Inverse Problem for Distributions of Dielectric Parameters

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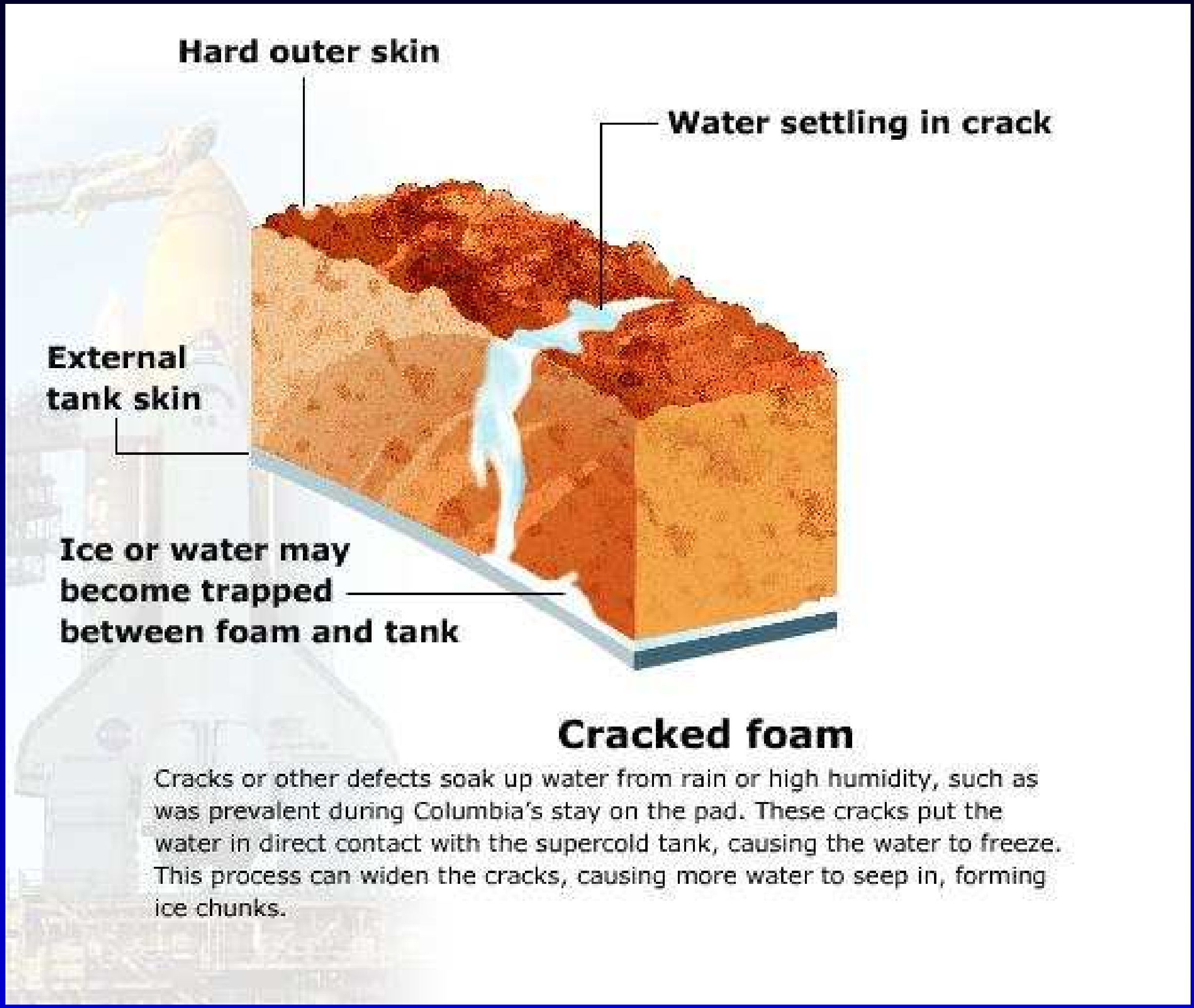
Motivating Application



The particular motivation for this research is the detection of defects in the insulating foam on the space shuttle fuel tanks in order to help eliminate the separation of foam during shuttle ascent.

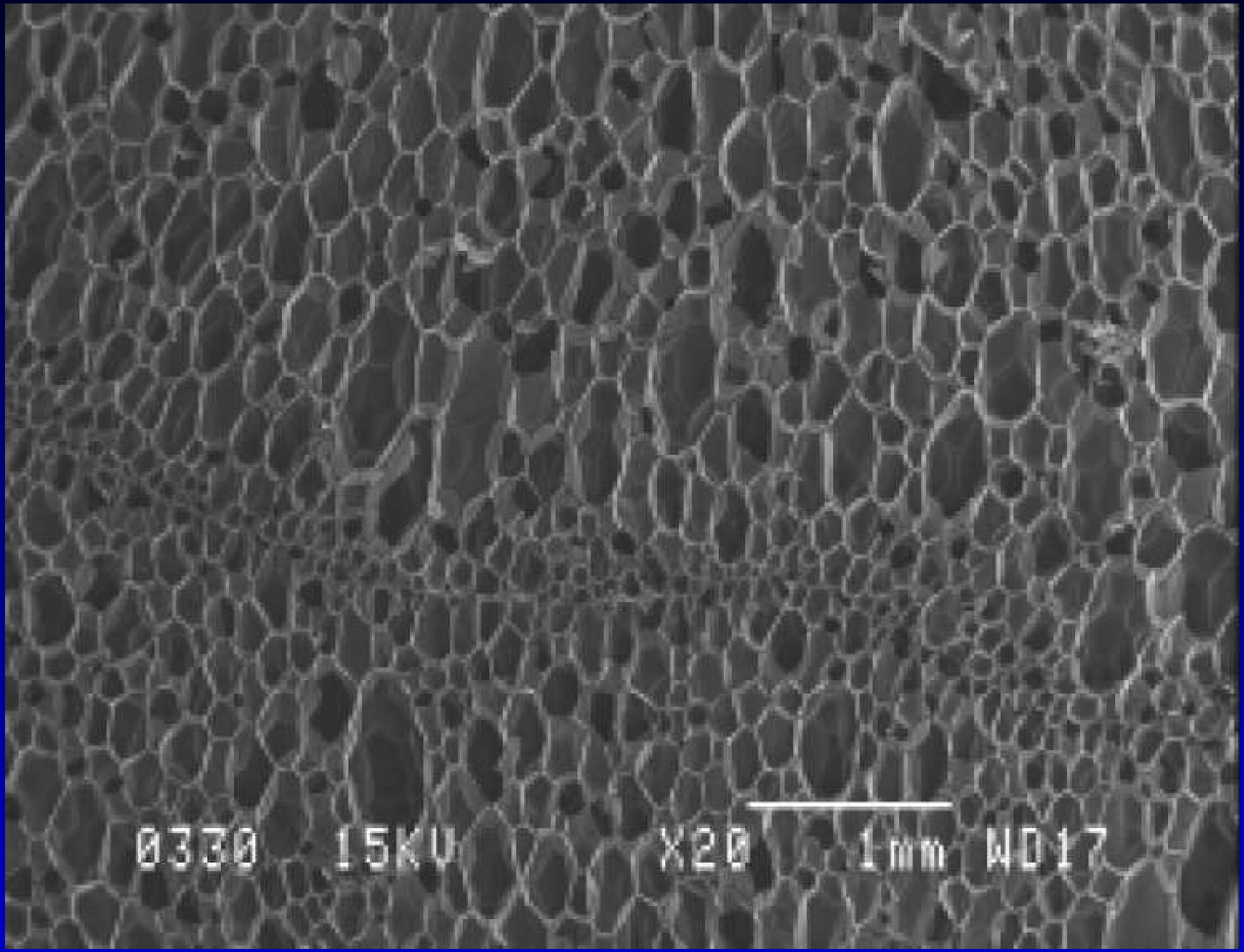
Our Contributions

- Gap Detection Inverse Problem
- Improved Modeling Approaches
  - **Distributions of Dielectric Properties**
  - Homogenization
- Modeling Knit Lines

