Stochastic Multiscale Analysis and Design

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Integrated DEsign Automation Laboratory (IDEAL)

http://ideal.mech.northwestern.edu/
Hierarchical Multiscale Design

Multiscale Design
Concurrent optimization of hierarchical materials and product designs across multiple scales, accounting for the multiscale nature of physical behavior and manufacturing restrictions.

### Bio-Multiscale System for Drug Delivery

- **Drug Molecules, Parylene, Atoms**
- **Drug loaded Nanodiamonds**
- **Integrated drug delivery device**
- **Cell apoptosis**

### Micro-Nano-Composites Structure

- **Nanoparticle Reinforced polymer (matrix/foam)**
- **Microstructure of enhanced fiber-matrix/foam system**
- **Composite structures**
- **Multiscale composite based consumer systems**

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[IDEAL Integrated D'Esign Automation Laboratory]
**Multiscale Micro-Nano-Composites Structure**

**Multiscale Design**

Example: Nano-Composite Aircraft

<table>
<thead>
<tr>
<th>Scale</th>
<th>Design Variables (potential)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 – atomistic</td>
<td>$\beta^4$ Matrix Material Properties</td>
</tr>
<tr>
<td>3 – nano</td>
<td>$\alpha^3$ Nano-particle volume fraction NP particle size distribution</td>
</tr>
<tr>
<td>2 – meso/micro</td>
<td>$\alpha^2$ Composite layer orientation $\beta^2$ Adhesive material properties</td>
</tr>
<tr>
<td>1 – milli</td>
<td>$\alpha^1$ Surface texture</td>
</tr>
<tr>
<td>0 – macro</td>
<td>$\alpha^0$ Wing geometry</td>
</tr>
</tbody>
</table>

**Performance**: Strength, weight, heat conductivity
Uncertainty Sources

**Type I: Parameterizable variability (Aleatory)**
- Uncertainty associated with model parameters, e.g., microstructure, material parameters, loading

**Type II: Unparameterizable variability (Epistemic)**
- Uncertainty due to the inadequate statistical descriptors/parameters, or lack of computing power

**Type III: Model/method errors (Epistemic)**
- Uncertainty caused by lack of knowledge, model simplification/approximation often manifested by homogenization when bridging between scales.
Design under Uncertainty

- Uncertainty Representation
- Efficient Uncertainty Propagation (robustness & reliability Assessments)
- Efficient Probabilistic Optimization
- Quantification of Model Uncertainty (model validation)
Stochastic Multiscale Computational Design Framework

Optimal designs of material and product

Probabilistic Optimization
Robust and reliability-based design, multilevel optimization

Operating conditions
Type I uncertainty

Multiscale design variables
\( \alpha \) and \( \beta \)

\( \alpha \) - Structure
\( \beta \) - Property

Proabilistic performance \( y^\theta \)

Macroscale product model

Multiscale simulations

Product

Type I & II uncertainties

Multiscale experiments

Bias-correlation

Type III Uncertainty
Model uncertainty

Bayesian calibration

Stochastic upscaling

Time

Type IV uncertainties

Multiscale simulations

Material

Stochastic multiscale constitutive relation
\[ \sigma = \sigma(\varepsilon(t), T(t), \theta) \]

Sub-Microscale Model

Microscale Model

Primary particle

Secondary particle

\( \beta_1 \)

\( \beta_2 \)

\( \beta_3 \)

\( \alpha_1 \)

\( \alpha_2 \)

\( \alpha_3 \)
Stochastic Multiscale Analysis and Design Methodology

• Predictive stochastic multiscale analysis
  – *Statistical material characterization*
  – *Stochastic constitutive theory (upscaling)*

• Managing complexity in multiscale design
  – *Multilevel optimization (target cascading)*
  – *Hierarchical statistical cause-effect analysis*

• Quantification of model uncertainty
  – *Combining computer simulations & physical experiments*
Statistical Material Characterization

**MATERIAL STRUCTURE**

- Microstructure
- Processing
- Composition

**MATERIAL PROPERTY**

- Mechanical testing (numerical, experimental)

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1. **SEM Image**
   - Microstructure imaging techniques (SEM, TEM, etc.)

