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

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

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

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"We":

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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

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

UQ and SA Issues:

• Is 6th order term required to accurately characterize material behavior?

• Note: Determines molecular structure
Quantum-Informed Continuum Models

Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Landau energy
    \[ \psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6 \]

UQ and SA Issues:

- Is 6\textsuperscript{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

\[ \psi(q) = \psi_\infty(G_e, G_c, \lambda_{\text{max}}) + \gamma(\eta, \beta, \gamma) \]

- Dissipative energy function \( \gamma \)
- Conserved hyperelastic energy function

\[ \psi^N_\infty = \frac{1}{6} G_c I_1 - G_c \lambda_{\text{max}}^2 \ln(3 \lambda_{\text{max}}^2 - I_1) + G_e \sum_j \left( \lambda_j + \frac{1}{\lambda_j} \right) \]

**Parameters:**

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

- \( G_c \): Crosslink network modulus
- \( G_e \): Plateau modulus
- \( \lambda_{\text{max}} \): 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 \( n = \lfloor \alpha \rfloor \). Consider \( \alpha \in [0, 1) \Rightarrow n = 1 \)

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

Issue: Singularity at upper integration limit requires delicate quadrature

- We employ hybrid Gaussian quadrature/analytic Riemann sum approximation

Collaborators: Graham Pash, Paul Miles
Shape Memory Alloy (SMA) Actuators and Sensors

Shape Memory Alloys:

- Catheters for Laser Ablation
- SMA Hinges for Solar Arrays
- Chevrons for Noise Reduction/Fuel efficiency

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

\[
\rho \dddot{\mathbf{u}} = \nabla \cdot \mathbf{\sigma} + \mathbf{F}
\]

\[
\nabla \cdot \mathbf{D} = 0, \quad \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}
\]

\[
\nabla \times \mathbf{E} = 0, \quad \mathbf{E} = -\nabla \varphi
\]

Continuum Energy Relations:

\[
P^\alpha = d_\alpha \mathbf{\sigma} + \chi^\alpha \mathbf{E} + P^\alpha_R
\]

\[
\varepsilon^\alpha = s^E \mathbf{\sigma} + d_\alpha \mathbf{E} + \varepsilon^\alpha_R
\]

Homogenized Energy Model (HEM):

\[
P = d(E, \mathbf{\sigma}) \mathbf{\sigma} + \chi^\mathbf{\sigma} \mathbf{E} + P_{\text{irr}}(E, \mathbf{\sigma})
\]

\[
\varepsilon = s^E \mathbf{\sigma} + d(E, \mathbf{\sigma}) \mathbf{E} + \varepsilon_{\text{irr}}(E, \mathbf{\sigma})
\]
Example: PZT-Based MFC and Robobee

Beam Model: 20 parameters

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

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

Homogenized Energy Model (HEM)

2nd Example: Robobee Drive Mechanism
Multiscale Model Development: Macro-Fiber Composites

**Strong Form:**

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

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

**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:**

\[
y_i = w^N(t_i, q) + \varepsilon_i, \quad i = 1, \ldots, n
\]

**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:
\[
\frac{dz}{dt} = f(t, z, u, q) + v_1(t)
\]
\[
y(t, q) = Cz(t, q) + v_2(t)
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UQ Formulation: e.g., average tip displacement
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\frac{dz}{dt} = f(t, z, q) + v_1(t)
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y(t) = \int_{\mathbb{R}^{20}} w^N(t, \bar{x}, q) \rho(q) dq
\]

Control Objectives:

• Determine optimal q; requires identifiability analysis.

• Construct reduced-order model for state z; e.g., POD, DMD.

