system, e.g., plane in the case $N=2$.
8. Find the MPP $\vec{\xi}_{MPP}$ of the new surrogate model y_{lin}.
9. Sample the system to get $y(t,\vec{\xi}_{MPP})$.
10. Among the last $(N+2)$ points find the best $(N+1)$ points in terms of the exact value of $y(t)$. Update the surrogate model y_{lin} by using the best $(N+1)$ points.
11. Find the next approximation of the failure probability by MC sampling the updated surrogate model.
12. Compare the previous and current estimates of the probabilities.
13. Stop if the difference between the estimates is smaller than a prescribed tolerance; otherwise repeat steps (7)-(12).

Outline

Future Work

- Multi-objective and multi-constraint robust optimization of the multi-reservoir river systems.
- Additional sources of uncertainty: price, demand forecast, wind generated power.
- Demonstration with actual historical data.
- Optimization-based domain decomposition (for parallel implementation).

References

LEON, A. S., KANASHIRO, E. A., & GONZÁLEZ-CASTRO, J. A. (2013) A fast approach for unsteady flow routing in complex river networks based on performance graphs, *Journal of Hydraulic Engineering*, **139**(3), pp. 284–295.

LEON, A. S., GIBSON, N. L., & GIFFORD-MIEARS, C. H. (2012), Toward reduction of uncertainty in complex multi-reservoir river systems, *Proceedings from the XIX International Conference on Water Resources*.

GIBSON, N. L., GIFFORD-MIEARS, C. H., LEON, A. S. & VASYLKIVSKA, V. (201X), Efficient Computation of Unsteady Flow in Complex River Systems with Uncertain Inputs, to appear in the *International Journal of Computer Mathematics*.

GIBSON, N. L., HOYLE, C., MCINTIRE, M. G. & VASYLKIVSKA, V. (20XX), Applying Robust Design Optimization to Large Systems, *in preparation*.