Sensitivity Analysis, Uncertainty Quantification, and Control Design for Smart Material Systems

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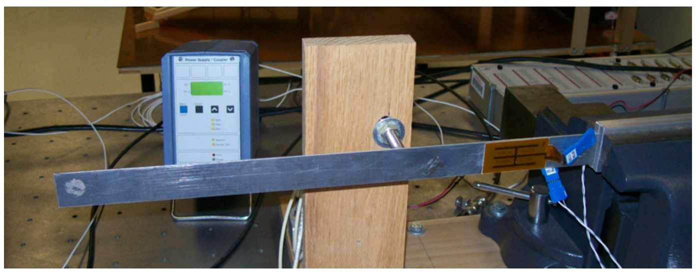
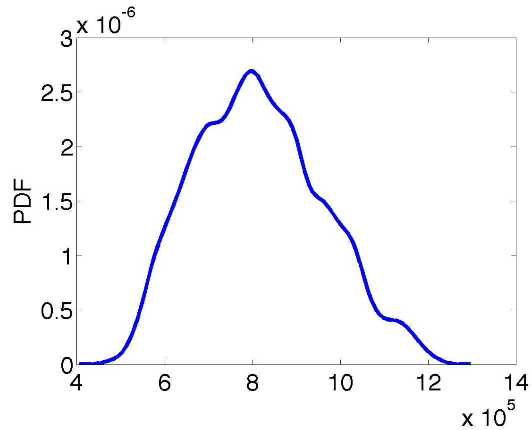
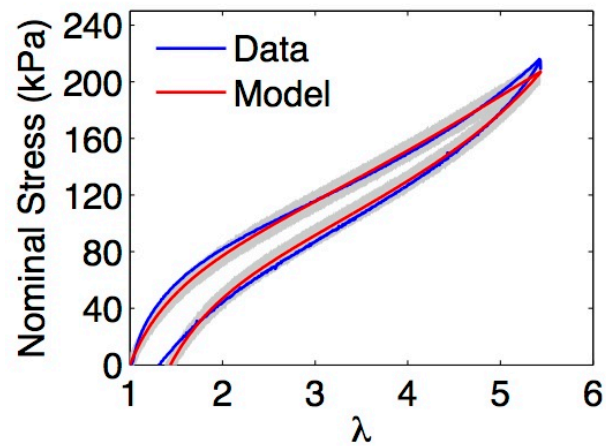


Experimental Errors



Parameter Uncertainty



Response Uncertainty

Essentially, all models are wrong, but some are useful, George E.P. Box, Industrial Statistician.

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DOE Consortium for Advanced Simulation of LWR (CASL)

NNSA Consortium for Nonproliferation Enabling Capabilities (CNEC)

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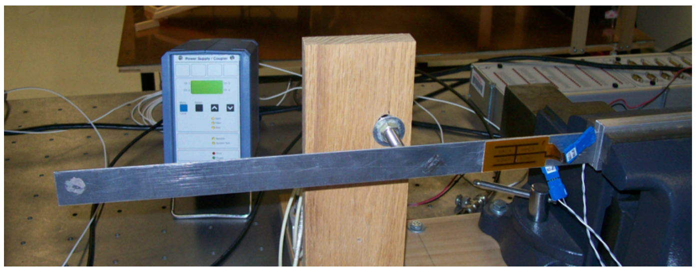
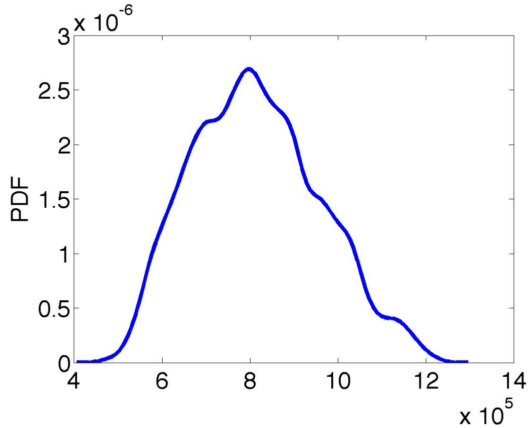
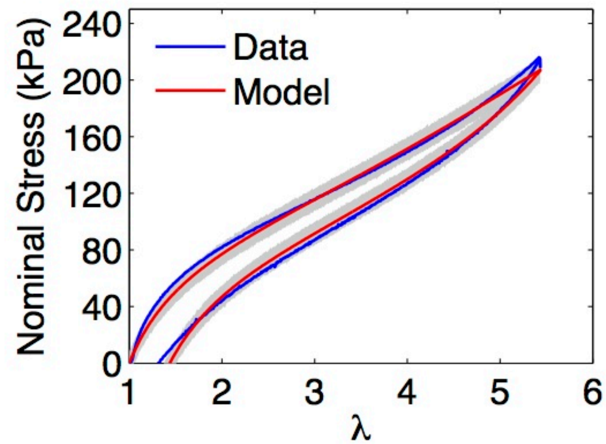


Experimental Errors



Parameter Uncertainty



Response Uncertainty

"We":

Nikolas Bravo, Nate Burch, John Crews, Jennifer Hannen, Zhengzheng Hu, Lider Leon, Jerry McMahan, Paul Miles, Graham Pash (NCSU)

Michael Hays, Billy Oates (Florida State University)

Alex Solomou (Texas A&M)

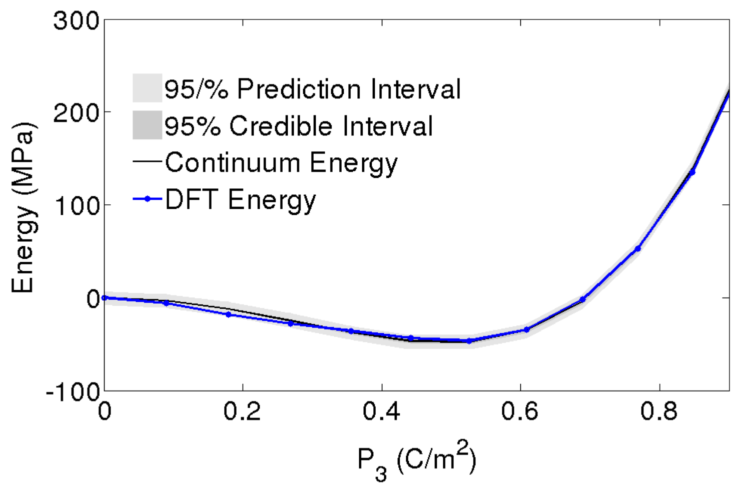
Max Morris (Iowa State University)

Example 1: Quantum-Informed Continuum Models

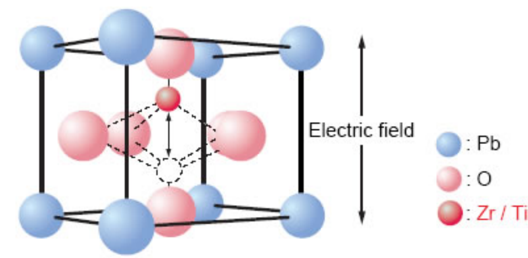
Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Landau energy

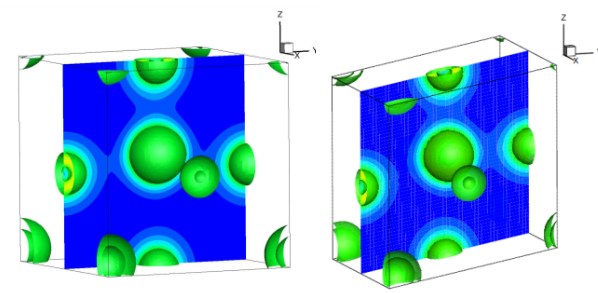
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$



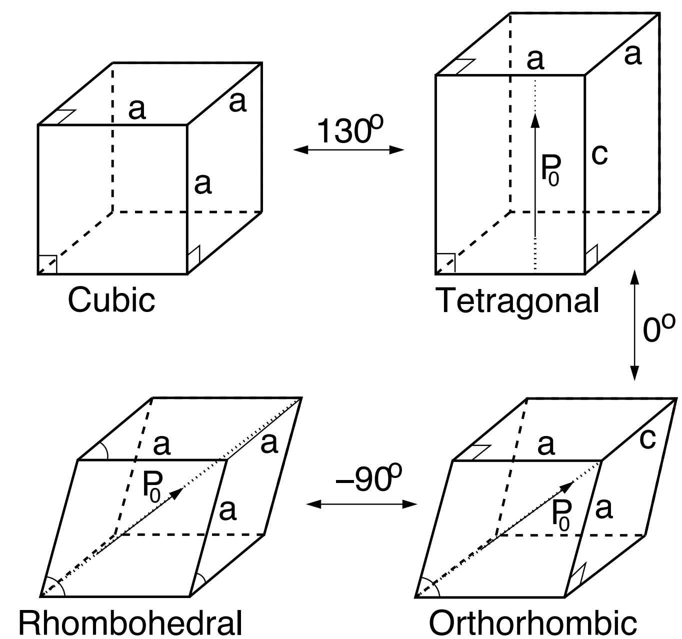
Landau energy



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation



UQ and SA Issues:

- Is 6^{th} order term required to accurately characterize material behavior?
- **Note:** Determines molecular structure

Quantum-Informed Continuum Models

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- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
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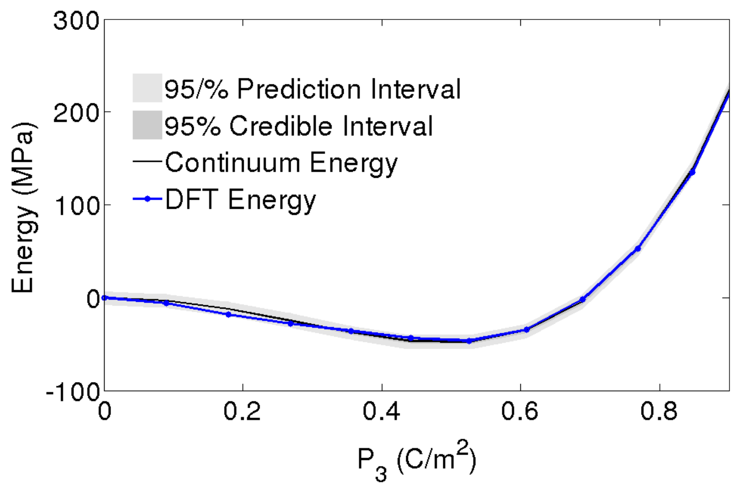
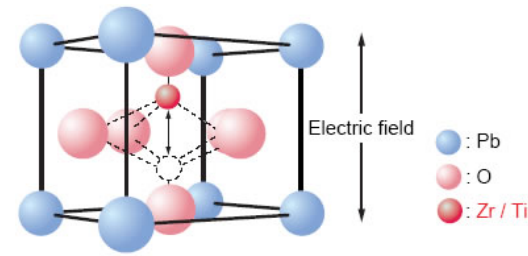
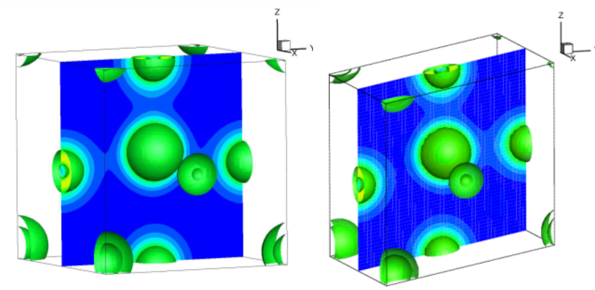


Landau energy



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation

UQ and SA Issues:

- Is 6^{th} order term required to accurately characterize material behavior?
- **Note:** Determines molecular structure

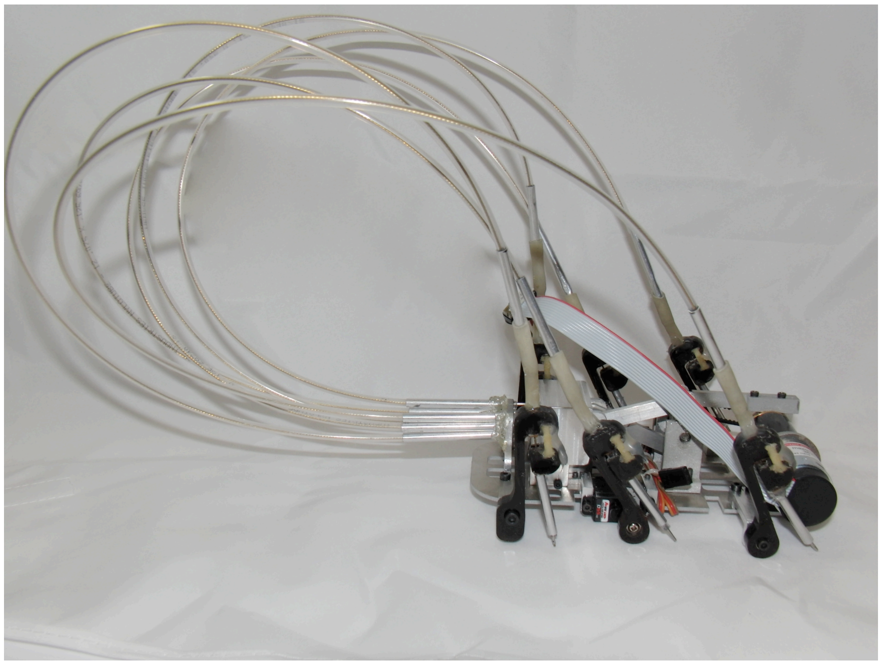
Broad Objective:

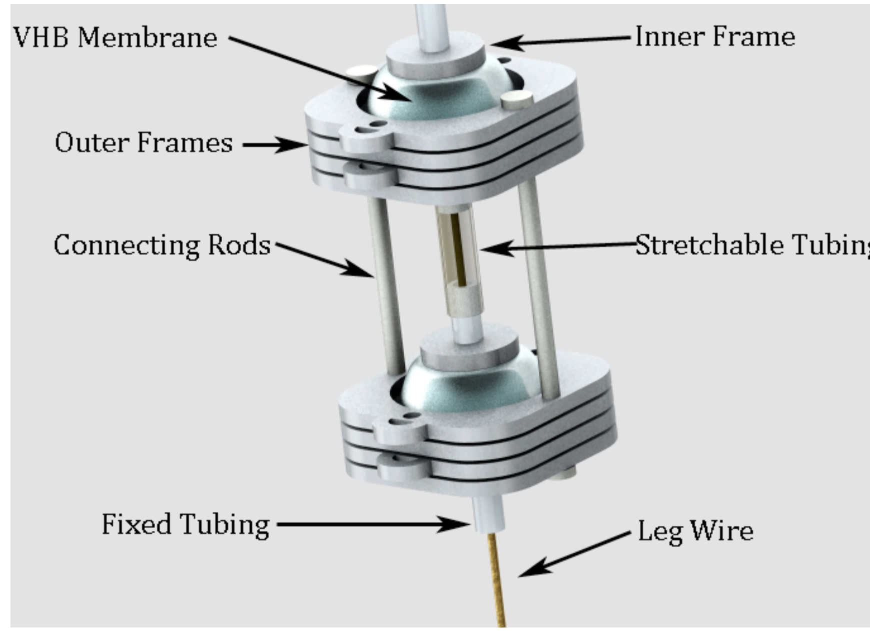
- Use UQ/SA to help bridge scales from quantum to system

Collaborators: Billy Oates, Paul Miles, Lider Leon

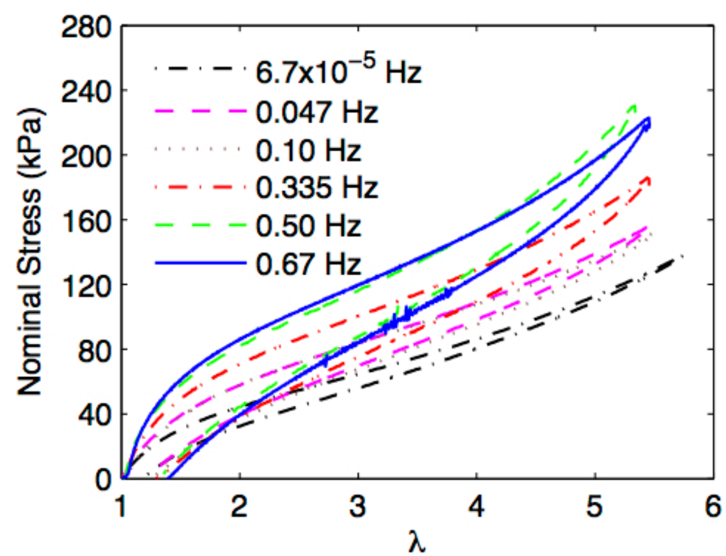
Example 2: Viscoelastic Material Models

Application: Adaptive materials for legged robotics





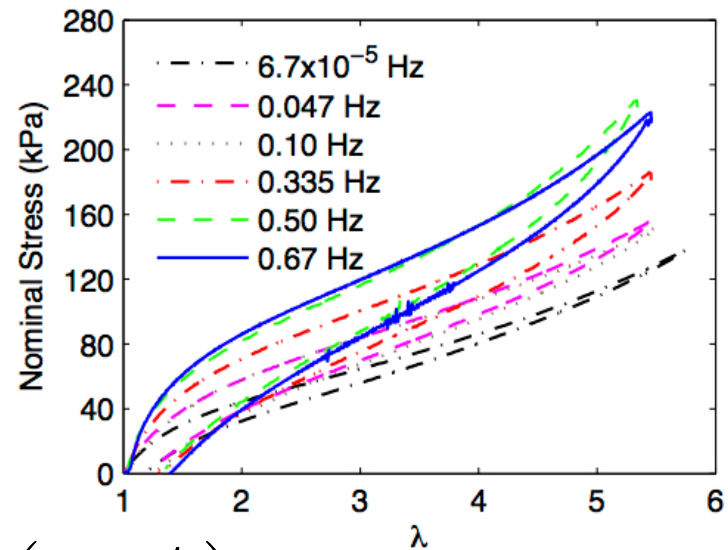
Material Behavior: Significant rate dependence



Collaborators: Billy Oates, Paul Miles, Michael Hays

Example: Viscoelastic Material Models

Material Behavior: Significant rate dependence



Finite-Deformation Model: Nonlinear, non-affine

$$\psi(q) = \psi_\infty(G_e, G_c, \lambda_{\max}) + \Upsilon(\eta, \beta, \gamma)$$

- Dissipative energy function Υ
- Conserved hyperelastic energy function

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

Parameters:

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

G_c: Crosslink network modulus

G_e: Plateau modulus

$\lambda_{\max}$: Max stretch effective affine tube

$[\eta, \beta, \gamma]$: Viscoelastic parameters

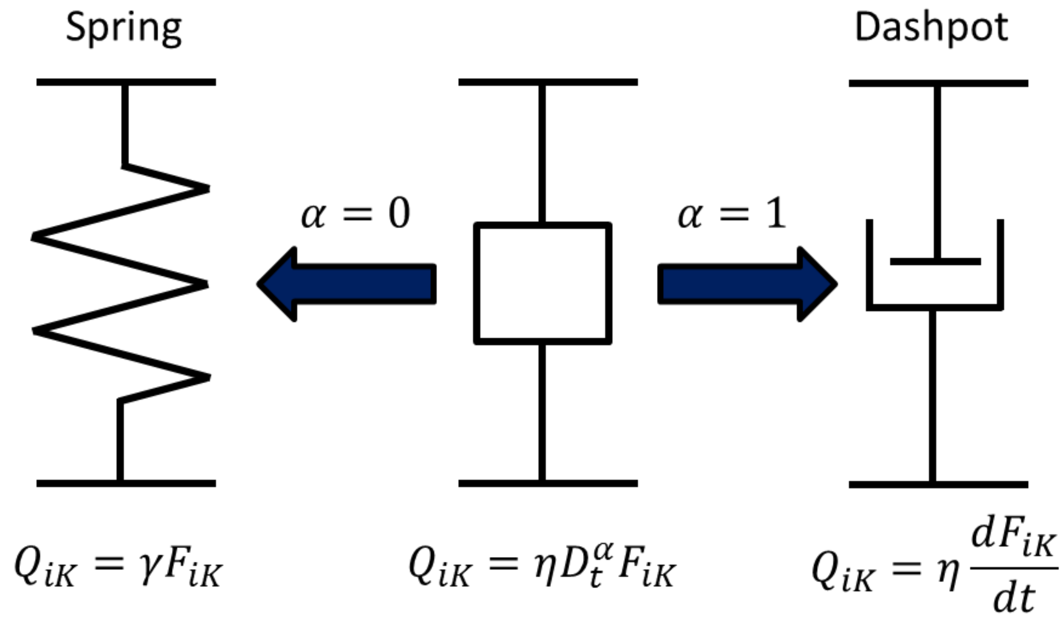
Uncertainty Quantification Goals:

- Quantify measurement errors.
- Quantify uncertainty in parameters.
- Use statistics to quantify accuracy of considered models.
- Employ fractional-order models to quantify rate-dependent hysteresis.