2. **Target**
   - Binary image construction via image processing algorithms

3. **Point correlation**
   - n-point correlation functions (2-point shown)

4. **Reconstruction**
   - Statistically equivalent microstructure reconstruction
   - Accuracy lost with simplified statistical description

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**Constitutive Relationship**

- Work primarily conducted by Y. Liu

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Integrated Design Automation Laboratory
Stochastic Constitutive Theory

For multiscale analysis, deterministic fine scale simulations create randomness

Macroscale, e.g.

Fine resolution statistical volume element realizations

Deterministic homogenization (standard constitutive modeling)

$$\langle S \rangle = f \left( \kappa, \langle \varepsilon \rangle, \langle \dot{\varepsilon} \rangle, \langle T \rangle, t, \ldots, SA \right)$$

Add randomness to constitutive law parameters

$$\langle S \rangle = f \left[ K \left( \omega, \langle \varepsilon \rangle, \langle \dot{\varepsilon} \rangle, \langle T \rangle, t, \ldots, SA \right) \right]$$

Specific form of stochastic constitutive theory

Fit set of phenomenological constitutive law parameters to SVE simulation results

Treat parameters as multivariate statistical distribution whose data are each realization

$$K(\theta) \sim f_K(\kappa, \theta)$$
High strength, porous 4330 steel alloy with microstructure

Random parameters (all follow uniform distribution)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N)</td>
<td>Number of particles</td>
</tr>
<tr>
<td>(D_i)</td>
<td>Void diameter</td>
</tr>
<tr>
<td>(NND)</td>
<td>Nearest neighbor distance</td>
</tr>
<tr>
<td>(X_i, Y_i)</td>
<td>Void center coordinates</td>
</tr>
</tbody>
</table>

Deterministic parameters

- \(BND = 0.06\) minimum distance from void to SVE boundary
- \(l = 1\) SVE simulation domain size

330 SVE simulations (30 minutes apiece)

Phenomenological Constitutive Model – Bamann Chiesa Johnson

\[
\sigma (\kappa, \varepsilon) = \left(1 - \phi\right)\left[\kappa_1 + \kappa_2 \tanh (\kappa_3 \varepsilon)\right]
\]

Damage a quadratic function of effective strain

\[\phi = \phi_0 + \kappa_4 \varepsilon + \kappa_5 \varepsilon^2\]

\[
\sigma [K(\theta), \varepsilon] = \left[1 - \left(\phi_0 + \kappa_4 \varepsilon + \kappa_5 \varepsilon^2\right)\right]\left[\kappa_1 + \kappa_2 \tanh (\kappa_3 \varepsilon)\right]
\]

Via stochastic constitutive theory, the 5 constitutive model parameters are assumed to have some unknown joint distribution.
Capturing Correlations of Coefficients in Stochastic Constitutive Relation

MARGINAL PROBABILITY DISTRIBUTIONS

SELECTED BIVARIATE SCATTER PLOTS

Copula approach (Schweizer and Wolff, 1981) links arbitrary marginal CDFs to multivariate dependence structures through correlation measure that depends on the copula type.

Polynomial chaos for non-Gaussian processes used to quantify joint statistical distribution
Copula method better captures the constitutive behavior observed in the sample of SVE simulations.

PCE method provides a highly conservative estimate on the upper bound of constitutive behavior.

Stochastic Multiscale Analysis and Design Methodology

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  – *Stochastic constitutive theory (upscaling)*

• Managing complexity in multiscale design
  – *Multilevel optimization (target cascading)*
  – *Hierarchical statistical cause-effect analysis*

• Quantification of model uncertainty
  – *Combining computer simulations & physical experiments*
Multi-level optimization is used for designing multiscale systems across various scales and disciplines.

