Bayesian Inference and Sensitivity Analysis for Multi-Scale Materials

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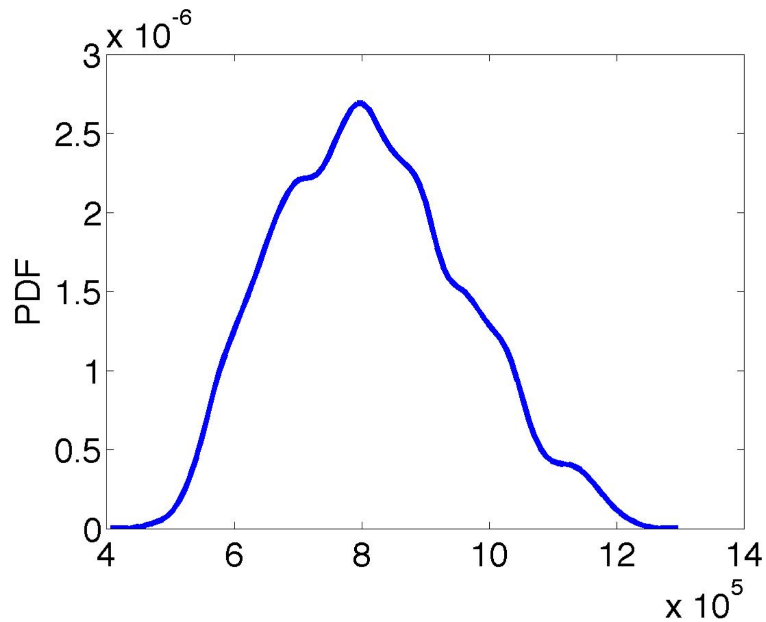

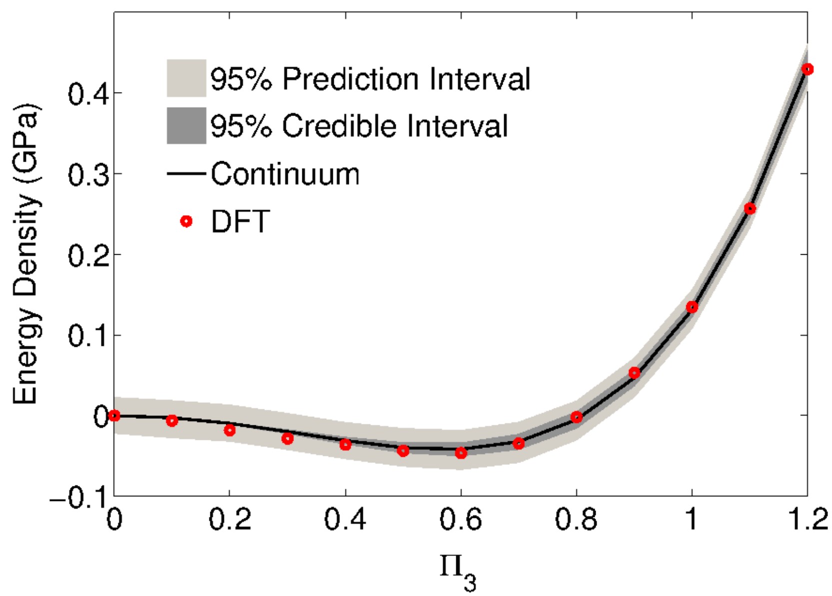

Support: DOE Consortium for Advanced Simulation of LWR (CASL)

NNSA Consortium for Nonproliferation Enabling Capabilities (CNEC)

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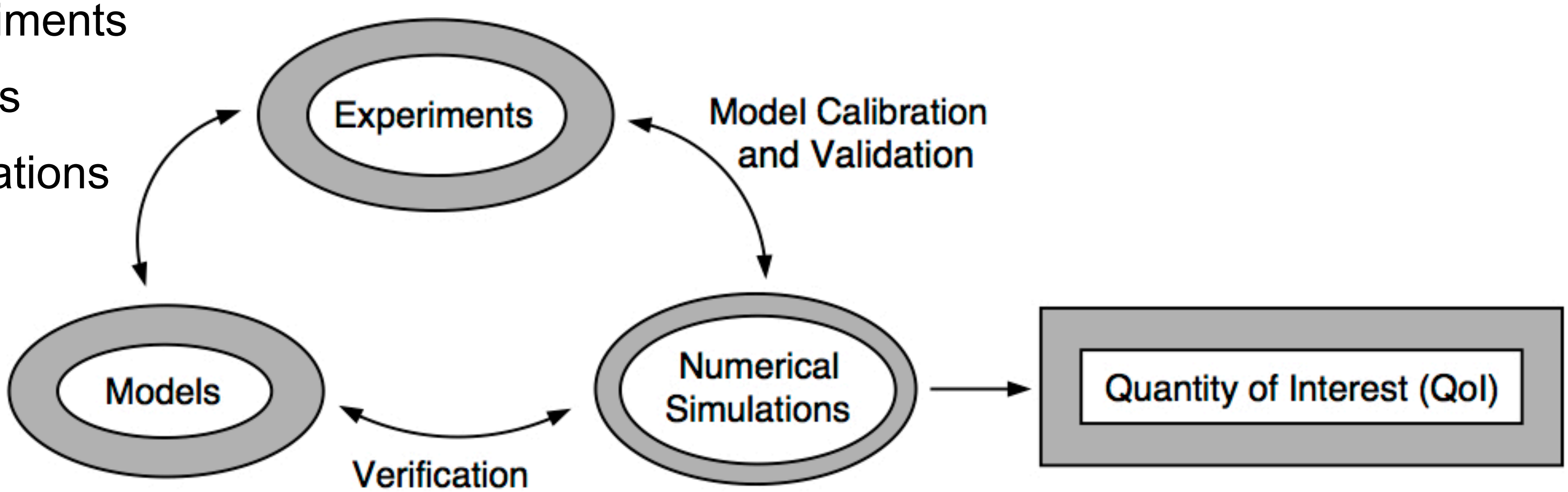
Predictive Science

Components: All involve uncertainty

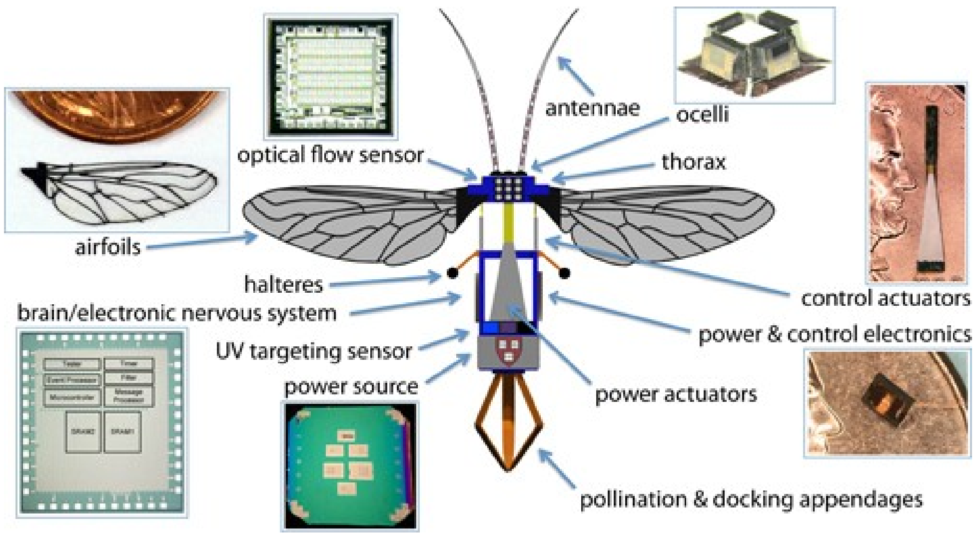
- Experiments
- Models
- Simulations



- *Experimental results are believed by everyone, except for the person who ran the experiment*, source anonymous, quoted by Max Gunzburger, Florida State University.
- *Essentially, all models are wrong, but some are useful,* George E.P. Box, Industrial Statistician.
- *Computational results are believed by no one, except the person who wrote the code*, source anonymous, quoted by Max Gunzburger, Florida State University.
- *I have always done uncertainty quantification. The difference now is that it is capitalized.* Bill Browning, Applied Mathematics Incorporated.

Example: PZT-Based Actuators and Sensors

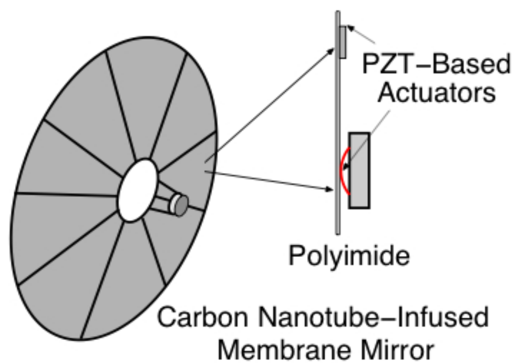
PZT: Robobee -- Rob Wood, Harvard University



Applications and Challenges:

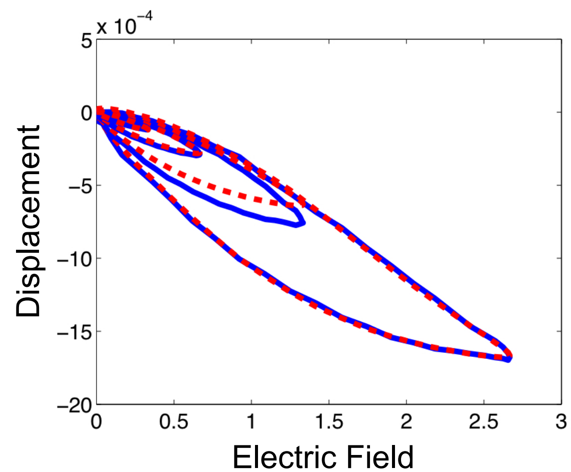
- Autonomous crop pollination
- Search and rescue
- Surveillance
- Weather and climate mapping
- Nonlinear and hysteretic dynamics