Example: Viscoelastic Material Models

Viscoelastic Constitutive Law:

$$Q_{iK} = \eta D_t^{\alpha} F_{iK}$$



Fractional Derivative:

- Riemann-Liouville definition

$$D_t^{\alpha}[f(t)] = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_0^t \frac{f(s)}{(t-s)^{\alpha+1-n}} ds$$

where $n = \lceil \alpha \rceil$. Consider $\alpha \in [0, 1) \Rightarrow n = 1$

$$D_t^{\alpha}[f(t)] = \frac{1}{\Gamma(n-\alpha)} \frac{d}{dt} \int_0^t \frac{f(s)}{(t-s)^{\alpha}} ds$$

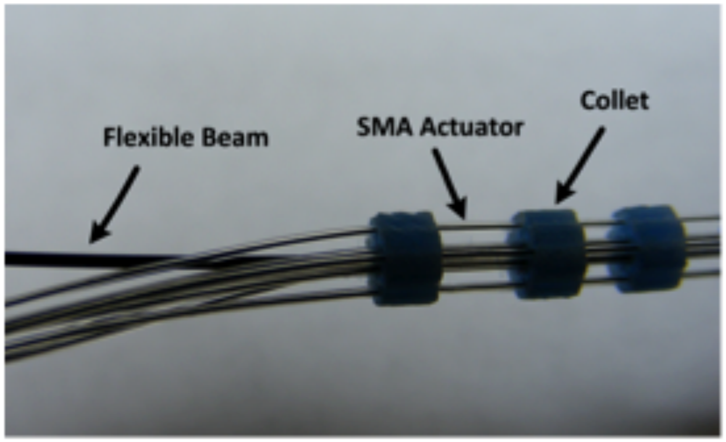
Collaborators: Graham Pash, Paul Miles

Issue: Singularity at upper integration limit requires delicate quadrature

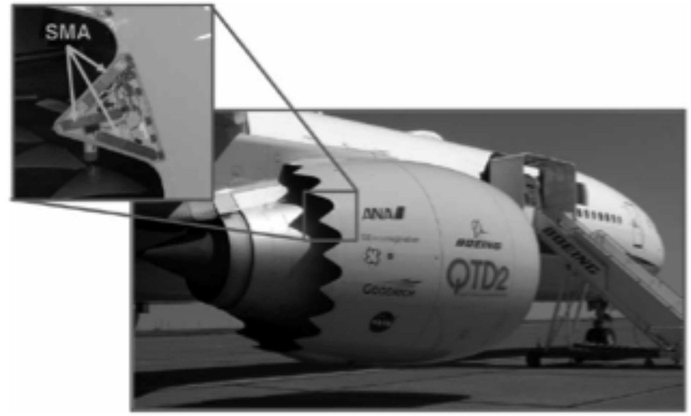
- We employ hybrid Gaussian quadrature/analytic Riemann sum approximation

Shape Memory Alloy (SMA) Actuators and Sensors

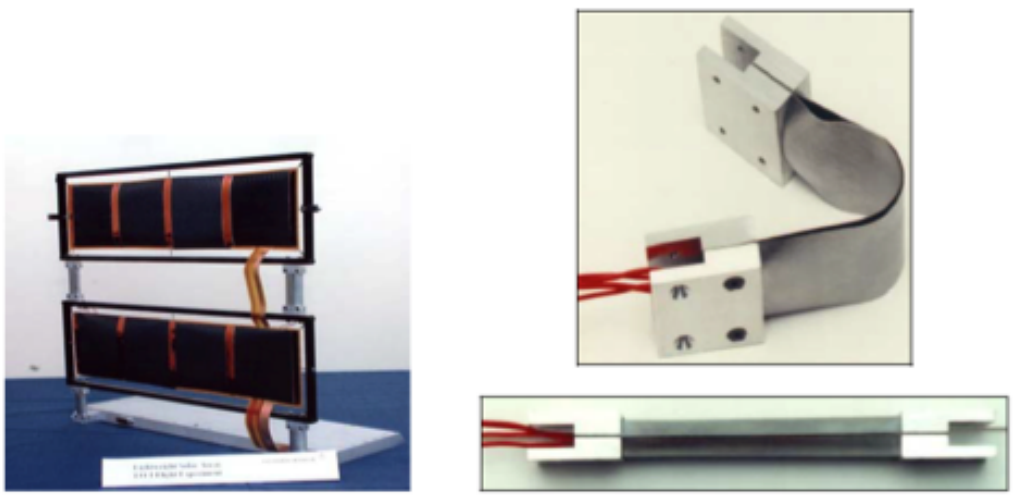
Shape Memory Alloys:



Catheters for Laser Ablation



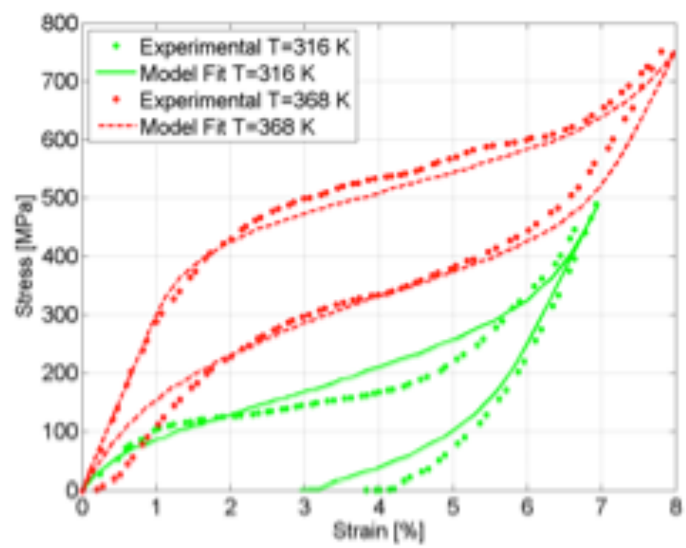
Chevrons for Noise Reduction/Fuel efficiency



SMA Hinges for Solar Arrays

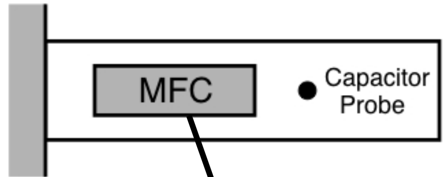
Properties and Challenges:

- High work densities
- Slow actuation rates (e.g., Hz)
- Hysteretic dynamics



Example 4: Multiscale Model Development

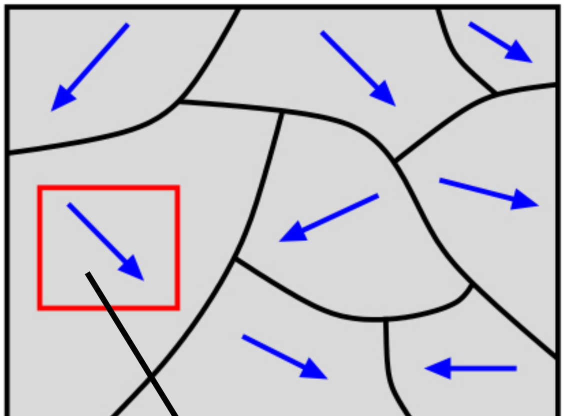
Example: PZT-Based Macro-Fiber Composites

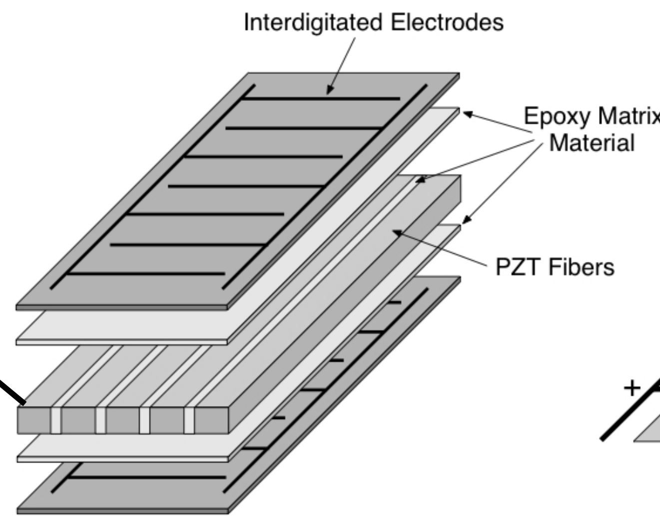


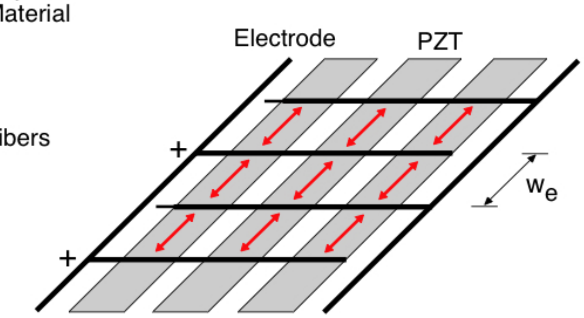
$$\rho \ddot{u} = \nabla \cdot \sigma + F$$

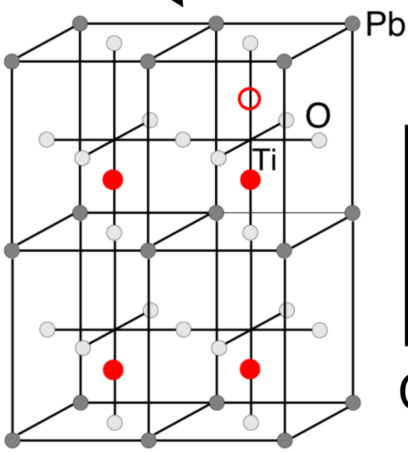
$$\nabla \cdot D = 0 \, , \;\; D = \varepsilon_0 E + P$$

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









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

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

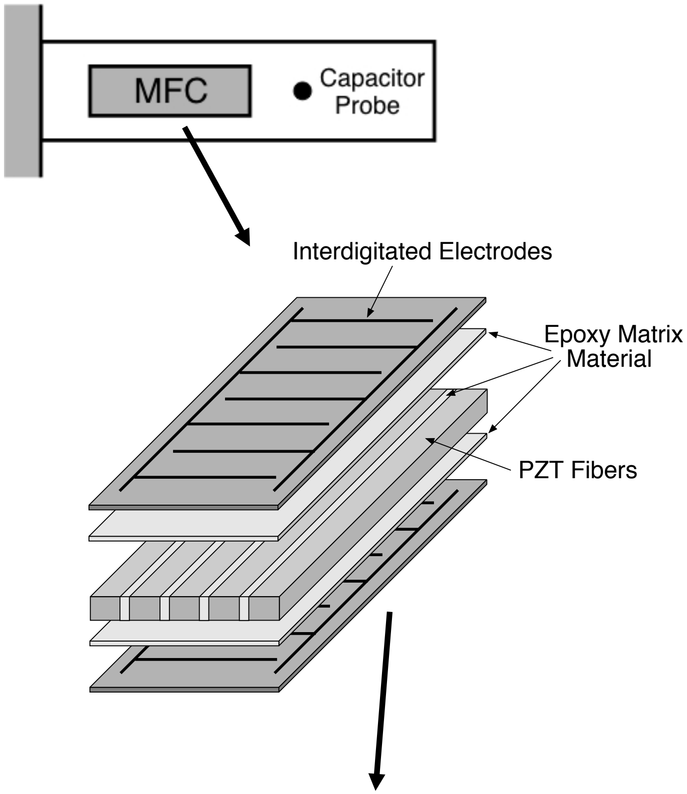
Continuum Energy Relations

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

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

Homogenized Energy Model (HEM)

Example: PZT-Based MFC and Robobee

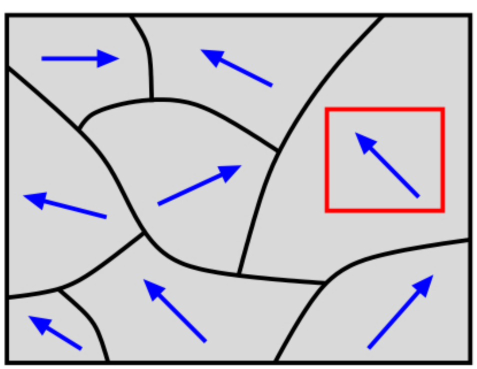


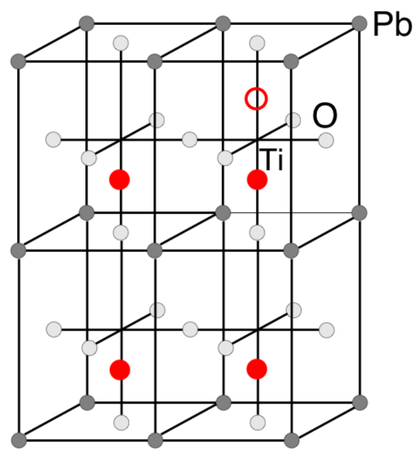
Beam Model: 20 parameters

$$\underline{\rho} \frac{\partial^2 w}{\partial t^2} + \underline{\gamma} \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0$$

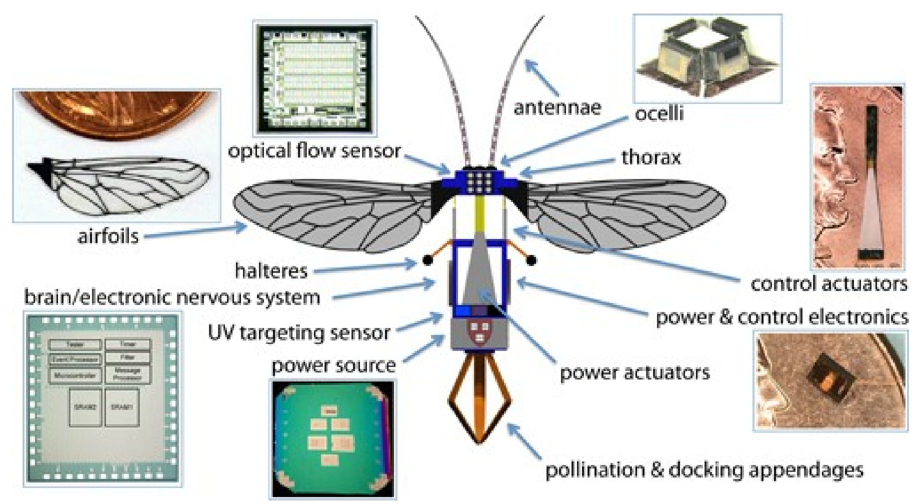
$$M = -\underline{c^E I} \frac{\partial^2 w}{\partial x^2} - \underline{c_D I} \frac{\partial^3 w}{\partial x^2 \partial t} - [\underline{k_1} e(E, \sigma_0) E + \underline{k_2} \varepsilon_{irr}(E, \sigma_0)] \chi_{MFC}(x)$$

Homogenized Energy Model (HEM)



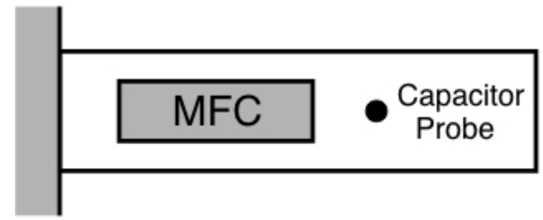


2nd Example: Robobee Drive Mechanism



Multiscale Model Development: Macro-Fiber Composites

Strong Form:



$$\rho(x)\frac{\partial^2 w(t,x)}{\partial t^2} - \gamma\frac{\partial w(t,x)}{\partial t} - \frac{\partial^2 M(t,x)}{\partial x^2} = 0$$

$$M(t,x) = -c^E I(x)\frac{\partial^2 w(t,x)}{\partial x}^2 - C_d I(x)\frac{\partial^3 w(t,x)}{\partial x^2 \partial t} + F(t,x,w)$$

Notes:

- Nonlinear, hysteretic and rate-dependent behavior incorporated in F(t,x,w)
- Consider tip displacement $w(t,\bar{x},q)$ where $q \in \mathbb{R}^{20}$ are model parameters; i.e., $y(t,q) = w(t,\bar{x},q)$.
- Employ Galerkin representation $w^N(t,x) = \sum_{i=1}^N w_i^N(t)\phi_i(x)$ in weak formulation to obtain finite-dimensional semi-discrete system where $z(t) = [w^N(t), \dot{w}^N(t)]$.

Control Formulation:

$$\frac{dz}{dt} = f(t,z,u,q) + v_1(t)$$

$$y(t,q) = Cz(t,q) + v_2(t)$$

Statistical Model:

$$y_i = w^N(t_i,q) + \varepsilon_i\ , \quad i = 1,\dots,n$$

UQ Formulation:

$$\frac{dz}{dt} = f(t,z,q) + v_1(t)$$

$$y(t) = \int_{\mathbb{R}^{20}} w^N(t,\bar{x},q)\rho(q)dq$$

E.g., Average tip displacement

Broad Control and UQ Objectives

Control Formulation:

$$\frac{dz}{dt} = f(t, z, u, q) + v_1(t)$$

$$y(t, q) = Cz(t, q) + v_2(t)$$

UQ Formulation: e.g., average tip displacement

$$\frac{dz}{dt} = f(t, z, q) + v_1(t)$$

$$y(t) = \int_{\mathbb{R}^{20}} w^N(t, \bar{x}, q)\rho(q)dq$$

Control Objectives:

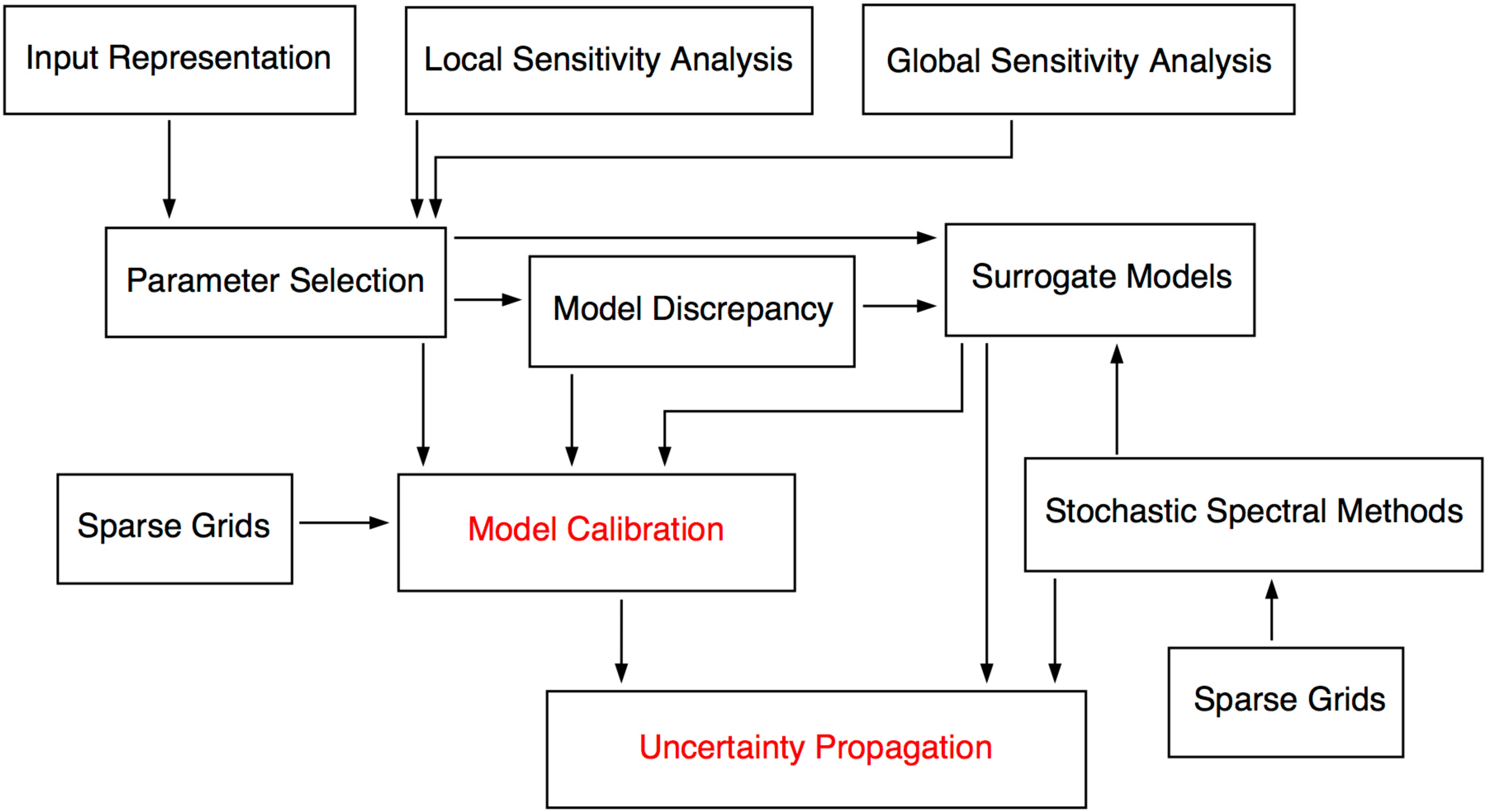
- Determine optimal q; requires identifiability analysis.
- Construct reduced-order model for state z; e.g., POD, DMD.
- Determine plant error Δ for robust control design.
- Construct state estimator $z_c(t)$.
- Compute feedforward or feedback controls; e.g., $u(t) = -kz_c(t)$.
- Note: Feedback not necessary if no uncertainties!

UQ Objectives:

- Determine identifiable parameter subsets or subspace; SA or active subspace techniques.
- Construct surrogate model; e.g., GP, regression, collocation, POD.
- Infer distributions (Bayesian) or estimators (frequentist) for q or q(x).
- Compute distributions or statistics for QoI. Analytic relations for stochastic Galerkin or collocation for certain distributions; e.g., Gaussian or uniform.

