Multi-Scale Fusion of Information for Uncertainty Quantification and Management in Large-Scale Simulations
To develop rigorous **theory, algorithms and software** for UQ management in a computationally scalable way.

To demonstrate how a mathematical framework that addresses the analysis of stochastic multiscale systems can be driven by **limited/gappy information**, thus leading to a revolutionary but realistic approach for capturing, harnessing and **exploiting stochasticity** in engineered systems.

To demonstrate the physical relevance and **broad applicability** of our framework through the consideration of multiple applications of interest to the USAF.
Multiscale Features and Uncertainty Sources

**Macroscale uncertainties**
- Initial and boundary conditions (e.g., Die shape)
- Location-specific microstructures
- Process parameters:
  - Temperature
  - Strain rate
  - etc.

**Mesoscale uncertainties**
- Topology
- Two-phase features
- Orientation
- Model Parameters: CRSS, etc.

**Microscale uncertainties**
- Particle size/volume fraction
- Particle shape
- Dislocation configuration
- Parameters: APB energy, etc.
Multiple Scattering Problem

Extension to different types of scatterers

\[ k = 3, \quad \theta_{\text{rcs}} = \frac{\pi}{2}, \phi_{\text{rcs}} \in [0, 2\pi] \]

\[ \theta_{\text{inc}} = \frac{\pi}{2}, \phi_{\text{inc}} \in [0, 2\pi] \]

Note - scatterers are not in plane
A Multi-Element Generalized Polynomial Chaos Approach to Analysis of Mobile Robot Dynamics under Uncertainty

Gaurav Kewlani, Karl Iagnemma

Dynamic Performance of a SCARA Robot Manipulator With Uncertainty Using Polynomial Chaos Theory

Philip Voglewede, Anton H. C. Smith, and Antonello Monti

Research @ MIT

Research @ Aachen

Fig. 8. Robot model for mobility analysis under uncertainty

Fig. 1. Schematic of the SCARA robot showing the geometric parameters and coordinate frames.
MEPCMP is a C++ package which can generate high-dimensional multi-element collocation points based on arbitrary probability density functions in each dimension. Example: a 3-D random variable

$\xi = (\xi_1, \xi_2, \xi_3)$  where $\xi_i$ are independent with density functions:

- $\frac{1}{\sqrt{2\pi}} e^{-x^2/2}$
- $\frac{1}{\sqrt{\pi}} e^{-x^2}$
- $0.25 - 0.5 e^{-x^2}$
- $0.75(1 - x^2)$

We first use function `Generate1DPoint()` to generate stochastic collocation points in each dimension, then use `GenerateTensor()`, `GenerateSparse()` or `GenerateANOVAD()` to obtain high-dimensional points based on different rules.

Download: http://sourceforge.net/projects/mepcmpackage/
Research Areas

I. Mathematical Analysis and Multiscale Formulation of SPDEs
   (Brown-Caltech-Cornell)

II. Numerical Solution of SPDEs
   (Brown-Cornell-Caltech)

III. Reduced-Order Modeling
   (MIT-Brown-Caltech)

IV. Multiscale Property Estimation
   (Cornell-MIT-Caltech)

V. Design & Control Under Uncertainty
   (MIT-Cornell-Brown)
Research Highlights

- **Mathematical Theory:** Quantization-renormalization of SPDEs; New evolution equations for joint-pdf of SPDEs; Nonlinear Malliavin calculus

- **Reduced Basis Methods (RBM):** Integral equations and multi-scattering problems; Robust design, parameter estimation, and model uncertainty

- **Adaptive ANOVA:** Convergence theory; Parameter compression and RBM; Fluid flows, porous media, multi-scattering

- **Bayesian Framework:** coarse-graining; Active learning + SPDEs; Adaptive SMC, dependent random variables, model uncertainty in inverse problems

- **Numerical SPDEs:** Data-driven stochastic multiscale method; Multiscale, multilevel MC, long-time integrators of SPDEs

- **Software:** MEPCM library; Reduced basis method libraries - RBOOMIT, RBAppMIT; Random poly-crystals - RPCrystal
Horn Problem Setup

Geometry Parameters:

- $L$ = Length of waveguide and flare
- $2a$ = waveguide width
- $b_1$ = height of 1st slice of flare from center
- $b_2$ = height of 2nd slice of flare from center
- $b$ = final height of flare from center

Boundaries:

- $\Gamma_{in}$ = waveguide inlet
- $\Gamma_N$ = internal and external horn walls
- $\Gamma_R$ = farfield circular boundary of radius $R$

Governing Equation: Helmholtz equation

$$\nabla^2 u + k^2 u = 0,$$

where $u$ is amplitude and $k$ is dimensionless wavenumber.