Distributions of Parameters

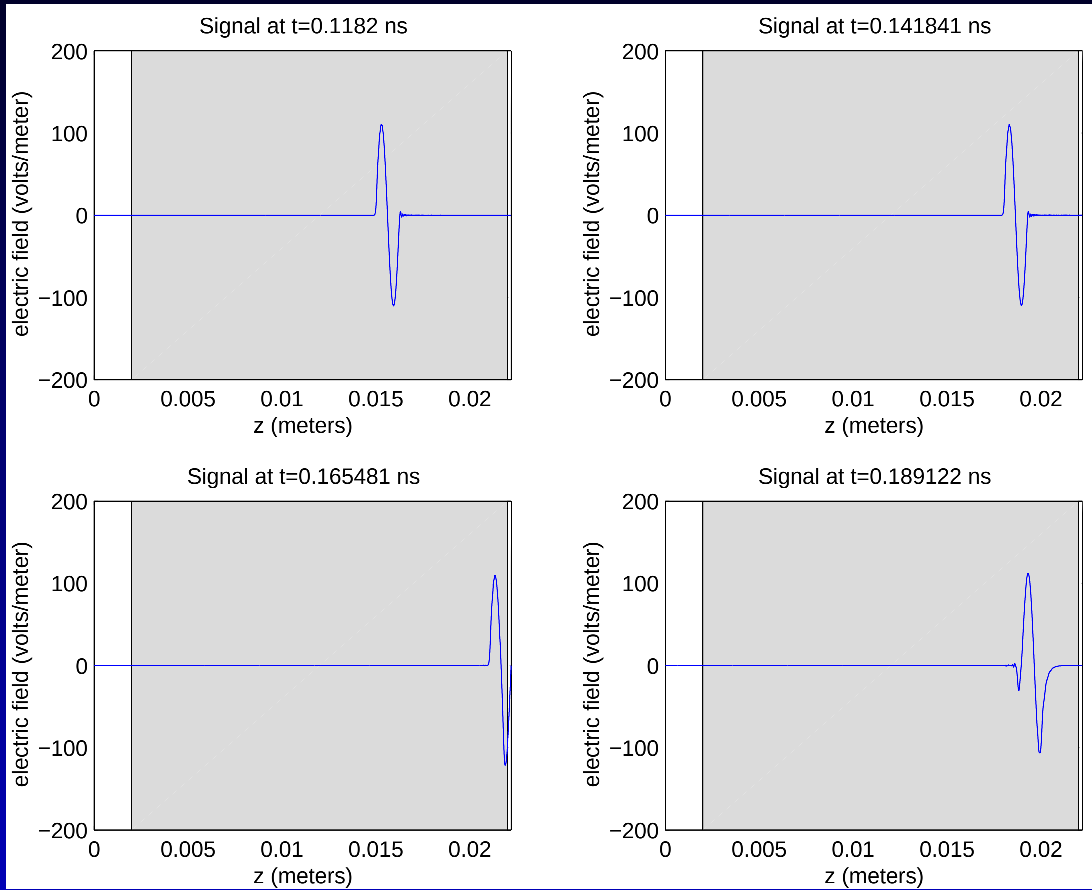
- Background
  - Interrogation Experiment
  - Maxwell's Equations
- Polarization with Distributions
  - Parameters
  - Mechanisms
- Well-posedness of Inverse Problem
- Sample Inverse Problem Results
  - Discrete Multiple Debye
  - Bi-gaussian Debye
  - High and low frequencies

Motivating Application



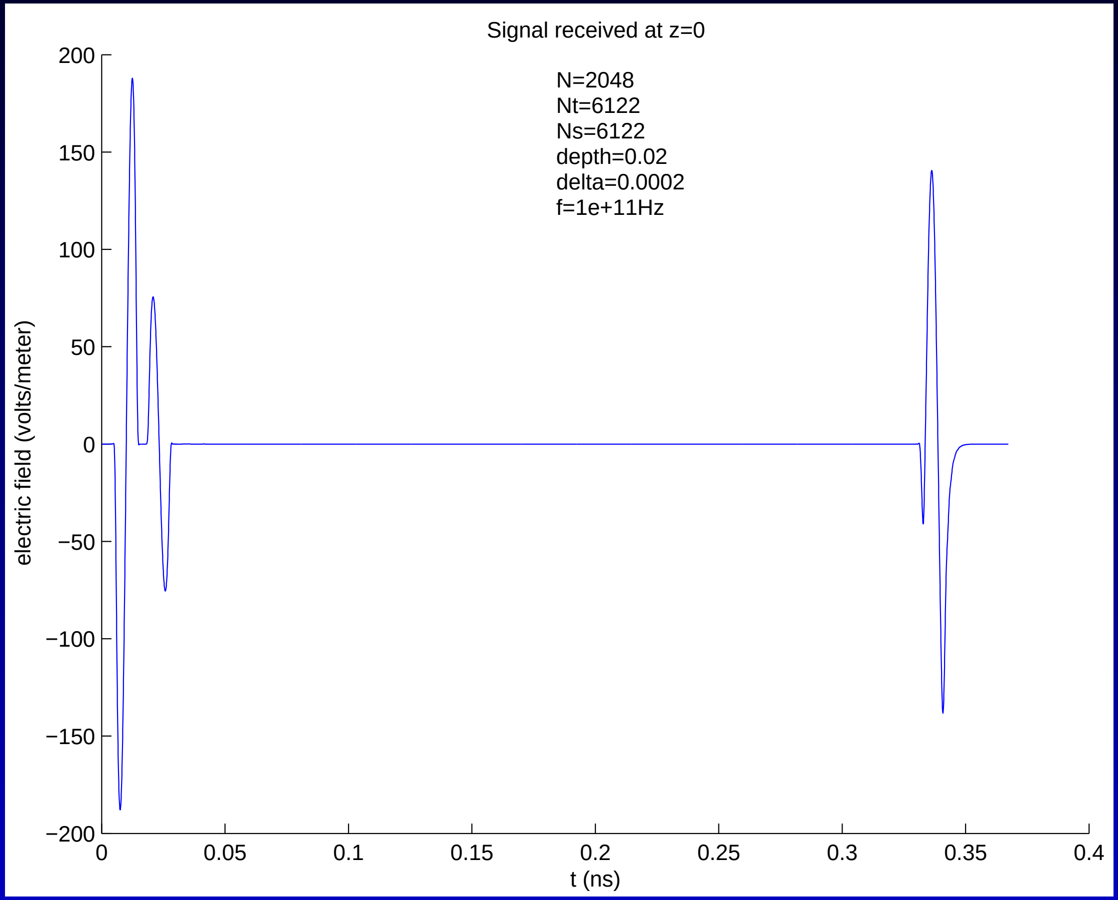
The SOFI is a complex mixture of gases and polyurethane. We account for multiple substances by allowing a variety of parameters in a single model.

