Large number of uncertainties in complex engineering simulations

Essential to take all uncertainties into account:
- Non-deterministic parameters in mathematical model
- Inherent variability in environment
- Stochastic fields in material properties

Monte Carlo (MC) simulation classical uncertainty quantification (UQ) method:
- Ensemble of simulations for randomly sampled parameter values
- High robustness for irregular response surfaces
- Order of convergence independent of the number of random input parameters
- Constant convergence rate of the order $O = 0.5$ only

MC leads to excessive computational costs in large-scale numerical simulations
Stochastic Collocation suffers from the curse of dimensionality

Stochastic Collocation\textsuperscript{1,2} (SC) more efficient alternative for MC:
\begin{itemize}
  \item Based on Gauss quadrature sampling and Lagrangian polynomial interpolation
  \item Spectral convergence for smooth responses
  \item Tensor product extension to multiple dimensions
  \item Exponential increase of number of samples
\end{itemize}

More efficient extensions of SC to higher dimensions:
\begin{itemize}
  \item Smolyak sparse grid formulations\textsuperscript{3,4}
  \item Dimension adaptive SC methods\textsuperscript{5,6}
  \item Local adaptive multi-element methods\textsuperscript{7,8,9}
\end{itemize}

Adaptive methods are promising approaches for efficient UQ in higher dimensions

Requirements for efficient local adaptive SC methods

Special attention for multi-element adaptive nature:
- Reuse all samples after $h$-refinements using nested quadrature rules
- Share samples at element boundaries with adjacent elements
- Establish quantitative robustness properties for discontinuous responses

Effectiveness of adaptive SC methods is determined to large extent by the $h$- and $p$-refinement measures

We consider the Simplex Stochastic Collocation (SSC) method with focus on:
- $h$-refinement measures
- $p$-refinement criterion
- Refinement stopping criterion
- Error convergence properties
- Quantitative robustness concepts
- Number of initial samples
- Non-hypercube probability spaces
Simplex Stochastic Collocation satisfies requirements for adaptive methods

First-degree Newton-Cotes quadrature in simplex elements:
• Piecewise linear interpolation of samples in vertexes of simplex elements
• Samples reused after refinements and shared with adjacent elements
• Local Extremum Diminishing (LED) robustness

Initial grid of 4 elements

Refined grid of 32 elements
SSC follows general formulation of local UQ methods

Consider computational problem for output of interest: \( u(x, t, \xi) \)

\[
L(x, t, \xi; u(x, t, \xi)) = S(x, t, \xi)
\]

With a set of \( n_\xi \) uncorrelated random parameters:

\[
\xi(\omega) = \{\xi_1(\omega_1), \ldots, \xi_{n_\xi}(\omega_{n_\xi})\} \in \Xi
\]

Find probability distribution and statistical moments of: 
\( u(x, t, \xi) \)

\[
\mu_{u_i}(x, t) = \int_\Xi u(x, t, \xi)^i f_\xi(\xi)d\xi
\]

Local UQ formulation:

\[
\mu_{u_i}(x, t) = \sum_{j=1}^{n_e} \int_{\Xi_j} u(x, t, \xi)^i f_\xi(\xi)d\xi
\]
SSC based on non-intrusive approximation of response surface

Approximate response surface $u(\xi)$ by interpolation $w(\xi)$ of samples $v = \{v_1, \ldots, v_{n_s}\}$ with number of samples $n_s$.
Non-intrusive UQ is combination of sampling and interpolation

UQ method $q$ consists of sampling method $g$ and interpolation method $h$.

$$w(\xi) = q(u(\xi)) = h(g(u(\xi)))$$

Sampling method $g$ selects sampling points $\xi_k$ for $k = 1, \ldots, n_s$ and returns sampled values $v = g(u(\xi))$ with $v_k = g_k(u(\xi)) = u(\xi_k)$

$$\mathcal{L}(x, t, \xi_k; v_k(x, t)) = S(x, t, \xi_k)$$

Interpolation $w(\xi) = h(v)$ results in piecewise polynomial function $w(\xi) = w_j(\xi)$ for $\xi \in \Xi_j$

$$\mu_{u_i}(x, t) \approx \mu_{w_i}(x, t) = \sum_{j=1}^{n_e} \int_{\Xi_j} w_j(x, t, \xi)^i f_{\xi}(\xi) d\xi$$
Construction piecewise polynomial response surface interpolation