✓ Cradle-to-Grave Application of our Methodology
The reflection coefficient at the inflow boundary $\Gamma_{in}$ is defined as

$$l_\omega = \frac{< p_\omega >_{in} - A}{A}$$

where $A$ is the amplitude of the incoming wave at $\Gamma_{in}$ and $p_\omega$ is the acoustic pressure at angular frequency $\omega$,

$$< p_\omega >_{in} = \frac{1}{a} \int_{\Gamma_{in}} p_\omega d\Gamma,$$

where $a$ is half the width of the waveguide.

The far-field directivity at an angle $\theta$ and frequency $\omega$ can be expressed as

$$p_{\infty}(\theta, \omega) = \frac{1 - i}{4 \sqrt{\pi} k} \int_{\Gamma_{out}} \exp(ik \hat{x} \cdot x) \left( ik \hat{x} \cdot \frac{x}{R_\Omega} + ik + \frac{1}{2R_\Omega} \right) p(x) d\Gamma(x)$$

where $\hat{x}$ is the unit vector at an angle of $\theta$ and $\hat{x}$ and $x$ are 2-dimensional vectors.
Assume that there is a randomness on the amplitude of the incoming wave:

\[ A = 1 + 0.5\xi, \]

where \( \xi \sim U[-1, 1] \).
An Integrated Methodology

I Application
physical problem

II Stochastic Description
\[ \frac{\partial^2 u_0}{\partial t^2} = A_0(u_0; \alpha_0) \]
\[ t \in [0, T] \text{ time variable} \]
\[ x_0 \in \Omega_0 \subset \mathbb{R}^{d_0} \text{ space variable} \]
\[ \alpha_0 \in D_0 \subset \mathbb{R}^{M_0} \text{ random variable/parameter} \]

III Parameter Dimension Reduction
\[ \Omega_0 \rightarrow \Omega \subset \mathbb{R}^d \]
\[ \alpha_0 \rightarrow \alpha \]
\[ D_0 \rightarrow D \subset \mathbb{R}^M \text{ with } M \ll M_0 \]
\[ A_0 \rightarrow A \]
\[ u_0 \rightarrow u \]

IV Sample Sparsification
\[ \{u(\alpha) \mid \alpha \in D\} \rightarrow \{u(\alpha_n), 1 \leq n \leq N\} \]
projection, collocation
\[ \downarrow u_N \]

V Characterization
\[ \{\alpha\} \text{ data} \]
noisy measurements \[ Q_{\text{meas}} \]
\[ \{\alpha\}_\text{data} \sim p_{\alpha}_\text{data} \]
\[ \downarrow u_N \]

VI Optimization and Control
\[ \beta \equiv \{\alpha\}_\text{design} \]
\[ \frac{\partial^2 u^*}{\partial t^2} = A(u^*; \{\alpha\}_\text{data}, \beta) \]
\[ + \min J(Q^*_N(u^*; \{\alpha\}_\text{data}, \beta); \beta) \]
\[ \downarrow \beta^{**} \]

Validation
\[ Q_N^{\beta} \pm \Delta_N \]
\[ \{\alpha\}_\text{design} \]

\[ Q \pm \Delta \]
\[ (\alpha) \]
We consider the following model problem for monochromatic waves in a random medium

$$\nabla^2 p + \left( 1 + \sigma \xi^2 \cos^2(nx) \cos^2(my) \right) \frac{\omega^2}{c^2} \diamond p = 0 \quad n, m \in \mathbb{N}$$

**NOTE:** The Wick product approximation modifies the form of the Helmholtz equation. In other works, differently from other stochastic methods (e.g. polynomial chaos), is it a stochastic approximation technique formulated at the level of the equation.

**Wick Product:**

$$\xi_\alpha \diamond \xi_\beta = C(\alpha, \beta) \xi_{\alpha+\beta}, \text{ where }$$

$$C(\alpha, \beta) = \sqrt{(\alpha + \beta)!/\alpha!\beta!}$$

Compare with:

$$\xi_\alpha \xi_\beta = C(\alpha, \beta) \xi_{\alpha+\beta} + \kappa, \text{ where }$$

$$\kappa = \sum_{\gamma<\alpha+\beta} \kappa_\gamma \xi_\gamma \implies$$
Theorem