Sample Signal Propagation



Snapshots of a windowed electromagnetic pulse with $f = 100GHz$ for the gap detection problem.

Sample Data Received



Reflected signal received at z=0 for the gap detection problem.

Sample Inverse Problem

Given data $\{\hat{E}\}_j$ taken at $z = 0$ and over times t_j, we seek to determine the parameters ν that will produce an E which will minimize a measure of the error, e.g.,

$$\mathcal{J}(\nu) = \sum_j \left(|E(0, t_j; \nu)| - |\hat{E}_j| \right)^2 .$$

Need an efficient way to simulate E given ν.

Maxwell's Equations

In the following, $\mathcal{D} = \Omega \cup \Omega_0$, where Ω is the domain occupied by the material and the ambient, Ω_0, is considered a vacuum.

In $(0, T) \times \mathcal{D}$:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \qquad \nabla \cdot \vec{D} = \rho, \qquad \vec{E}(0, \vec{x}) = 0,$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}, \qquad \nabla \cdot \vec{B} = 0, \qquad \vec{H}(0, \vec{x}) = 0.$$

On $(0, T) \times \partial\mathcal{D}$:

$$\vec{E} \times \vec{n} = 0.$$

Constitutive Relations

In the domain $\mathcal{D}$ we assume the following relations:

$$\vec{D} = \epsilon_0 \epsilon_r \vec{E} + \vec{P},$$
$$\vec{B} = \mu_0 \vec{H},$$
$$\vec{J} = \sigma \vec{E} I_\Omega + \vec{J}_s,$$

where $\epsilon_r = 1 + \chi$ is the relative permittivity, and $\vec{P}$ is the dielectric polarization:

$$\vec{P}(t, \vec{x}) = g \star \vec{E}(t, \vec{x}) = \int_0^t g(t - s, \vec{x}; \nu) \vec{E}(s, \vec{x}) ds,$$

where g is a general dielectric response function (DRF), and ν is some parameter set.

DRF Examples

- Debye model

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

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

- Lorentz model

$$g(t,\vec{x}) = \epsilon_0\omega_p^2/\nu_0 \;\; e^{-t/2\tau} sin(\nu_0 t)$$

- Cole-Cole model (defined via the Laplace transform)

$$\begin{aligned} g(t,\vec{x}) &= \mathcal{L}^{-1}\left\{\frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{1+(s\tau)^\alpha}\right\} \\ &= \frac{1}{2\pi i}\int_{\zeta-i\infty}^{\zeta+i\infty} \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{1+(s\tau)^\alpha} e^{st} ds \end{aligned}$$

Distributions of Parameters

To account for the possible effect of multiple parameter sets ν, consider

$$h(t, \vec{x}; F) = \int_{\mathcal{N}} g(t, \vec{x}; \nu) dF(\nu),$$

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

$$\vec{P}(t, \vec{x}) = \int_0^t h(t - s, \vec{x}) \vec{E}(s, \vec{x}) ds.$$

Multiple Mechanisms

We may further generalize the polarization law to allow for multiple mechanisms

$$K(t,\vec{x};G,F)=\int_{\mathcal{G}}\int_{\mathcal{N}} g(t,\vec{x};\nu)dF(\nu)dG(g).$$

Then the polarization becomes:

$$\vec{P}(t,\vec{x};G,F)=\int_0^t K(t-s,\vec{x};G,F)\vec{E}(s,\vec{x})ds,$$

where $F\in\mathfrak{P}(\mathcal{N})$ and $G\in\mathfrak{P}(\mathcal{G})$. (See [BG05b] for more details.)

1D Model

$$\mu_0\epsilon_0\epsilon_r\ddot{E} + \mu_0 I_\Omega \ddot{P} + \mu_0\sigma I_\Omega \dot{E} - E'' = -\mu_0 \dot{J}_s \quad \text{in } \mathcal{D},$$

$$[\dot{E} - cE']_{z=0} = [E]_{z=1} = 0,$$

$$E(0,z) = \dot{E}(0,z) = 0 \qquad \text{in } \mathcal{D},$$

$$P(t,z) = \int_0^t h(t-s,z;F)E(s,z)ds,$$

$$h(t,z) = \int_{\mathcal{N}} g(t,z;\nu)dF(\nu).$$

Assumptions:

- Uniformity in y, propagation in the z direction
- Zero charge density ($\rho = 0$)
- Single polarization mechanism

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Weak Form

Converting our system to weak form we have:

$$\left\langle \ddot{E}, \phi \right\rangle + \left\langle \gamma \dot{E}, \phi \right\rangle + \langle \beta E, \phi \rangle + \left\langle c^2 E', \phi' \right\rangle +$$

$$\left\langle \int_0^t \alpha(t-s,\cdot) E(s,\cdot) ds, \phi \right\rangle + c\dot{E}(t,0)\phi(0) = \langle \mathfrak{J}, \phi \rangle \, ,$$

where,

$$\gamma(z) = \frac{1}{\epsilon_0} I_\Omega \left[\sigma(z) + h(0,z;F) \right],$$

$$\beta(z) = \frac{1}{\epsilon_0} I_\Omega \dot{h}(0,z;F),$$

$$\alpha(t,z) = \frac{1}{\epsilon_0} I_\Omega \ddot{h}(t,z;F).$$

Well-Posedness

- [BBL00]: existence and uniqueness
- [BG05]: continuous dependence on F in the Prohorov metric, e.g.,

$$|\dot{E}^n - \dot{E}|_{L^2([0,T],H)} + |E^n - E|_{L^2([0,T],V)} \\ \leq \nu|\alpha_n - \alpha|_{L^2} T e^{\nu T}.$$

- Similar arguments hold for γ and β
- Therefore $F \to (E, \dot{E})$ is continuous from $\mathfrak{P}(\mathcal{N})$ to $L^2([0,T],V) \times L^2([0,T],H)$.