Polynomial interpolation \( w_j(\xi) \) of order \( p \) through the samples \( v_j = \{ v_{k_j,0}, \ldots, v_{k_j,N} \} \) at sampling points \( \{ \xi_{k_j,0}, \ldots, \xi_{k_j,N} \} \) in element \( \Xi_j \)

\[
N + 1 = \frac{(n_\xi + p)!}{n_\xi!p!}
\]

\[
\begin{bmatrix}
\Psi_{j,0}(\xi_{k_j,0}) & \Psi_{j,1}(\xi_{k_j,0}) & \cdots & \Psi_{j,N}(\xi_{k_j,0}) \\
\Psi_{j,0}(\xi_{k_j,1}) & \Psi_{j,1}(\xi_{k_j,1}) & \cdots & \Psi_{j,N}(\xi_{k_j,1}) \\
\vdots & \vdots & \ddots & \vdots \\
\Psi_{j,0}(\xi_{k_j,N}) & \Psi_{j,1}(\xi_{k_j,N}) & \cdots & \Psi_{j,N}(\xi_{k_j,N})
\end{bmatrix}
\begin{bmatrix}
c_{j,0} \\
c_{j,1} \\
\vdots \\
c_{j,N}
\end{bmatrix}
= 
\begin{bmatrix}
v_{k_j,0} \\
v_{k_j,1} \\
\vdots \\
v_{k_j,N}
\end{bmatrix}
\]

SSC satisfies Local Extremum Diminishing (LED) robustness

Well-established robustness concept:
- Spatial discretizations of finite volume CFD methods
- Diminishes values of extrema over time
- No unphysical values due to overshoots and undershoots near shock discontinuities in physical space

Extension to probability space:
- Interpolation diminishes values of extrema of the samples
- No non-zero probabilities for unphysical realizations due to overshoots and undershoots in the interpolation of the samples in each of the elements

First-degree SSC approximation satisfies LED property:

\[ \min_{\xi_j} w_j(\xi) \geq \min_{\xi_j} u(\xi) \land \max_{\xi_j} w_j(\xi) \leq \max_{\xi_j} u(\xi) \]

Higher-degree SSC uses Local Extremum Conserving (LEC) limiter for polynomial degree to satisfy LED robustness:

\[ \min_{\xi_j} w_j(\xi) = \min v_j \land \max_{\xi_j} w_j(\xi) = \max v_j \]
Error estimates based on hierarchical surpluses

Define local error in response surface approximation as:

\[ \varepsilon(\xi) = w(\xi) - u(\xi) \]

Exactly known at creation of a new simplex in terms of hierarchical surplus at new sampling point:

\[ \tilde{\varepsilon}_j = \varepsilon(\xi_{k_j,\text{ref}}) \]

with

\[ \varepsilon(\xi_{k_j,\text{ref}}) = w(\xi_{k_j,\text{ref}}) - u(\xi_{k_j,\text{ref}}) = w(\xi_{k_j,\text{ref}}) - v_{k_j,\text{ref}} \]

Estimate of the error after refinement using the definition of the order of convergence:

\[ \mathcal{O} = \frac{\log(\tilde{\varepsilon}_j/\hat{\varepsilon}_j)}{\log(2)} \]

is:

\[ \hat{\varepsilon}_j = \frac{\tilde{\varepsilon}_j}{2^\mathcal{O}} = \frac{\tilde{\varepsilon}_j}{2^{\frac{p+1}{n_{\xi}}}} \]
Suitable for refinement measure and stopping criterion

Error estimate, for example, for the mean:

\[ \hat{\varepsilon}_\mu = \sum_{j=1}^{n_e} \Omega_j \hat{\varepsilon}_j \]

with

\[ \Omega_j = \int_{\Xi_j} f_\xi(\xi) d\xi \quad \sum_{j=1}^{n_e} \Omega_j = 1 \]

RMS error more suitable as basis for refinement and stopping criteria, which leads to:

\[ \hat{\varepsilon}_{\text{rms}} = \sqrt{\sum_{j=1}^{n_e} \Omega_j \hat{\varepsilon}_j^2} \]

Reliable stopping criterion:
• Conservative error estimate
• Smoother convergence behavior than moment integral quantities
Suitable for refinement measure and stopping criterion

