Treating Modeling Uncertainty in Multiscale Methods.

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Workshop on Uncertainty Quantification for Multiscale Stochastic Systems and Applications
1 Motivation

2 Multiscale Material Models

3 Multiscale UltraDeep Sea Drilling

4 Conclusions
Acknowledgment

- Jianyu Li (Tianjin University)
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Outline

1 Motivation

2 Multiscale Material Models

3 Multiscale UltraDeep Sea Drilling

4 Conclusions
Motivation

Error Budget

\[ U = \hat{U}_{h,d,p,m} + \left( \epsilon_{h|d,p,m} + \epsilon_{p|d,m} + \epsilon_{d|m} + \epsilon_{m} \right) \]

Limits on Predictability: Must be quantified

- \( \epsilon_{h|d,p,m} \): can be reduced through better numerics.
- \( \epsilon_{p|d,m} \): can be reduced through better statistics.
- \( \epsilon_{d|m} \): can be reduced through better data.
- \( \epsilon_{m} \): can be reduced through better models.
Observations from elementary statistics

CLT: average out the noise

- $X \sim \chi^2_d$

$$X = \sum_{i=1}^{d} \xi_i^2, \quad \xi_i \sim N(0, 1)$$

- $T \sim t_d$

$$T = \frac{1}{d} \sum_{i=1}^{d} \xi_i, \quad \xi_i \sim N(0, 1)$$

Reverse-engineer CLT:
Features matter: away from mean-field theories

Given coarse observable, construct a functional model from the finer scales:

$$X = f(\xi_1, \ldots, \xi_d) = f(\xi)$$
Rethink Data, Models and Risks

Models: Degrees of freedom back in fashion.
Reverse perspectives on Central Limit Theorems:

\[ X \stackrel{\Leftarrow}{\longrightarrow} \{\xi\} \quad T \stackrel{\Leftarrow}{\longrightarrow} \{\xi\} \]

Given observations and physics, find the statistical DOF.

Polynomial Chaos
First: decide/identify the root cause of uncertainty.
Second: relate everything to this root cause.

Risk
Is dynamic, function of data, and mathematical and statistical models.
Rethink Data, Models and Risks

**Models:** Degrees of freedom back in fashion.

Reverse perspectives on Central Limit Theorems:

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Motivation

Probabilistic Models

Construct Probabilistic Models

- Assume some model for the measure of $K$, parameterized by $\omega$:
  \[ f_K(k; \omega) \]

- Invoke enough constraints from data to evaluate $\omega$.
  - Kernel density estimation
  - Maximum Likelihood
  - Moment matching
  - Maximum Entropy
  - Bayes rule

Common Approach; constraints from data
Ignores additional knowledge (from physics?) about $K$. 
Motivation

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Ignores additional knowledge (from physics?) about $K$. 
Probabilistic Models

I/O models with random dynamics

$K$ is a function of fine scale behavior, which could be characterized, independently, through experiments.

Postulate dependence of $K$ on fine scale random parameters:

$$K = f(\xi_1, \cdots, \xi_d)$$

We embed ourselves in a $d$-dimensional space.

- The functional form of $f$ must be estimated from observations of $K$.
- Joint probability measure of $\xi$ must be estimated.
- We have accomplished a hierarchical decomposition.
Probabilistic Models

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Polynomial Chaos

Blame uncertainty in $\alpha$ on $\xi$:

$$\alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_i(x) \Psi_i(\xi(\omega))$$
Polynomial Chaos

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Motivation

Polynomial Chaos

Blame uncertainty in $\alpha$ on $\xi$:

$$\alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_i(x) \psi_i(\xi(\omega))$$

CONSTRAINTS

$\{\alpha_i\}$

DATA

PHYSICS

MATH

FIRST PRINCIPLES

$\xi_1$

$\xi_2$

$\cdots$

$\xi_d$

$\alpha(\xi_1, \cdots, \xi_d)$
Blame uncertainty in $\alpha$ on $\xi$:

$$\alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_i(x) \psi_i(\xi(\omega))$$
Motivation