- **Cascading targets** to lower level
- **Convergence** of targets and response is achieved at the end of the process

- Analytical Target Cascading (ATC) \((Kim\ et.\ al.,\ 2003)\)
- Probabilistic ATC (PATC) \((Kokkolaras\ et\ al.\ 2004;\ Liu\ et\ al.\ 2005)\)
- PATC with correlated subsystems \((Xiong\ et\ al.\ 2009)\)
Example - Multiscale Bracket Design

**Multiscale Design Solutions**

$S_c$ (GPa)

- 0.258
- 0.260
- 0.265
- 0.269
- 0.270

**Material microstructure solutions** ($PVF_3, N_3$)

- 0.0300, 3.0000
- 0.0343, 3.0000
- 0.0300, 3.8098
- 0.0300, 3.8163
- 0.0300, 3.0000
- 0.0418, 4.0944
- 0.0500, 4.9826
- 0.0300, 3.7667
- 0.0300, 3.7787
- 0.0300, 3.8429
- 0.0524, 5.0095
- 0.0300, 3.7285
- 0.0300, 3.8964
- 0.0300, 3.7297
- 0.0789, 3.0000
- 0.1095, 6.0229
- 0.0300, 4.0143
- 0.0435, 4.8733
- 0.0632, 3.0000
- 0.0705, 4.1363
- 0.0832, 5.2942
- 0.0986, 5.5558
- 0.0478, 7.0000

- **Unique solutions for small $S_c$; Multiple solutions of material microstructure for large $S_c$**
- **New aluminum alloy achieves reduction of stress concentrations by re-distribution of loads after yielding in the plastic range**
Hierarchical Statistical Sensitivity Analysis (HSSA) Method

Features:

(1) SSA is applied to submodels at each level with top-down sequence;

(2) The global Statistical Sensitivity Index (SSI) are aggregated from the local SSA at each level.

(3) Aggregation formulation considers submodel dependencies

HSSA Results


\[ \text{SSI}_R + \text{SSI}_{PVF} > 0.75 \]
Predictive Science (PS) - the application of verified and validated computational simulations to predict the response of complex systems, particularly in cases where routine experimental tests are not feasible.

Engineering Design (ED) - the process of devising a system, component or process to meet desired needs.

Certificate Requirements: 3 core courses + 2 electives

- Modeling, Simulation, and Computing
- Computational Design
- PS&ED 510 Seminar

http://psed.tech.northwestern.edu/
RESEARCH OBJECTIVE

Integrate contemporary materials and structure analysis & design principles to create products with better functionality as passive energy dissipation devices. Through exploring the codependent physics in the material (nano, micro) and continuum (meso, macro) domains, automated design techniques utilize experimental data, structural concepts, and atomistic and continuum simulations to consider mutual design issues across disparate scales in length and time. The end mission of the project is to use the integrated design approach to unlock new devices for earthquake protection, with a specific focus on historic buildings.

BENCHMARK PROBLEM

- Preliminary material and structural design of slit steel damper
- Optimal combination of material & geometry sought
- Dissipation occurs through metal yielding
- Material/structure integration through constitutive relationship

Class of secondary hardened Martensitic steel is considered to exploit transformation plasticity. Materials design provides optimal constitutive relationship for energy dissipation.
RESEARCH OBJECTIVE

The rapid development of industry in recent decades greatly raises the demand of high-performance structural materials to survive severe mechanical loadings. Our objective is to provide some insight to materials behavior of Metal Polymer laminates composites, and come up with novel designs. With impact resistance improved and other advantages maintained, such designed materials will have a broad spectrum of applications, including aircrafts, automobiles, armors, electronic devices and helmets.

MATERIAL SELECTION

The properties of composites significantly depend on their constitutive components. To obtain some insight from existing MPLCs, we need to relate their general properties to materials selection. Based on the desirable performance, we will make a list of primary and secondary properties taken into account with comprehensive consideration. We will follow the ideas from Ashby and use CES EduPack.

FUNCTION-ORIENTED OPTIMIZATION

Divide the structure into functional layers

Concept design of each layer

Adjust ratio of each functional layer

- Shielding layer
- Supporting layer
- Anti-trauma layer
Stochastic Multiscale Analysis and Design Methodology

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  – Stochastic constitutive theory (upscaling)

• Managing complexity in multiscale design
  – Multilevel optimization (target cascading)
  – Hierarchical statistical cause-effect analysis

• Quantification of model uncertainty
  – Combining computer simulations & physical experiments
Model Updating and Uncertainty Quantification

Model Refinement

Computer Model \( y^m(x, \theta) \)

Additional Sampling

Computer Simulations \( y^m(x^m, \theta^m) \)

Physical Experiments \( y^e(x^e) \)

Model Updating (calibration and bias-correction)

Validation

Satisfying?