Steps in Uncertainty Quantification

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

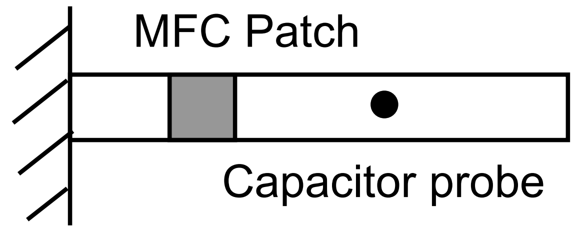


Deterministic Model Calibration

Example: MFC

$$\underline{\rho}\frac{\partial^2 w}{\partial t^2} + \underline{\gamma}\frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0$$

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



Macro-Fiber Composite

Homogenized Energy Model (HEM)

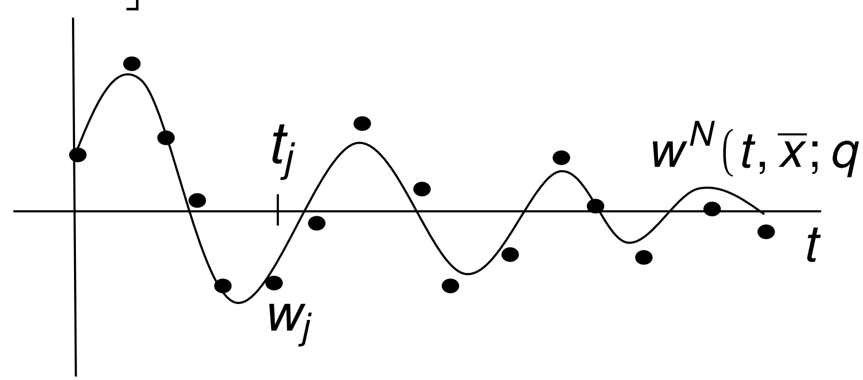
Parameters: $q = [q_{beam}, q_{hys}]$

Note: 20 parameters

- HEM $q_{hys} = [P_R^+, \varepsilon_R^+, \varepsilon_R^{90}, \chi^\sigma, d_+, \widetilde{\gamma}, \tau_{90}, \tau_{180}, \mu_c, \sigma_c^2, \sigma_I^2]$
- Beam: $q_{beam} = \left[\overline{\rho}, \widehat{\rho}, \overline{c^E I}, \widehat{c^E I}, \overline{c_D I}, \widehat{c_D I}, \gamma, k_1, k_2,\right]$

Point Estimates: Ordinary least squares

$$q^0 = \arg\min_q \frac{1}{2}\sum_{j=1}^{N}\left[w_j - w^N(t_j,\bar{x},q)\right]^2$$

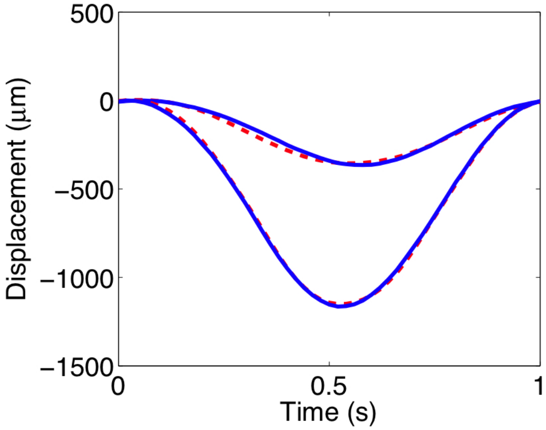


Deterministic Model Calibration

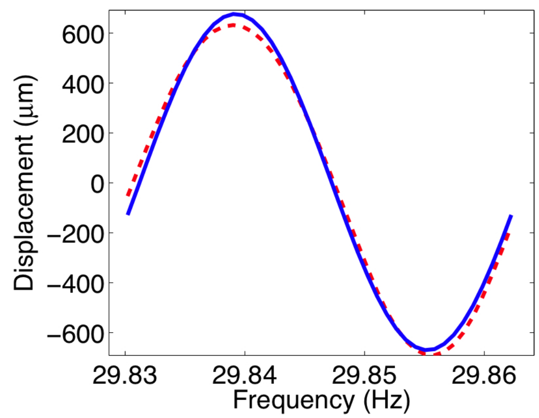
Representative Parameter Values:

d_+ (m/V)	σ_I (V/m)	τ_{180} (s)
478.10×10^{-12}	6.47×10^{6}	2.80×10^{-3}

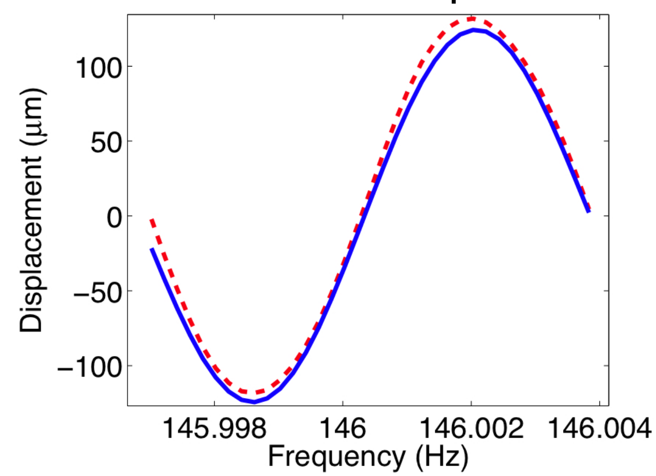
1 Hz Input
(400, 800 VDC)



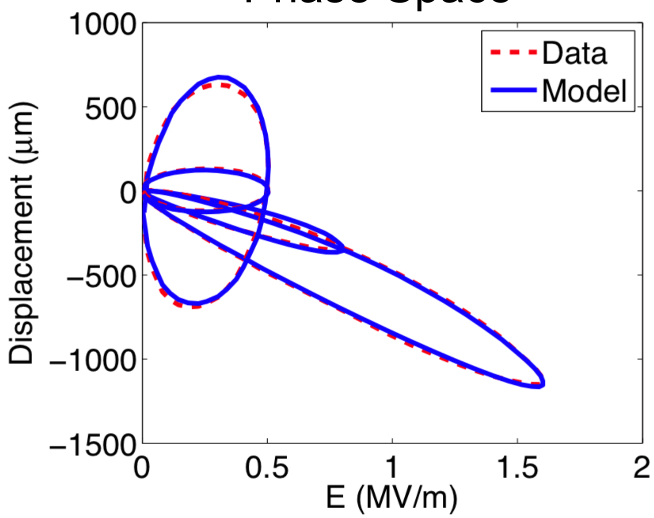
30 Hz Input



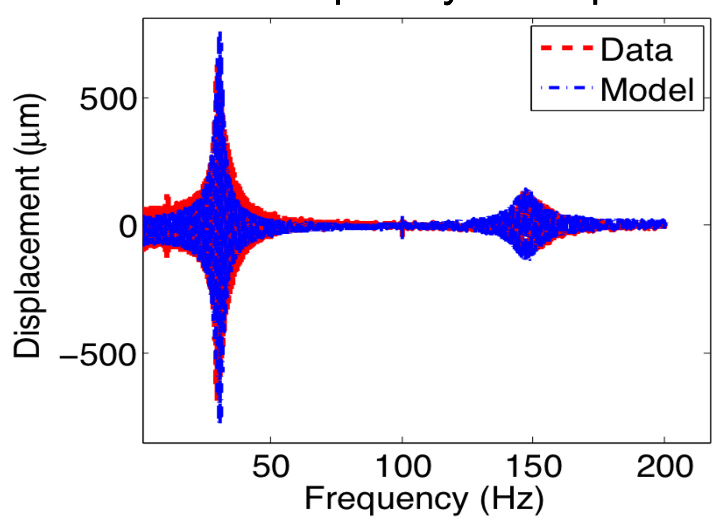
146 Hz Input



Phase Space



Frequency Sweep



Note: Point estimates but no quantification of uncertainty in:

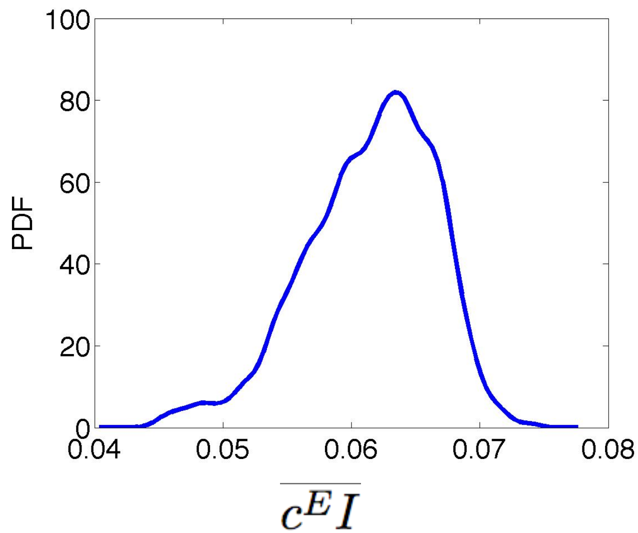
- Model
- Parameters
- Data

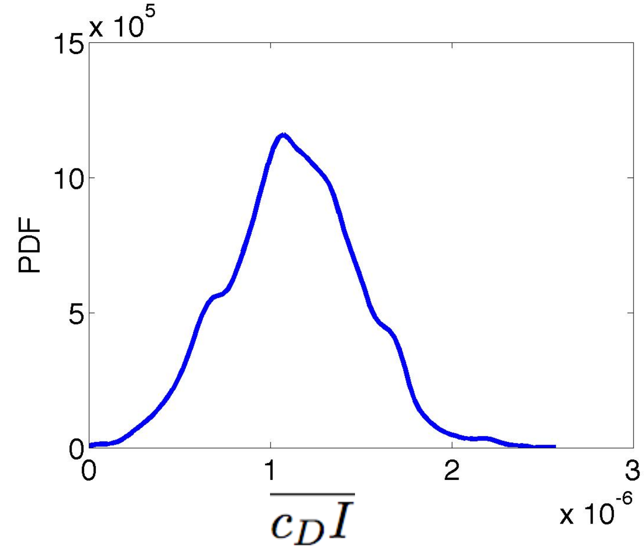
Collaborators: Zhengzheng Hu, Michael Hays, Nate Burch, Billy Oates

Objective for Uncertainty Quantification

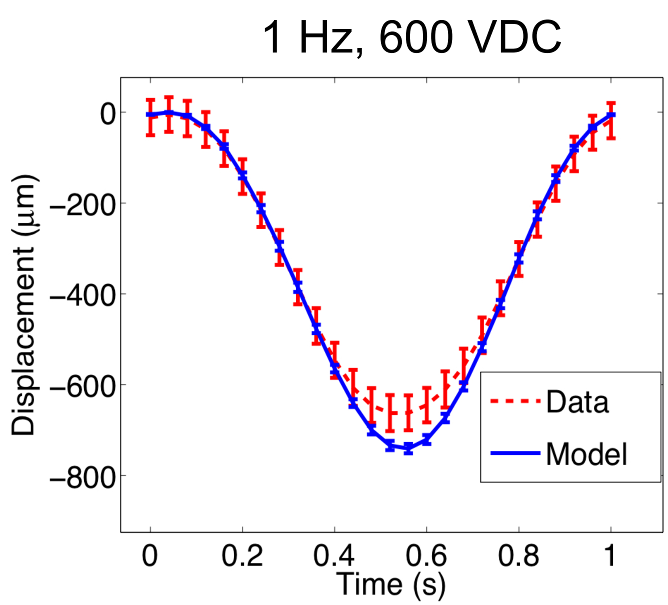
Goal: Replace point estimates with distributions or credible intervals

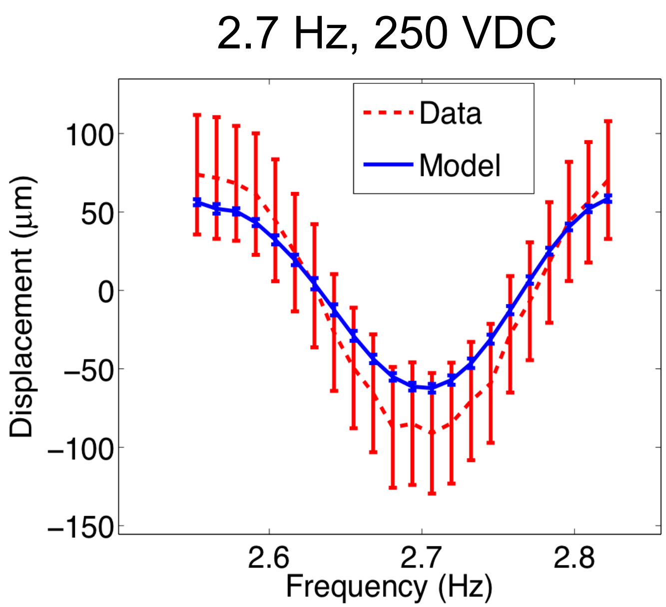
E.g., Parameter Densities





E.g., Response Intervals



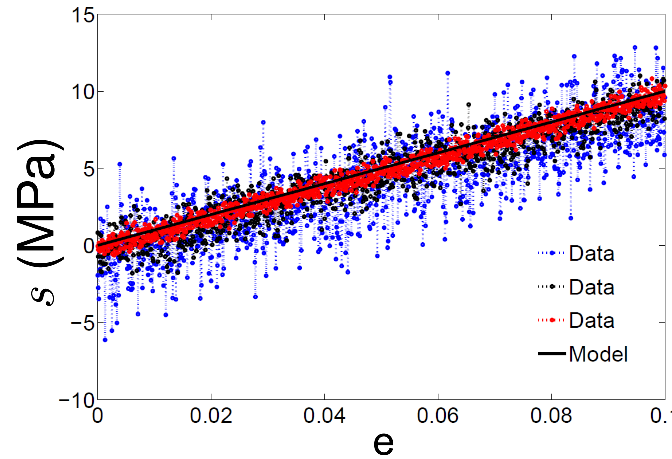


Bayesian Inference: Motivation

Example: Displacement-force relation (Hooke's Law)

$$s_i = Ee_i + \varepsilon_i \ , \ \ i = 1, \dots, N$$

$$\varepsilon_i \sim N(0, \sigma^2)$$



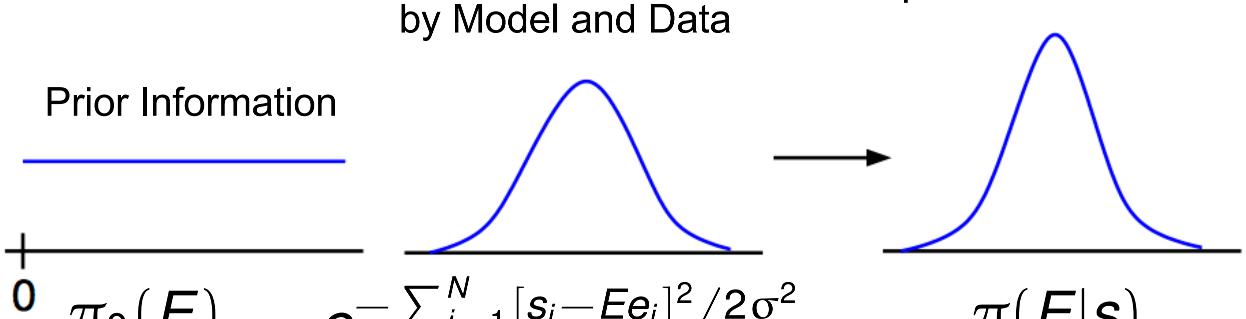
Parameter: Stiffness E

Strategy: Use model fit to data to update prior information

Prior Information

Information Provided by Model and Data

Updated Information



$$\pi_0(E) \qquad e^{-\sum_{i=1}^{N}[s_i - Ee_i]^2/2\sigma^2} \qquad \pi(E|s)$$

Data

Model

Non-normalized Bayes' Relation:

$$\pi(E|s) = e^{-\sum_{i=1}^{N}[s_i - Ee_i]^2/2\sigma^2}\pi_0(E)$$

Bayesian Inference: Motivation

Bayes' Relation: Specifies posterior in terms of likelihood and prior

Likelihood: $e^{-\sum_{i=1}^{N}[s_i - Ee_i]^2/2\sigma^2}$, $q = E$

$\upsilon = [s_1, \ldots, s_N]$

Posterior Distribution

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

Prior Distribution

Normalization Constant

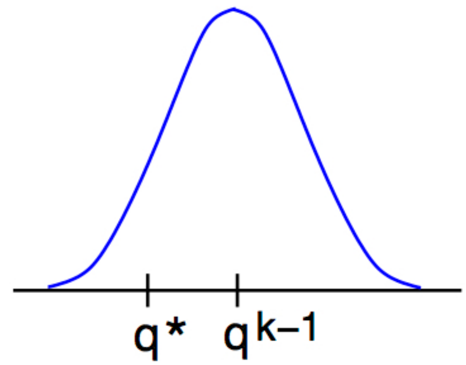
- Prior Distribution: Quantifies prior knowledge of parameter values
- Likelihood: Probability of observing a data given set of parameter values.
- Posterior Distribution: Conditional distribution of parameters given observed data.

Problem: Can require high-dimensional integration

- e.g., MFC Model: p = 20!
- Solution: Sampling-based Markov Chain Monte Carlo (MCMC) algorithms.
- Metropolis algorithms first used by nuclear physicists during Manhattan Project in 1940's to understand particle movement underlying first atomic bomb.

Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006] – MATLAB, Python



1. Determine $q^0 = \arg\min_q \sum_{i=1}^{N} [\upsilon_i - f(t_i, q)]^2$
2. For $k = 1, \cdots, M$
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   (b) Compute likelihood

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

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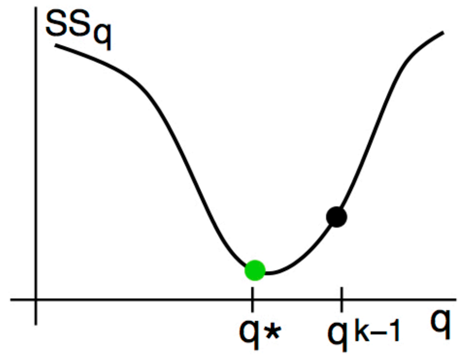

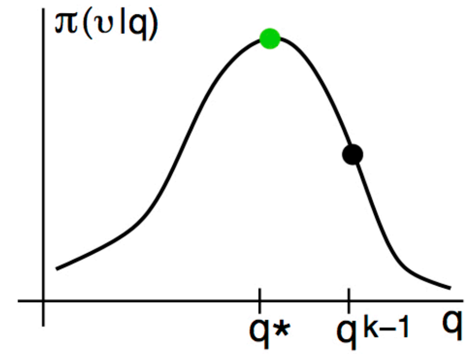

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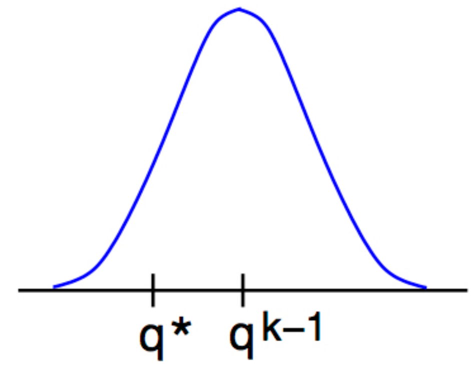

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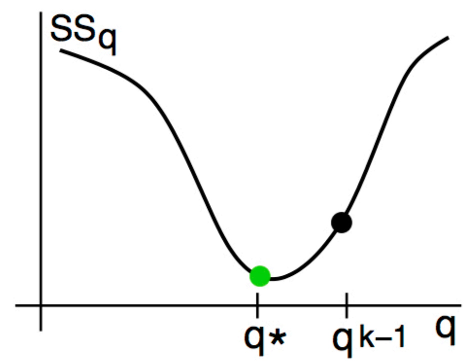