Inverse Problem for F

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

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

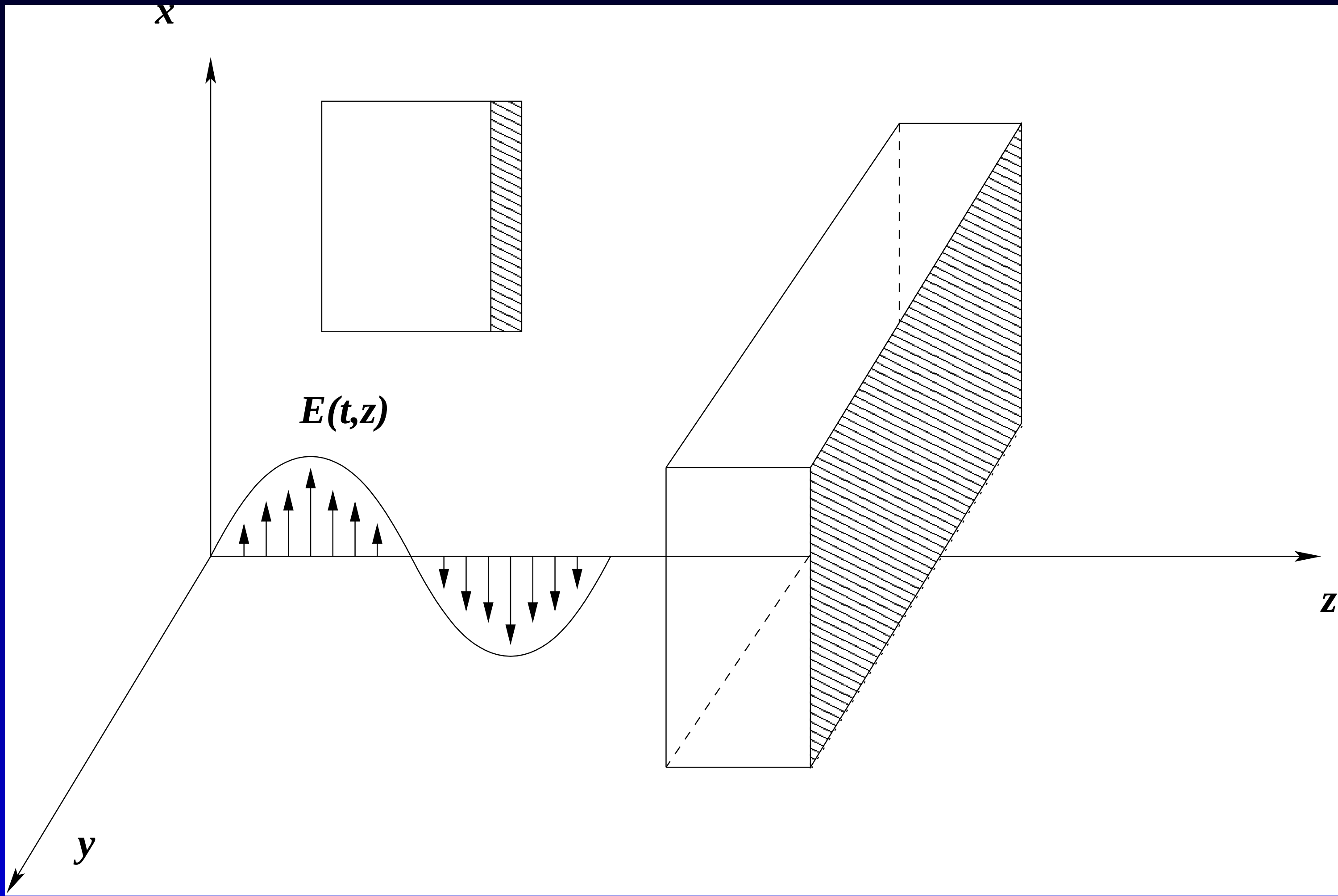
where, for example,

$$\mathcal{J}(F) = \sum_j \left(|E(0, t_j; F)| - |\hat{E}_j| \right)^2.$$

Stability of Inverse Problem

- Continuity of $F \to (E, \dot{E}) \implies$ continuity of $F \to \mathcal{J}(F)$
- Compactness of $\mathcal{N} \implies$ compactness of $\mathfrak{P}(\mathcal{N})$ with respect to the Prohorov metric
- Therefore, minimum of $\mathcal{J}(F)$ over $\mathfrak{P}(\mathcal{N})$ exists

Distribution Inverse Problem



$$J_s(t,z) = \delta_0(z)\sin(\omega t) I_{[0,t_f]}(t)$$

1D Maxwell's Equations

$$\mu_0\epsilon_0\epsilon_r\ddot{E} + \mu_0 I_\Omega \ddot{P} + \mu_0\sigma I_\Omega \dot{E} - E'' = -\mu_0 \dot{J}_s \qquad \text{in } \Omega \cup \Omega_0$$

$$\tau\dot{P} + P = \epsilon_0(\epsilon_s - \epsilon_\infty)E \qquad \text{in } \Omega$$

$$[\dot{E} - cE']_{z=0} = 0$$

$$[E]_{z=1} = 0$$

$$E(0,z) = \dot{E}(0,z) = 0$$

$$P(0,z) = 0$$

where

$$J_s(t,z) = \delta_0(z) sin(\omega t) I_{[0,t_f]}(t)$$

and

$$\epsilon_r = (1 + (\epsilon_\infty - 1)I_\Omega).$$

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Finite Element Method in Space

The resulting system of differential equations in semi-discrete form can be written

$$M_1\ddot{e} + M_2\dot{e} + M_3 e + \lambda^2\bar{p} = \eta_0 J \tag{1}$$

$$\dot{\bar{p}} + \lambda\bar{p} = \epsilon_d \lambda M^\Omega e. \tag{2}$$

where $\eta_0{=}\sqrt{\mu_0/\epsilon_0}$, $\epsilon_d{=}\epsilon_s - \epsilon_\infty$, $\lambda{=}1/c\tau$, e and p are vectors representing the approximate values of E and P respectively at the nodes z_i, $\bar{p}{=}M^\Omega p$ where M^Ω is the mass matrix integrated only over Ω.

Finite Difference in Time (p)

Our finite difference approximation for (2) is

$$\bar{p}_{n+1} = \bar{p}_n + \frac{\lambda \Delta t}{1 + \lambda \Delta t \theta} (\epsilon_d M^\Omega e_{n+\theta} - \bar{p}_n) \qquad (3)$$

where $[e_n]_j = E(t_n, z_j)$, $[\bar{p}_n]_j = M^\Omega P(t_n, z_j)$, $z_j = jh$, and $e_{n+\theta} = \theta e_n + (1-\theta) e_{n+1}$ is a weighted average of e_n and e_{n+1} for relaxation to help with stability of the method.

Finite Difference in Time (e)

Applying second order central differencing with averaging to (1) gives

$$A_1 e_{n+2} = A_2 e_{n+1} + A_3 e_n + \Delta t^2 \eta_0 J_{n+1} - \lambda^2 \Delta t^2 \bar{p}_{n+1}.$$

Also, approximating E with its Taylor expansion around t_0=0 and applying the initial conditions and ODE we get

$$E(t_1, z) \approx -\frac{\Delta t^2}{2} \mu_0 \dot{J}_s(0, z).$$

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Numerical Discretization

- Second order FEM in space
  - piecewise linear splines
- Second order FD in time
  - Crank-Nicholson (P)
  - Central differences (E)
  - $e_n \longrightarrow p_n \longrightarrow e_{n+1} \longrightarrow p_{n+1} \longrightarrow \cdots$
- E equation implicit, LU factorization used