Macro-Fiber Composites (MFC)



Applications and Challenges:

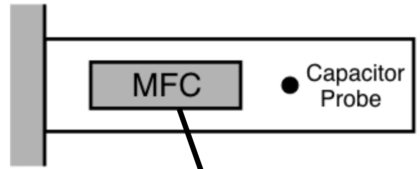
- Deployment/control of membrane mirrors
- Shape modification, flow control
- kHz to MHz response rates
- Nonlinear and hysteretic dynamics



Energy Harvesting: Several platforms

Multiscale Homogenized Energy Model (HEM) Development

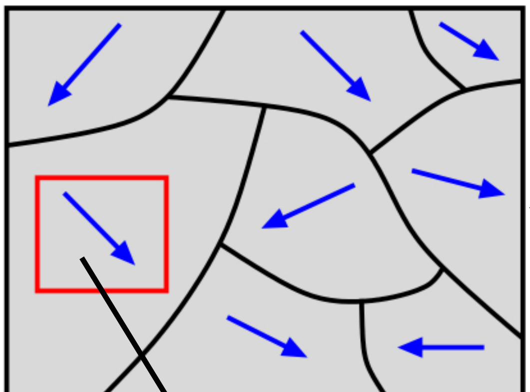
Example: PZT-Based Macro-Fiber Composite

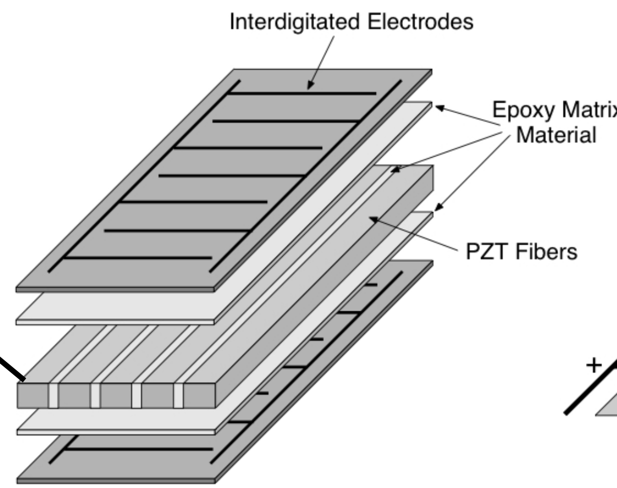


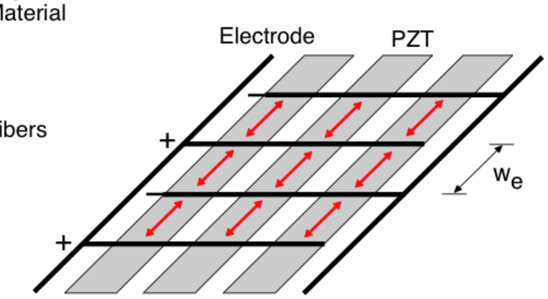
$$\rho \ddot{u} = \nabla \cdot \sigma + F$$

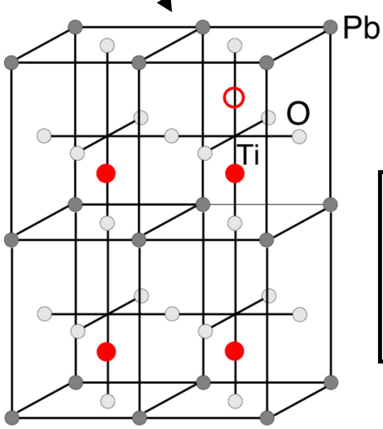
$$\nabla \cdot D = 0\,, \;\; D = \varepsilon_0 E + P$$

$$\nabla \times E = 0\,, \;\; E = -\nabla \varphi$$









$$P^\alpha = d_\alpha \sigma + \chi_\alpha^\sigma E + P_R^\alpha$$

$$\varepsilon^\alpha = s_\alpha^E \sigma + d_\alpha E + \varepsilon_R^\alpha$$

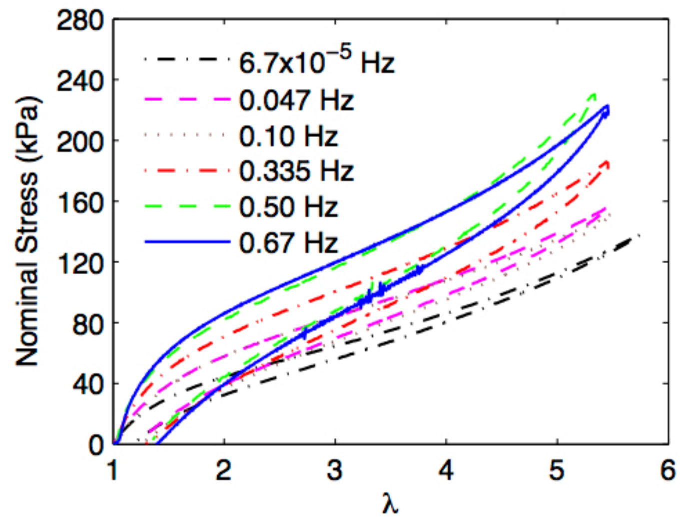
$$P = d(E,\sigma)\sigma + \chi^\sigma E + P_{irr}(E,\sigma)$$

$$\varepsilon = s^E \sigma + d(E,\sigma)E + \varepsilon_{irr}(E,\sigma)$$

Collaboration: Billy Oates (FSU), Zhengzheng Hu (NCSU)

Example: Viscoelastic Material Models

Collaboration: Billy Oates, Paul Miles, Michael Hays (FSU)



Material Behavior: Significant rate dependence

Finite-Deformation Model: Nonlinear non-affine

$$\Upsilon_L = \sum_\alpha \left[\frac{1}{2}\gamma^\alpha (F_{iK} - \Gamma_{iK}^\alpha)(F_{iK} - \Gamma_{iK}^\alpha) \right]$$

$$\psi_\infty^N = \frac{1}{6} G_c I_1 - G_c \lambda_{\max}^2 \ln\left(3\lambda_{\max}^2 - I_1\right) + G_e \sum_j \left(\lambda_j + \frac{1}{\lambda_j}\right)$$

Parameters: Nonlinear non-affine model

$$q = [G_e, G_c, \lambda_{\max}, \eta, \beta, \gamma]$$

$$q = [\eta, \beta, \gamma] \;, \; \text{Fixed hyperelastic parameters}$$

G_c: Crosslink network modulus

G_e: Plateau modulus

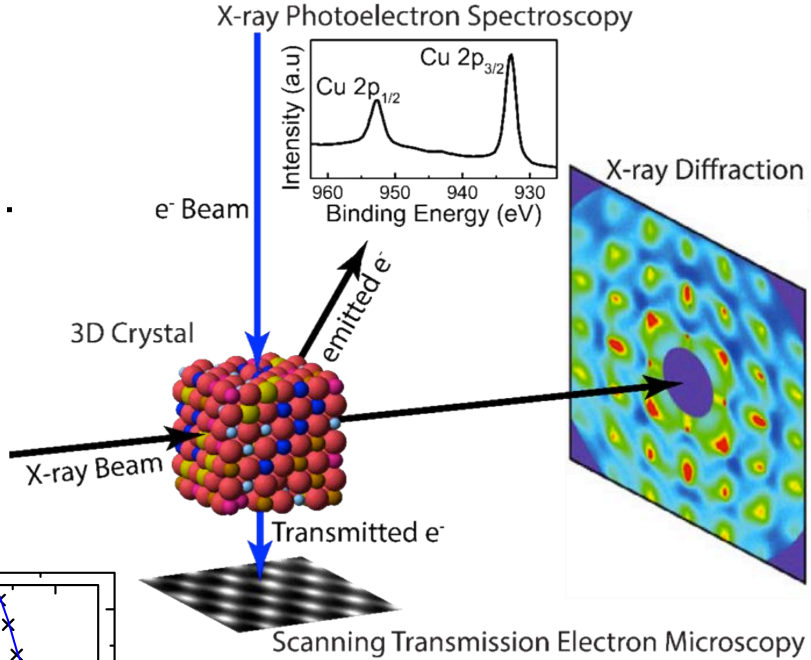
$\lambda_{\max}$: Maximum stretch of effective affine tube

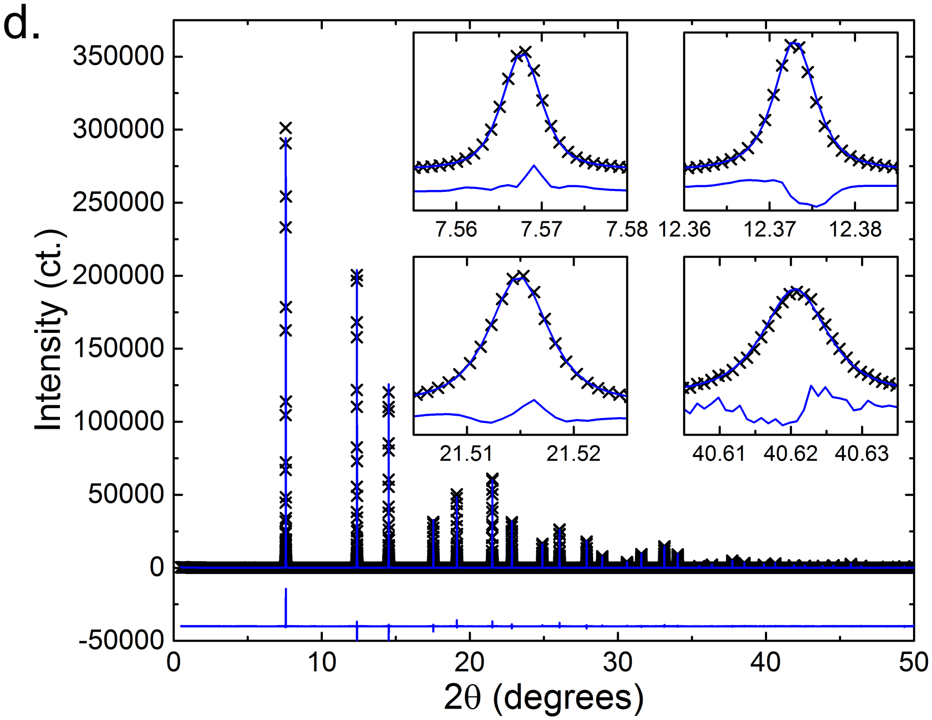
Example: X-Ray Crystallography

Properties:

- Reveal relative positions of atoms, their atomic number, types of chemical bonds, etc..
- Applications: determination of of DNA structure, design of pharmaceuticals, etc..

