Roles of Uncertainty Quantification in Materials Science

Part 2 of 2

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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
Bayesian Model Calibration for Viscoelastic Model

Full Parameter Set:

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

**Note:** Several parameter pairs appear non-identifiable in the sense they are not uniquely determined by the response.
Parameter Selection Techniques

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

Example: Simple harmonic oscillator

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

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

Note: Parameter sets \( q = [m, c, k, f_0] \) and \( q = [1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}] \) yield same states

Solution: Reformulate problem as

\[ \frac{d^2 z}{dt^2} + C \frac{dz}{dt} + K z = F_0 \cos(\omega_F t) \]

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

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

Techniques:

- Linear algebra analysis;
  - e.g., SVD or QR algorithms
- Sensitivity analysis
- Active Subspaces

Second Issue: Nuclear neutronics problems can have 1,000,000 parameters but only 25-50 are influential.
Global Sensitivity Analysis

Example: Portfolio model

\[ Y = c_1 Q_1 + c_2 Q_2 \]

Note:

- \( Q_1 \) and \( Q_2 \) represent hedged portfolios
- \( c_1 \) and \( c_2 \) amounts invested in each portfolio

Take

\[ c_1 = 2, \quad c_2 = 1 \]

\[ Q_1 \sim N(0, \sigma_1^2) \text{ with } \sigma_1 = 1 \]

\[ Q_2 \sim N(0, \sigma_2^2) \text{ with } \sigma_2 = 3 \]

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

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

subject to

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

Then

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

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

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

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

**Variance:**

\[
D_i = \int_0^1 f_i^2(q_i) \, dq_i
\]

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

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

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

**Sobol Indices:**

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

\[
S_{T_i} = S_i + \sum_{j=1}^{p} S_{ij}
\]
Morris Screening

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

Elementary Effect:

$$d_i^j = \frac{f(q^j + \Delta e_i) - f(q^j)}{\Delta}$$

$i^{th}$ parameter, $j^{th}$ sample

$$\Delta \in \left\{ \frac{1}{\ell - 1}, \ldots, 1 - \frac{1}{\ell - 1} \right\}$$

$\ell$ is level

Global Sensitivity Measures: $r$ samples

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

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

SIR Model:

\[
\frac{dS}{dt} = \delta N - \delta S - \gamma k IS, \quad S(0) = S_0
\]

\[
\text{Susceptible}
\]

\[
\frac{dI}{dt} = \gamma k IS - (r + \delta)I, \quad I(0) = I_0
\]

\[
\text{Infectious}
\]

\[
\frac{dR}{dt} = rI - \delta R, \quad R(0) = R_0
\]

\[
\text{Recovered}
\]

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

Assumed Parameter Distribution:

\[
\gamma \sim \mathcal{U}(0, 1), \quad k \sim \text{Beta}(\alpha, \beta), \quad r \sim \mathcal{U}(0, 1), \quad \delta \sim \mathcal{U}(0, 1)
\]

Infection Coefficient \quad Interaction Coefficient \quad Recovery Rate \quad Birth/death Rate

Response:

\[
y = \int_0^5 R(t, q) dt
\]
SIR Disease Example

SIR Model:

\[
\frac{dS}{dt} = \delta N - \delta S - \gamma k IS , \quad S(0) = S_0
\]  
Susceptible

\[
\frac{dI}{dt} = \gamma k IS - (r + \delta)I , \quad I(0) = I_0
\]  
Infectious

\[
\frac{dR}{dt} = r I - \delta R , \quad R(0) = R_0
\]  
Recovered

Typical Realization:
SIR Disease Example

Global Sensitivity Measures:

<table>
<thead>
<tr>
<th>Measure</th>
<th>$\gamma$</th>
<th>$k$</th>
<th>$r$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_i$</td>
<td>0.0997</td>
<td>0.0312</td>
<td>0.7901</td>
<td>0.1750</td>
</tr>
<tr>
<td>$S_{T_i}$</td>
<td>$-0.0637$</td>
<td>$-0.0541$</td>
<td>0.5634</td>
<td>0.2029</td>
</tr>
<tr>
<td>$\mu_i^* \times 10^3$</td>
<td>0.2532</td>
<td>0.2812</td>
<td>2.0184</td>
<td>1.2328</td>
</tr>
<tr>
<td>$\sigma_i \times 10^3$</td>
<td>0.9539</td>
<td>1.6245</td>
<td>6.6748</td>
<td>3.9886</td>
</tr>
</tbody>
</table>

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

Note: Can fix non-influential parameters
Steps in Uncertainty Quantification

Surrogate Models: Similar goals and strategies as used for control implementation
Surrogate Models

**Problem:** Difficult to obtain sufficient number of realizations of discretized PDE models for Bayesian model calibration and uncertainty propagation.