Polynomial Chaos

Blame uncertainty in $\alpha$ on $\xi$ and $\eta$:

$$
\alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_i(x, \eta) \psi_i(\xi) 
$$

Constraints

Data
Physics
Math
First Principles

$\xi_1$
$\xi_2$
$\vdots$
$\xi_d$

$\{\alpha_i\}$

$\alpha(\xi_1, \cdots, \xi_d)$
Polynomial Chaos

Blame uncertainty in $\alpha$ on $\xi$ and $\eta$:

$$\alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_{ij}(x) \psi_i(\xi(\omega)) \psi_j(\eta(\omega))$$
**Versatile Representations:**

By changing

- dimension
- order
- coefficient values

can come very close to any probability measure.

**Stable representations:**

Continuous dependence on parameters
Coupled Systems

PDF at Interfaces

\[ Q(f_1, f_2, f_3) \]
Coupled Systems

PCE at Interfaces

![Diagram showing coupled systems with variables and relationships]

WHITE NOISES:
SUBSCALE VARIABILITY
+ MODEL/INFORMATION UNCERTAINTY
Motivation

Coupled Systems

Updating Probabilistic Models of Subsystems

WHITE NOISES:
SUBSCALE VARIABILITY
+
MODEL/INFORMATION UNCERTAINTY
Coupled Systems

Updating Probabilistic Models of QoI

\[ Q(\xi, \eta, \zeta) \]

WHITE NOISES:
SUBSCALE VARIABILITY
+
MODEL/INFORMATION UNCERTAINTY

\( X_1(\xi) \)
\( X_2(\xi) \)
\( X_3(\eta, \xi) \)

\( \xi \quad \eta \quad \zeta \)
Polynomial Chaos

\[ \alpha(x, \omega) = \sum_{i=0}^{\infty} \alpha_i(x) \Psi_i(\xi(\omega)) \]

Note
- Must estimate \( \alpha_i \) constrained by information:
  - experimental constraints:
    - \( \xi \) captures endogenous sources of uncertainty.
  - physics constraints:
    - \( \alpha \) depends on \( \xi \) through a conservation law that must be honored.
- Dimension of \( \xi \) reflects complexity of the process \( \alpha \).
- Probability measure of \( \xi \) determines the geometry in which analysis and approximation are carried out.
We embed the problem in a high-dimensional space

Mean field approaches:
First order approximations smears out fluctuations.
Sacrificing reality for simplicity.

Modern approaches
Consistent with modern sensors and computers.
Challenges are computational, mathematical, and logical.
Outline

1. Motivation
2. Multiscale Material Models
3. Multiscale UltraDeep Sea Drilling
4. Conclusions
Multiscale Material Models

Lightweight Vehicle

Design of Composite Car

Figure 1. Schematic of manufacturing steps for common LCM processes (a) Resin Transfer Molding (RTM) (b) RTM Light (c) Vacuum Assisted Resin Transfer Molding (VARTM) and (d) membrane VARTM.

Figure 2. Racetracking as observed experimentally. The infused box images are assembled from experimental videos of individual sides. Resin "races" through channels formed in sharp corners by gaps between reinforcement and mold.

Figure 7. Unit cell RVE model of interlaced yarns in the woven fabric composite with (a) geometric characteristic parameters (b) 3D RVE model for permeability calculations.
Multiple Scales

- Macro scale Simulator (LS-DYNA)
- Micro scale Simulator (MDS)
- Manufacturing Simulator (PAM-DISTORTION)
- Manufacturing Simulator (PAM-RTM)

Boundary Conditions

Update

Structural Tests

Micro Tests

RTM Tests

\[ Q(p, \theta) \]
Multiscale Material Models

Multiple Scales

\[ \theta^c \]

Macro scale Simulator (LS-DYNA)