• Determine plant error \( \Delta \) 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

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

\[ M = -c_E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} \]

\[ - [k_1 e(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)] \chi_{MFC}(x) \]

Homogenized Energy Model (HEM)

Parameters: \( q = [q_{\text{beam}}, q_{\text{hys}}] \)

- HEM \( q_{\text{hys}} = [P_R^+, \varepsilon_R^+, \varepsilon_R^{90}, \chi^\sigma, d_+, \tilde{\gamma}, \tau_{90}, \tau_{180}, \mu_c, \sigma_c^2, \sigma_l^2] \)

- Beam: \( q_{\text{beam}} = [\bar{\rho}, \bar{\rho}, \bar{c}E I, \bar{c}E I, \bar{c}_D I, \bar{c}_D I, \gamma, k_1, k_2, ] \)

Point Estimates: Ordinary least squares

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

Representative Parameter Values:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_+$ (m/V)</td>
<td>$478.10 \times 10^{-12}$</td>
</tr>
<tr>
<td>$\sigma_l$ (V/m)</td>
<td>$6.47 \times 10^6$</td>
</tr>
<tr>
<td>$\tau_{180}$ (s)</td>
<td>$2.80 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

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)

\[ s_i = E e_i + \varepsilon_i, \quad i = 1, \ldots, N \]
\[ \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \]

Parameter: Stiffness \( E \)

Strategy: Use model fit to data to update prior information

\[
\begin{align*}
\pi_0(E) & \quad \text{Prior Information} \\
\pi(E|s) = e^{-\sum_{i=1}^{N} [s_i - E e_i]^2 / 2\sigma^2} & \quad \text{Updated Information} \\
\end{align*}
\]

Non-normalized Bayes’ Relation:

\[
\pi(E|s) = e^{-\sum_{i=1}^{N} [s_i - E e_i]^2 / 2\sigma^2} \pi_0(E)
\]
Bayesian Inference: Motivation

**Bayes’ Relation:** Specifies posterior in terms of likelihood and prior

\[ \pi(q|\nu) = \frac{\pi(\nu|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\nu|q)\pi_0(q) dq} \]

- **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.

\[ e^{-\sum_{i=1}^{N} [s_i - Ee_i]^2 / 2\sigma^2}, \quad q = E \nu = [s_1, \ldots, s_N] \]
Delayed Rejection Adaptive Metropolis (DRAM)

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

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

2. For $k = 1, \cdots, M$
   (a) Construct candidate $q^* \sim N(q^{k-1}, V)$
   (b) Compute likelihood
      \[ SS_{q^*} = \sum_{i=1}^{N} [u_i - f(t_i, q^*)]^2 \]
      \[ \pi(u|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2} \]
   (c) Accept $q^*$ with probability dictated by likelihood
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**Algorithm:** [Haario et al., 2006] – MATLAB, Python

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Delayed Rejection Adaptive Metropolis (DRAM)

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

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

2. For \( k = 1, \cdots, M \)
   (a) Construct candidate \( q^* \sim N(q^{k-1}, V) \)
   (b) Compute likelihood

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

(c) Accept \( q^* \) with probability dictated by likelihood
Example: Viscoelastic Material Models

**Material Behavior:** Significant rate dependence

**Finite-Deformation Model:** Nonlinear, non-affine

\[
\psi(q) = \psi_{\infty}(G_e, G_c, \lambda_{\text{max}}) + \gamma(\eta, \beta, \gamma)
\]

- Dissipative energy function \(\gamma\)
- Conserved hyperelastic energy function

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

**Parameters:**

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

- \(G_c\): Crosslink network modulus
- \(G_e\): Plateau modulus
- \(\lambda_{\text{max}}\): Max stretch effective affine tube

**[\(\eta, \beta, \gamma]\): Viscoelastic parameters**

**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.

Initial Focus
Viscoelastic Model

Reduced Parameter Set:

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

**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

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

\[
\frac{d\lambda}{dt} = 0.335 \text{ Hz}
\]

\[
\frac{d\lambda}{dt} = 0.67 \text{ Hz}
\]
Prediction Intervals for the Viscoelastic Model