Objective: Use Bayesian analysis to quantify uncertainty associated with Rietveld model and background.

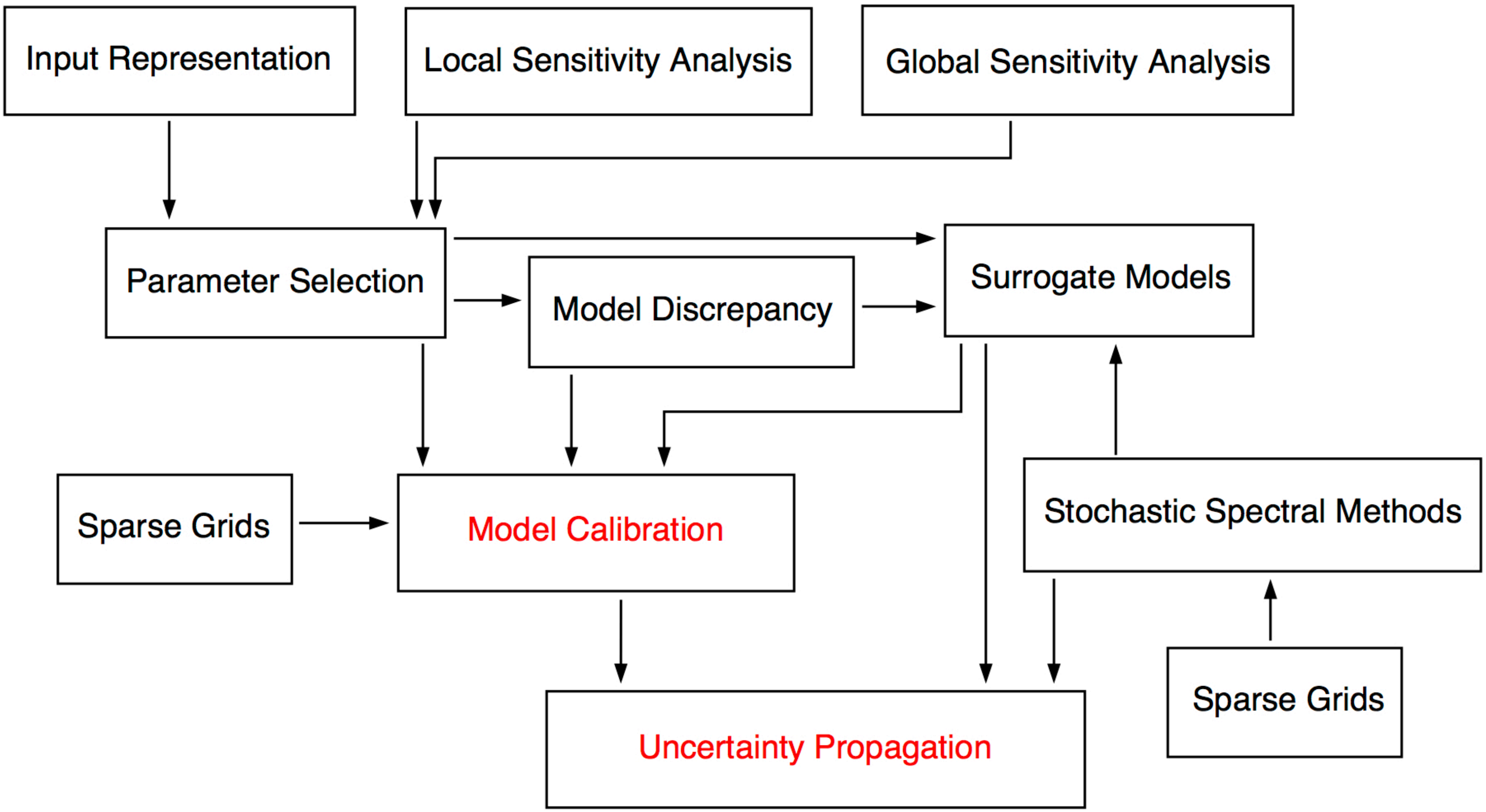




Collaboration: C. Fancher, J. Jones, Z. Han, B. Reich, A. Wilson, I. Levin, K. Page

Steps in Uncertainty Quantification

Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.

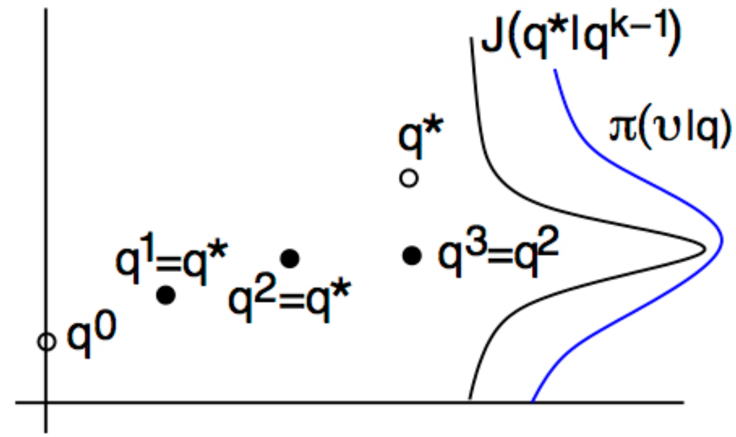


Bayesian Model Calibration

Bayesian Model Calibration:

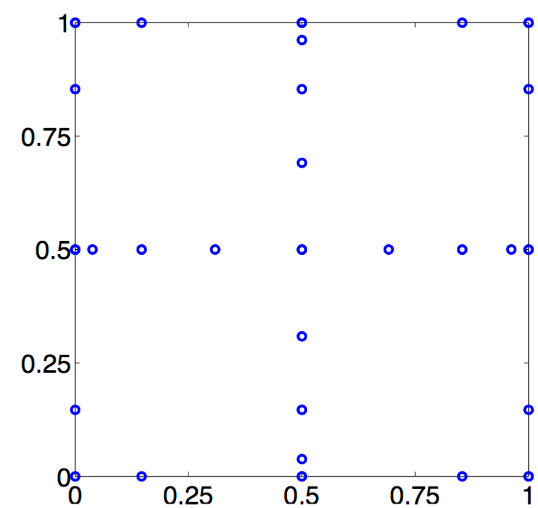
- Parameters considered to be random variables with associated densities.

$$\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}$$



Problem:

- Often requires high dimensional integration;
  - e.g., p = 18 for MFC model
    - HEM: $q_{hys} = [P_R^+, \varepsilon_R^+, \varepsilon_R^{90}, \chi^\sigma, d_+, \gamma, \tau_{90}, \tau_{180}, \mu_c, \sigma_c^2, \sigma_I^2]$
    - Beam: $q_{beam} = [\overline{\rho}, \widehat{\rho}, \overline{c^E I}, \widehat{c^E I}, \overline{c_D I}, \widehat{c_D I}, \gamma_v, k_2]$
  - p = thousands to millions for neutron transport models for nuclear power plant design



Strategies:

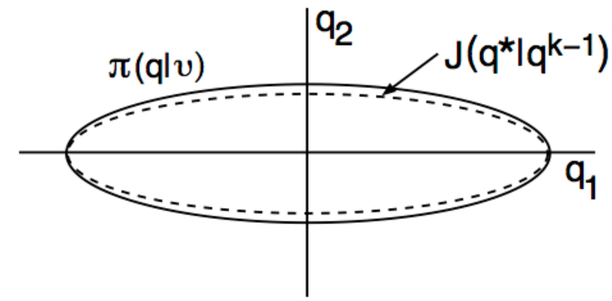
- Sampling methods (Metropolis algorithms)
- Sparse grid quadrature techniques

Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006]

Proposal Distribution

$$J(q^*|q^{k-1}) = N(q^{k-1}, V)$$



1. Determine $q^0 = \arg\min_q \sum_{i=1}^{N} [\upsilon_i - f(t_i, q)]^2$

2. Construct covariance estimate V

3. For $k = 1, \cdots, M$

   (a) Construct candidate

   $$q^* \sim N(q^{k-1}, V)$$

   (b) Compute

   $$SS_{q^*} = \sum_{i=1}^{N} [\upsilon_i - f(t_i, q^*)]^2$$

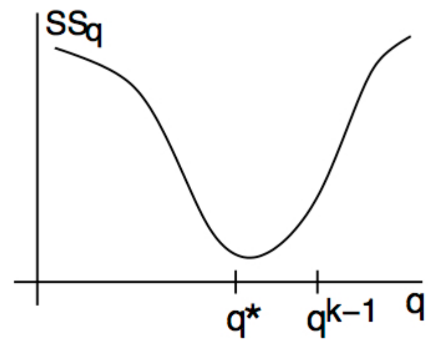
   $$\pi(\upsilon|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}$$