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0
\]
\[
\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho} \nabla p - g \hat{k} - 2\Omega \times v
\]
\[
\rho c_v \frac{\partial T}{\partial t} + p \nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k \nabla T) + \rho \dot{q}(T, p, \rho)
\]
\[
p = \rho RT
\]
\[
\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho) , \ j = 1, 2, 3,
\]
\[
\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho) , \ j = 1, \ldots, J,
\]

**Solution:** Construct surrogate models

- Also termed data-fit models, response surface models, emulators, meta-models
- Projection-based models often called reduced-order models
Surrogate Models: Motivation

**Example:** Consider the model

\[
\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(q)
\]

Boundary Conditions

Initial Conditions

with the response

\[
y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t, x, y, z; q) \, dx \, dy \, dz \, dt
\]

**Notes:**
- Requires approximation of PDE in 3-D
- What would be a simple surrogate?
Surrogate Models

Example: Consider the model

\[
\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(q)
\]

Boundary Conditions

Initial Conditions

with the response

\[
y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t, x, y, z; q) \, dx \, dy \, dz \, dt
\]

Surrogate: Quadratic

\[
y_s(q) = (q - 0.25)^2 + 0.5
\]
Data-Fit Models

Notes:

• Often termed response surface models, emulators, meta-models;
• Rely on interpolation or regression;
• Data can consist of high-fidelity simulations or experiments.
• Common techniques: polynomial models, kriging (Gaussian process regression), stochastic collocation.

Strategy: Consider high fidelity model

\[ y = f(q) \]

with M model evaluations

\[ y_m = f(q^m), \ m = 1, \ldots, M \]

Statistical Model: \( f_s(q) \): Emulator for \( f(q) \)

\[ y_m = f_s(q^m) + \varepsilon_m, \ m = 1, \ldots, M \]
Data-Fit Models – Polynomial Emulator

**Quadratic Emulator:** Regression

\[ f_s(q; \beta) = \beta_0 + \beta_1 q + \beta_2 q^2 \]

**Deterministic System:** \( y_{obs} = X \beta \)

\[
\begin{bmatrix}
  y_1 \\
  \vdots \\
  y_M
\end{bmatrix}
= 
\begin{bmatrix}
  1 & q^1 & (q^1)^2 \\
  \vdots & \vdots & \vdots \\
  1 & q^M & (q^M)^2
\end{bmatrix}
\begin{bmatrix}
  \beta_0 \\
  \beta_1 \\
  \beta_2
\end{bmatrix}
\]

**Least Squares Estimate:**

\[ \beta = [X^T X]^{-1} X^T y_{obs} \]

**Notes:**

- Good choice for optimization;
- Accurate approximation may require high-order polynomials;
- Does not provide uncertainty bounds for uncertainty quantification.
Data-Fit Models – Stochastic Collocation

**Strategy:** Consider high fidelity model

\[ y = f(q) \]

with \( M \) model evaluations

\[ y_m = f(q^m), \ m = 1, \ldots, M \]

**Collocation Surrogate:**

\[ y_s(q) = f_s(q) = \sum_{m=1}^{M} y_m L_m(q) \]

where \( L_m(q) \) is a Lagrange polynomial, which in 1-D is represented by

\[ L_m(q) = \prod_{\substack{j=0 \atop j \neq m}}^{M} \frac{q - q^j}{q^m - q^j} = \frac{(q - q^1) \cdots (q - q^{m-1})(q - q^{m+1}) \cdots (q - q^M)}{(q^m - q^1) \cdots (q^m - q^{m-1})(q^m - q^{m+1}) \cdots (q^m - q^M)} \]

**Note:**

\[ L_m(q^j) = \delta_{jm} = \begin{cases} 0 & , \ j \neq m \\ 1 & , \ j = m \end{cases} \]

**Result:** \( y_s(q^m) = f(q^m) \)

**Note:** Method is nonintrusive and treats code as blackbox.
Surrogate Models – Grid Choice

Example: Consider the Runge function \( f(q) = \frac{1}{1 + 25q^2} \) with points

\[ q^j = -1 + (j - 1) \frac{2}{M_1}, \quad j = 1, \ldots, M_1 + 1 \]
Surrogate Models – Grid Choice

Example: Consider the Runge function \( f(q) = \frac{1}{1 + 25q^2} \) with points

\[ q^j = -1 + (j - 1) \frac{2}{M_1}, \quad j = 1, \ldots, M_1 + 1 \]

\[ q^j = -\cos \frac{\pi(j - 1)}{M_1 - 1}, \quad j = 1, \ldots, M_1 \]
Sparse Grid Techniques

**Tensored Grids:** Exponential growth

**Sparse Grids:** Same accuracy

\[
\begin{array}{c|c|c|c}
 p & R_\ell & \text{Sparse Grid } \mathcal{R} & \text{Tensored Grid } R = (R_\ell)^p \\
\hline
 2 & 9 & 29 & 81 \\
 5 & 9 & 241 & 59,049 \\
10 & 9 & 1581 & > 3 \times 10^9 \\
50 & 9 & 171,901 & > 5 \times 10^{47} \\
100 & 9 & 1,353,801 & > 2 \times 10^{95} \\
\end{array}
\]
Steps in Uncertainty Quantification