Boundary Conditions

Update

Structural Tests

Cross-scale Updates

Micro Tests

RTM Tests

Manufacturing Simulator (PAM-DISTORTION)

Upscale \( p^c \)

Manufacturing Simulator (PAM-RTM)

Upscale \( p^f \)

Micro scale Simulator (MDS)

Upscale \( p^m \)

Upstream

\[ Q(p, \theta) \]
Multiscale Material Models

Multiple Scales

Macro scale Simulator (LS-DYNA) → $Q(p, \theta)$

Micro scale Simulator (MDS) → $p^c$

Manufacturing Simulator (PAM-RTM) → $p^m$

Update

Structural Tests

Manufacturing Simulator (PAM-DISTORTION)

Boundary Conditions

Cross-scale Updates

Fiber tow width in Material 4A

Fiber tow thickness in Material 4A

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Multiple Scales

- Fibers and resin in tow
- Tows and resin in lamina
- 8 layers of laminae in laminate
- Upscaling
- Homogenized tow
- Homogenized lamina
- Homogenized laminate

Mathematical expressions:
- $S_a = D_a + d_a$
- $S_b = D_b + d_b$
- $D_f$
- $D_a$
- $D_b$
- $d_a$
- $d_b$
- $D_{fa}$
- $D_{fb}$

R. Ghanem (USC)
Multiple Scales

\[ \xi^0 = f^1(\xi^0) \]

\[ \xi^n = (\xi^{n-1}, p^n) \]
Multiple Scales

\[ \xi^0 \]

FINEST SCALE DETAIL

\[ \xi^0 = f^1(\xi^0) \]

COARSE SCALE PROPERTIES

\[ \xi^n = (\Pi_n \xi^{n-1}, p^n) \]

PROJECTED UPSCALED DETAIL

\[ \xi^n = f^{n+1}(\hat{\xi}^n) \]

COARSE SCALE PROPERTIES

\[ \xi^n = (\Pi_n \xi^{n-1}, p^n) \]

UPSACLING

\[ \Pi_n \xi^{n-1} \]

\[ \xi^{n+1} \]

\[ p^n \]

\[ f^{n+1} \]

\[ \hat{\xi}^n \]

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Multiscale Material Models

Multiple Scales

\[ \xi^0 \]

FINEST SCALE DETAIL

\[ \xi^n = f^n(\xi^0) \]

COARSE SCALE PROPERTIES

\[ \xi^n = (\Pi^n \zeta^{n-1}, p^n) \]

PROJECTED UPSCALED DETAIL

\[ \zeta^n = f^{n+1}(\xi^n) \]

COARSE SCALE PROPERTIES

\[ S_b = D_b + d_b \]

\[ S_a = D_a + d_a \]

\[ D_a = 3.47 \quad 0.74 \quad 6.2 \quad 45.4\% \]

\[ d_a = 0.505 \quad 0.01 \quad 1.0 \quad 56.6\% \]

\[ D_b = 0.27 \quad 0.12 \quad 0.42 \quad 32.1\% \]
Multiscale Material Models

PC of coarse scale in terms of fine scale

- Parameter Gyz, PC order = 2
  - SGC level 1
  - SGC level 2
  - SGC level 3

- Parameter Gyz, PC order = 3
  - SGC level 1
  - SGC level 2
  - SGC level 3

- Parameter Gyz, PC order = 4
  - SGC level 1
  - SGC level 2
  - SGC level 3

- Parameter Gyz, PC order = 5
  - SGC level 1
  - SGC level 2
  - SGC level 3
PC of coarse scale in terms of fine scale
Example of upscaling the elasticity matrix of the laminate.
Uncertainty in material processing stage (RTM)

Uncertainty propagation in 13D

Uncertainty in \((K_1^{(0)}, K_2^{(0)}, K_3^{(0)}, K_{cha}^{(0)}, \phi, T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8)\).
Results

Figure: pdf of the fill time.