Not Satisfied

Additional Sampling

Satisfied

Prediction within intended region

Updated model for design

Bias Correction and Calibration

\[ y^e(x) = y^m(x, \theta) + \delta(x) + \epsilon \]

Variable Inputs \hspace{1cm} Computer Model \hspace{1cm} Experimental Error

Experimental Prediction \hspace{1cm} Unknown Parameters \hspace{1cm} Bias Correction Function

Kennedy and O'Hagan (2001)
Gaussian Processes (GP) for Lack of Data

- Representation assuming the function is a multivariate normal distribution
- Reflects uncertainty between sample points
- Written as:

\[ f(x) \sim \mathcal{GP}(m(x), K(x, x')) \]

Mean of the Gaussian process

\[ m(x) = h(x)\beta \]

\( \beta \): Parameters for polynomial regression of the mean

\( h(x) \): Polynomials used to represent the mean

Covariance function of the Gaussian process

\[ K(x, x') = r(x - x') \]

\[ r(x - x') = \sigma^2 \exp\left(- \sum_{i=1}^{d} \omega_i (x - x')^2\right) \]

Correlation of the distance between two points, \( x \) and \( x' \)

Hyperparameters

\[ \beta, \sigma^2, \omega \]
Modular Bayesian Approach

- Computer simulations \( y^m \)
- Physical experiments \( y^e \)

**Model Updating**
- Estimation of hyperparameters of GP
- Posterior distributions of calibration parameters

**Updated Model**
- Distributions for prediction based on posterior and GP model

\[
y^m(x^m, \theta^m) \rightarrow \hat{\beta}_1, \hat{\sigma}_1, \hat{\omega}_1 \rightarrow \hat{y}^m(x, \theta) \rightarrow \text{GP} \rightarrow \hat{\beta}_2, \hat{\sigma}_2, \hat{\omega}_2 \rightarrow \hat{\delta}(x) \rightarrow \hat{\lambda} \rightarrow \hat{\epsilon} \rightarrow y^e(x^e)
\]

Bayes Theorem

\[
p(\theta | \hat{\omega}, \hat{\beta}, \hat{\sigma}, \hat{y}^m, \hat{y}^e)
\]

**Responses:**
- Random

\[
y^e(x^e) = \hat{y}^m(x, \theta) + \hat{\delta}(x) + \hat{\epsilon}
\]

Blast Resistant Fiber Reinforced Plastic (FRP) Sandwich

Experiment Setup
- Flyer plate thickness and velocity, and time
- Gas gun
- Shock frame
- Projectile
- Specimen

FE Model
- Specimen Damage Maps

Displacement
- $u^m = y^m(x, \theta)$
- $u^e = y^e(x)$

Assume well calibrated model

Collaboration with Prof. H. Espinosa

Figures provided by Ravi Bellur Ramaswamy

Time (µs)
- 0
- 100
- 200
- 300
- 400
- 500

Deflection (mm)
- 0
- 2
- 4
- 6
- 8
- 10
- 12
- 14
- 16

- 3150 Pa/s experimental
- 1500 Pa/s experimental
- 3150 Pa/s
- 1500 Pa/s
Nanodiamond (ND) Drug Delivery System

\[
\theta
\]
(unknown but fixed inputs)

% of Atoms on Surface of ND for Drug Attachment

\[
x
\]
(known inputs)

pH

MD Simulations

Collaboration with Prof. W. K. Liu and Prof. D. Ho
Incremental Forming Process

Experiments

Simulations

\[ \Delta z \] (known inputs)

\[ \theta \] (unknown but fixed inputs)

\( m \) – damage \( \beta \) – weakening evolution parameter

Fracture Depth

Collaboration with Prof. Jian Cao
Observations

1. Model calibration/updating insights into the computer model
   - Discrepancy function – capture missing physics
   - Calibration parameters – accurate identification is needed to be used in larger simulation system

2. Implementation of modular Bayesian process suffered from:
   - Computationally expensive posterior distribution
   - Confounding between calibration parameters
   - Confounding between bias function and calibration parameters
Identifiability (Lancaster 2004)