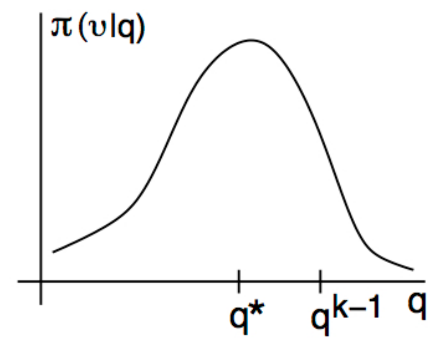
   (c) Compute

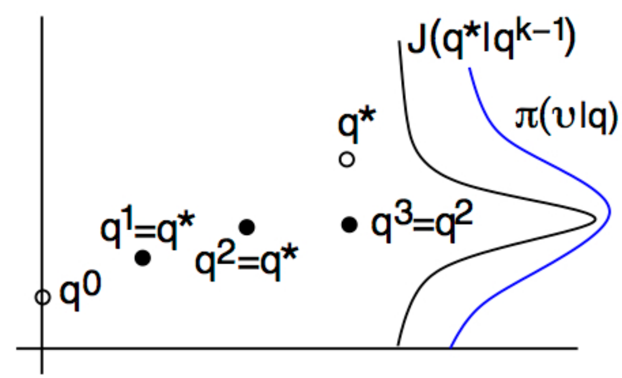
   $$\alpha(q^*|q^{k-1}) = \min\left(1, e^{-[SS_{q^*} - SS_{q^{k-1}}]/2\sigma^2}\right)$$

   (f) Accept q^* with probability α

4. Update covariance as samples accepted

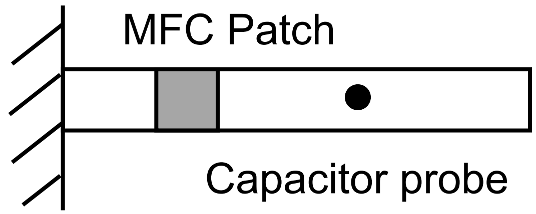






Bayesian Model Calibration for Macro-Fiber Composite

Experimental Structure:

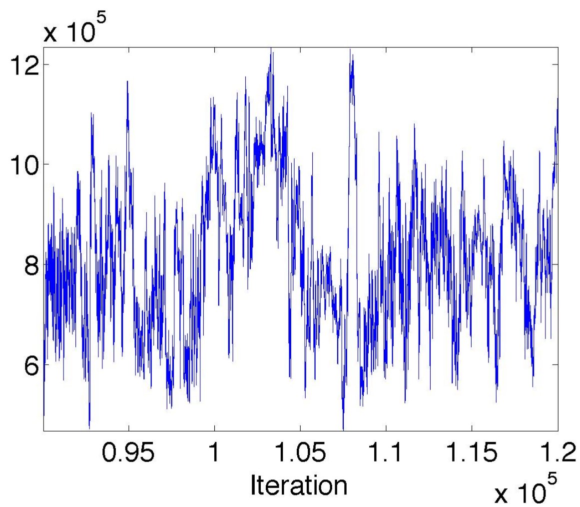


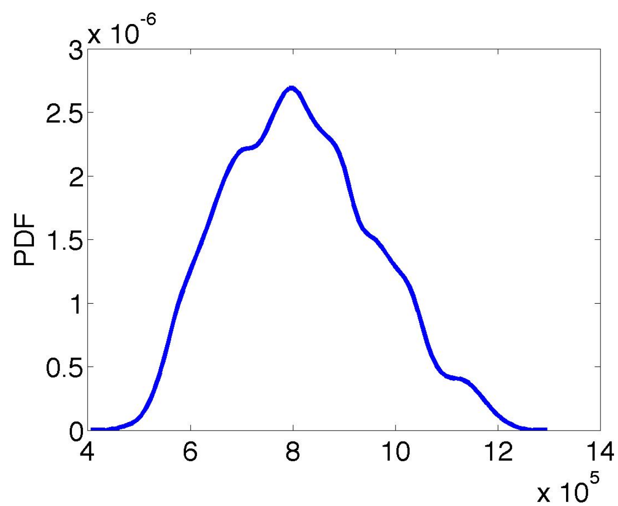
Beam Model:

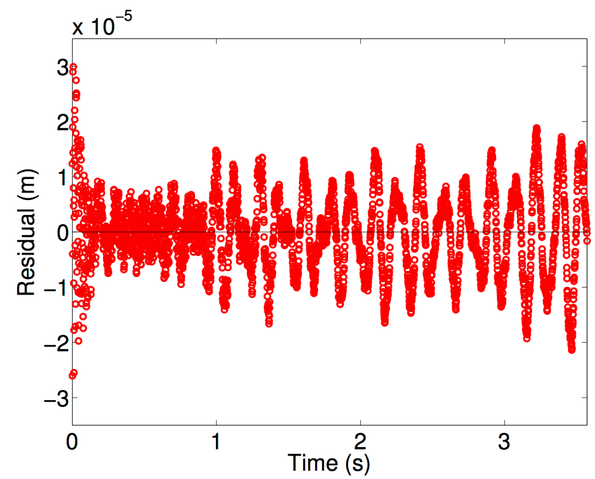
$$\rho \frac{\partial^2 w}{\partial t^2} - \frac{\partial^2 M}{\partial x^2} = f$$

$$M = -c^E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} - [k_1 e(E,\sigma_0)E + k_2 \varepsilon_{irr}(E,\sigma_0)]\, \chi_{MFC}(x)$$

Representative DRAM Results: (18 parameters, 32 states)





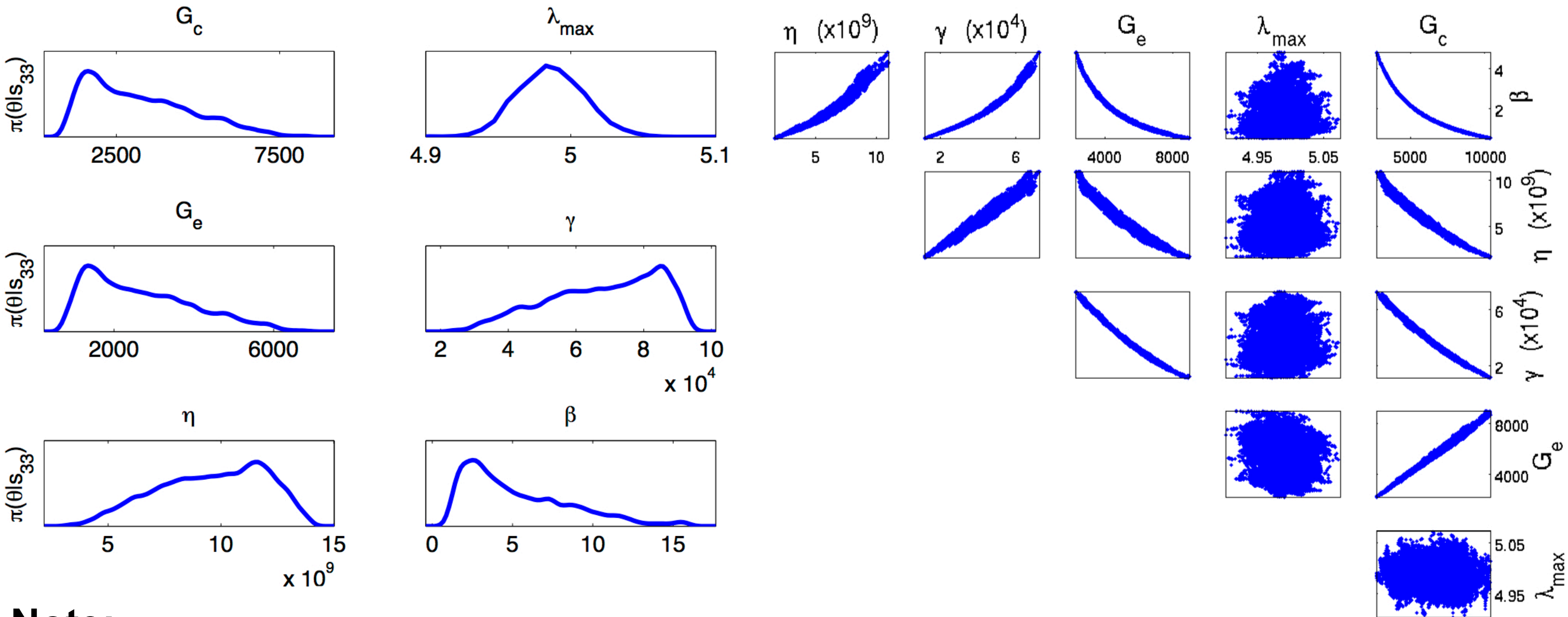


Correlated Residuals

Bayesian Model Calibration for Viscoelastic Model

Full Parameter Set: Nonlinear non-affine model

$$q = [G_e, G_c, \lambda_{\max}, \eta, \beta, \gamma]$$



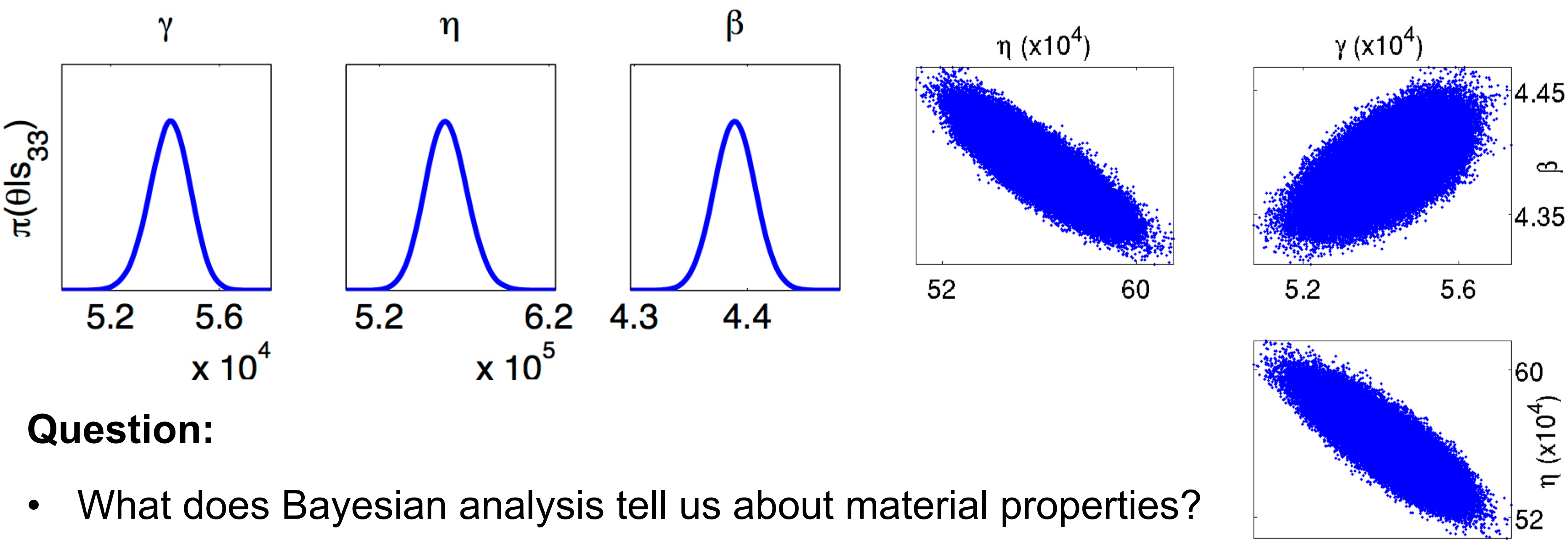
Note:

- Several parameter pairs appear non-identifiable in the sense they are not uniquely determined by the response.