- 1D Adaptation
- 2D Adaptation
Adaptation: $\eta = A\xi$

- Numerical RTM model (PAM-RTM) evaluated 57 times; Gaussian part computation (27 times) + 1D adaptation computation (9 times) + 2D adaptation computation (21 times)
- Dominant $\eta$ direction is

$$\eta(\xi) = -0.95226259 \, K_1^{(0)}(\xi_1) - 0.21606623 \, K_2^{(0)}(\xi_2) - 0.00269772 \, K_3^{(0)}(\xi_3) - 0.00377367 \, K_{cha}^{(0)}(\xi_4) - 0.00640321 \, \phi(\xi_5) - 0.00641398 \, T_1(\xi_6) - 0.02025733 \, T_2(\xi_7) - 0.02158714 \, T_3(\xi_8) + 0.04207637 \, T_4(\xi_9) - 0.04635585 \, T_5(\xi_{10}) + 0.0593152 \, T_6(\xi_{11}) + 0.06031331 \, T_7(\xi_{12}) - 0.18562338 \, T_8(\xi_{13})$$
**Figure:** Realizations of the pressure at the sensors.
Adapted Bases: $\eta = A\xi$
Leveraging structure in high-dimensional geometry

**Fill time of resin transfer molding**

<table>
<thead>
<tr>
<th>Method</th>
<th>Number of function evaluations</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Monte Carlo</td>
<td>Computationally prohibitive</td>
<td>PDF, not functional map.</td>
</tr>
<tr>
<td>2 PCE with quadrature</td>
<td>$n^d(2^{18})$</td>
<td>Functional map from input to output.</td>
</tr>
<tr>
<td>3 PCE with Sparse Grid</td>
<td>$&lt; n^d$ (10,597 for level 3)</td>
<td>Functional map from input to output.</td>
</tr>
<tr>
<td>4 PCE with adapted basis</td>
<td>46</td>
<td>Adapted to specific QoI.</td>
</tr>
</tbody>
</table>
Embedded Quadrature
Leveraging structure in high-dimensional geometry

Probabilities of events are integrals over the basic random variables:
Downselect the gauss quadratures from the high-dimensional space using $l_1$ regularization on the weights.
What to do with evidence?

Data can be acquired on several scales, often separately.
- Data can be used to calibrate the finer scales.
- Data can be used to validate the upscaling process.

Validating Upscaling
- We use models of random tensors to capture theoretical constraints on bounds of tensors.
- Statistical comparisons of these models against models upscaled through models.
- Stochastic sensitivity to understand the discrepancy.
Constrain the probabilistic model of the heterogeneous material with this information: \( \mathcal{G} = \{G \in \mathbb{M}_n^+: G_l < G < G_u\} \)

\[
\begin{align*}
\int_{\mathcal{G}} p_G(G) dG &= 1 \\
\int_{\mathcal{G}} \ln[\det(G - G_l)] p_G(G) dG &= g_l \\
\int_{\mathcal{G}} \ln[\det(G_u - G)] p_G(G) dG &= g_u
\end{align*}
\]
MaxEnt Distribution of Bounded Random Matrix: Using Lagrange Multipliers, we maximize the following Lagrangian:

\[
\mathcal{L}(p_c, \lambda_l, \lambda_u) = -H(p_c) + (\lambda_0 - 1) \left[ \int_{\mathcal{G}} p_c(G) \, dG - 1 \right] \\
+ \lambda_l \left[ \int_{\mathcal{G}} \ln[\det(G - G_l)] \times p_c(G) \, dG - g_l \right] \\
+ \lambda_u \left[ \int_{\mathcal{C}} \ln[\det(G_u - G)] \times p_c(G) \, dG - g_u \right],
\]
MaxEnt Distribution of Bounded Random Matrix:

\[ p_G(G) = \frac{\det(G - G_l)^{a-(N+1)/2} \det(G_u - G)^{b+(N+1)/2}}{\beta_N(a, b) \det(G_u - G_l)^{(a+b)-(N+1)/2}} \]