The Helmholtz-Wick propagator defined in the previous slide has a unique solution \( \{ \hat{p}_j \} \in H^1 \) if \( \omega^2/c^2 \) is not an eigenvalue of the following problem

\[
-\nabla^2 p - \lambda \left( 1 + \sigma \xi^2 \cos^2(nx) \cos^2(ny) \right) p = 0
\]

with boundary conditions

\[
p = 0
\]

\[
\frac{\partial p}{\partial n} = 0
\]
From a **theoretical analysis** of the Helmholtz-Wick propagator it can be shown that an optimal rescaling of the chaos modes $\hat{p}_k(x,y)$ is in the form of $C^k$ where $C(\sigma) = \sigma/2$. Thus, we construct the **renormalized field** $p_r(x,y;\xi)$

$$p_r(x,y;\xi) = \sum_{k=0}^{P} \frac{\hat{p}_k(x,y)}{C(\sigma)^k} H_k(\xi)$$

**Optimal rescaling as function of the perturbation magnitude**
Combining RBM and ANOVA

- Parametric Compression via ANOVA:

- 8 parameters, describing wall impedance in horn
Based on ANOVA sensitivity indices we conclude:

Two boundaries are responsible for >99% of all variation in output - allows for a compression to 2 parameters.
Adaptive ANOVA - Effect of Roughness

Perturbation of Far-Field Directivity

![Graphs showing perturbation of far-field directivity for waveguides with different dimensions.]

Waveguide – 7 dimensions
(MC: 50,000; SG2: 113; ANOVA: 67)

Waveguide – 102 dimensions
(MC: 50,000; SG2: 21,013; ANOVA: 529)
Figure: Real part of the mean solution of the Horn problem (left) and variance curve (right). The grid size is $h_l = 0.25 \cdot 2^{-l}$. Because of the multiscale feature, we run 40000 MC simulations on the finest grid of level 3, i.e., $h_3 = 0.03125$, to resolve the problem and denote this MC solution as our mean function $\mathbb{E} [u]$. 
robust objective \[ \min \mu(b_1, b_2) + \sigma(b_1, b_2) \]
design variables \[ b_1, b_2 \] for piecewise linear flare
uncertain parameters \[ k \sim U[1.3, 1.5] \quad Z_t, Z_b \sim U[1, 100] \]
high-fidelity model RB model, \( N = 118 \)
low-fidelity model RB model, \( N = 20 \)

<table>
<thead>
<tr>
<th></th>
<th>Robust Solution</th>
<th>Point Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>At ( k=1.4, Z_t=Z_b=50 )</td>
<td>0.054</td>
<td>0.013</td>
</tr>
<tr>
<td>( \mu^* )</td>
<td>0.083</td>
<td>0.11</td>
</tr>
<tr>
<td>( \sigma^* )</td>
<td>0.044</td>
<td>0.054</td>
</tr>
</tbody>
</table>

- **Multifidelity approach required 5.5 times fewer high-fidelity model evaluations than single-fidelity optimization.**
Next: RBM for Systems

Component to System: Muffler with Reflection Rooms

\[ P = 16 \] Parameters

Patera, Huynh, Knezevic, Eftang

AFOSR MURI
Karhunen–Loève (KL) expansion has been widely used for model reduction of stochastic processes and random fields.

\[ a(x, \omega) \approx E[a(x, \omega)] + \sum_{i=1}^{n} \sqrt{\lambda_i} \phi_i(x) \eta_i(\omega) \]

with \( E[\eta_i] = 0 \) \( E[\eta_i \eta_j] = \delta_{ij} \)

The KL coefficients, \( \eta_i \), generally have nonstandard distributions determined by the data. Thus, it is desirable to represent them with standard random variables, e.g. \( i.i.d. \) normal variables, using generalized polynomial chaos expansion (GPCE).

\[ \eta = \sum_{\alpha} \gamma_{\alpha} \Psi_{\alpha}(\xi) \]

where \( \gamma_{\alpha} = \int g(\xi) \Psi_{\alpha}(\xi) p(\xi) d\xi \) and \( \eta = g(\xi) \)

However, it is challenging to take account of the dependence between KL coefficients in GPCE.
We construct a Bayesian network (BN) for KL coefficients and learn its structure using a constraint-based algorithm. It runs local hypothesis tests to identify a dependency model for random variables. The learned conditional independence (CI) are viewed as constraints on the final model structure.