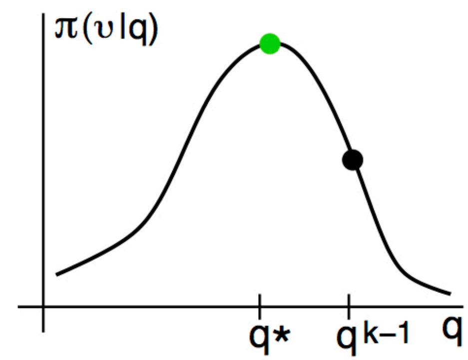

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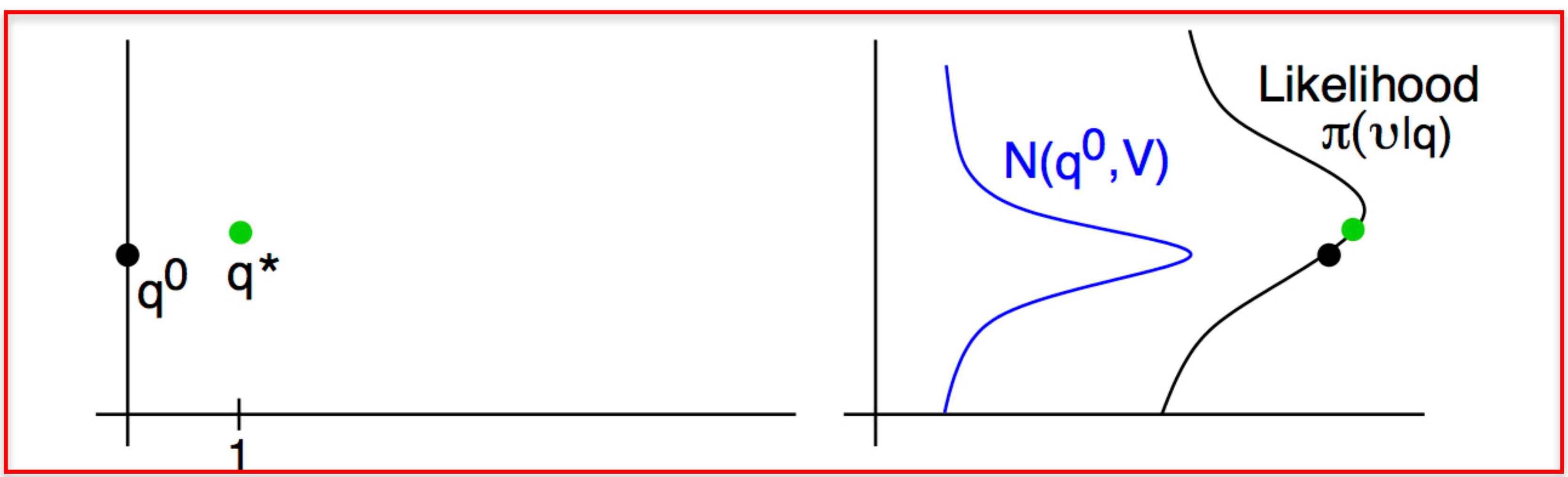

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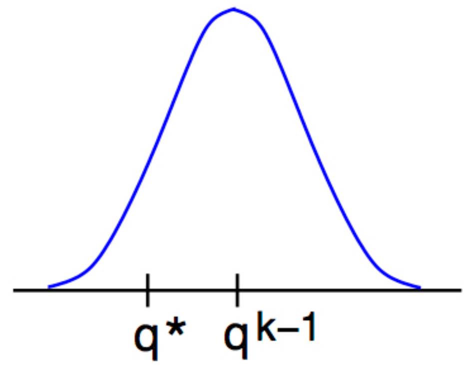

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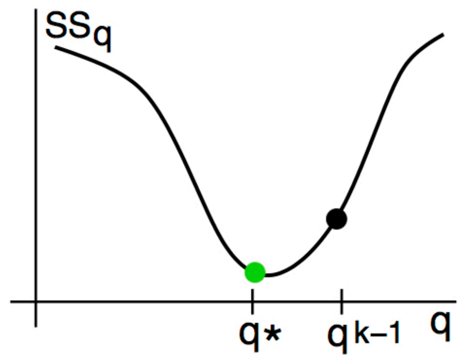

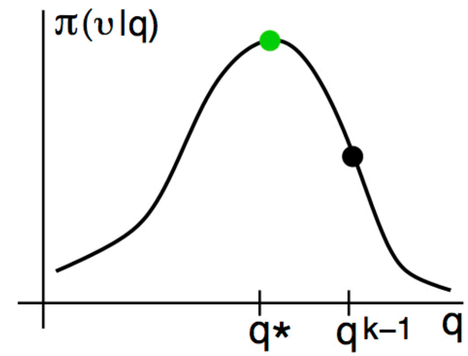

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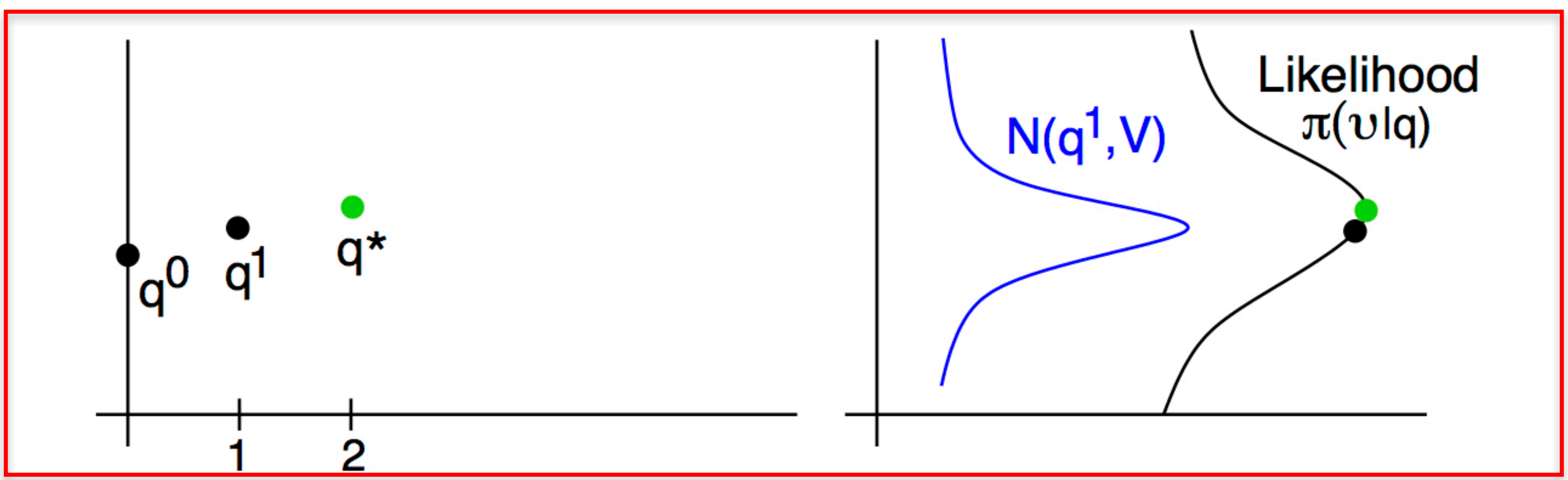

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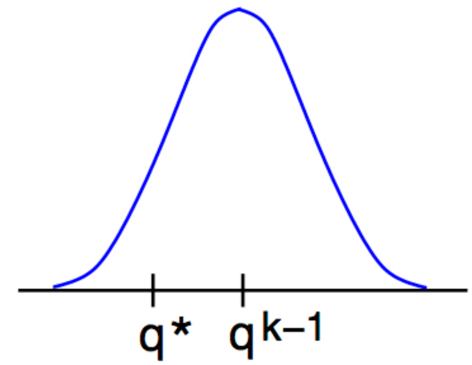

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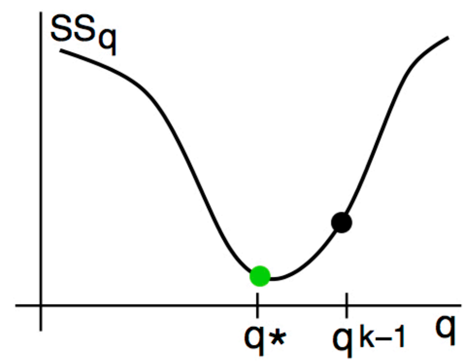

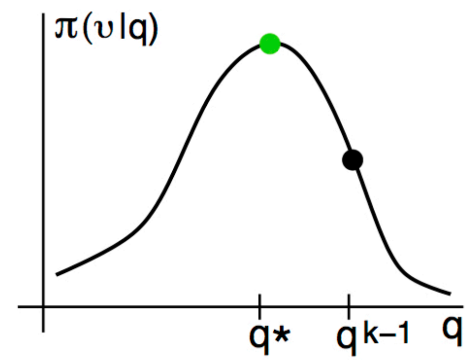

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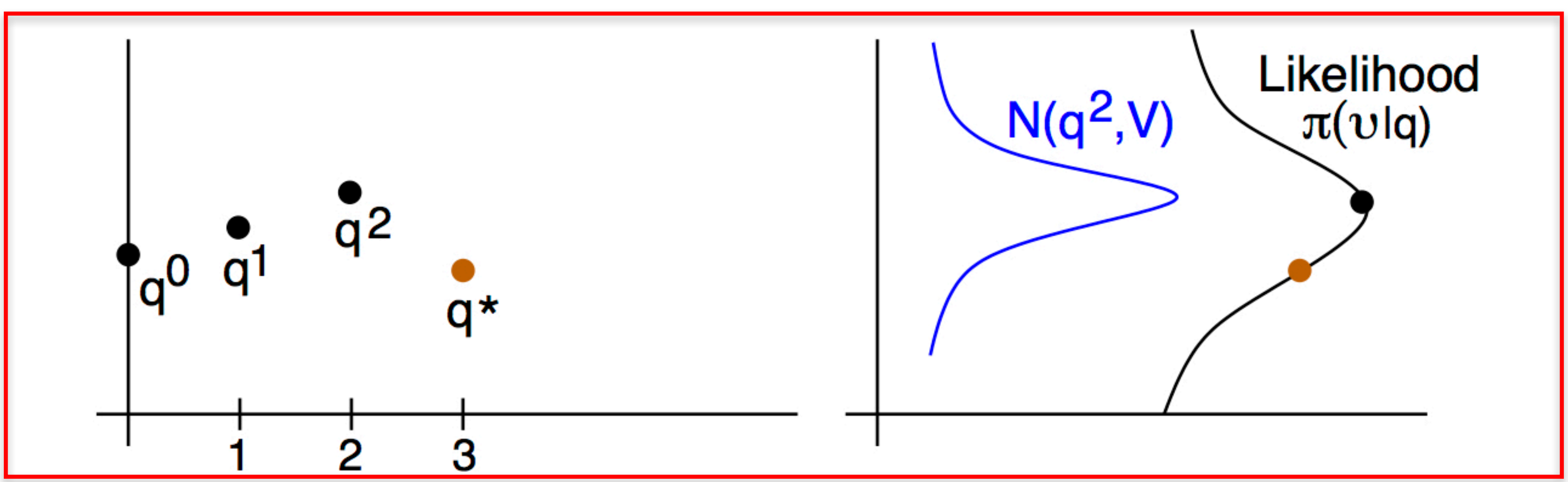

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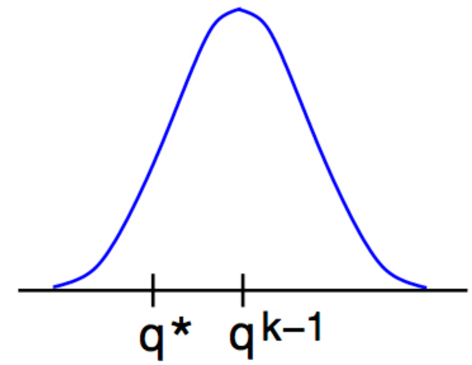

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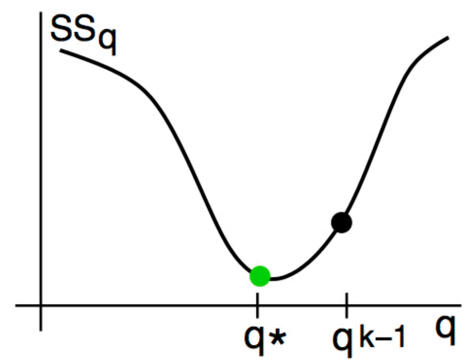

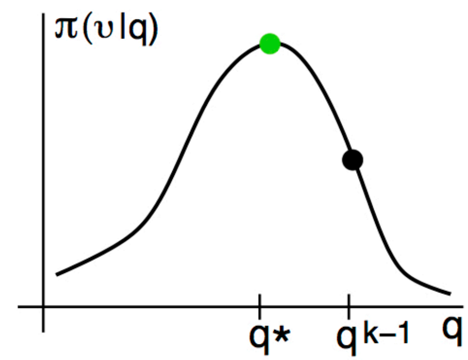

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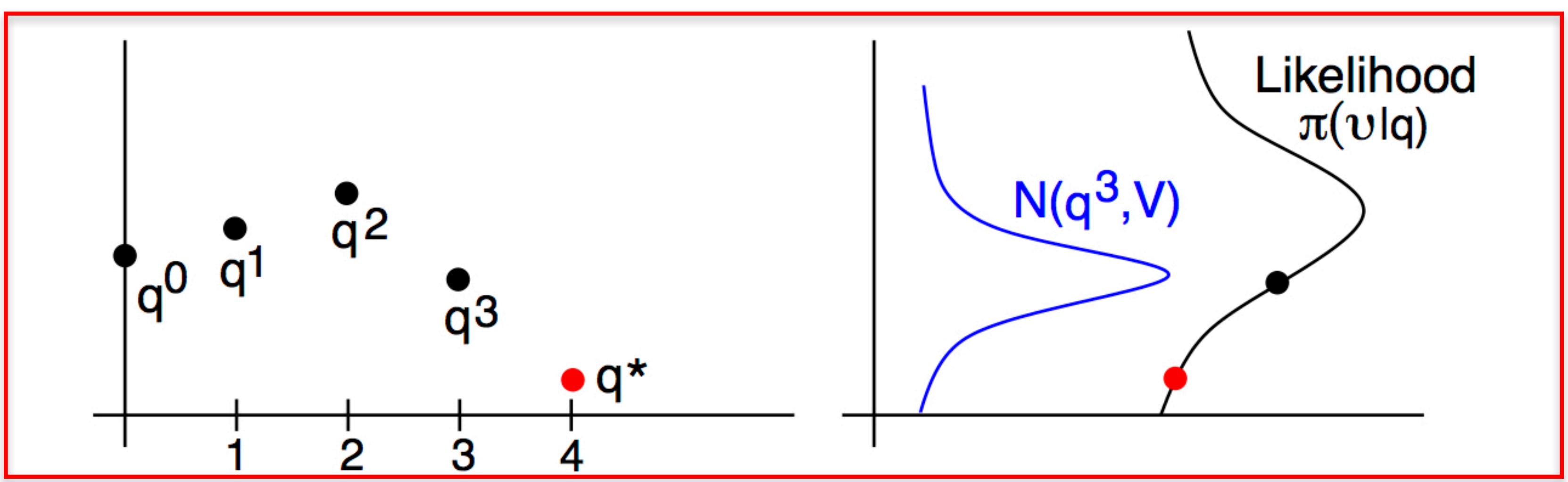

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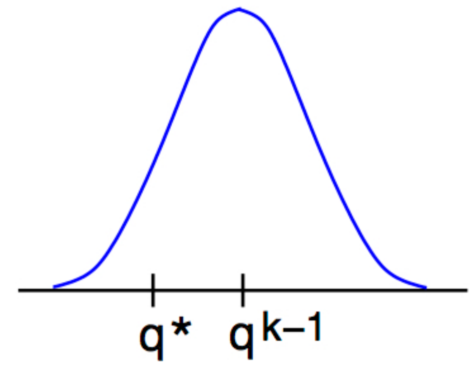

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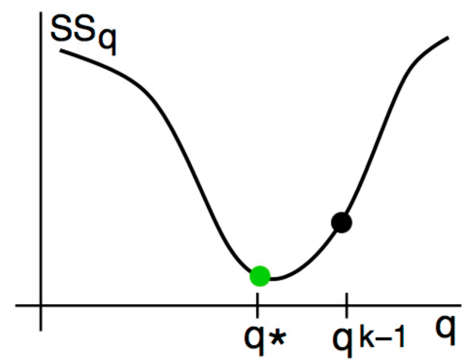

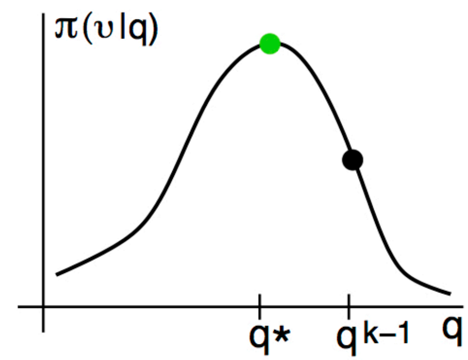

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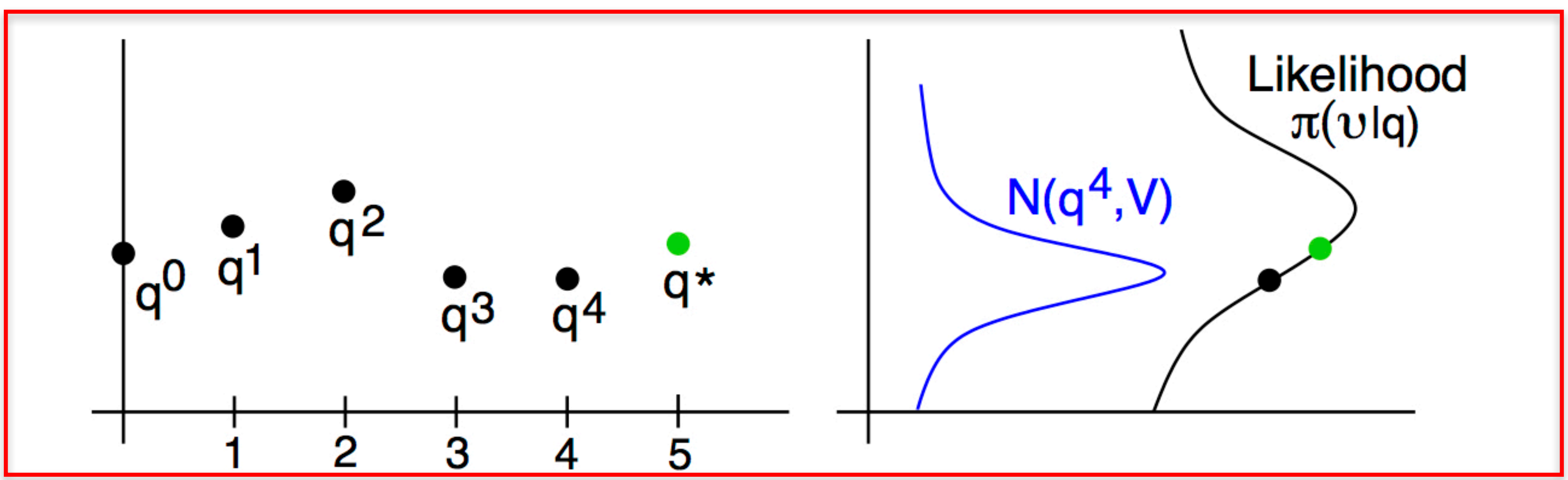


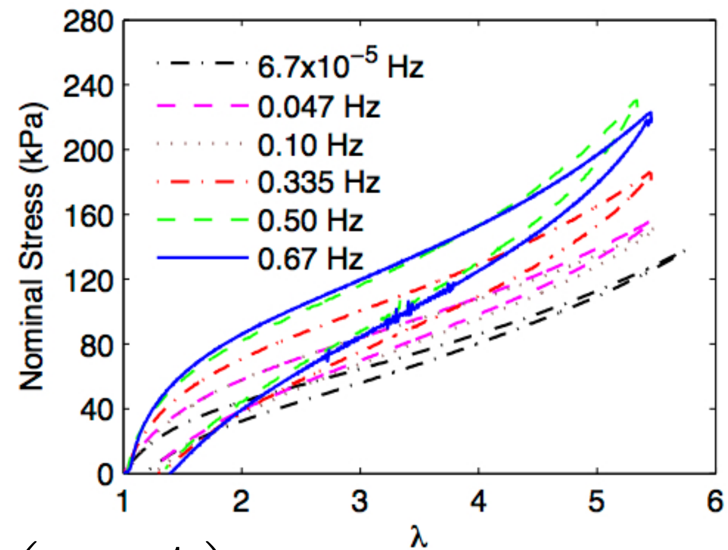
Example: Viscoelastic Material Models

Material Behavior: Significant rate dependence

Finite-Deformation Model: Nonlinear, non-affine

$$\psi(q) = \psi_\infty(G_e, G_c, \lambda_{max}) + \Upsilon(\eta, \beta, \gamma)$$

- Dissipative energy function Υ
- Conserved hyperelastic energy function



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

Parameters:

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

G_c: Crosslink network modulus

G_e: Plateau modulus

λ_{max}: Max stretch effective affine tube

$\boxed{[\eta, \beta, \gamma]\text{: Viscoelastic parameters}}$ Initial Focus

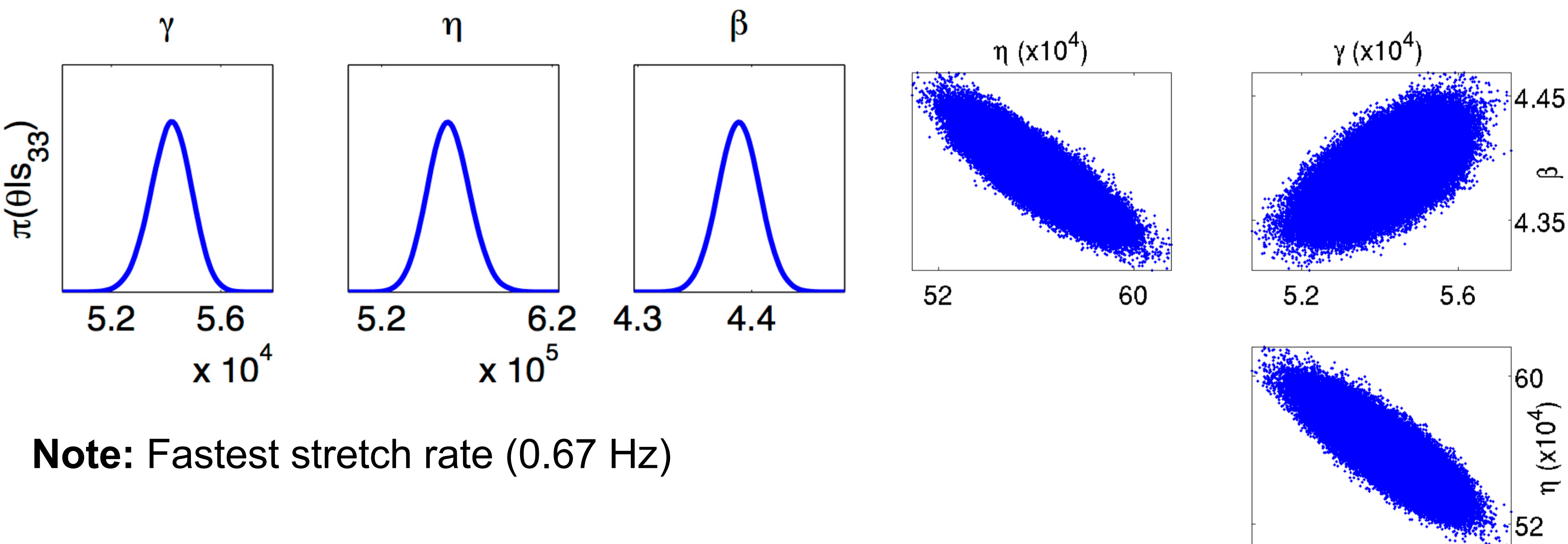
UQ Goals:

- Quantify uncertainty in parameters.
- Use UQ for model selection
  - E.g., linear versus nonlinear.
- Quantify models' predictive capabilities for range of stretch rates.