Bayesian Model Calibration for Viscoelastic Model

Reduced Parameter Set:

$$q = [\eta, \beta, \gamma] \ , \ \text{Fixed hyperelastic parameters}$$



Question:

- What does Bayesian analysis tell us about material properties? Moduli and stretch parameters not informed by data. Fix at values inferred for low stretch rate for validation at higher rates.

Goal:

- Use global sensitivity analysis or parameter subset selection to determine nonidentifiable or noninfluential parameters before Bayesian analysis.

Monte Carlo Construction of Prediction Intervals

Advantages:

• No additional cost for DRAM if interpolating.

• Does not require independent parameters.

• Does not require Gaussian or uniform densities.

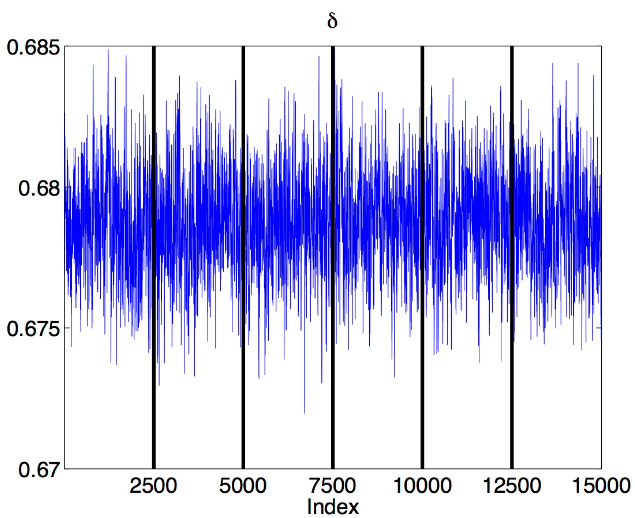
• Incorporates both parameter and measurement uncertainties.

Disadvantages:

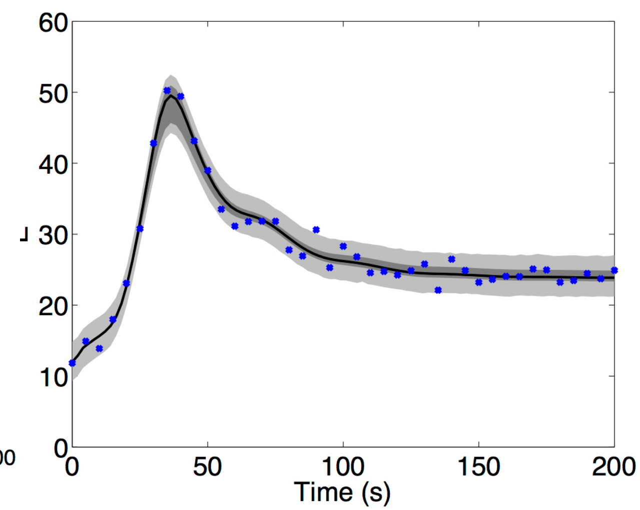
• Slow convergence rate $\mathcal{O}(1/\sqrt{M})$

• 100-fold more evaluations required to gain additional place of accuracy.

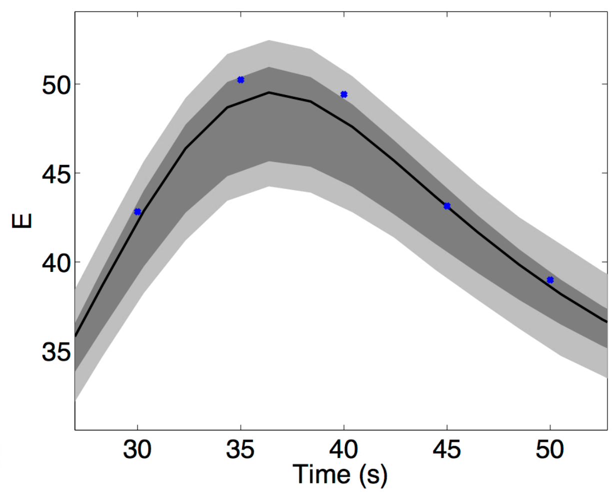
• Computationally prohibitive for many PDE and often requires surrogates or advanced numerical techniques … Talk with Max Gunzburger.



Samples from Chain



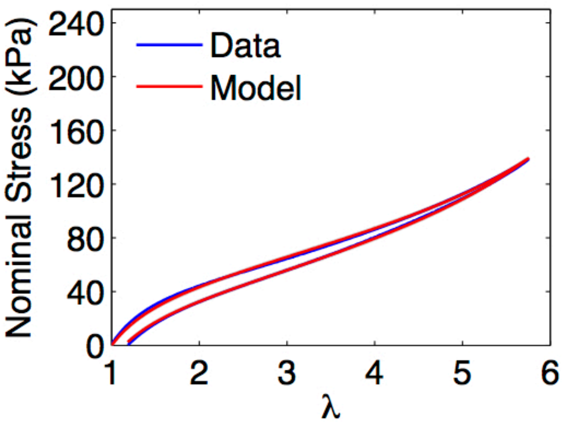
Data, Credible Intervals and Prediction Intervals

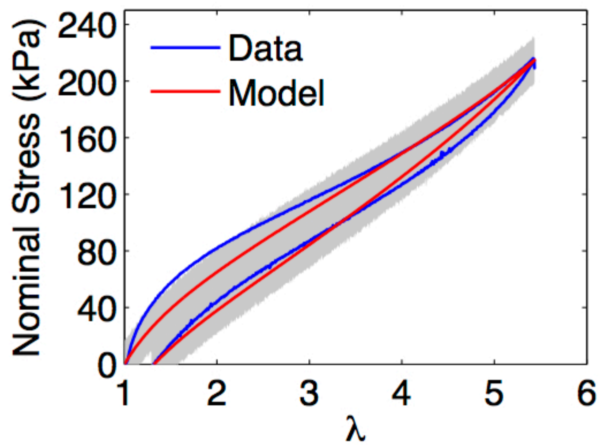


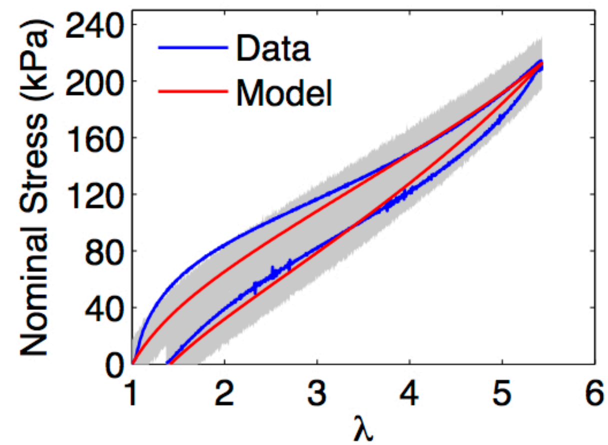
Non-Gaussian Credible and Prediction Intervals

Prediction Intervals for the Viscoelastic Model

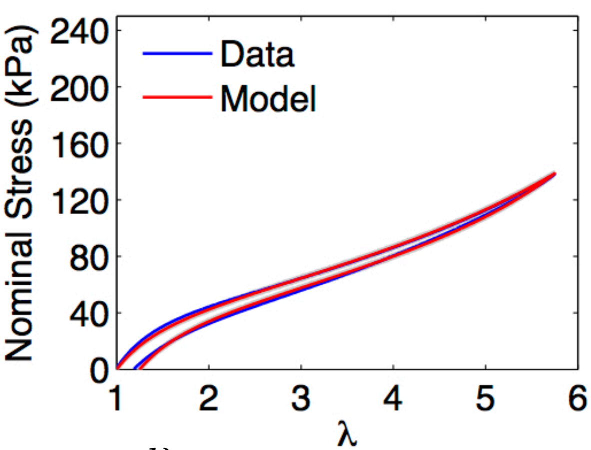
Linear Non-Affine Model:



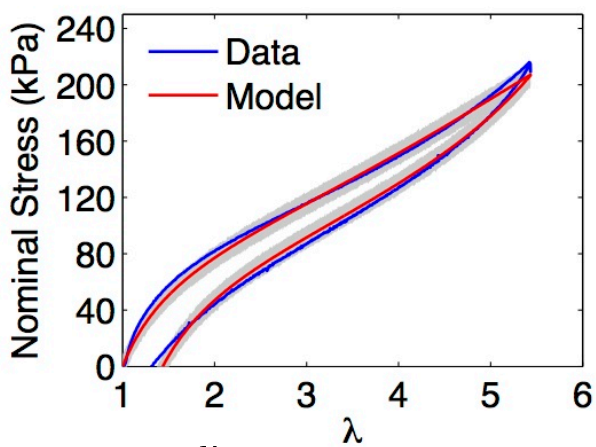




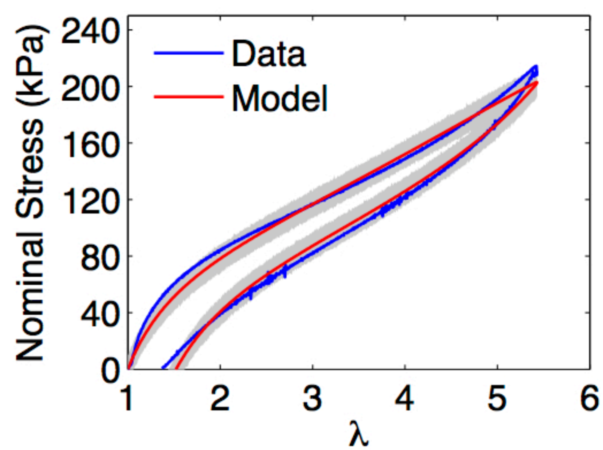
Nonlinear Non-Affine Model:



$$\frac{d\lambda}{dt} = 6.7 \times 10^{-5} \text{ Hz}$$



$$\frac{d\lambda}{dt} = 0.335 \text{ Hz}$$

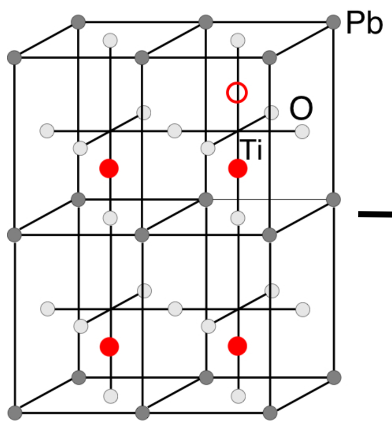


$$\frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

Bayesian Calibration Using Heterogeneous Multiscale Data

Current Directions and Challenges:

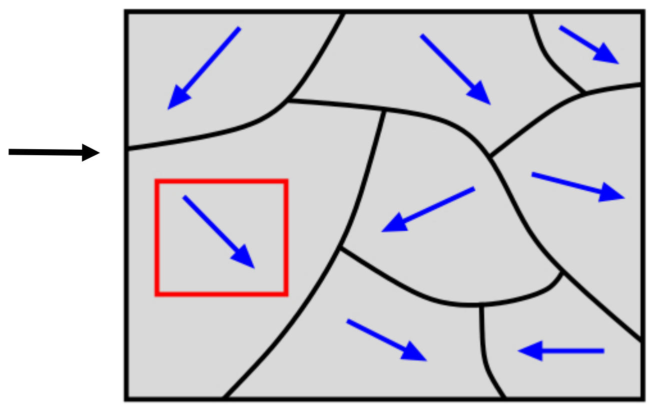
- How do we combine heterogeneous data – e.g., strain and polarization?
  - Bayesian melding to modify priors and likelihoods …
- How do we combine data from disparate spatial/temporal scales – e.g., atomistic and continuum?
  - Bayesian networks and trees …



Atomistic Data

- DFT simulations: W Oates
- Diffraction measurements: J. Jones

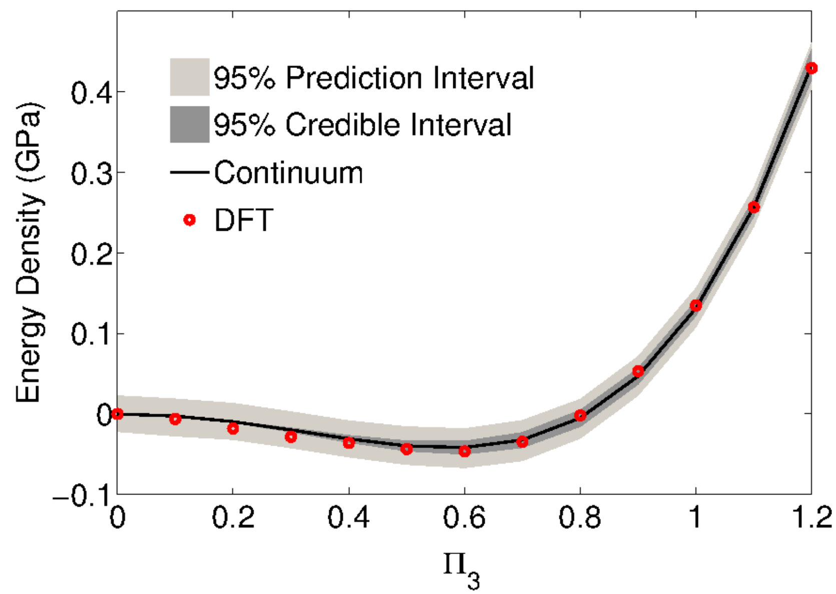
Goal: Calibrate continuum model



Continuum Data

- Polarization
- Strain

DFT Informed Continuum



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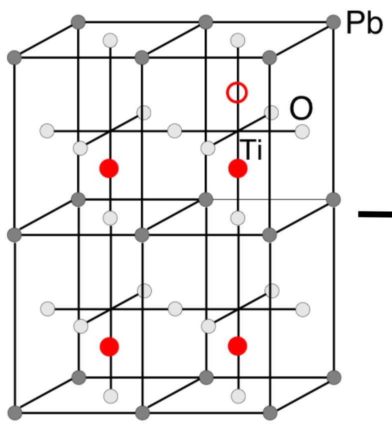

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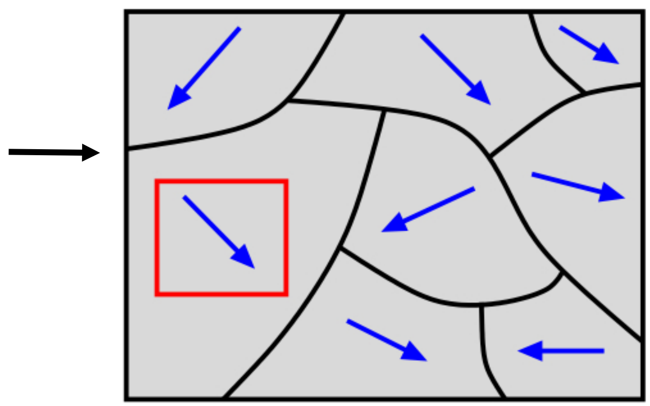

Continuum Data

- Polarization
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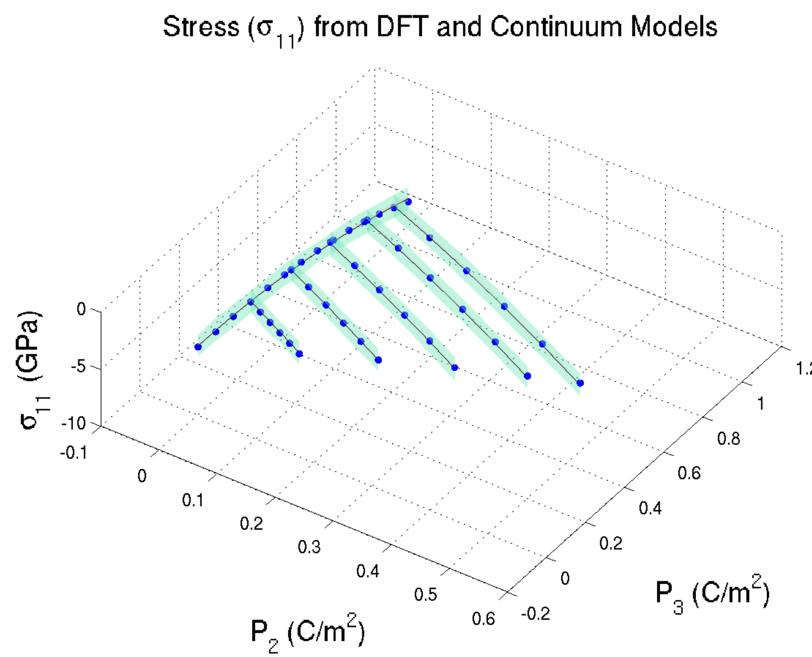
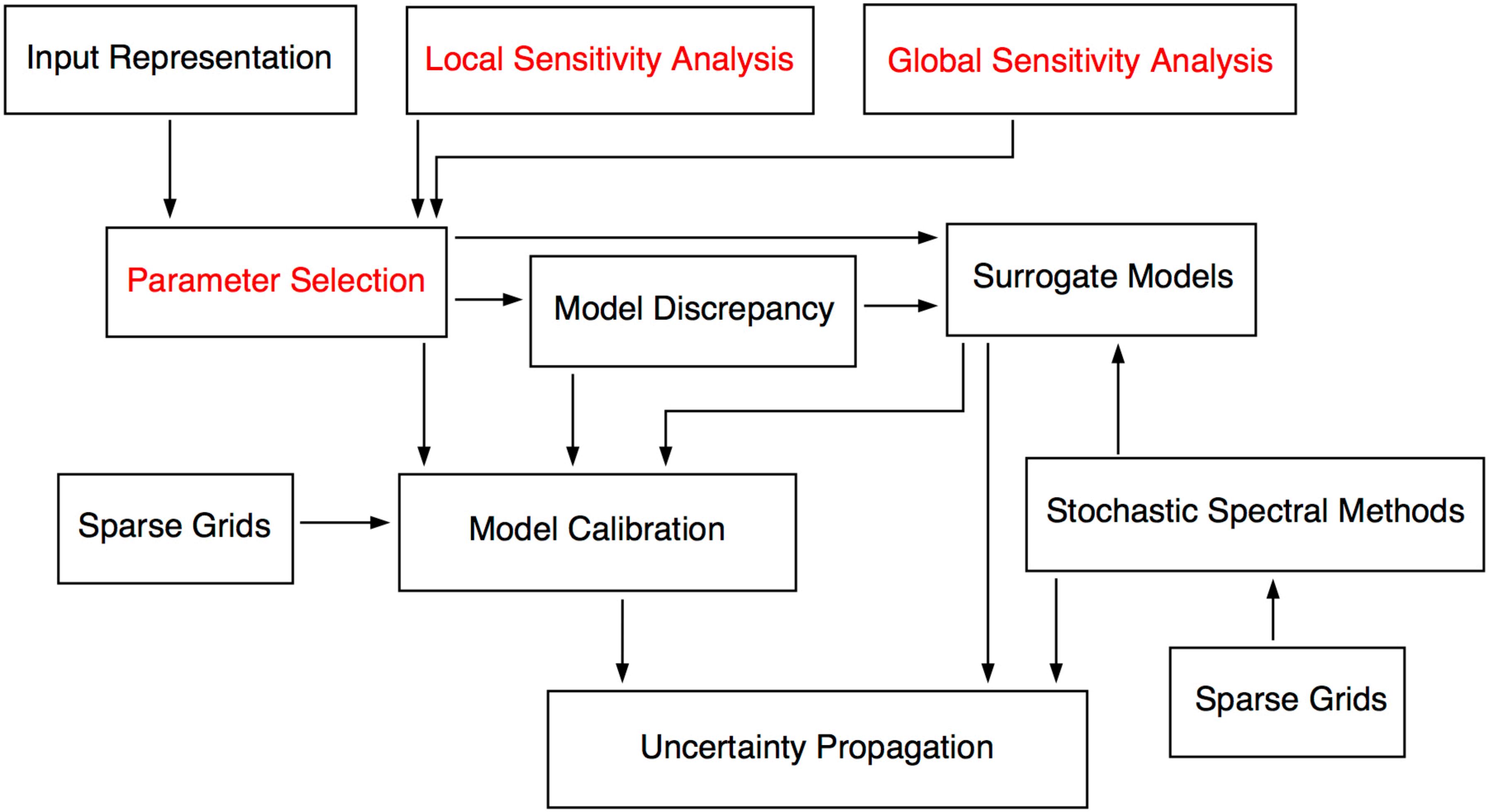