A System is not identifiable if different values of the model parameters are equally probable

\[ y^e(x) = y^m(x, \theta) + \delta(x) + \varepsilon \]

Two equally plausible solutions for \( \theta \) and bias function
Multi-Response Gaussian Process (MR GP)

\[ \text{vec}(y(x)) \sim \text{GP}(\text{vec}(H\beta), \Sigma \otimes R(x,x)) \]

Define MR GP for computer simulations and bias function

\[
\begin{align*}
\text{vec}(y^m(x,\theta)) & \sim \text{GP}(\text{vec}(H_1(x,\theta)\beta_1), \Sigma_1 \otimes C_1 \{(x,\theta),(x,\theta)\}) \\
\text{vec}(\delta(x)) & \sim \text{GP}(\text{vec}(H_2(x)\beta_2), \Sigma_2 \otimes C_2 \{x,x\})
\end{align*}
\]

MR GP Based on Conti and O’Hagan (2010)
**Simply Supported Beam Example**

**Objective:** Find Young’s modulus ($\theta$) and missing physics of the physical experiments

**Problem:** Identifiability

---

**Inputs**
- $x$: Force
- $\theta$: Young’s Modulus

**Computer Simulations**
- FEA with simplified material model

**Physical Experiments**
- FEA with elaborate material model

**Responses used for calibration**
- $y^m(x, \theta)$: Computer simulations
- $y^e(x)$: Physical Experiments

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**Cross Section of Beam**

**Objective:** Find Young’s modulus ($\theta$) and missing physics of the physical experiments

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Simply Supported Beam Calibration

\[ y_1: \text{ Angle of deflection at the end of the beam (radians)} \]
\[ y_2: \text{ Internal energy (Joules)} \]

- **Single Response** \((y_1)\): Angle of deflection at the end of the beam (radians)
- **Single Response** \((y_2)\): Internal energy (Joules)
- **Multiple Responses** \((y_1 \text{ and } y_2)\)

Note experimental prediction is not shown because it is accurate in all cases for the amount of experimental data used.
Calibration with Different Responses

\(y_3\): Total strain at the midpoint of the beam (mm)

\(y_4\): Plastic strain at the midpoint of the beam (mm)

- True Bias Function
- Pred. Mean of Bias Function
- 95 % CI

**Single Response (\(y_3\))**

**Single Response (\(y_4\))**

**Multiple Responses (\(y_3\) and \(y_4\))**

\[ \delta_3(x) \]

\[ \delta_4(x) \]

\[ \delta_3(x) \]

\[ \delta_4(x) \]

\[ \theta (\text{GPa}) \]

\[ \theta (\text{GPa}) \]

\[ \theta (\text{GPa}) \]

- True Cal. Parameter
- Posterior PDF
Benefits of Designed Experiments for Calibration

Computer Model:
\[ y_i^m(x, \theta) = \sin(\theta x) \]
\( \theta \in [1, 4] \quad x \in [0, \pi] \)

Experimental Function:
\[ y_i^e(x) = \sin(\theta_{\text{true}} x) + 0.1e^x - 0.05x^2 + \varepsilon_i \]
\( \varepsilon_i \sim N(0, \lambda I) \quad \theta_{\text{true}} = 3.1 \quad \lambda = 0 \)

Initial Data Set

Add \( x = 2.75 \)

Add \( x = 0.5 \)

Experimental Prediction

Bias Function

Posterior \( \theta \)
Closure – Research Challenges

• **Stochastic multiscale analysis**
  • How to identify critical macroscopic property/performance that are sensitive to microscopic variability – value of information, resource allocation in uncertainty management.
  • We don’t know what is critical until we model it correctly
  • Capture the right correlation (space, time) to gain the usefulness of data

• **Stochastic multiscale design**
  • How to efficiently build constitutive relations for a range of design
  • Concurrent topology and material design

• **Quantification of model uncertainty**
  • Criterion for identifiability prior to experiments
  • Design of experiments for improved identifiability

Acknowledgement: NSF grants CMMI-0928320, CMMI-0758557, and Goodyear Tire Company