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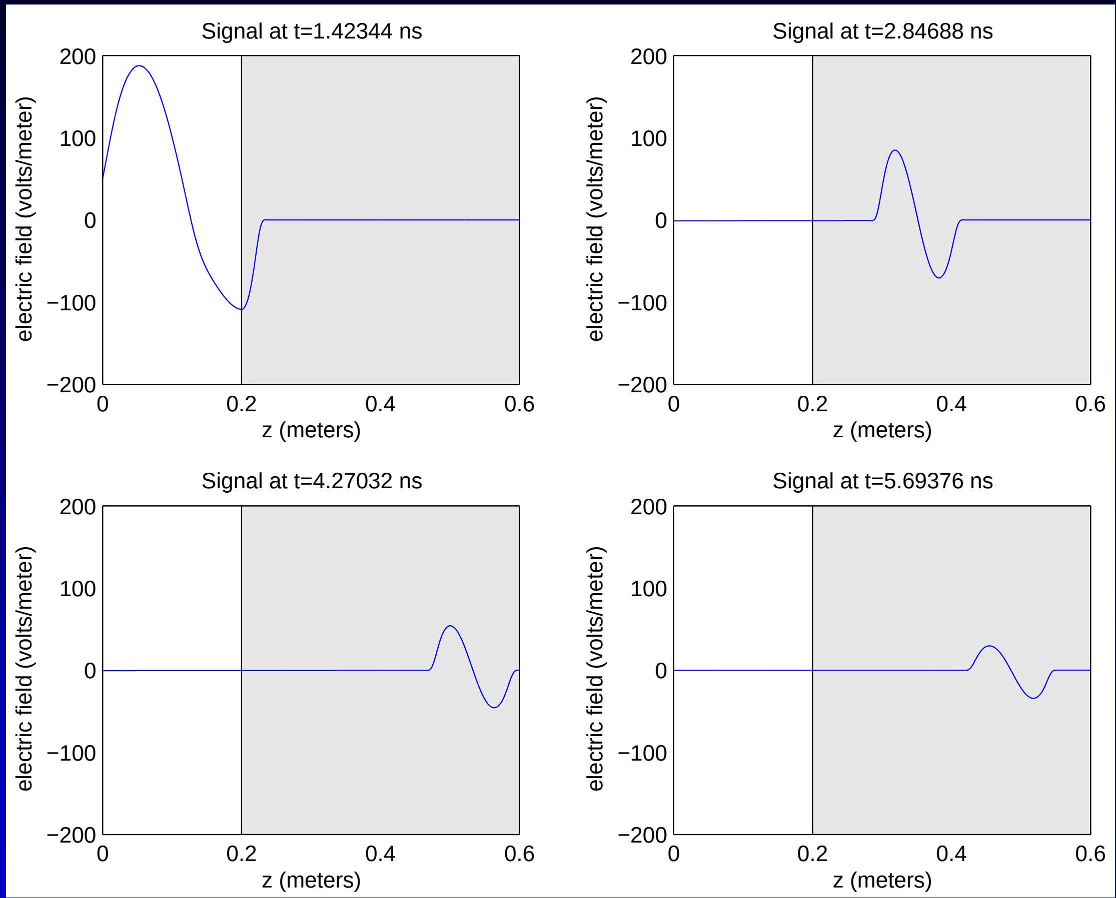
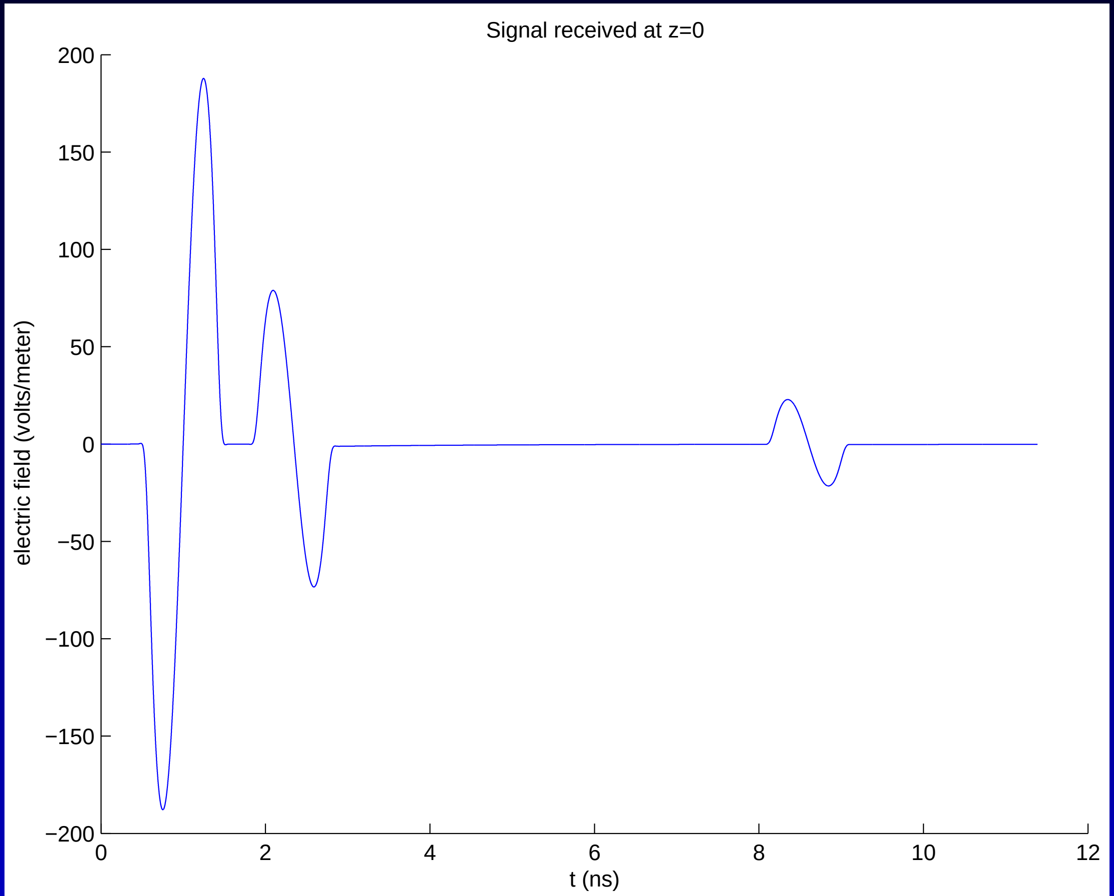
Sample Simulation



Forward simulation of a windowed electromagnetic pulse with $f{=}1GHz$ incident on a Debye medium of width $d{=}.4m$ with a metal backing. Note that $J_s(t,z) = \delta(z)sin(\omega t)I_{[0,t_f]}(t)$.

Sample Data



Reflected signal received at z=0.