Notes:
- \( a, b \) are obtained from the MaxEnt optimization.
- Efficient sampling algorithms have been developed for this distribution.
- Each realization \( G \) of the random matrix is obtained through an inverse analysis from experimental measurements of the mechanical field.
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Objective
Data from BOEM: Bureau of Ocean Data Management

Given:
- BOEM Data
- Physics

Infer:
- Fluxes at seafloor under different operating conditions
Objective

Data from BOEM: Bureau of Ocean Data Management

Infer:
Fluxes at seafloor under different operating conditions

R. Ghanem (USC)
UQ @ IPAM
January 21, 2015
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Complexity

Gulf of Mexico Geologic Divisions

<table>
<thead>
<tr>
<th>Shelf</th>
<th>Deepwater</th>
<th>Ultra Deepwater</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-600 ft</td>
<td>600-5,000 ft</td>
<td>5,000-10,000 ft+</td>
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</table>

- Plio.-Pleistocene
- Allochthonous Salt Canopy
- Fold and Thrust Belts
- M.- U. Miocene
- L. Miocene
- Eocene-Paleocene
- Cretaceous
- Basement
Complexity
Multiscale Knowledge

Physics Constraints
- At scale of each reservoir: Multiphase flow in porous medium.
- At scale of wellbore at location of interest

Poorly understood constraints
- local geological fluctuations
- global geological fluctuations
Diffusion Metric

A Markov chain with controlled step evolving on the data set will eventually discover intrinsic distances between data points.

Spiral has intrinsic dimension of 1.

Torus has intrinsic dimension of 2.
Decomposition of uncertainty:

\[
\alpha(\omega) = f(\underbrace{\xi_1, \cdots, \xi_n}_{\text{Aleatoric Uncertainty}}, \underbrace{\xi_{n+1}, \cdots, \xi_m}_{\text{Model/Data Uncertainty}})
\]

\[
= \sum_{ijkl} \alpha_{ijkl}(x) \psi_i(\xi_1) \psi_j(\xi_2) \psi_k(\xi_3) \psi_l(\xi_4)
\]

- \(\xi_1\) uncertainty at scale of reservoir (polynomial chaos).
- \(\xi_2\) uncertainty at scale of field (lease) (Gaussian process interpolation).
- \(\xi_3\) uncertainty at scale of Gulf of Mexico (Gaussian Process with Diffusion metric from data).
- \(\xi_4\) uncertainty in wellbore performance at target site.
Decomposition of uncertainty:

\[ \alpha(\omega) = f(\xi_1, \cdots, \xi_n, \xi_{n+1}, \cdots, \xi_m) \]

\[ = \sum_{ijkl} \alpha_{ijkl}(x) \psi_i(\xi_1) \psi_j(\xi_2) \psi_k(\xi_3) \psi_l(\xi_4) \]

- \( \xi_1 \) uncertainty at scale of reservoir (polynomial chaos).
- \( \xi_2 \) uncertainty at scale of field (lease) (Gaussian process interpolation).
- \( \xi_3 \) uncertainty at scale of Gulf of Mexico (Gaussian Process with Diffusion metric from data).
- \( \xi_4 \) uncertainty in wellbore performance at target site.
Multiscale UltraDeep Sea Drilling

Sample Results

![Graph showing probability density functions](image)

- Predicted pdf of q
- Actual pdf of q
- pdf of q from "Preliminary Estimate"

Flow rate on day one (q) in bbl

Probability density f(q)
Outline

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Comments: Constraints are building blocks UQ models

Mathematical constraints:
- sum of rows equal 1.
- satisfy a governing equation

Physics constraints:
- bounds on elasticity
- symmetry and conservation laws
- behavior across interfaces

Data constraints:
- Statistics
- Manifolds
References