Viscoelastic Model

Reduced Parameter Set:

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



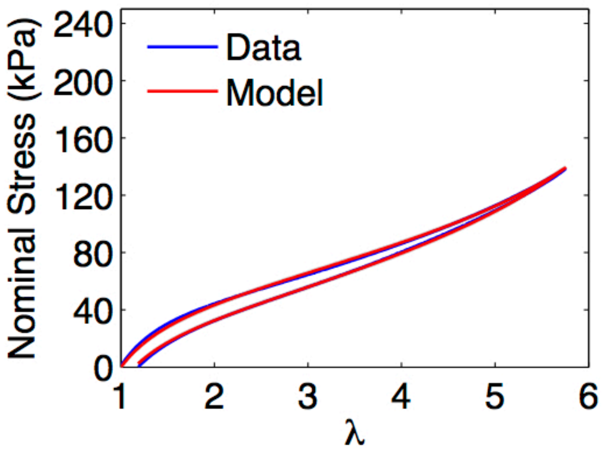
Note: Fastest stretch rate (0.67 Hz)

Question: How do we quantify uncertainty in response (stress)?

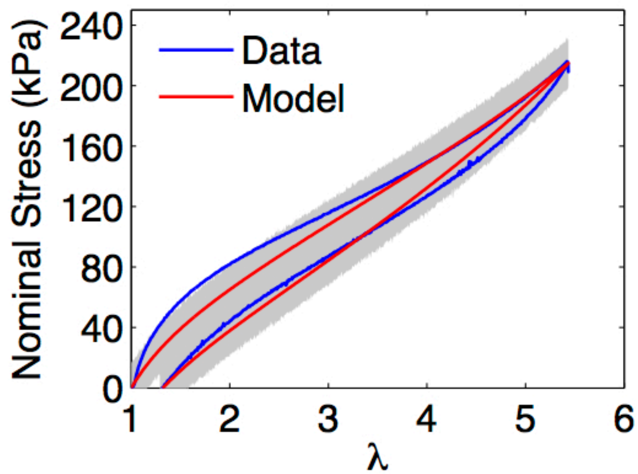
Solution: Propagate parameter and measurement uncertainties through model.

Prediction Intervals for the Viscoelastic Model

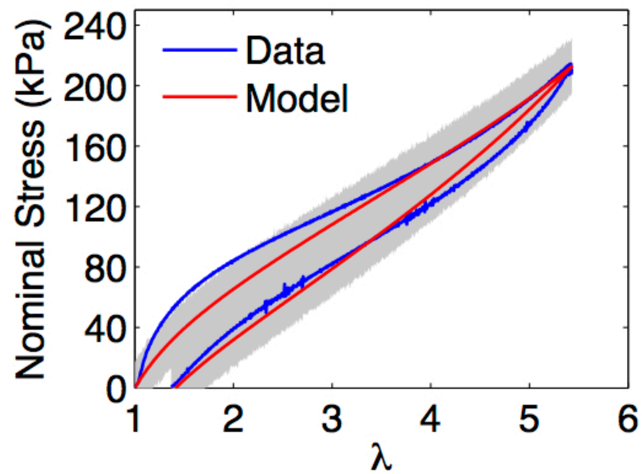
Linear Non-Affine Model: Not accurate for predicting higher stretch rates



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



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



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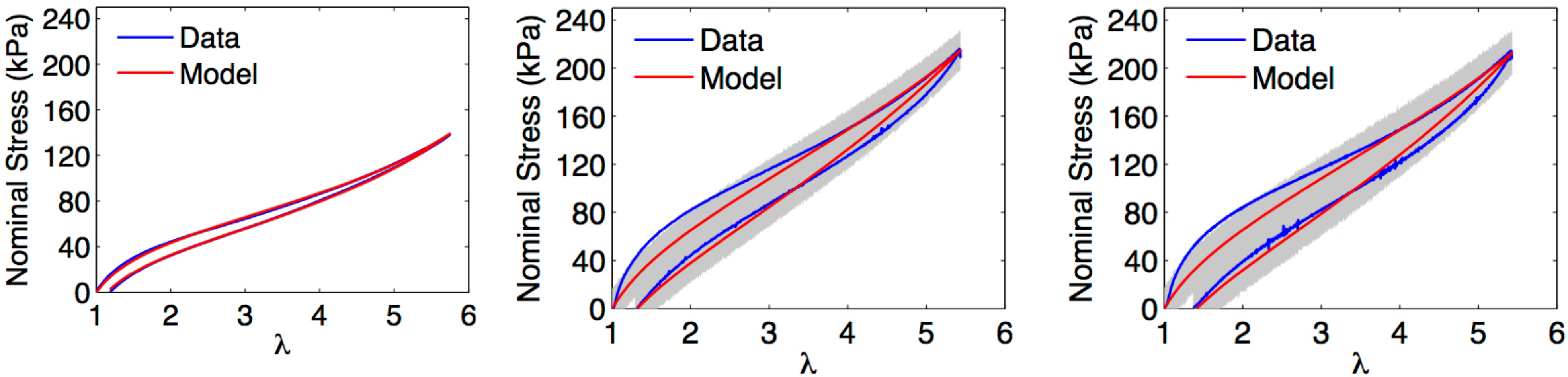
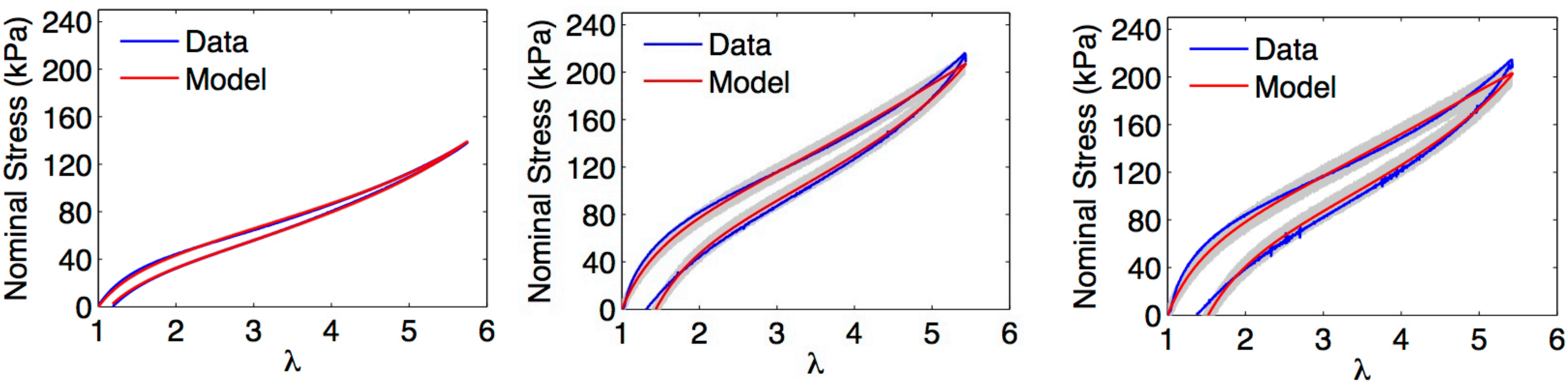
Prediction Intervals for the Viscoelastic Model

Linear Non-Affine Model:



Nonlinear Non-Affine Model: Significantly more accurate over range of stretch rates!



$$\frac{d\lambda}{dt} = 6.7 \times 10^{-5} \text{ Hz} \qquad \frac{d\lambda}{dt} = 0.335 \text{ Hz} \qquad \frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

Prediction Intervals for the Viscoelastic Model

Linear Viscoelasticity:

- Fractional-order relation

$$Q_{iK} = \eta D_t^{\alpha} F_{iK}$$

- C – Calibrated
- P - Predicted

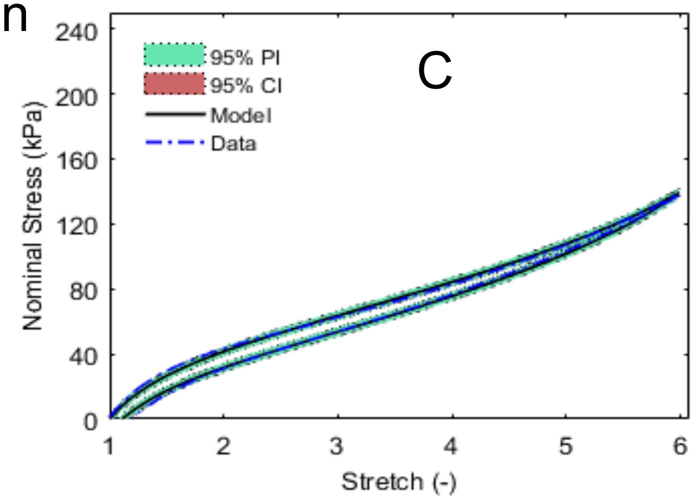
Note:

$\bar{\eta} = 35.3$

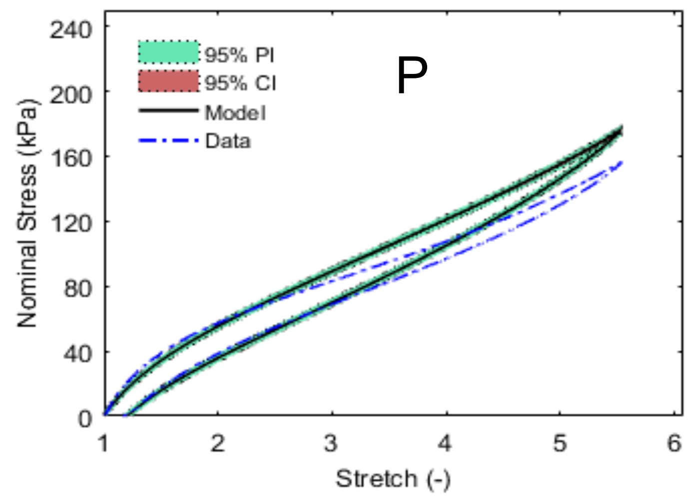
$\bar{\alpha} = 0.12$

Collaborators: Billy Oates, Paul Miles

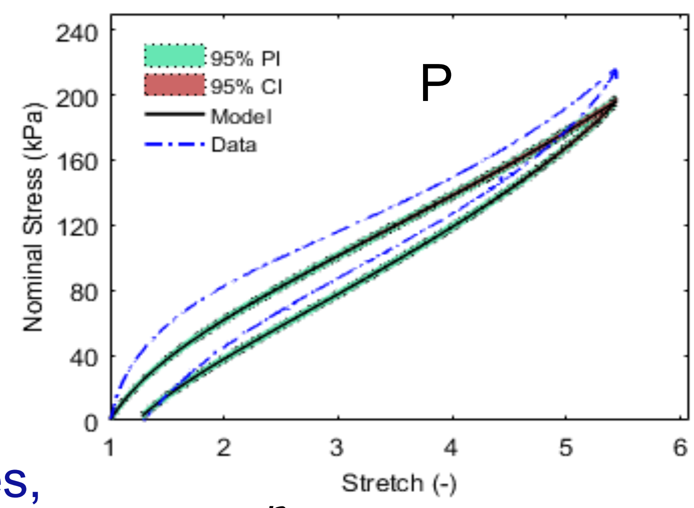
Calibrated Rate (1/s): 6.7×10^{-5}



$$\frac{d\lambda}{dt} = 6.5 \times 10^{-5} \text{ Hz}$$



$$\frac{d\lambda}{dt} = 0.0472 \text{ Hz}$$



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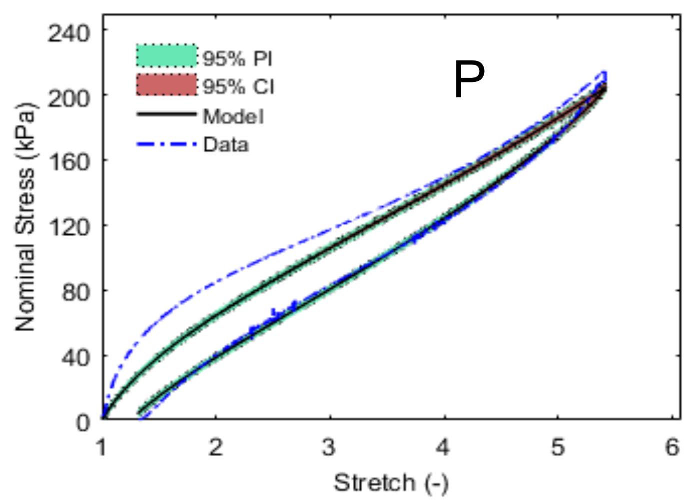


$$\frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

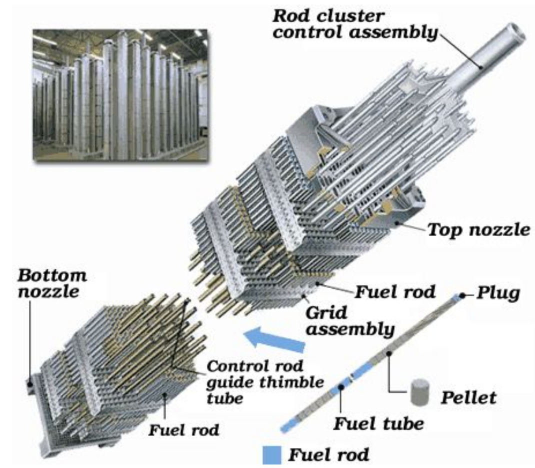
Use of Prediction Intervals: Nuclear Power Plant Design

Subchannel Code (COBRA-TF): numerous closure relations, ~70 parameters

e.g., Dittus—Boelter Relation

$$Nu = 0.023 Re^{0.8} Pr^{0.4}$$

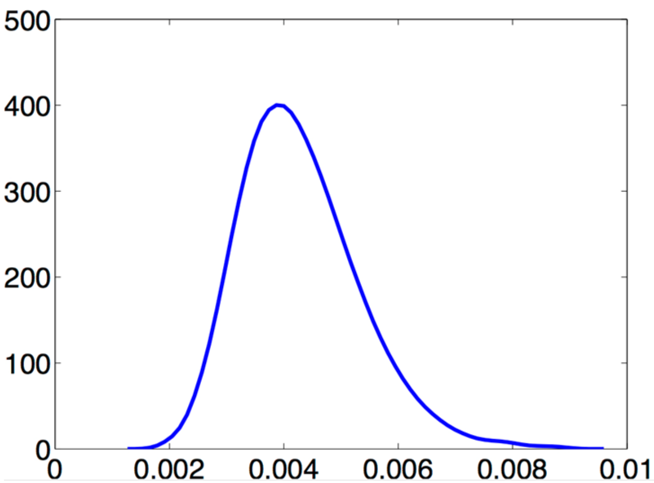
Nu: Nusselt number
Re: Reynolds number
Pr: Prandtl number



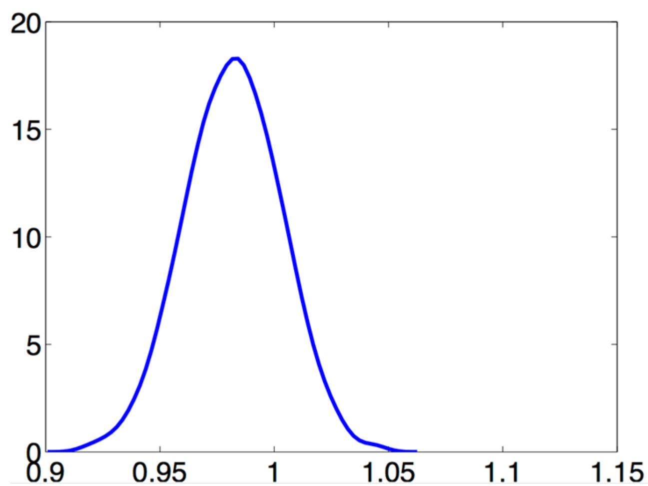
Industry Standard: Employ conservative, uniform, bounds

i.e., [0, 0.046], [0, 1.6], [0,0.8]

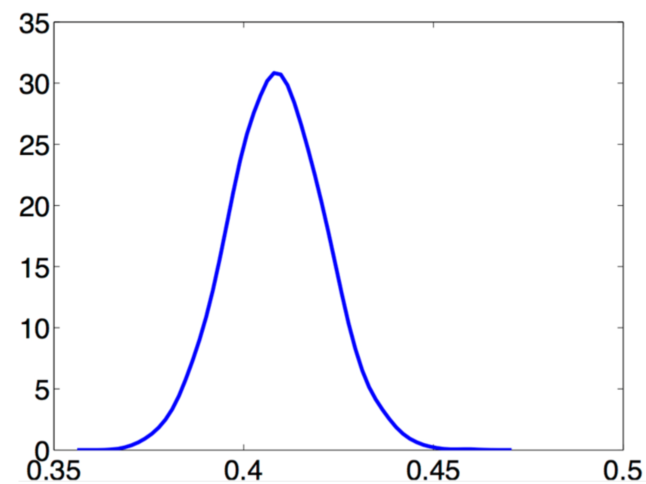
Bayesian Analysis: Employ conservative bounds as priors



$2\sigma \approx 0.0035$



$2\sigma \approx 0.06$

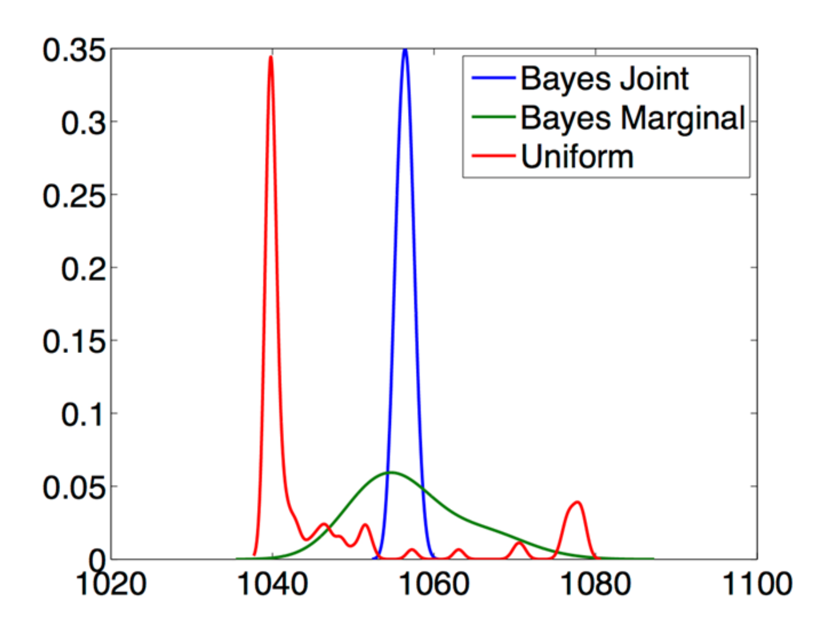


$2\sigma \approx 0.03$

Note: Substantial reduction in parameter uncertainty

Use of Prediction Intervals: Nuclear Power Plant Design

Strategy: Propagate parameter uncertainties through COBRA-TF surrogate to determine uncertainty in maximum fuel temperature



Notes:

- Temperature uncertainty reduced from 40 degrees to 5 degrees
- Can run plant 20 degrees hotter, which significantly improves efficiency