Discrete Distribution Example

- Mixture of two Debye materials with τ_1 and τ_2
- Total polarization a weighted average

$$P = \alpha_1 P_1(\tau_1) + \alpha_2 P_2(\tau_2)$$

- Corresponds to the discrete probability distribution

$$dF(\tau) = \left[\alpha_1 \delta(\tau_1) + \alpha_2 \delta(\tau_2)\right] d\tau$$

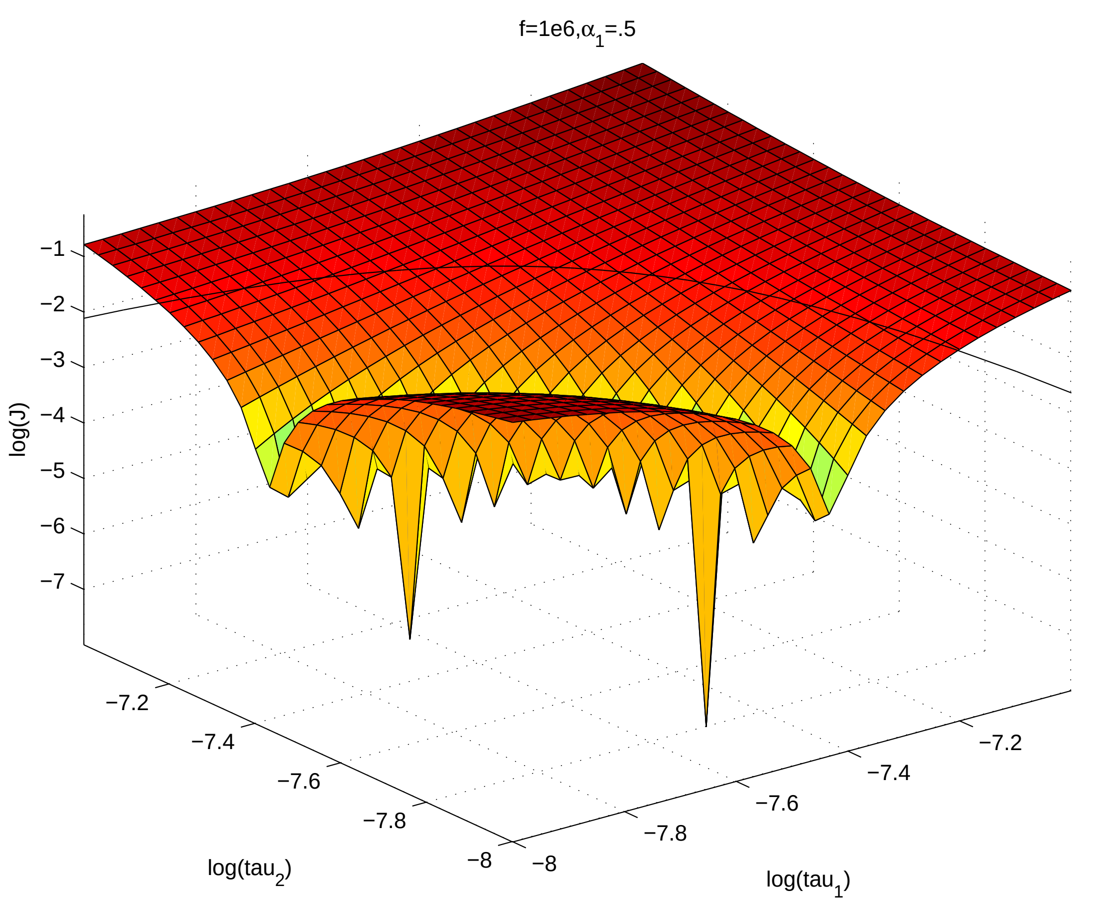
Discrete Distribution Inverse Problem

- Assume the proportions α_1 and $\alpha_2 = 1 - \alpha_1$ are known.
- Define the following least squares optimization problem:

$$\min_{(\tau_1,\tau_2)} \mathcal{J} = \min_{(\tau_1,\tau_2)} \sum_j \left| |E(t_j, 0; (\tau_1, \tau_2))| - |\hat{E}_j| \right|^2,$$

where $\hat{E}_j$ is *synthetic* data generated using (τ_1^*, τ_2^*) in our simulation routine.

Discrete Distribution J using $10^6 Hz$



The solid line above the surface represents the curve of constant $\tilde{\tau} := \alpha_1\tau_1 + (1-\alpha_1)\tau_2$. Note: $\omega\tilde{\tau} \approx .15 < 1$.

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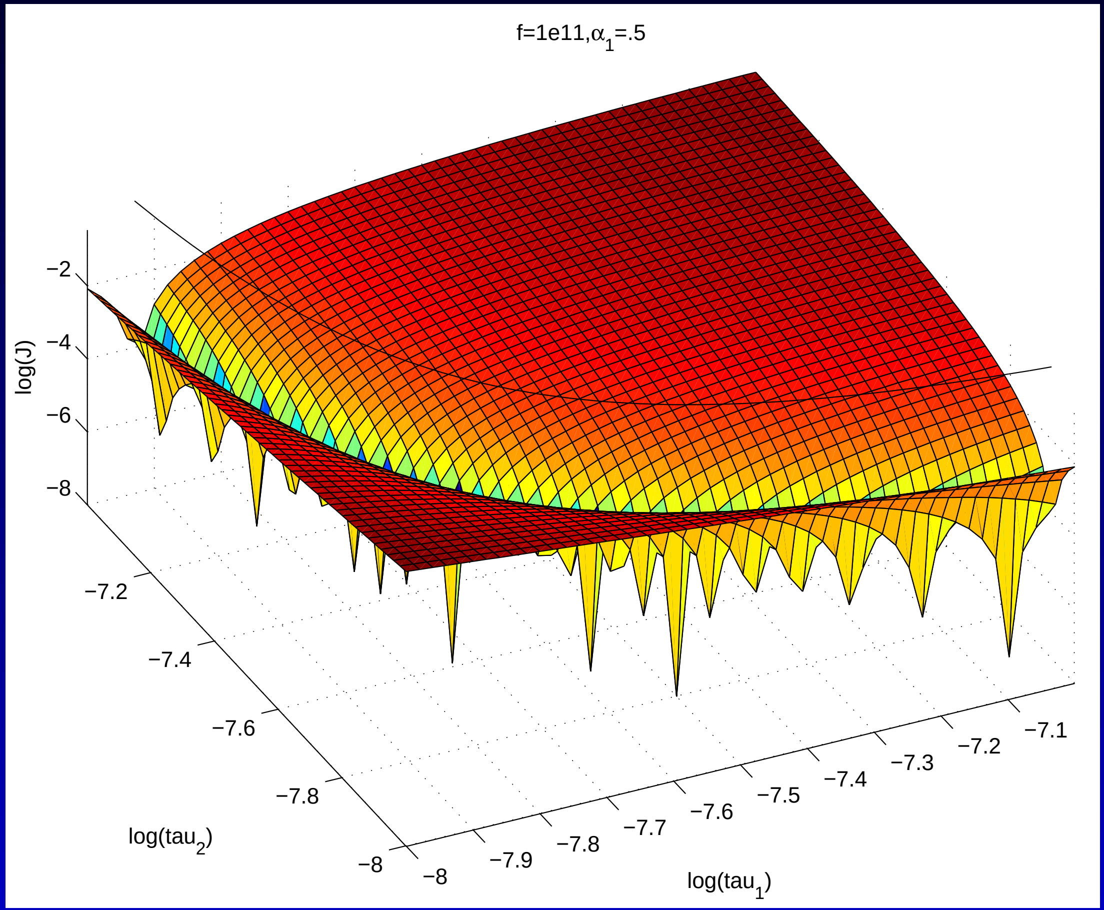
Inverse Problem Results $10^6 Hz$

	τ_1	τ_2	$\tilde{\tau}$
Initial	3.95000e-8	1.26400e-8	2.60700e-8
LM	3.19001e-8	1.55032e-8	2.37016e-8
Final	3.16039e-8	1.55744e-8	2.37016e-8
Exact	3.16000e-8	1.58000e-8	2.37000e-8

- Levenberg-Marquardt converges to curve of constant $\tilde{\tau}$
- Traversing curve results in accurate final estimates

Discrete Distribution J using $10^{11} Hz$



The solid line above the surface represents the curve of constant $\tilde{\lambda} := \frac{1}{c\tilde{\tau}} = \frac{\alpha_1}{c\tau_1} + \frac{\alpha_2}{c\tau_2}$. Note: $\omega\tilde{\tau} \approx 15000 > 1$.