**Linear Non-Affine Model:**

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

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

- \( \frac{d\lambda}{dt} = 0.335 \text{ Hz} \)
- \( \frac{d\lambda}{dt} = 6.7 \times 10^{-5} \text{ Hz} \)
- \( \frac{d\lambda}{dt} = 0.67 \text{ Hz} \)
Prediction Intervals for the Viscoelastic Model

**Linear Viscoelasticity:**

- Fractional-order relation
  \[ Q_{ik} = \eta D_t^\alpha F_{ik} \]
- C – Calibrated
- P - Predicted

**Note:**

\[ \bar{\eta} = 35.3 \]
\[ \bar{\alpha} = 0.12 \]

**Calibrated Rate (1/s):** \( 6.7 \times 10^{-5} \)

**Predicted Rates:**

\[ \frac{d\lambda}{dt} = 6.5 \times 10^{-5} \text{ Hz} \]
\[ \frac{d\lambda}{dt} = 0.0472 \text{ Hz} \]
\[ \frac{d\lambda}{dt} = 0.335 \text{ Hz} \]
\[ \frac{d\lambda}{dt} = 0.67 \text{ Hz} \]

**Collaborators:** Billy Oates, Paul Miles
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

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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**Ramification:** Savings of 10 billion dollars per year for US power plants
Use of Prediction Intervals: Nuclear Power Plant Design

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

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

**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

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

**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:
\[
\frac{dz}{dt} = f(t, z, u, q) + v_1(t)
\]
\[
y(t, q) = Cz(t, q) + v_2(t)
\]

Control Objectives:
- Determine optimal \(q\); requires identifiability analysis.
- Construct reduced-order model for state \(z\); e.g., POD, DMD.
- Determine plant error \(\Delta\) 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 Formulation: e.g., average tip displacement
\[
\frac{dz}{dt} = f(t, z, q) + v_1(t)
\]
\[
y(t) = \int_{\mathbb{R}^n} w^N(t, \bar{x}, q) \rho(q) dq
\]

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

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

\[z(0) = z_0, \quad \frac{dz}{dt}(0) = z_1\]

**Problem:** Parameters \( q = [m, c, k, f_0] \) and \( q = [1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}] \) yield same displacements.
Parameter Selection Techniques

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

Solution: Reformulate problem as

\[ \ddot{z} + C \dot{z} + Kz = F_0 \cos(\omega_F t) \]

\[ z(0) = z_0, \quad \frac{dz}{dt}(0) = z_1 \]

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

\[
\sigma = E e + c \frac{de}{dt}
\]

**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:**

\[
\frac{\partial \sigma}{\partial E} = e = 0.001
\]

\[
\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1
\]

**Conclusion:** Model most sensitive to damping parameter \( c \)
Sensitivity Analysis: Motivation

Example: Linear elastic constitute relation

\[ \sigma = Ee + c \frac{de}{dt} \]

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\[ \frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1 \]

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 constitutive relation

\[ \sigma = E e + c \frac{de}{dt} \]

**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:** \( Y = f(q) \)

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

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

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

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

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

**Sobol’ Indices:**

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

**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 4\(^{th}\) or 6\(^{th}\)-order Landau energy?

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

**Parameters:**

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

**Global Sensitivity Analysis:**

<table>
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**Conclusion:** \(\alpha_{111}\) insignificant and can be fixed
Global Sensitivity Analysis

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**Conclusion:**

\( \alpha_{111} \) insignificant and can be fixed

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

---

![Graphs showing distributions of different parameters](image-url)
Global Sensitivity Analysis

Example: Quantum-informed continuum model

Question: Do we use $4^{th}$ or $6^{th}$-order Landau energy?