Input Representation → Parameter Selection → Model Discrepancy → Model Calibration → Uncertainty Propagation

Local Sensitivity Analysis → Parameter Selection → Model Discrepancy

Global Sensitivity Analysis → Surrogate Models

Sparse Grids → Parameter Selection → Model Calibration

Stochastic Spectral Methods

Sparse Grids
Quantification of Model Discrepancy – Thin Beam

“Essentially all models are wrong, but some are useful” George E.P. Box

Example: Thin beam driven by PZT patches

Euler-Bernoulli Model: For all $\phi \in V$

$$
\int_0^L \left[ \rho(x) \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} \right] \phi dx + \int_0^L \left[ YI(x) \frac{\partial^2 w}{\partial x^2} + cI(x) \frac{\partial^3 w}{\partial x^2 \partial t} \right] \phi'' dx
$$

$$
= k_p V(t) \int_{x_1}^{x_2} \phi'' dx
$$

with

$$
\rho(x) = \rho h b + \rho_p h_p b_p \chi_p(x), \quad YI(x) = YI + Y_p I_p \chi_p(x)
$$

$$
cI(x) = cI + c_p I_p \chi_p(x)
$$

Note: 7 parameters, 32 states

Statistical Model:

$$
Y_i = y(t_i; q) + \delta(t_i) + \varepsilon_i
$$

$$
y(t_i; q) = w(t_i, \bar{x}; q)
$$
Quantification of Model Discrepancy – Thin Beam

**Example:** Good model fit

\[ Y_i = y(t_i; q) + \delta(t_i) + \varepsilon_i \]

**Problem:** Measurement errors not iid

![Residuals vs Time](residuals.png)

![Model Fit to Data](model_fit.png)
Quantification of Model Discrepancy – Thin Beam

**Example:** Good model fit

\[ Y_i = y(t_i; q) + \delta(t_i) + \varepsilon_i \]

**Problem:** Measurement errors not iid

**Result:** Prediction intervals wrong

**Approaches:**
- GP Model: Inaccurate for extrapolation
- Control-based approaches
- Illustrate first for heat example
- Return to beam in a bit
Quantification of Model Discrepancy – Heat Equation

Example: Steady state heat model

\[
\frac{d^2 T_s}{dx^2} = \frac{2(a + b)}{ab} \frac{h}{k} \left[ T_s(x) - T_{amb} \right]
\]

\[
\frac{dT_s}{dx}(0) = \frac{\Phi}{k}, \quad \frac{dT_s}{dx}(L) = \frac{h}{k} \left[ T_{amb} - T_s(L) \right]
\]

Problem: Correlated residuals

Solution: Consider statistical model

\[
Y_i = T_s(x_i; q) + \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i
\]
Example: Steady state heat model

\[
\frac{d^2 T_s}{dx^2} = \frac{2(a+b)}{ab} \frac{h}{k} [T_s(x) - T_{amb}]
\]
\[
\frac{dT_s}{dx}(0) = \frac{\Phi}{k}, \quad \frac{dT_s}{dx}(L) = \frac{h}{k} [T_{amb} - T_s(L)]
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Quantification of Model Discrepancy – Heat Equation

**Example:** Steady state heat model

\[
\frac{d^2 T_s}{dx^2} = \frac{2(a + b)}{ab} \frac{h}{k} [T_s(x) - T_{amb}]
\]

\[
\frac{dT_s}{dx} (0) = \frac{\Phi}{k}, \quad \frac{dT_s}{dx} (L) = \frac{h}{k} [T_{amb} - T_s(L)]
\]

**Issue:** Confounding between physical and phenomenological components

\[ Y_i = T_s(x_i; q) + \delta(x_i) + \varepsilon_i \]

**Example:** Purely phenomenological

\[ Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \beta_4 x_i^4 + \varepsilon_i \]

**Result:** Cannot provide extrapolatory predictions

**Conclusion:** Must incorporate prior information about physical parameters and model discrepancy term.
Quantification of Model Discrepancy – Thin Beam

Partial Solution: “Optimize” calibration interval
• Use damping/frequency domain results to guide.

Note: We have substantially extended calibration regime.
Concluding Remarks

Notes:

• UQ requires a synergy between applied mathematics, statistics, and domain sciences.

• Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.

• Goal is to predict model responses with quantified and reduced uncertainties.

• Parameter selection is critical to isolate identifiable and influential parameters.

• Due to complexity of models, surrogate models are required for many applications.

• Codes and packages: Sandia Dakota, R, MATLAB, Python, nanoHUB

• *Prediction is very difficult, especially if it’s about the future,* Niels Bohr.

• Algorithms and techniques are new and evolving.