Inverse Problem Results $10^{11} Hz$

	τ_1	τ_2	$\tilde{\lambda}$
Initial	3.95000e-8	1.26400e-8	0.174167
LM	4.08413e-8	1.41942e-8	0.158333
Final	3.16038e-8	1.57991e-8	0.158333
Exact	3.16000e-8	1.58000e-8	0.158333

- Levenberg-Marquardt converges to curve of constant $\tilde{\lambda}$
- Traversing curve results in accurate final estimates

Volume Proportions

Above we assumed the relative volume proportions of each material (α_1 and $1 - \alpha_1$) were known. However, for problems where the geometry allows interrogation with angular frequencies above and below the critical $\tilde{\tau}^{-1}$ value we can, in theory, determine the volume proportions as well.

Volume Proportion Example

- Using $f = 10^6 Hz$, we converge to $\tilde{\tau}$ even when α_1 is not known!
- Using $\tilde{\tau}$, eliminate α_1:

$$\alpha_1 = \frac{\tilde{\tau} - \tau_2}{\tau_1 - \tau_2}.$$

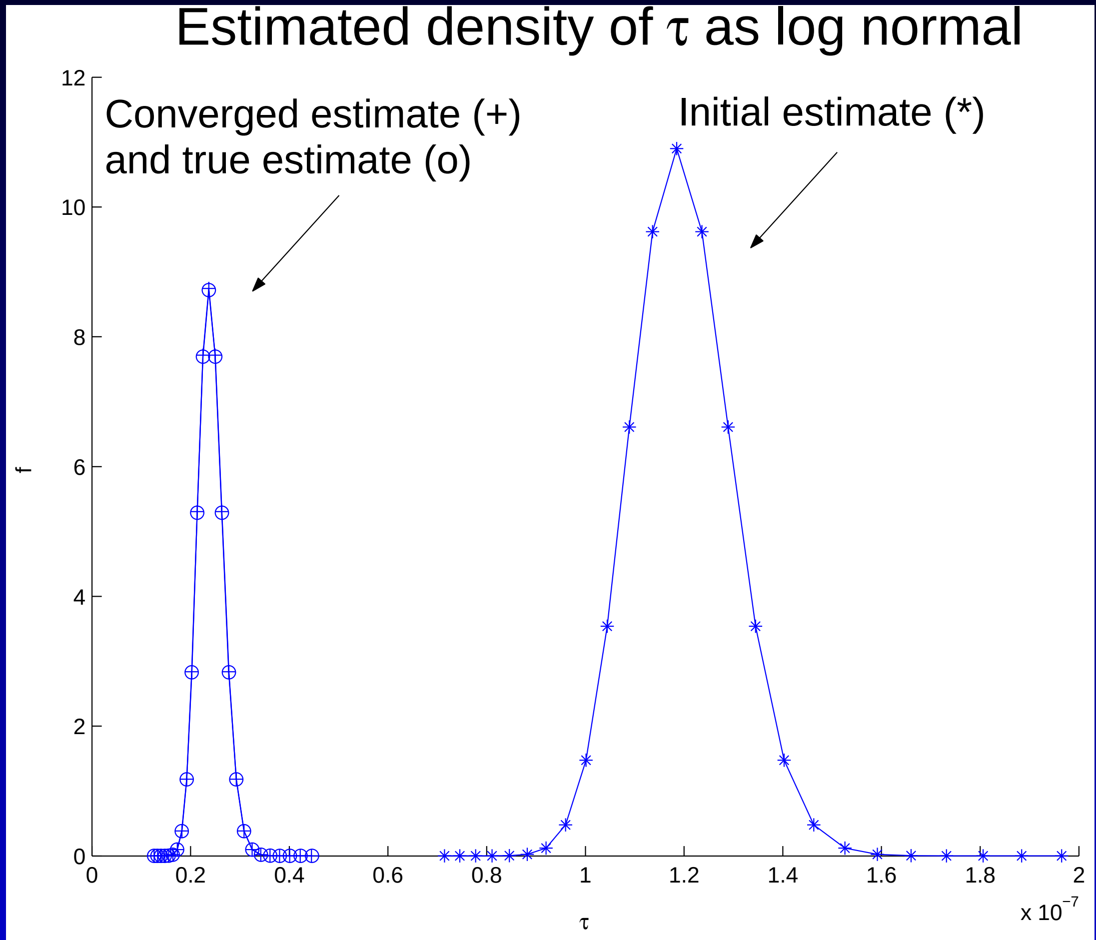
- Interrogating with $f = 10^9 Hz$ is a two parameter inverse problem

Results using $10^6 Hz$ and $10^9 Hz$

	τ_1	τ_2	α_1	$\tilde{\tau}$	$\tilde{\lambda}$
Initial	1.58000e-7	3.16000e-9	0.999900	1.57985e-7	0.0212146
10^6	2.12522e-8	8.82441e-9	0.687959	1.73742e-8	0.225925
10^9	3.13819e-8	1.57826e-8	0.102596	1.73830e-8	0.200566
Exact	3.16000e-8	1.58000e-8	0.100000	1.73800e-8	0.200556

- Using $f = 10^6 Hz$ Levenberg-Marquardt converges to curve of constant $\tilde{\tau}$
- Using $f = 10^9 Hz$ with α_1 fixed by $\tilde{\tau}$ Levenberg-Marquardt converges to curve of constant $\tilde{\lambda}$
- Traversing $\tilde{\lambda}$ curve results in accurate final estimates

Gaussian Distribution



Results of inverse problem applied to a log-normal distribution of relaxation times.