Use of Prediction Intervals: Nuclear Power Plant Design

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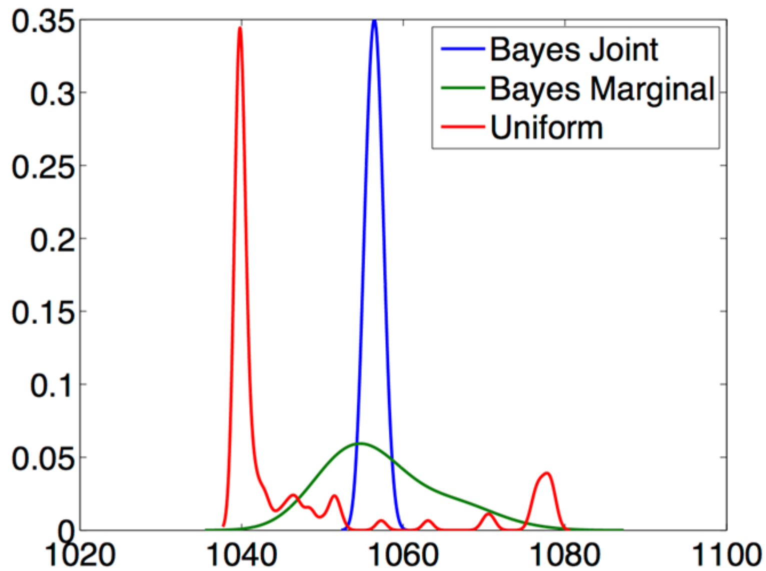

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Ramification: Savings of 10 billion dollars per year for US power plants

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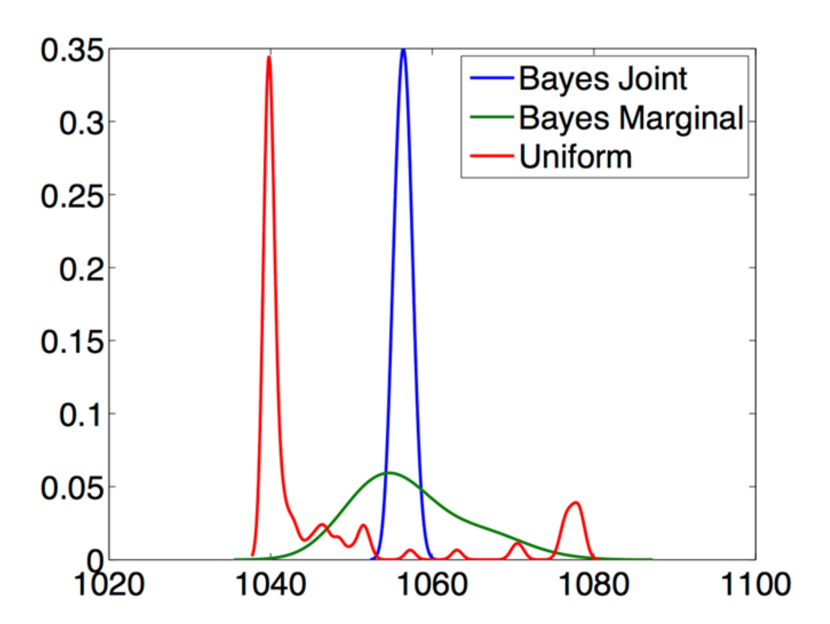

Notes:

- Temperature uncertainty reduced from 40 degrees to 5 degrees
- Can run plant 20 degrees hotter, which significantly improves efficiency

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Issues:

- We considered only one of many closure relations
- Nuclear regulatory commission takes years to change requirements and codes

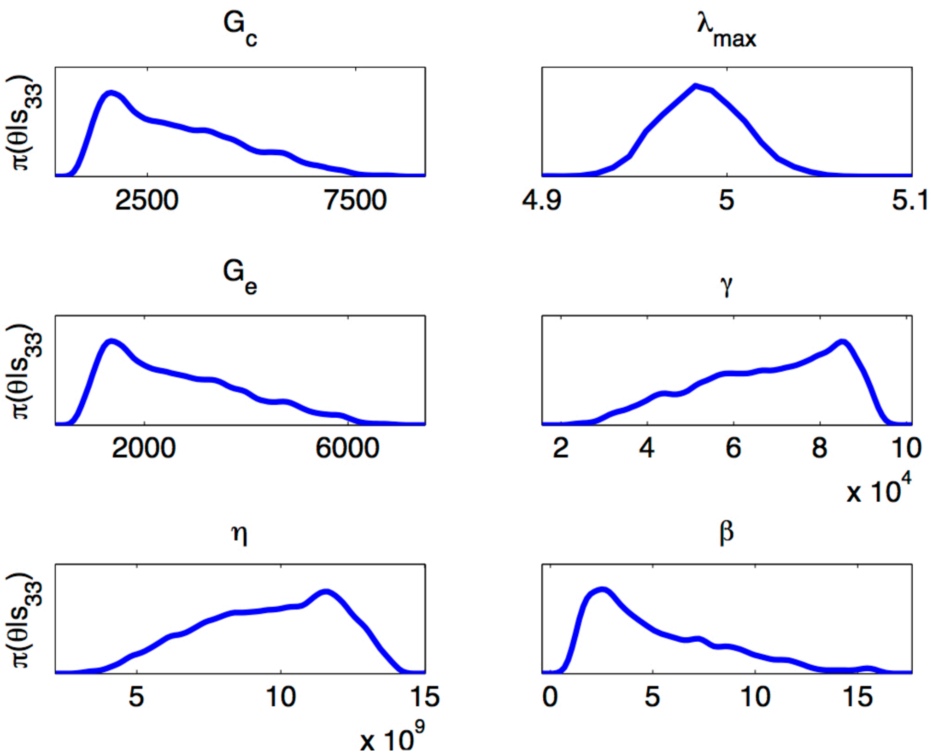
Good News: We are now working with Westinghouse to reduce uncertainties.

Note: Requires construction and verification of surrogate models.

Uncertainty Quantification Challenges

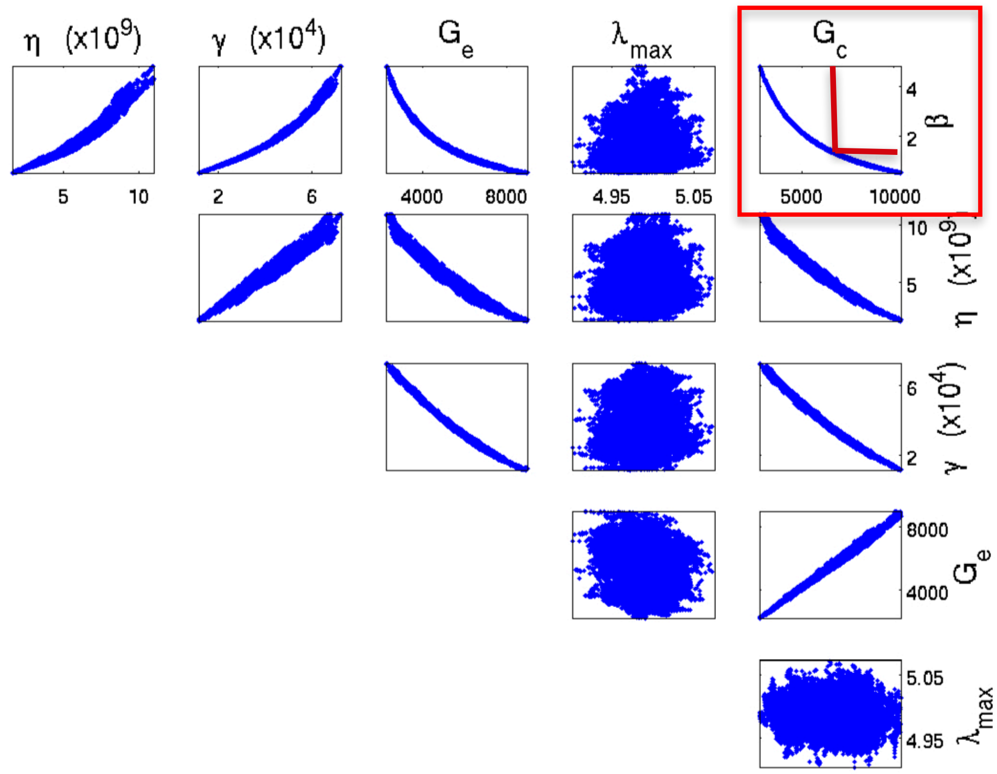
Viscoelastic Material Model: Full Parameter Set

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



Marginal Posterior Densities

Joint Posterior Densities



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

Broad Control and UQ Objectives

Control Formulation:

$$\frac{dz}{dt} = f(t, z, u, q) + v_1(t)$$

$$y(t, q) = Cz(t, q) + v_2(t)$$

UQ Formulation: e.g., average tip displacement

$$\frac{dz}{dt} = f(t, z, q) + v_1(t)$$

$$y(t) = \int_{\mathbb{R}^{20}} w^N(t, \bar{x}, q)\rho(q)dq$$

Control Objectives:

- Determine optimal q; requires identifiability analysis.
- Construct reduced-order model for state z; e.g., POD, DMD.
- Determine plant error Δ for robust control design.
- Construct state estimator $z_c(t)$.
- Compute feedforward or feedback controls; e.g., $u(t) = -kz_c(t)$.
- Note: Feedback not necessary if no uncertainties!

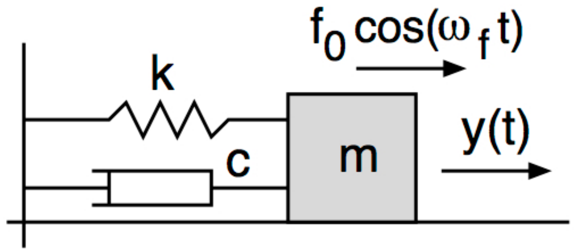
UQ Objectives:

- Determine identifiable parameter subsets or subspace; GSA or active subspace techniques.
- Construct surrogate model; e.g., GP, regression, collocation, POD.
- Infer distributions (Bayesian) or estimators (frequentist) for q or q(x).
- Compute distributions or statistics for QoI. Analytic relations for stochastic Galerkin or collocation for certain distributions; e.g., Gaussian or uniform.

Parameter Selection Techniques

First Issue: Parameters often not *identifiable* in the sense that they are uniquely determined by the data.

Example: Spring model



$$m\frac{d^2z}{dt^2} + c\frac{dz}{dt} + kz = f_0\cos(\omega_F t)$$

$$z(0) = z_0 \; , \; \frac{dz}{dt}(0) = z_1$$

Problem: Parameters $q = [m, c, k, f_0]$ and $q = \left[1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}\right]$ yield same displacements

Parameter Selection Techniques

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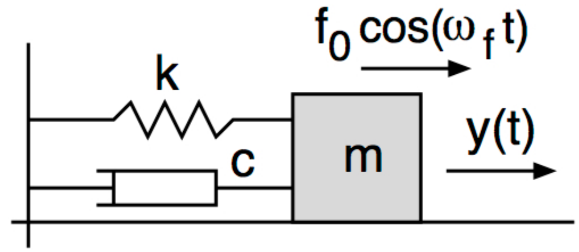
Example: Spring model

$$\underline{m}\frac{d^2z}{dt^2} + \underline{c}\frac{dz}{dt} + \underline{kz} = \underline{f_0}\cos(\omega_F t)$$

$$z(0) = z_0 \ , \ \frac{dz}{dt}(0) = z_1$$



Problem: Parameters $q = [m, c, k, f_0]$ and $q = \left[1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}\right]$ yield same displacements

Solution: Reformulate problem as

$$\frac{d^2z}{dt^2} + \underline{C}\frac{dz}{dt} + \underline{Kz} = \underline{F_0}\cos(\omega_F t)$$

$$z(0) = z_0 \ , \ \frac{dz}{dt}(0) = z_1$$

where $C = \frac{c}{m}, K = \frac{k}{m}$ and $F_0 = \frac{f_0}{m}$

Techniques for General Models:

- Linear algebra analysis;
  - e.g., SVD or QR algorithms
- Global Sensitivity analysis
- Parameter subset selection
- Active subspaces: Identifiable subspaces from control

Sensitivity Analysis: Motivation

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100,\ c = 0.1,\ e = 0.001,\ \frac{de}{dt} = 0.1$

Question: To which parameter E or c is stress most sensitive?

Local Sensitivity Analysis:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\boxed{\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1}$$

Conclusion: Model most sensitive to damping parameter c

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Conclusion: Model most sensitive to damping parameter c

Limitations:

- Does not accommodate potential uncertainty in parameters.
- Does not accommodate potential correlation between parameters.
- Sensitive to units and magnitudes of parameters.

Global Sensitivity Analysis

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100,\ c = 0.1$

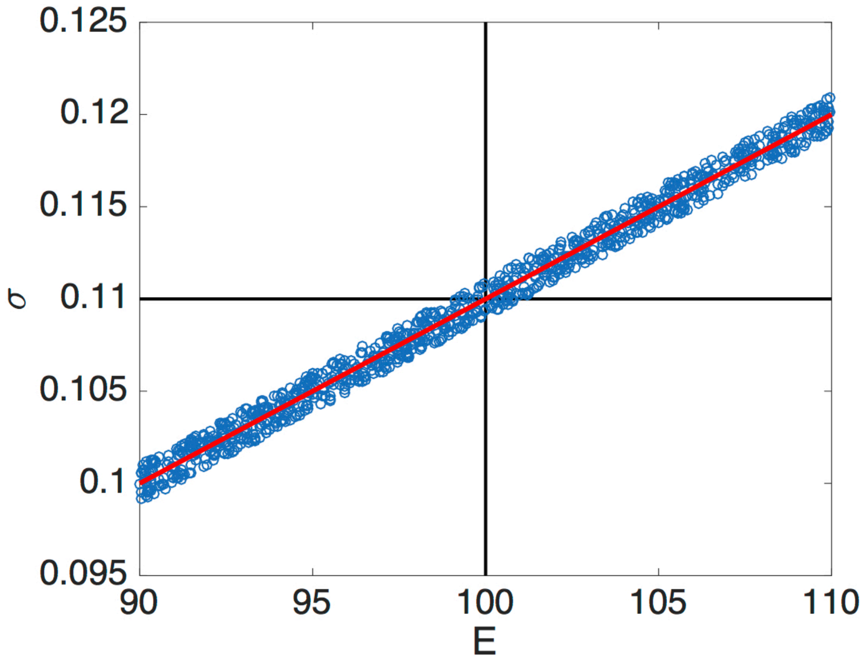
Uncertainty: 10% of nominal values

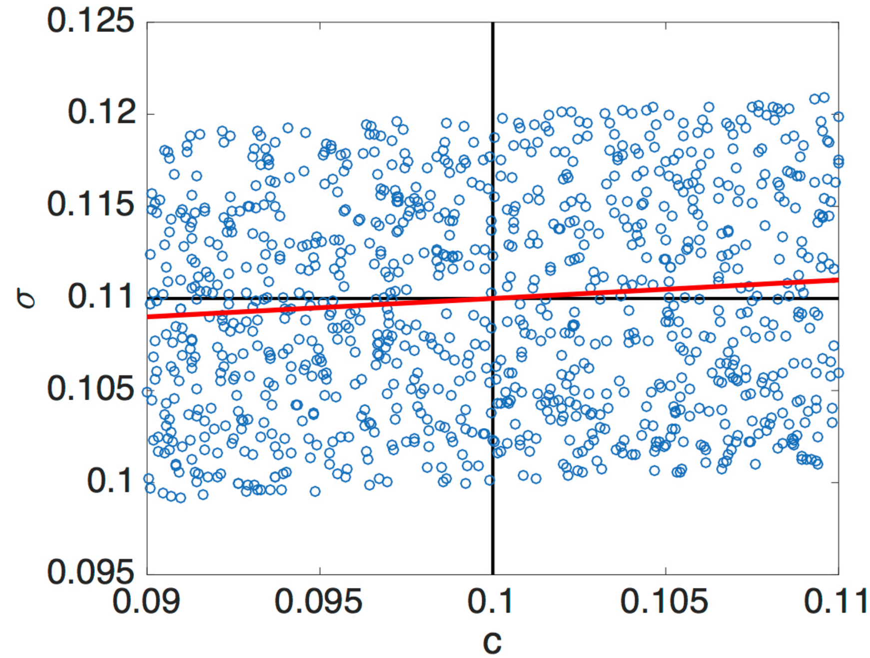
$$E \sim \mathcal{U}(90, 110)\ ,\ c \sim \mathcal{U}(0.09, 0.11)$$

Local Sensitivities:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1$$





Global Sensitivity: E is more influential

Global Sensitivity Analysis: Analysis of Variance (ANOVA)

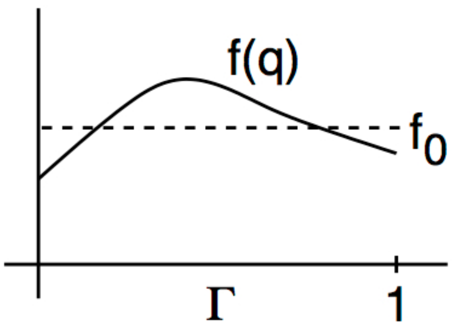
Sobol' Representation: $Y = f(q)$

$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{i\leqslant i<j\leqslant p} f_{ij}(q_i, q_j) + \cdots + f_{12\cdots p}(q_1, \ldots, q_p)$$

$$= f_0 + \sum_{i=1}^{p} \sum_{|u|=i} f_u(q_u)$$

where

$$f_0 = \int_\Gamma f(q)\rho(q)dq = \mathbb{E}[f(q)]$$



$$f_i(q_i) = \mathbb{E}[f(q)|q_i] - f_0$$

$$f_{ij}(q_i, q_j) = \mathbb{E}[f(q)|q_i, q_j] - f_i(q_i) - f_j(q_j) - f_0$$

Typical Assumption: $q_1, q_2, \ldots, q_p$ independent. Then

$$\int_\Gamma f_u(q_u) f_v(q_v)\rho(q)dq = 0 \quad \text{for } u \neq v$$

$$\Rightarrow \text{var}[f(q)] = \sum_{i=1}^{p} \sum_{|u|=i} \text{var}[f_u(q_u)]$$

Sobol' Indices:

$$S_u = \frac{\text{var}[f_u(q_u)]}{\text{var}[f(q)]} \quad , \quad T_u = \sum_{v\subseteq u} S_v$$

Note: Magnitude of S_i, T_i quantify contributions of q_i to $\text{var}[f(q)]$

Global Sensitivity Analysis

Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

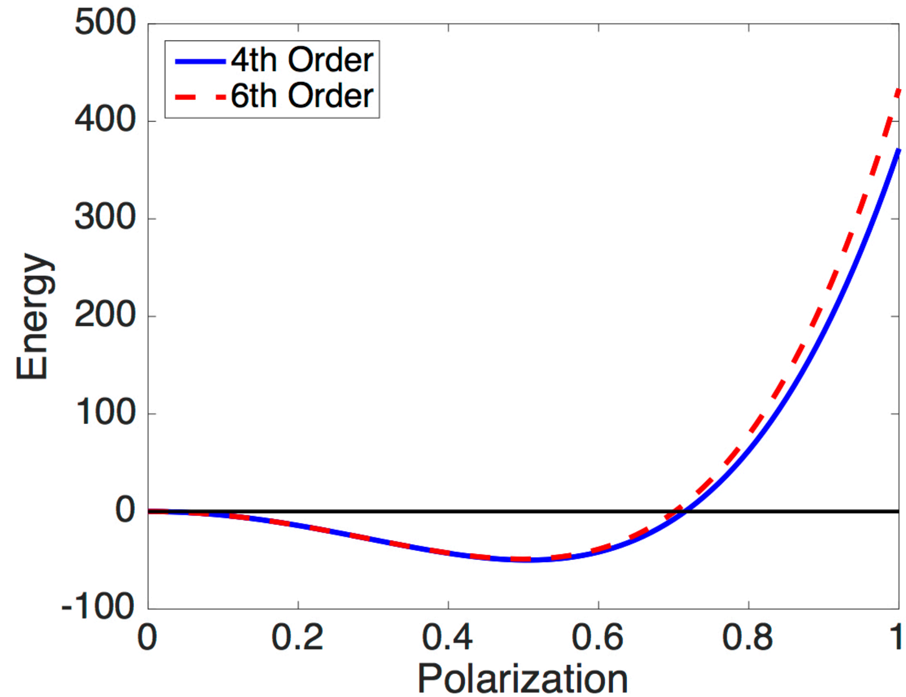
$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03



Conclusion: α_{111} insignificant and can be fixed

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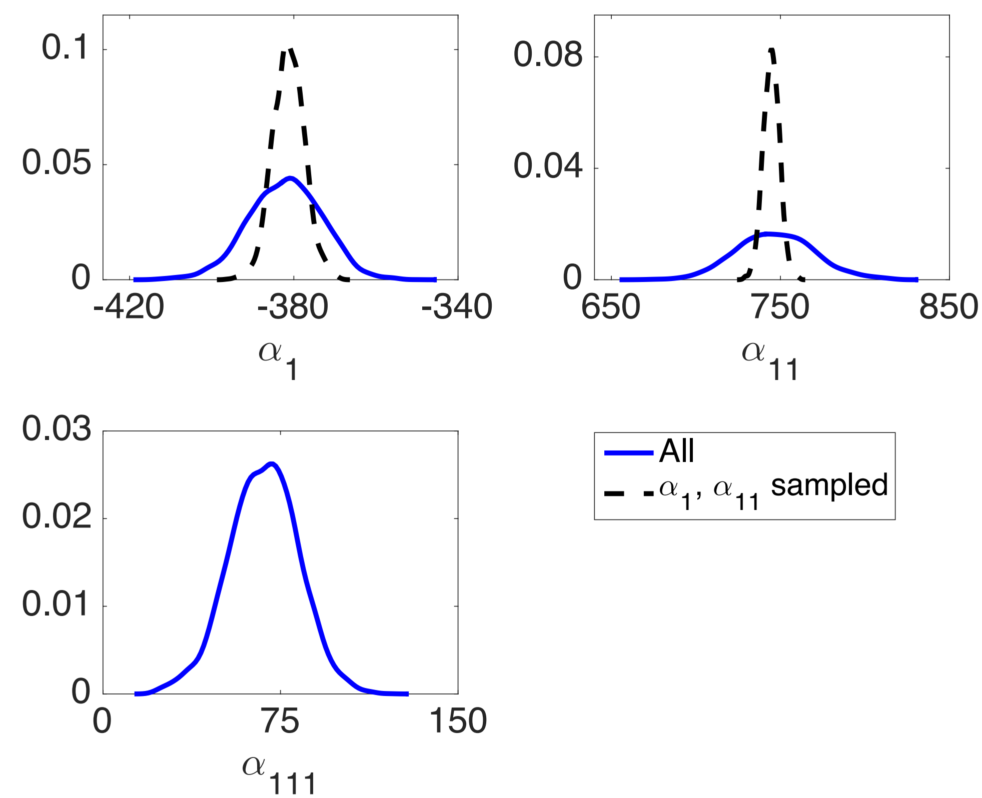
Problem: We obtain different distributions when we perform Bayesian inference with fixed non-influential parameters