RMS error also basis for local refinement measures as summation of non-negative terms in the elements:

$$\hat{\varepsilon}_{\text{rms}} = \sqrt{\sum_{j=1}^{n_e} \Omega_j \varepsilon_j^2}$$

Resulting solution-based refinement measure:

$$\hat{\varepsilon}_{\text{rms}_j} = \Omega_j \varepsilon_j^2$$

And alternative refinement measure can be derived from:

$$O_j = \frac{\log(\varepsilon_j/\varepsilon_0)}{\log(\Xi_j)}$$

$$\varepsilon_j \sim \Xi_j^{O_j}$$

$$\Xi_j = \frac{1}{\Xi} \int_{\Xi_j} d\xi$$

Such that:

$$\hat{\varepsilon}_{\text{rms}_j} = \Omega_j \Xi_j^{2O_j}$$
Second-order convergence for first-degree Newton-Cotes quadrature

Test function with $\xi$ standard uniform $U(0, 1)$

$$u(\xi) = \arctan(\xi \cdot \xi^* - \xi_1^*)$$

and $\xi^* = \{\xi_1^*, \ldots, \xi_n^*\} \in [0, 1]^{n_\xi}$

**Function of elements**

**Function of samples**
Decreasing average number of samples per element

- Because of samples on boundaries of the elements
- Asymptotic average number of samples per element = 1
Error estimates slightly conservative prediction of error

- Because of conservative nature of hierarchical surpluses
- Leads to reliable stopping criterion
Error estimates slightly conservative prediction of error

- Local error estimate forms convex hull of local error
- Suitable for $h$-refinement measure
Curse of dimensionality

Increasing number of uncertain parameters up to 8:

- Decreasing order of convergence with increasing number of uncertainties
- Convergence lower than $O = 0.5$ of MC for more than 4 uncertain parameters

**Order of convergence**

<table>
<thead>
<tr>
<th>$n_\xi$</th>
<th>function of $n_s$</th>
<th>function of $n_e$</th>
<th>$O = \frac{2}{n_\xi}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.023</td>
<td>2.003</td>
<td>2.000</td>
</tr>
<tr>
<td>2</td>
<td>1.081</td>
<td>1.006</td>
<td>1.000</td>
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<tr>
<td>3</td>
<td>0.748</td>
<td>0.641</td>
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<td>4</td>
<td>0.577</td>
<td><strong>0.472</strong></td>
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<tr>
<td>5</td>
<td>0.541</td>
<td>0.395</td>
<td>0.400</td>
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<tr>
<td>6</td>
<td>0.405</td>
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<td>7</td>
<td>0.180</td>
<td>0.311</td>
<td>0.286</td>
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<tr>
<td>8</td>
<td>0.038</td>
<td>0.371</td>
<td>0.250</td>
</tr>
</tbody>
</table>
Higher-degree polynomial interpolation

Counteracts decreasing order of convergence using:

- Higher-degree Newton-Cotes quadrature samples
- In addition to samples at vertices of the elements

*Initial grid, \( p = 2 \)\n
*Initial grid, \( p = 4 \)\n
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Criterion for selecting the polynomial degree

Order of convergence follows relation:\textsuperscript{1,2}

\[ O = \frac{(p + 1)}{n_{\xi}} \]

Criterion for polynomial degree as function of number of uncertain parameters:
- In principle a constant order of convergence
- Increase polynomial degree \( p \) according to

\[ p = O n_{\xi} - 1 \]

- Higher order of convergence than MC

Constant order of convergence with increasing dimensionality

- Use p-criterion: \( p = \mathcal{O}n_{\xi} - 1 \)
- Higher degree polynomial interpolation essential for efficient UQ for multiple uncertainties

**Order of convergence**

<table>
<thead>
<tr>
<th>( p )</th>
<th>( n_{\xi} )</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.023</td>
<td>1.081</td>
<td>0.748</td>
<td></td>
</tr>
<tr>
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<tr>
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<td></td>
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<tr>
<td>4</td>
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<tr>
<td>5</td>
<td>6.333</td>
<td>3.074</td>
<td>1.984</td>
<td></td>
</tr>
</tbody>
</table>
Fast increase initial number of samples

Another special property of Monte Carlo simulation:

- Initial approximation using $n_{\text{SMC init}} = 1$ samples
- Independent of the number of uncertainties $n_\xi$

Fast increase initial number of samples for Newton-Cotes quadrature:

- Tensorial grid of samples in multiple dimensions
- Increasing average number of samples per element
- Especially with relation $p = \Theta n_\xi - 1$

*Initial number of samples and asymptotic average number of samples per element*
Randomized refinement sampling

Improves efficiency for multiple uncertainties to superlinear convergence:

- Random sampling location at refinement of an element
- In sub-simplex for good spread of the samples

Flexibility of simplexes to discretize random samples using Delaunay triangulation:

- Random sampling effective approach in higher dimensions
- Naturally avoids tensor grid in multiple dimensions

Random sampling in sub-simplex

Delaunay triangulation
Higher-degree interpolation stencils

Higher-degree interpolation essential for efficient UQ with multiple uncertainties:

- Impractical to reuse higher-degree Newton-Cotes quadrature
- Higher-degree stencils of vertexes of surrounding elements
- Stencils constructed based on nearest neighbor principle

Local Extremum Diminishing robustness property maintained:

- Reduce stencil based on a Local Extremum Conserving (LEC) limiter
- Robust approximation of discontinuities

$ n_a = 3 \text{ for } p = 1 $  \quad \quad \quad \quad \quad \quad n_s = 15 \text{ for } p = 4 $  

$ n_s = 6 \text{ for } p = 2 $
Superlinear convergence rate

Efficiency increased to superlinear convergence:
- Increasing polynomial order with increasing number of samples
- Up to two orders of magnitude less samples than NC quadrature

Initial number of samples significantly lower than NC quadrature
- Average number of samples per element decreases with dimension
- Still exponential increase of initial number of samples
- Sampling in the vertices of the hypercube probability space

Randomized refinement (RR) and Newton-Cotes (NC) sampling

<table>
<thead>
<tr>
<th>$n_E$</th>
<th>$n_E/n_0$</th>
<th>$n_{init}$</th>
</tr>
</thead>
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<tr>
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<td>4.59</td>
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<tr>
<td>4</td>
<td>-</td>
<td>341</td>
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</tbody>
</table>

Initial number of samples and asymptotic average number of samples per element
Essentially Extremum Diminishing extrapolation

Achieves linear increase of the initial number of samples:
- Vertices of hypercube probability space not used as samples
- Introduces the need for extrapolation
- Extending the approximation in nearest interpolation element

Extrapolation changes robustness to Essentially Extremum Diminishing (EED):
- Quantitative robustness in terms of upper bound of probability of unphysical predictions
- Converges to ED robustness for increasing number of elements
Linear increase of initial number of samples

Essentially Extremum Diminishing extrapolation:

- Linear increase initial number of samples
- Initially faster convergence owing to better spread of the samples
- Asymptotically comparable error convergence behavior

<table>
<thead>
<tr>
<th>$n_\xi$</th>
<th>$n_{s_{\text{init}}}$</th>
<th>ED</th>
<th>EED</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
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<tr>
<td>8</td>
<td>257</td>
<td>257</td>
<td>9</td>
</tr>
</tbody>
</table>
Comparable results for non-uniform input distributions

Convergence for non-uniform distributions is essential

Discretization parameter space for weighted interpolation:
- Moderately higher density of samples at higher probabilities
- Good coverage of the domain for accurate interpolation

Convergence does not primarily depend on type of distribution:
- Faster convergence for beta distribution on same domain [0,1]
- Slower convergence for normal distribution with same standard deviation
Non-hypercube probability spaces with correlated uncertainties

Examples of non-hypercube probability spaces:

- Uncertainties with constraints and truncated parameter spaces
- Physical system unrealizable outside probability domain

Simplex elements with extrapolation flexible for discretizing non-hypercube domains:

- Superlinear error convergence behavior unaffected
- Convergence even faster owing to smaller domain than hypercube example

Monte Carlo integration  
SSC discretization  
Error convergence
Conclusions

Simplex Stochastic Collocation multi-element UQ method:
- Local Extremum Diminishing (LED) robustness
- Superlinear convergence rate using randomized refinement sampling
- Linear increase initial number of samples using EED extrapolation
- Flexibility for discretizing non-hypercube probability spaces

Reliable refinement measures and stopping criteria:
- h-refinement measures based on absolute and relative error estimate
- p-criterion for in principle a constant order of convergence
- Reliable stopping criterion based on conservative error estimate
Thank you

Questions?