Bi-gaussian Distribution of $\log\tau$

- Bi-gaussian distribution with means μ_1 and μ_2 and with standard deviations σ_1 and σ_2:

$$dF(\tau) = \alpha_1 d\hat{F}(\tau;\mu_1,\sigma_1) + (1-\alpha_1)d\hat{F}(\tau;\mu_2,\sigma_2),$$

where

$$d\hat{F}(\tau;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\frac{1}{\ln 10}\frac{1}{\tau}\exp\left(-\frac{(\log\tau-\mu)^2}{2\sigma^2}\right)d\tau,$$

- Corresponding inverse problem:

$$\min_{q=(\mu_1,\sigma_1,\mu_2,\sigma_2)} \sum_j \left| |E(t_j,0;q)| - |\hat{E}_j| \right|^2.$$

Bi-gaussian Results with $10^6 Hz$

case	μ_1	σ_1	μ_2	σ_2	$\tilde{\tau}$
Initial	1.58001e-7	0.036606	3.16002e-9	0.0571969	8.1201e-8
μ_1,μ_2	4.27129e-8	0.036606	4.24844e-9	0.0571969	2.36499e-8
Final	3.09079e-8	0.0136811	1.63897e-8	0.0663628	2.37978e-8
Exact	3.16000e-8	0.0457575	1.58000e-8	0.0457575	2.37957e-8

- Levenberg-Marquardt converges to curve of constant $\tilde{\tau}$
- Traversing curve results in accurate final estimates

Note: for this continuous distribution,

$$\tilde{\tau} = \int_{\mathcal{T}} \tau dF(\tau).$$

Bi-gaussian Results with $10^{11} Hz$

case	μ_1	σ_1	μ_2	σ_2	$\tilde{\lambda}$
Initial	1.58001e-7	0.036606	3.16002e-9	0.0571969	0.538786
μ_1,μ_2	1.58001e-7	0.036606	1.12595e-8	0.0571969	0.158863
Final	3.23914e-8	0.0366059	1.56020e-8	0.0571968	0.158863
Exact	3.16000e-8	0.0457575	1.58000e-8	0.0457575	0.158863

- Levenberg-Marquardt converges to curve of constant $\tilde{\lambda}$
- Traversing curve results in accurate final estimates

Note: for this continuous distribution,

$$\tilde{\lambda} = \int_{\mathcal{T}} \frac{1}{c\tau} dF(\tau).$$

Comments on Inverse Problems

- We have shown well-posedness of the problem for determining distributions of dielectric parameters
- Our estimation methods worked well for discrete distributions
- Our estimation methods worked well for the continuous uniform distribution and gaussian distributions
- We are currently only able to determine the means in the bi-gaussian distributions, the data is relatively insensitive to the standard deviations

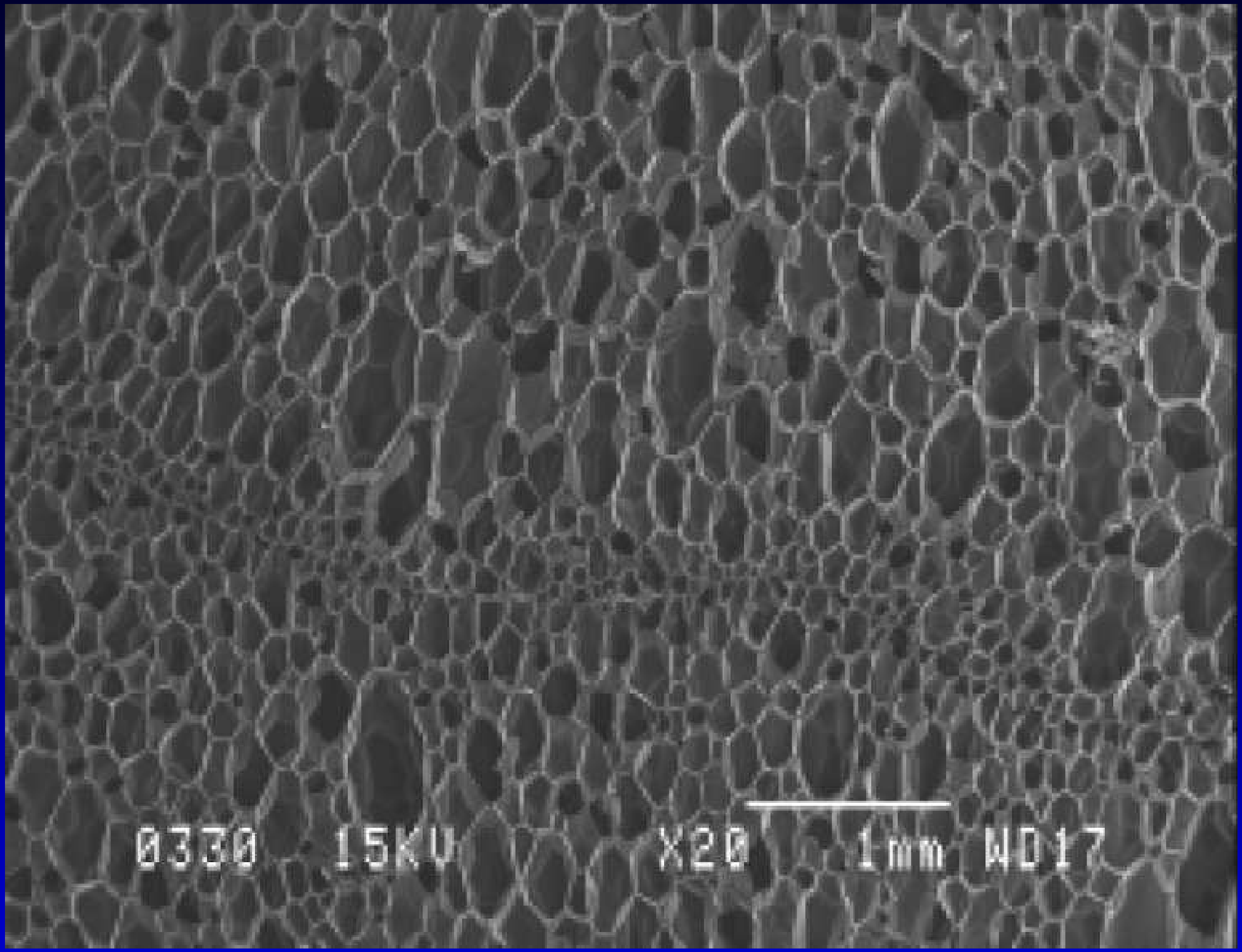
Homogenization

- A good fit when $\tilde{\lambda}$ (or $\tilde{\tau}$) is constant suggests using a single τ, even for the bi-gaussian case
- This modeling approach concludes that the "effective" parameter should be $\tilde{\tau}$
- We have considered a more elaborate homogenization method based on "period unfolding".
- This approach allows us to use information about the periodic structure, i.e., hexagonal cells.
- See [B-05] for details.

Summary

- Distributions of dielectric mechanisms and parameters
  - Theoretical foundation established
  - Sample problems worked well for certain distributions
  - Suggests applying homogenization techniques (in progress!)

SOFI under 20X magnification



Cured Layer

As the top of each layer cures, a thin line is formed which is of higher density (i.e., is comprised of smaller, more tightly packed polyurethane cells).

Modeling Knit Lines

- The speed of propagation in the domain is

$$c(\vec{x}) = \frac{c_0}{n(\vec{x})} = \sqrt{\frac{1}{\epsilon(\vec{x})\mu_0}},$$

  where c_0 is the speed in a vacuum and n is the index of refraction.
- We model knit lines by changing the index of refraction, thus effectively the speed in that region.

Future Directions

- Modeling approaches
  - Mixtures of polarization models
  - Consider frequency dependence in choice of mechanisms
  - Separate scattering mechanism to match attenuation observed in data
  - Compare simulations using distributions to those using homogenization techniques
  - Perform more experiments to validate method
  - Consider fractional order polarization models (Cole-Cole)
  - Fit model to data (may require *new* model)
  - Separate mechanism to match high attenuation observed
- Knit lines
  - Move to Higher Dimensions:
  - Need to consider oblique angles

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