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Problem:

- Parameters correlated
- Cannot fix α_{111}

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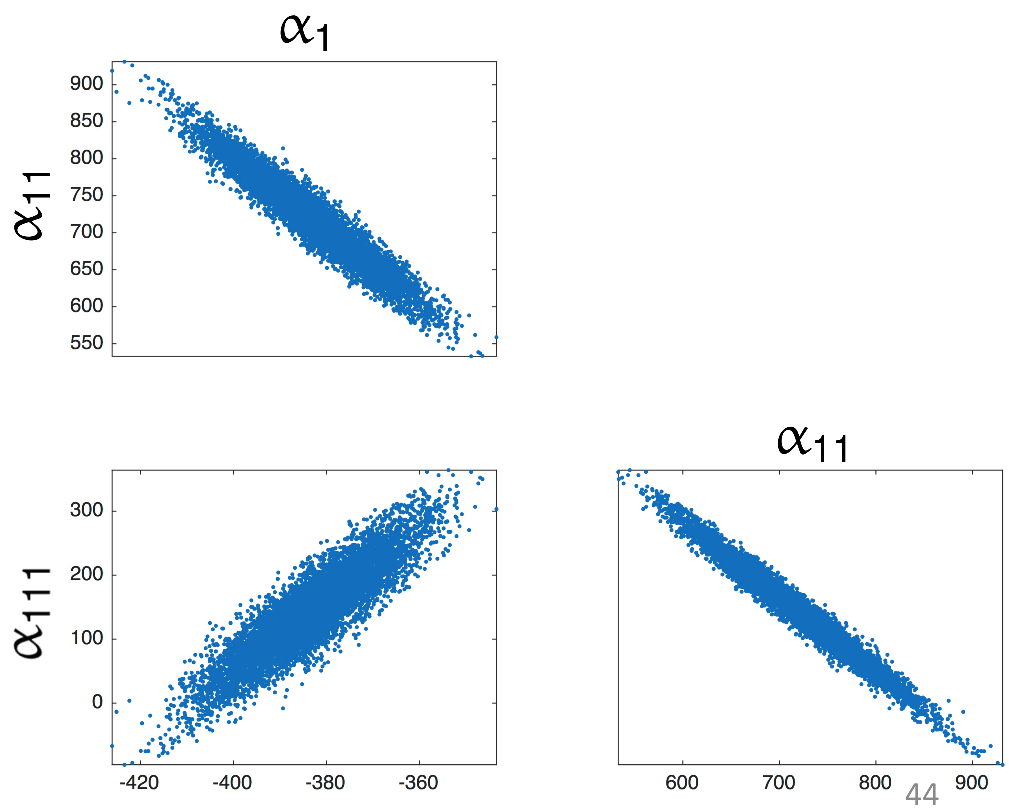
	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03

Solution: Must accommodate correlation



Global Sensitivity Analysis: Analysis of Variance (ANOVA)

Sobol' Representation:

$$f(q) = f_0 + \sum_{i=1}^{p} \sum_{|u|=i} f_u(q_u)$$

One Solution: Take variance to obtain

$$\text{var}[f(q)] = \sum_{i=1}^{p} \sum_{|u|=i} \text{cov}[f_u(q_u), f(q)]$$

Sobol' Indices:

$$S_u = \frac{\text{cov}[f_u(q_u), f(q)]}{\text{var}[f(q)]}$$

Pros:

- Provides variance decomposition that is analogous to independent case

Cons:

- Indices can be negative and difficult to interpret
- Often difficult to determine underlying distribution
- Monte Carlo approximation often prohibitively expensive.

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Sobol' Indices:

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Alternatives:

- Parameter subset selection
- Construct active subspaces
  - Often effective in high-dimensional spaces; e.g., p = 7700 reduced to 5-D active subspace for neutronics example

Pros:

- Provides variance decomposition that is analogous to independent case

Cons:

- Indices can be negative and difficult to interpret
- Often difficult to determine underlying distribution
- Monte Carlo approximation often prohibitively expensive.

One Solution: Parameter Subset Selection

Consider

$$\psi(P_i, q) \approx \psi(P_i, q^*) + \nabla_q \psi(P_i, q^*) \Delta q$$

where

$$\nabla_q \psi(P_i, q^*) = \left[\frac{\partial \psi}{\partial \alpha_1}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{11}}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{111}}(P_i, q^*) \right]$$

Functional: Since $\upsilon_i \approx \psi(P_i, q^*)$

$$\begin{aligned} J(q) &= \frac{1}{n} \sum_{i=1}^{n} [\upsilon_i - \psi(P_i, q)]]^2 \\ &\approx \frac{1}{n} \sum_{i=1}^{n} [\nabla_q \psi(P_i, q^*) \cdot \Delta q]^2 \\ &= \frac{1}{n} (\chi \Delta q)^T (\chi \Delta q) \end{aligned}$$

Sensitivity Matrix:

$$\chi(q^*) = \begin{bmatrix} \frac{\partial \psi}{\partial \alpha_1}(P_1, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_1, q^*) \\ \vdots & ... & \vdots \\ \frac{\partial \psi}{\partial \alpha_1}(P_n, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_n, q^*) \end{bmatrix}$$

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

One Solution: Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

Note: $\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable

Note: Estimator for covariance matrix

$$V = s^2 \left[\chi^T \chi\right]^{-1} = \begin{bmatrix} \text{var}(q_1) & \text{cov}(q_1, q_2) & \cdots & \text{cov}(q_1, q_n) \\ \text{cov}(q_2, q_1) & \text{var}(q_2) & \text{cov}(q_2, q_3) & \\ \vdots & & & \vdots \\ \text{cov}(q_n, q_1) & \cdots & \cdots & \text{var}(q_n) \end{bmatrix}$$

Ramification: Incorporates underlying distribution

One Solution: Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

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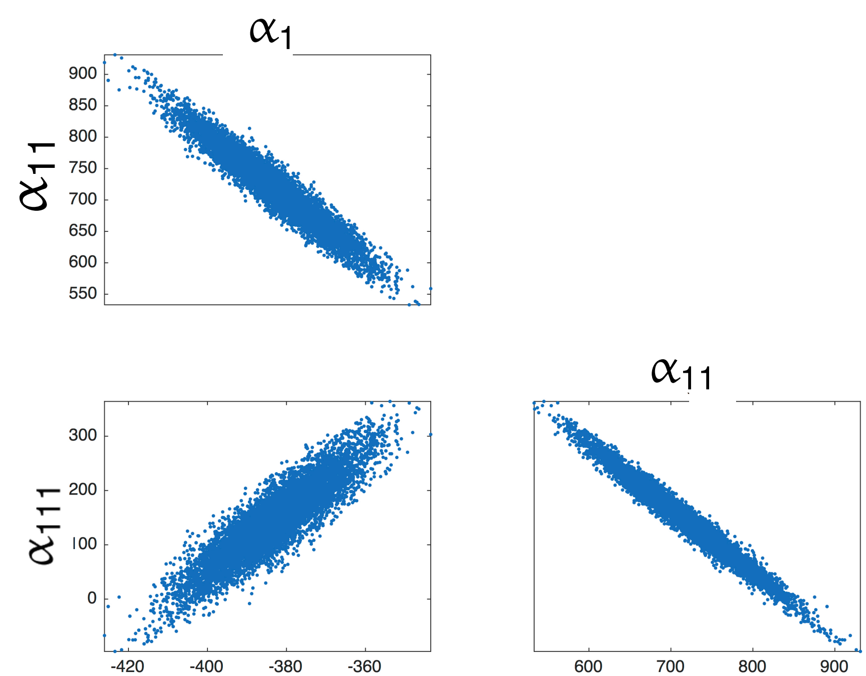
Example:

$$\psi(P, q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

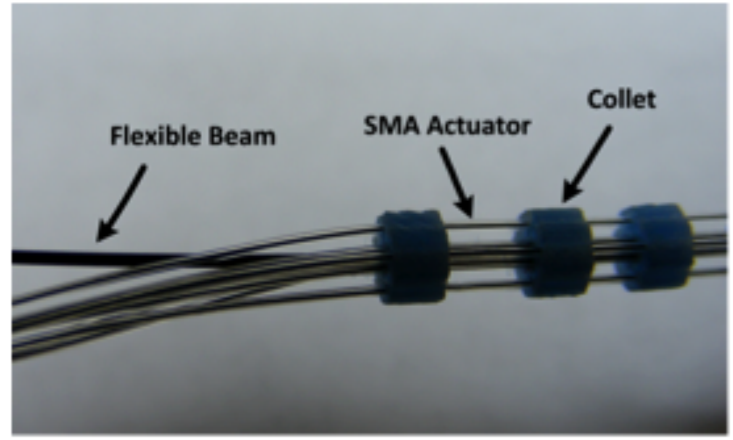


Result: rank($\chi^T\chi$) = 3 so all parameters identifiable

Parameter Selection for SMA Model

Constitutive Model:

$$f(\sigma, T, q) = \varepsilon$$



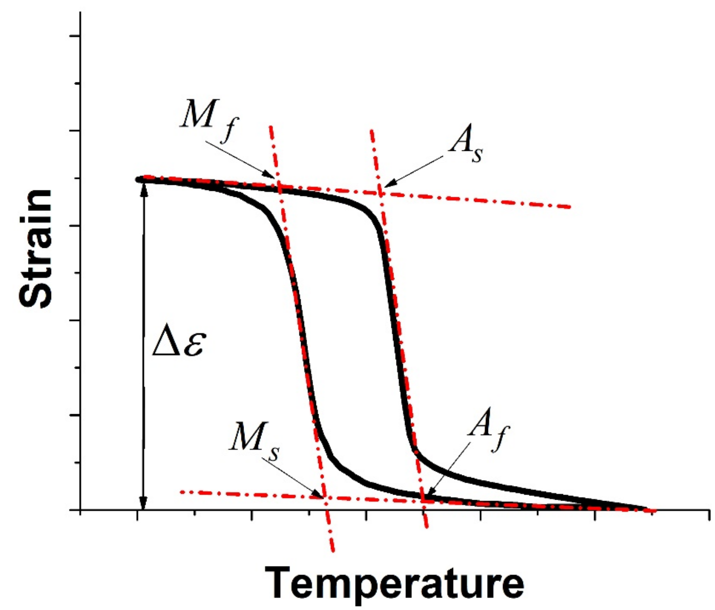
Independent Variables:

- Stress: σ
- Temperature: T

14 Parameters:

$$q = [E_a, E_m, A_s, A_f, M_s, M_f, C_a, C_m, H_{\max}, k_t, n_1, n_2, n_3, n_4]$$

Output: Strain ε



Note:

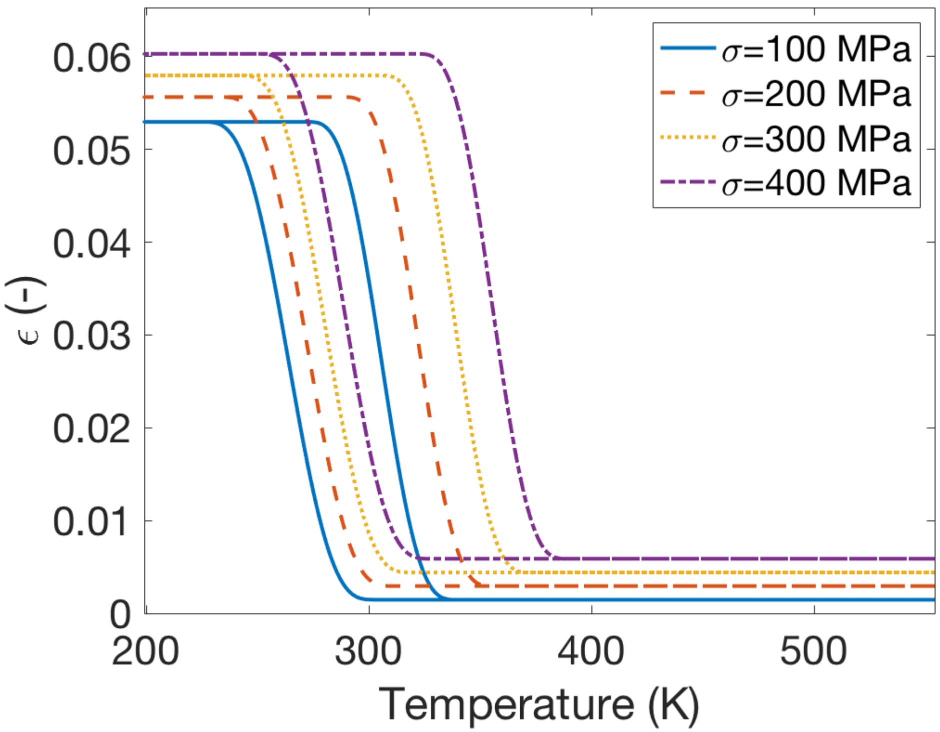
- Parameter subset selection yields 8 identifiable parameters

$$q^{id} = [A_s, A_f, M_s, M_f, C_a, C_m, H_{\max}, k_t]$$

Bayesian Inference for SMA Model

Notes:

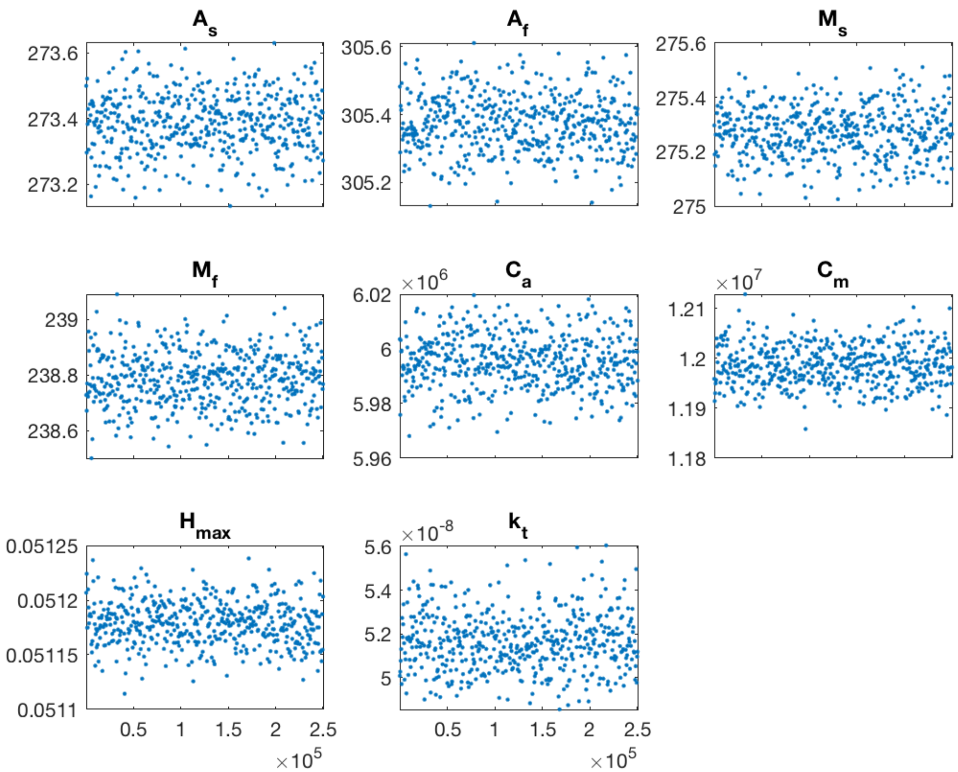
- Perform Bayesian inference for the 8 identifiable parameters
- Experimental data at four prestress levels

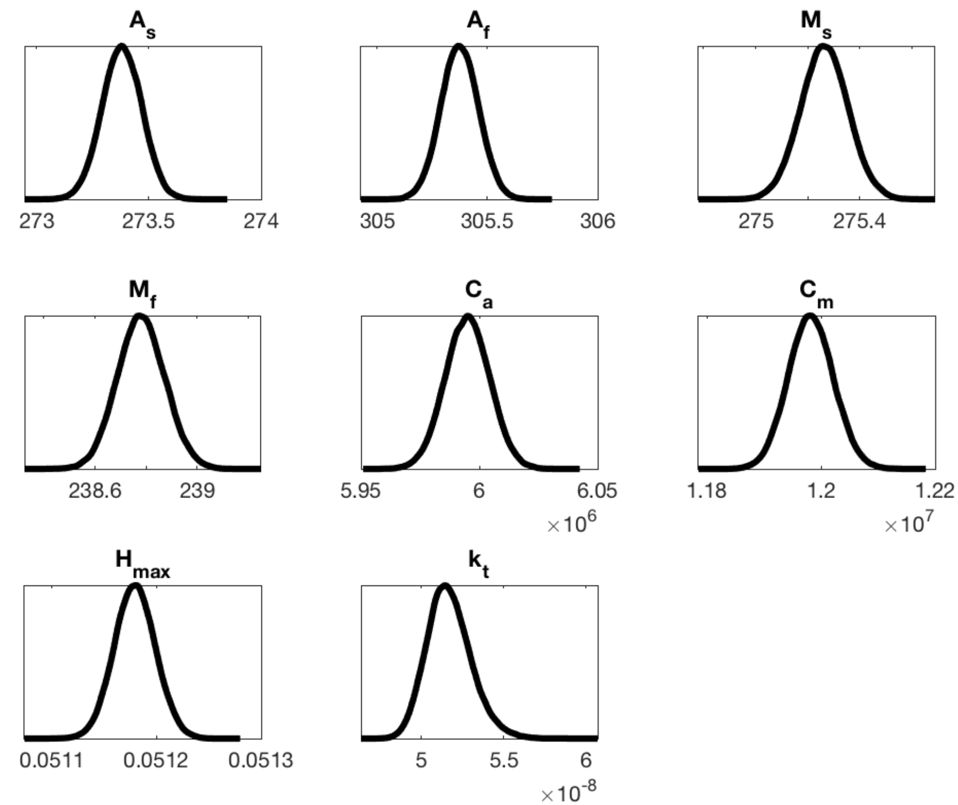


Collaborators: Paul Miles, Alex Solomou

Bayesian Inference for SMA Model

Chains and Marginal Distributions:

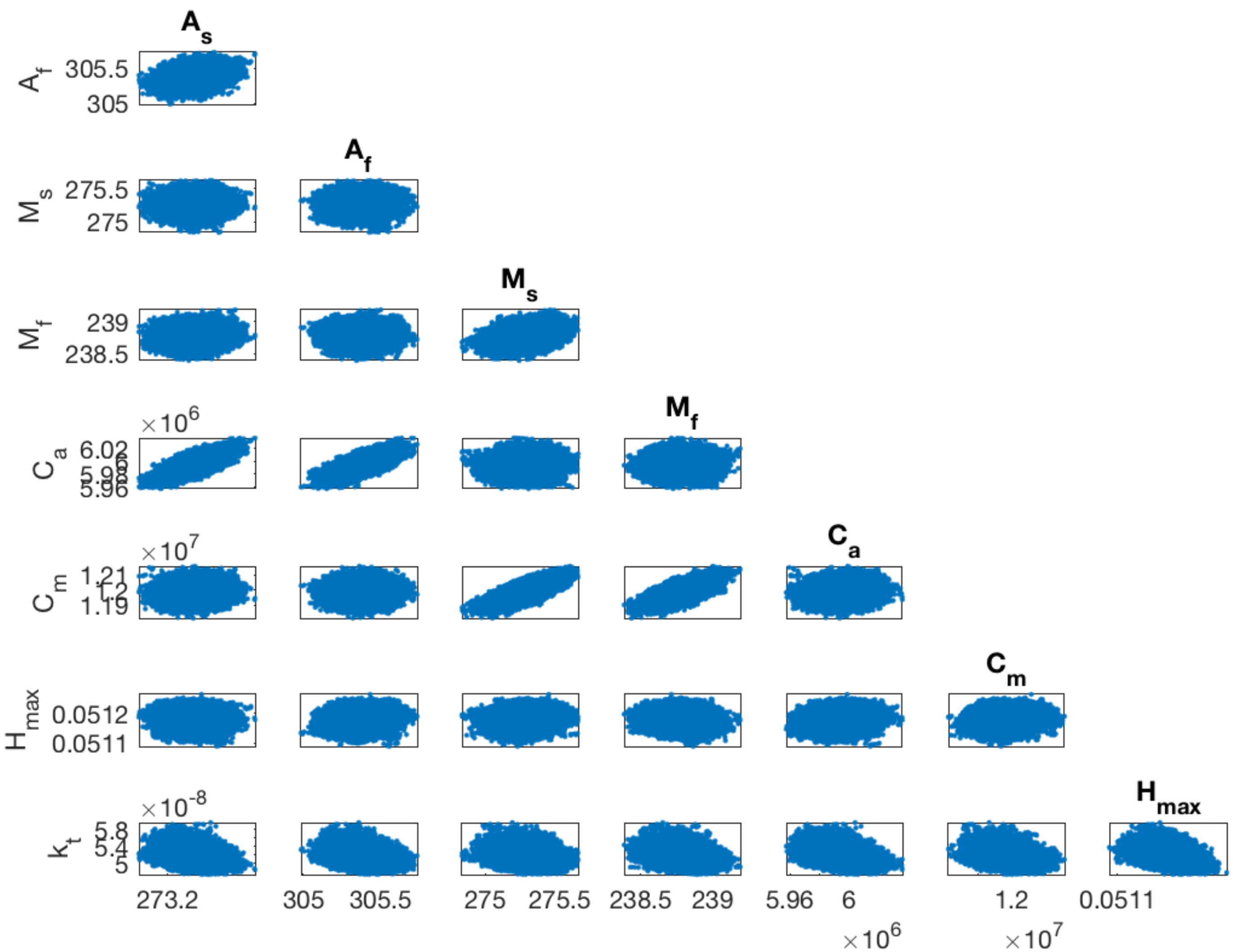




Bayesian Inference for SMA Model

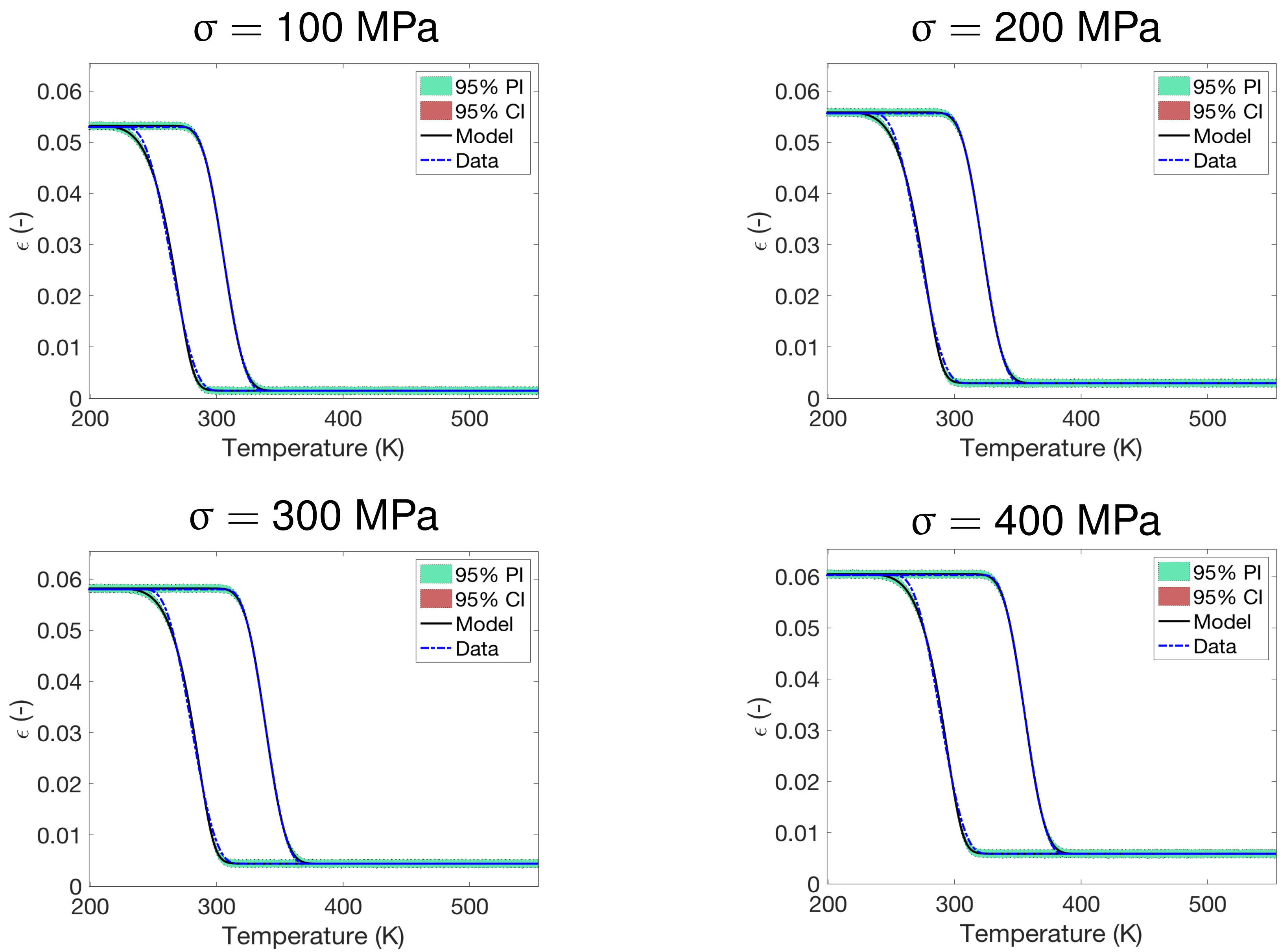
Pairwise Distributions:

- Delayed Rejection Adaptive Metropolis (DRAM) correctly infers correlation structure



Uncertainty Propagation for SMA Model

Uncertainty Propagation: 95% credible and prediction intervals



Broad Control and UQ Objectives

Control Formulation:

$$\frac{dz}{dt} = f(t, z, u, q) + v_1(t)$$

$$y(t, q) = Cz(t, q) + v_2(t)$$

UQ Formulation: e.g., average tip displacement

$$\frac{dz}{dt} = f(t, z, q) + v_1(t)$$

$$y(t) = \int_{\mathbb{R}^{20}} w^N(t, \bar{x}, q)\rho(q)dq$$

Control Objectives:

- Determine optimal q; requires identifiability analysis.
- Construct reduced-order model for state z; e.g., POD, DMD.
- Determine plant error Δ for robust control design.
- Construct state estimator $z_c(t)$.
- Compute feedforward or feedback controls; e.g., $u(t) = -kz_c(t)$.
- Note: Feedback not necessary if no uncertainties!

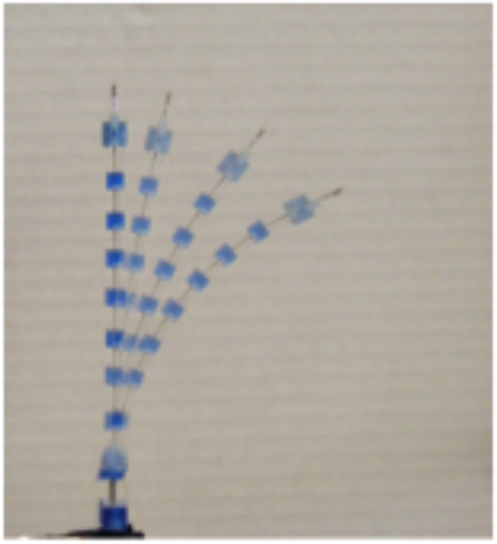
UQ Objectives:

- Determine identifiable parameter subsets or subspace; GSA or active subspace techniques.
- Construct surrogate model; e.g., GP, regression, collocation, POD.
- Infer distributions (Bayesian) or estimators (frequentist) for q or q(x).
- Compute distributions or statistics for QoI. Analytic relations for stochastic Galerkin or collocation for certain distributions; e.g., Gaussian or uniform.

Role of Uncertainty Quantification for Control Design

Strategy:

- Robust control provides control authority in presence of parameter uncertainty and plant disturbances.
- Use Bayesian inference and UQ to quantify uncertainties.

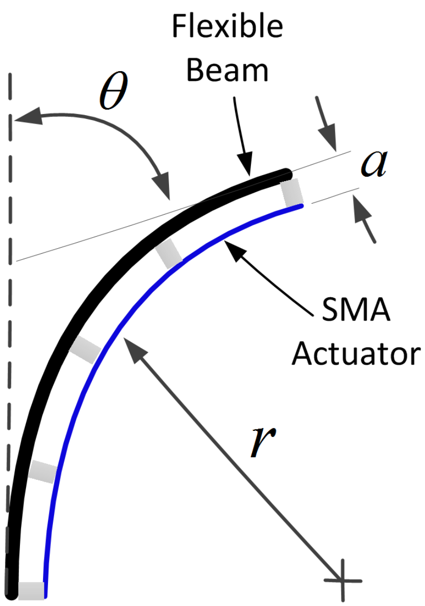


Experimental Device

Example: Robotic SMA catheter actuated by Joule heating

- Bending angle: $\theta(t) = \frac{A_c L}{a}\left[\varepsilon_p - \varepsilon(t)\right]$
- Strain quantified by Homogenized Energy Model (HEM)

$$\varepsilon(t) = \int_0^\infty \int_{-\infty}^\infty \overline{\varepsilon}\left[\sigma(t) + \sigma_I, T(t); \sigma_R\right] \nu_R(\sigma_R)\nu_I(\sigma_I) d\sigma_I d\sigma_R$$

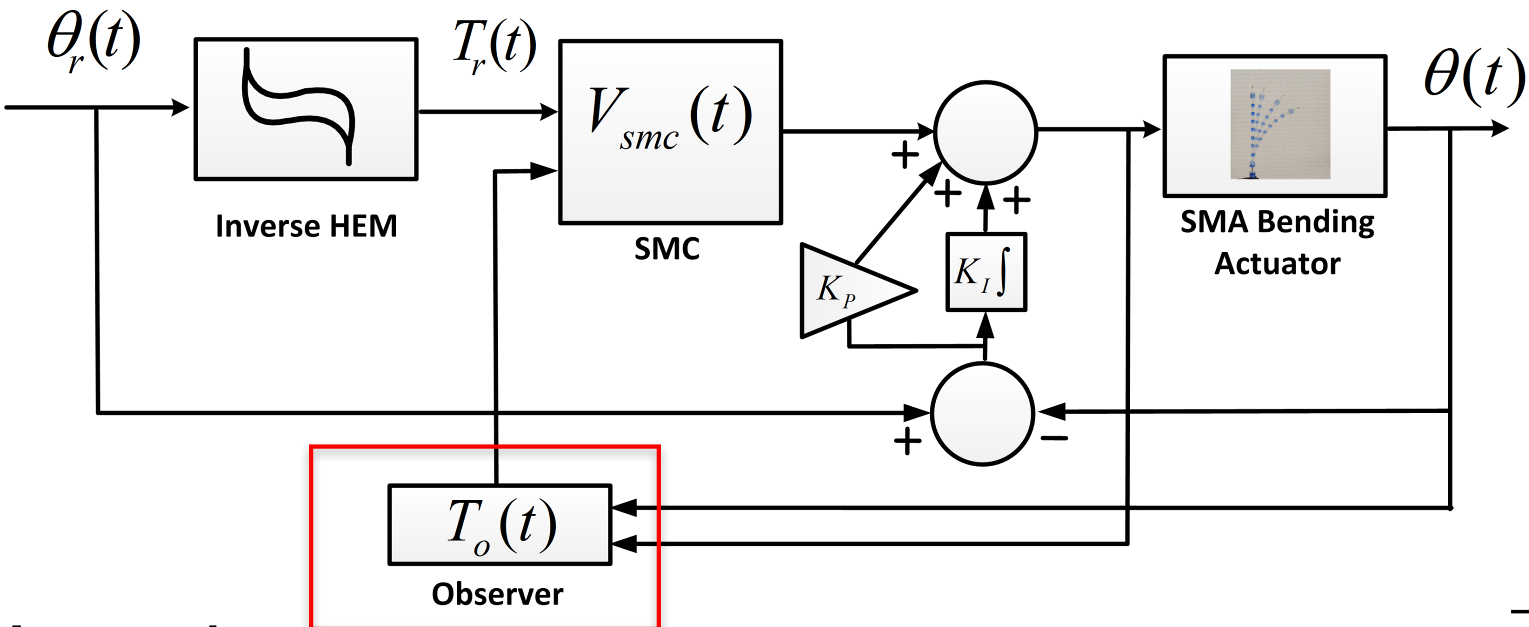


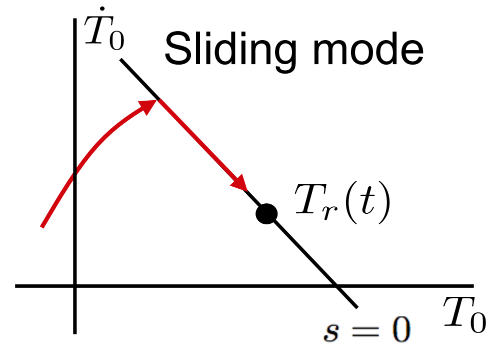
- Heat transfer model

$$\frac{dT}{dt}(t) = -\underline{h}\left[T(t) - T_\infty\right] + \underline{\gamma} u(t) + \underline{H}\left[\frac{dx_{M^+}}{dt}(t) + \frac{dx_{M^-}}{dt}(t)\right]$$

- Control input: Power $u(t)$

Sliding Mode Control Design



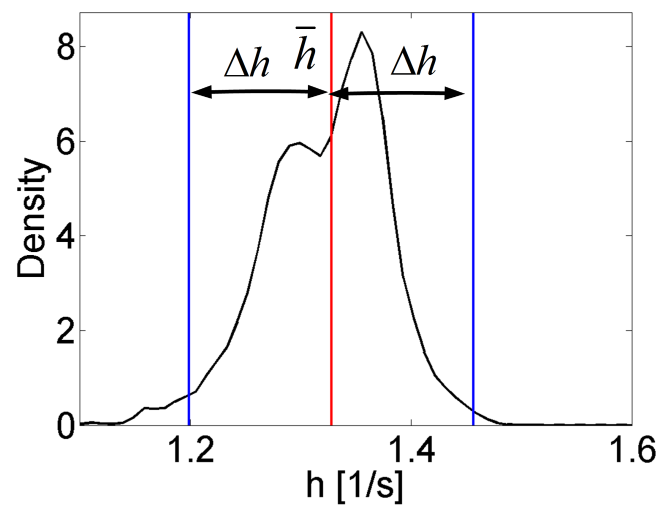


Approach:

- Inverse HEM converts reference bending angle to reference temperature
- Sliding mode controller (SMC) regulates temperature to reference temperature
- Temperature estimated using observer:

$$\frac{dT_0}{dt}(t) = -\underline{h}[T_0(t) - T_\infty] + \underline{\gamma} u(t) + \cdots$$

$$h = \overline{h} + \Delta h \, , \; \gamma = \overline{\gamma} + \Delta\gamma$$

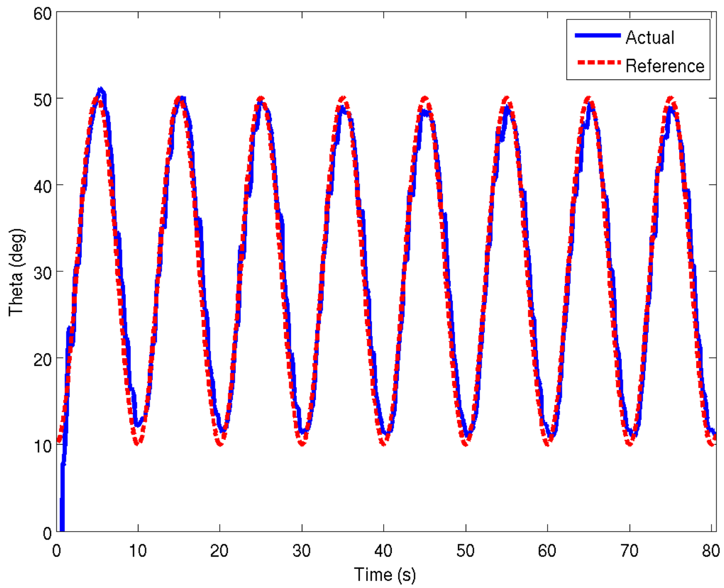


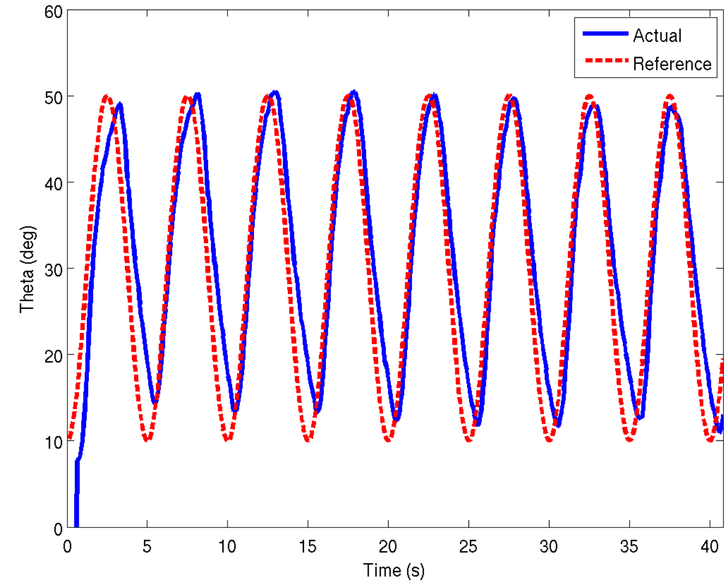
- Control augmented with Proportional-Integral (PI)

Experimental Control Results

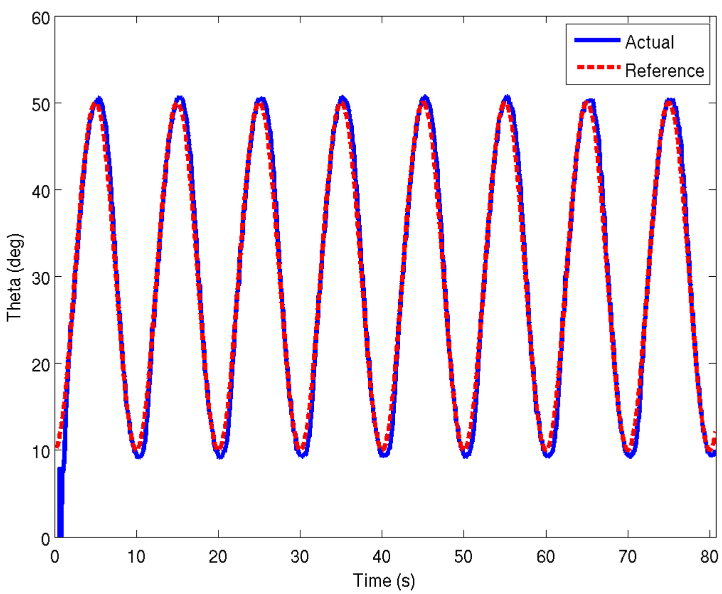
0.1 Hz Sine Wave | 0.2 Hz Sine Wave

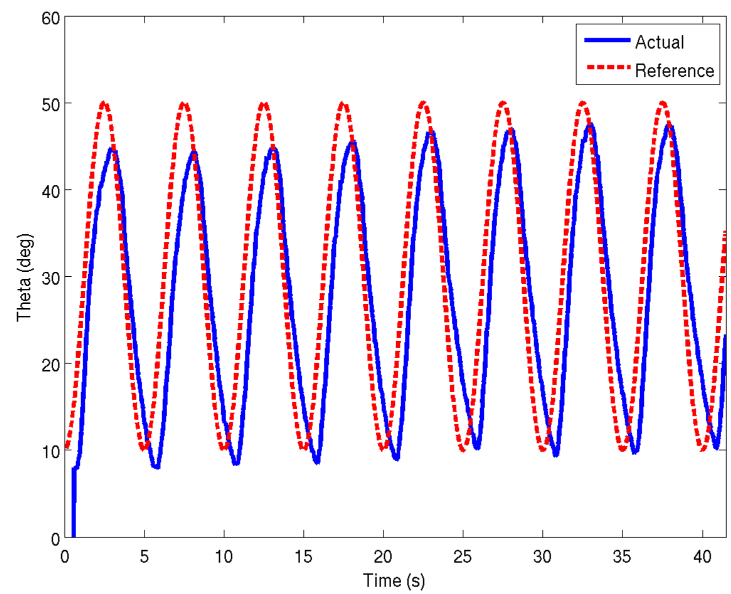
Sliding Mode





PID





Collaborators: John Crews, Jerry McMahan, Jennifer Hannen

Concluding Remarks

Notes:

- UQ requires a synergy between domain science, applied mathematics, and statistics.
- Model calibration, model selection, uncertainty propagation and experimental design natural in a Bayesian framework.
- Goal: Predict model responses with quantified and reduced uncertainties.
- Parameter selection critical to isolate identifiable and influential parameters.
- Surrogate models critical for computationally intensive simulation codes; e.g., essentially all PDE.
- Significant synergies between control theory and Uncertainty Quantification.
- Codes and packages: MATLAB, Python, R, nanoHUB, Sandia Dakota.
- *Prediction is very difficult, especially if it's about the future*. Niels Bohr.