Steps in Uncertainty Quantification



Parameter Selection: Required for models with unidentifiable or noninfluential inputs

- e.g., Nuclear neutron transport codes can have 100,000 inputs

Global Sensitivity Analysis

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

Note:

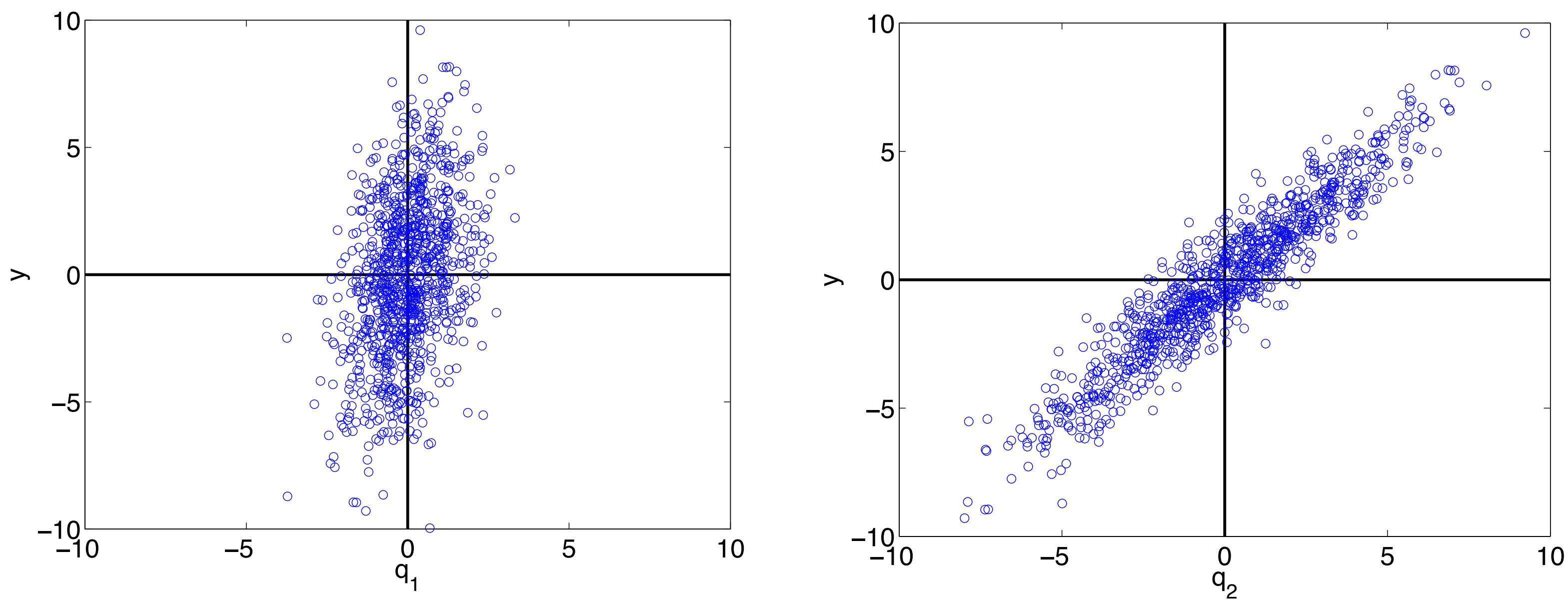
- Q_1 and Q_2 represent hedged porfolios
- c_1 and c_2 amounts invested in each portfolio

Take

$$c_1 = 2\ ,\ c_2 = 1$$

$Q_1 \sim N(0, \sigma_1^2)$ with $\sigma_1 = 1$

$Q_2 \sim N(0, \sigma_2^2)$ with $\sigma_2 = 3$



Local Sensitivities:

$$s_i \equiv \frac{\partial Y}{\partial Q_i} \Rightarrow s_1 = 2 > s_2 = 1$$

Solutions:

- Response correlation
- Variance methods
- Random sampling of local sensitivities

Variance-Based Methods

Sobol Representation: For now, take $Q_i \sim \mathcal{U}(0,1)$ and $\Gamma = [0,1]^p$

Take

$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{1 \le i < j \le p} f_{ij}(q_i, q_j)$$

Analogy: Taylor or Fourier series

subject to

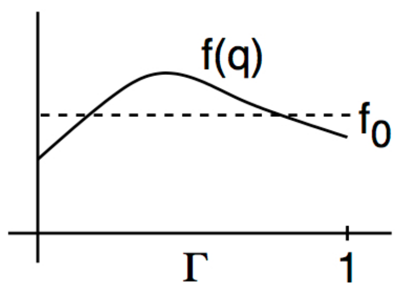
$$\int_0^1 f_i(q_i)dq_i = \int_0^1 f_{ij}(q_i, q_j)dq_i = \int_0^1 f_{ij}(q_i, q_j)dq_j = 0$$

Analogy:

- Derivatives for Taylor
- Orthogonality of sines and cosines for Fourier

Then

$$f_0 = \int_\Gamma f(q)dq$$



$$f_i(q_i) = \int_{\Gamma^{p-1}} f(q)dq_{\sim i} - f_0$$

Notation: $q_{\sim i} = [q_1, \cdots, q_{i-1}, q_{i+1}, \cdots, q_p]$

$$f_{ij}(q_i, q_j) = \int_{\Gamma^{p-2}} f(q)dq_{\sim\{ij\}} - f_i(q_i) - f_j(q_j) - f_0$$

Variance-Based Methods

Variances:

$$D_i = \int_0^1 f_i^2(q_i)dq_i$$

$$D_{ij} = \int_0^1 \int_0^1 f_{ij}^2(q_i, q_j)dq_i dq_j$$

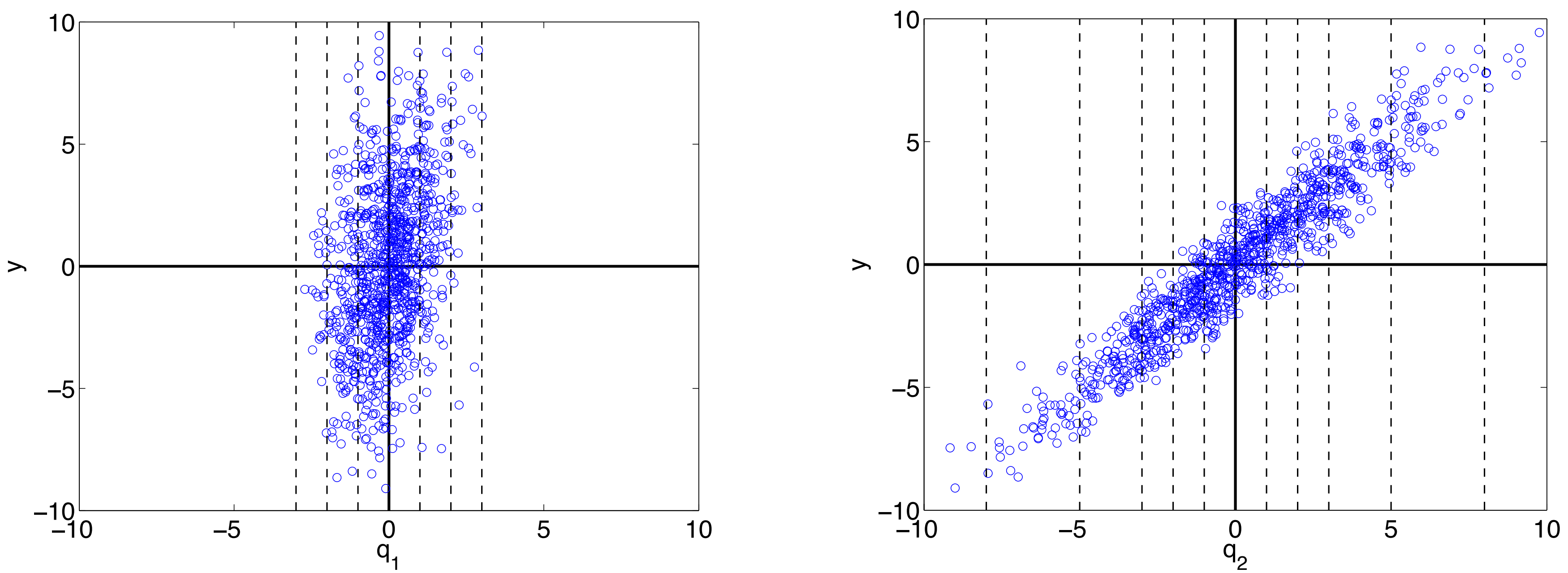
$$D = \text{var}(Y) = \int_\Gamma f^2(q)dq - f_0^2$$