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

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Problem:

- Parameters correlated
- Cannot fix $\alpha_{111}$

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.
Global Sensitivity Analysis: Analysis of Variance (ANOVA)

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

**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
One Solution: Parameter Subset Selection

Consider

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

where

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

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

$$
J(q) = \frac{1}{n} \sum_{i=1}^{n} \left[ \nu_i - \psi(P_i, q) \right]^2
$$

$$
\approx \frac{1}{n} \sum_{i=1}^{n} \left[ \nabla_q \psi(P_i, q^*) \cdot \Delta q \right]^2
$$

$$
= \frac{1}{n} (\chi \Delta q)^T (\chi \Delta q)
$$

Note:

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

Sensitivity Matrix:

$$
\chi(q^*) = \begin{bmatrix}
\frac{\partial \psi}{\partial \alpha_1}(P_1, q^*) & \frac{\partial \psi}{\partial \alpha_{11}}(P_1, q^*) \\
\vdots & \vdots & \vdots \\
\frac{\partial \psi}{\partial \alpha_1}(P_n, q^*) & \frac{\partial \psi}{\partial \alpha_{11}}(P_n, q^*)
\end{bmatrix}
$$
One Solution: Parameter Subset Selection

Note:
\[ J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q \]

Strategy: Take \( \Delta q \) to be eigenvector of \( \chi^T \chi \) 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
\[ V = s^2 [\chi^T \chi]^{-1} = \begin{bmatrix}
\text{var}(q_1) & \text{cov}(q_1, q_2) & \cdots & \text{cov}(q_1, q_n) \\
\text{cov}(q_2, q_1) & \text{var}(q_2) & \text{cov}(q_2, q_3) \\
\vdots & & \ddots & \vdots \\
\text{cov}(q_n, q_1) & \cdots & \cdots & \text{var}(q_n)
\end{bmatrix} \]

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 \( \Delta q \) to be eigenvector of \( \chi^T \chi \) Fisher Information

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\( \lambda \approx 0 \Rightarrow \) Perturbations \( J(q^* + \Delta q) \approx 0 \)
\[ \Rightarrow \text{Nonidentifiable} \]

**Example:**

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

Parameters:

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

**Result:** \( \text{rank}(\chi^T \chi) = 3 \) so all parameters identifiable
Parameter Selection for SMA Model

Constitutive Model:

\[ f(\sigma, T, q) = \varepsilon \]

Independent Variables:

- Stress: \( \sigma \)
- 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 \( \varepsilon \)

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

\[ \sigma = 100 \text{ MPa} \]

\[ \sigma = 200 \text{ MPa} \]

\[ \sigma = 300 \text{ MPa} \]

\[ \sigma = 400 \text{ MPa} \]
Broad Control and UQ Objectives

**Control Formulation:**

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

\[
y(t, q) = Cz(t, q) + v_2(t)
\]

**Control Objectives:**

- Determine optimal q; requires identifiability analysis.
- Construct reduced-order model for state z; e.g., POD, DMD.
- Determine plant error \( \Delta \) 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 Formulation:** e.g., average tip displacement

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

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

**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.

Example: Robotic SMA catheter actuated by Joule heating

• Bending angle: $\theta(t) = \frac{A_c L}{a} [\varepsilon_p - \varepsilon(t)]$
• Strain quantified by Homogenized Energy Model (HEM)
  \[\varepsilon(t) = \int_0^\infty \int_{-\infty}^\infty \bar{\varepsilon} [\sigma(t) + \sigma_l, T(t); \sigma_R] \nu_R(\sigma_R) \nu_I(\sigma_I) d\sigma_I d\sigma_R\]
• Heat transfer model
  \[\frac{dT}{dt}(t) = -h [T(t) - T_\infty] + \gamma u(t) + H \left\{ \frac{dx_{M+}}{dt}(t) + \frac{dx_{M-}}{dt}(t) \right\}\]
• 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:
  \[
  \frac{dT_0}{dt}(t) = -h[T_0(t) - T_\infty] + \gamma u(t) + \cdots
  \]
  \[h = \bar{h} + \Delta h, \quad \gamma = \bar{\gamma} + \Delta \gamma\]
- Control augmented with Proportional-Integral (PI)
Experimental Control Results

0.1 Hz Sine Wave

0.2 Hz Sine Wave

Collaborators: John Crews, Jerry McMahan, Jennifer Hannen
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.