Null hypothesis $H_o : Y \perp Z \mid X \iff H_o : \Pr\{p_{Y|X,Z}(y \mid x,z) = p_{Y|X}(y \mid x)\} = 1$

**Step 1:**
For neighboring nodes A and C, make CI test for $A \perp C \mid S$ where $S \in \text{Adjacence}(A) \setminus \{C\} = \{B, D, E\}$

i.e. test $p(A, C \mid B)$  
$p(A, C \mid D)$  
$p(A, C \mid E)$

Since $A \perp C \mid B$
remove edge A-C
Multiple Correlated Random Processes

- **Covariance structure of two random processes**

\[
\begin{align*}
\langle f_1(t) \rangle &= \langle f_2(t) \rangle = 0 \\
\langle f_1(t), f_1(s) \rangle &= C_1(t, s), \quad \langle f_2(t), f_2(s) \rangle = C_2(t, s) \\
\langle f_1(t), f_2(s) \rangle &= C_3(t, s)
\end{align*}
\]

**Expansion with single r.v. set**

\[
\begin{align*}
f_1(t) &= \sum_k \sqrt{\lambda_k} \| \phi_k(t) \| \hat{\phi}_k(t) \xi_k, \\
f_2(t) &= \sum_k \sqrt{\lambda_k} \| \psi_k(t) \| \hat{\psi}_k(t) \xi_k
\end{align*}
\]

Assemble the covariance matrix as \( C \),

\[
\langle \tilde{v}(t), \tilde{v}(s) \rangle = C = \begin{bmatrix} C_1 & C_3 \\ C_3 & C_2 \end{bmatrix},
\]

where \( \tilde{v}(t) = [f_1(t); f_2(t)] \).

Find the eigenpair of \( C \),

\[
\{ \tilde{v}_k(t), \lambda_k \} \quad \tilde{v}_k(t) = [\phi_k(t); \psi_k(t)]
\]

**Expansion with different r.v. sets**

\[
\begin{align*}
f_1(t) &= \sum_k \sqrt{\lambda_k} \phi_k(t) \xi_k, \\
f_2(t) &= \sum_k \sqrt{\gamma_k} \psi_k(t) \eta_k
\end{align*}
\]

Compute the K-L expansion of each process from \( C_1 \) and \( C_2 \).

Then give correlation between r.v. sets as

\[
\langle \xi_k, \eta_m \rangle = c_{km} \quad \text{by projection},
\]

\[
c_{km} = \frac{1}{\sqrt{\lambda_k \gamma_m}} \int \int C_3(t, s) \phi_k(t) \psi_m(s) dt ds
\]
### Multiple Correlated Random Processes

<table>
<thead>
<tr>
<th>Expansion with single r.v. set</th>
<th>Expansion with different r.v. sets</th>
</tr>
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<tbody>
<tr>
<td>• Need less number of random variables</td>
<td>• Usually need more random variables</td>
</tr>
<tr>
<td>• Easily extended to multiple processes</td>
<td>• Cost : projection to the basis (integration)</td>
</tr>
<tr>
<td>• Cost : solving an eigen-problem</td>
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**Constraint for Covariance kernel (in single r.v. set)**

- Assembled matrix must be Positive Definite.

- e.g. Condition to correlation time for two random process with exponential Covariance kernel, 
  \[ C_i(t, s) = \frac{D_i}{\tau_i} e^{\left(-\frac{|t-s|}{\tau_i}\right)}, \quad i = 1, 2, 3 \]  
  (let \( c_i = \frac{1}{\tau_i} \))

Eigenvalues can be computed by solving

\[
\lambda \phi''(t) = (-2c_1 + c_1^2 \lambda) \phi(t) + (-2c_3 + c_3^2 \lambda) \psi(t), \\
\lambda \psi''(t) = (-2c_3 + c_3^2 \lambda) \phi(t) + (-2c_2 + c_2^2 \lambda) \psi(t),
\]

with boundary conditions

\[
\phi'(0) - c_1 \phi(0) - c_3 \psi(0) = 0, \quad \phi'(T) + c_1 \phi(T) + c_3 \psi(T) = 0, \\
\psi'(0) - c_3 \phi(0) - c_2 \psi(0) = 0, \quad \psi'(T) + c_3 \phi(T) + c_2 \psi(T) = 0.
\]

⇒ Constraint for correlation length : 

\[
\frac{1}{\tau_1} + \frac{1}{\tau_2} < \frac{2}{\tau_3}
\]
More to Do…

✓ From MC to gPC to ANOVA to Quantization…

✓ From single components to systems; (RBM & UQ)

✓ UQ for inverse problems (new PI: Y. Marzuk, MIT)

✓ Model validation; non-parametric uncertainty

✓ Time-propagation of high-dimensional systems

✓ Realistic inputs; industrial complexity apps
Education: 8 Postdocs & 13 PhD students

J. Eftang, MIT
Adaptive ROM

P. Huynh, MIT
Model Validation

D. Knezevic, MIT
ROM Errors

J. Park, Brown
Quant/NL Filt

B. Stamm, Brown
ROM/Integral

D. Venturi, Brown
PDF/Quant

S. Zhang, Brown
ROM/ANOVA

Z. Zhang, Caltech,
Data-Driven-Mscale