Sobol Indices:

$$S_i = \frac{D_i}{D} \quad , \; S_{ij} = \frac{D_{ij}}{D} \quad , \; i, j = 1, \cdots p$$

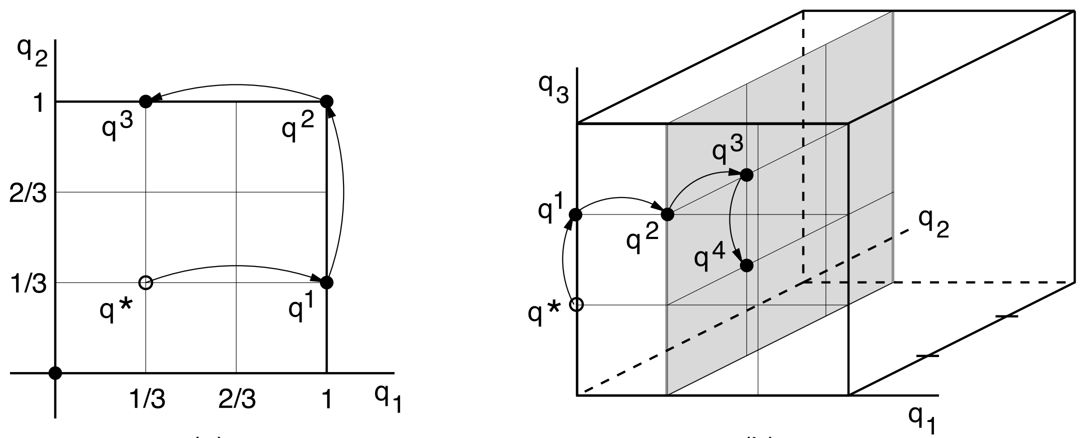
$$S_{T_i} = S_i + \sum_{j=1}^p S_{ij}$$

Statistical Interpretation: $D_i = \text{var}[\mathbb{E}(Y|q_i)] \Rightarrow S_i = \dfrac{\text{var}[\mathbb{E}(y|q_i)]}{\text{var}(Y)}$



Morris Screening

Example: Consider uniformly distributed parameters on $\Gamma = [0,1]^p$



(a) (b)

Elementary Effect:

$$d_i^j = \frac{f(q^j + \Delta e_i) - f(q^j)}{\Delta} \quad i^{th} \text{ parameter, } j^{th} \text{ sample}$$

$$\Delta \in \left\{ \frac{1}{\ell - 1}, \cdots, 1 - \frac{1}{\ell - 1} \right\} \quad \ell \text{ is level}$$

Global Sensitivity Measures: r samples

$$\mu_i^* = \frac{1}{r} \sum_{j=1}^{r} |d_i^j(q)|$$

$$\sigma_i^2 = \frac{1}{r-1} \sum_{j=1}^{r} \left(d_i^j(q) - \mu_i \right)^2 \;,\; \mu_i = \frac{1}{r} \sum_{j=1}^{r} d_i^j(q)$$

SIR Disease Example

SIR Model:

$$\frac{dS}{dt} = \delta N - \delta S - \gamma k I S \quad , \; S(0) = S_0$$ Susceptible

$$\frac{dI}{dt} = \gamma k I S - (r + \delta) I \quad , \; I(0) = I_0$$ Infectious

$$\frac{dR}{dt} = rI - \delta R \quad , \; R(0) = R_0$$ Recovered

Note: Parameter set $q = [\gamma, k, r, \delta]$ is not identifiable

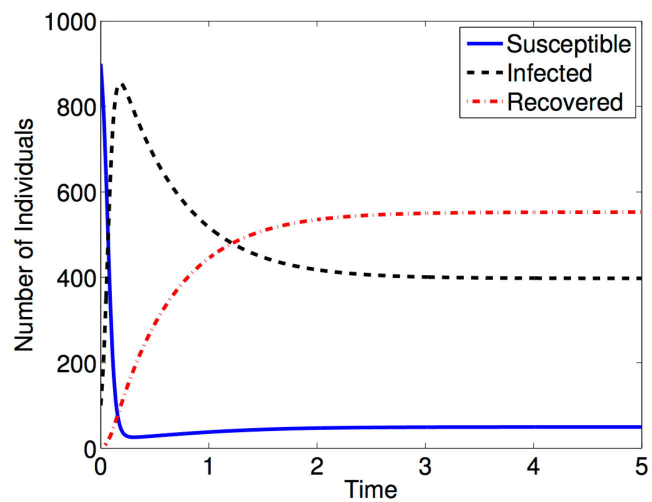
Assumed Parameter Distribution:

$$\gamma \sim \mathcal{U}(0,1) \; , \; k \sim \text{Beta}(\alpha, \beta) \; , \; r \sim \mathcal{U}(0,1) \; , \; \delta \sim \mathcal{U}(0,1)$$

Infection Coefficient — Interaction Coefficient — Recovery Rate

Response:

$$y = \int_0^5 R(t,q)dt$$

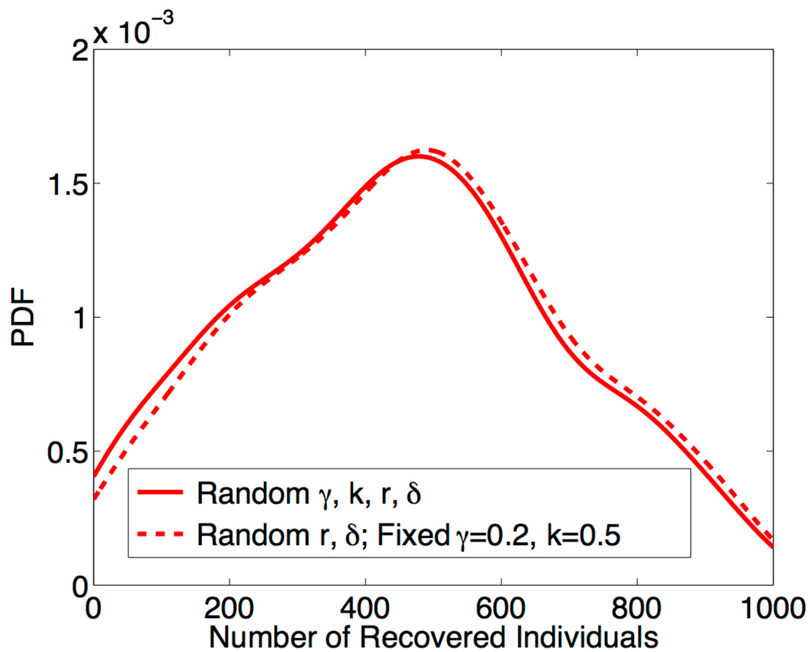


SIR Disease Example

Global Sensitivity Measures:

		γ	k	r	δ
	S_i	0.0997	0.0312	0.7901	0.1750
Sobol	S_{T_i}	-0.0637	-0.0541	0.5634	0.2029
	μ_i^* $(\times 10^3)$	0.2532	0.2812	2.0184	1.2328
Morris	σ_i $(\times 10^3)$	0.9539	1.6245	6.6748	3.9886

Result: Densities for $R(t_f)$ at $t_f = 5$



Note: Can fix non-influential parameters

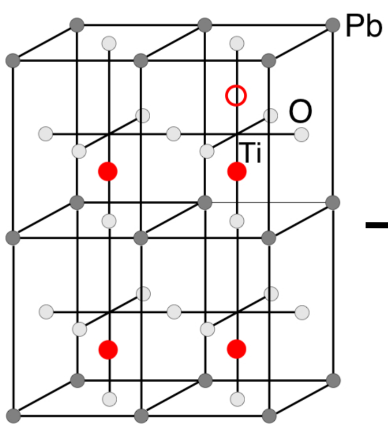
Sensitivity Analysis Using Heterogeneous Multiscale Data

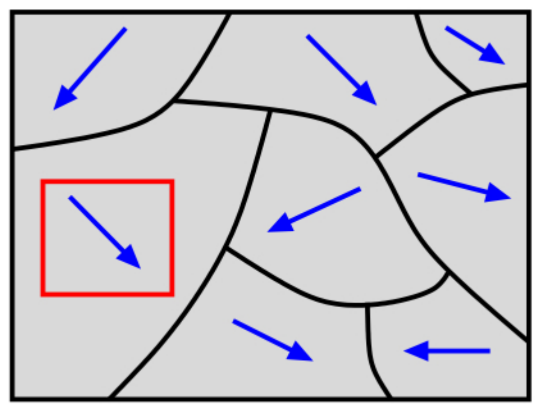
Current Directions and Challenges:

- How do we combine heterogeneous responses – e.g., strain and polarization?
  - One Approach: Pseudo-response

$$y = \omega_1 y^s + \omega_2 y^p \ , \ \omega_1, \omega_2 \quad \text{Random}$$

- How do we combine responses from disparate spatial/temporal scales – e.g., atomistic and continuum?





Atomistic Responses

- DFT simulations

Continuum Responses

- Polarization y^p
- Strain y^s

Concluding Remarks

Notes:

- Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.
- Parameter selection is critical to isolate identifiable and influential parameters.
- Due to complexity of models, surrogate models are required for many applications.
- Research issues and challenges for SA and UQ
  - Data and model fusion for heterogeneous data; e.g., strain, polarization and energy.
  - Data and model fusion across very disparate spatial and temporal scales; e.g., atomistic to macroscopic.
- Quantification of model discrepancy or bias is difficult but critical, especially when extrapolating.
- *Prediction is very difficult, especially if it's about the future*, Niels Bohr (or Yogi Berra).