Stochastic decomposition methods

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Introduction

- In Lecture 1, an example of a stochastic ODE was considered and GPCE was shown to exhibit exponential convergence in approximating stochastic solutions at early times. However, the absolute error may increase gradually in time and become unacceptably large for long-term integration.

- In addition, for discontinuous dependence or singularity of the solution on the input random data, GPCE may converge very slowly or fail to converge even in short-time.

- To remedy these problems, we have already introduced the collocation methods based on the piecewise linear interpolation. Another popular method is the so-called multi-element (ME) based method.

- This method decomposes the random space into several small subdomain, like the finite element discretization, and then solve the original stochastic problem in each region.
Introduction

- Another problem is the *curse of dimensionality*. As shown in earlier lectures, the number of terms in gPC expansion grows exponentially with the increasing of stochastic dimensions. So in general, GPCE is suitable for low dimensional stochastic problem.

- Although by using Smolyak algorithm and adaptive construction of the sparse grids, the stochastic collocation methods alleviates the *curse of dimensionality* to some extent, it still can not solve very large dimensional problem (>10) or the computation is unrealistic (huge number of collocation points). In addition, the convergence rate deteriorates with the increasing of dimensions due to the logarithmic terms in the error estimate.

- A possible remedy to this problem is to **decompose the high dimensional** problem to several lower dimensional problem through the so called high dimensional model representation technique (HDMR).

- Both methods decompose the original large problem into several small sub-problems. Thus, we give these methods the name “Stochastic decomposition methods”.

Introduction

- After generating the small sub-problems from either decomposition method, we can use any stochastic method to solve them such as GPCE or collocation method.

  - Multi-wavelet (Wiener Haar) method (O.P.L.Maitre et al., 2004a, 2004b)
  
  
  
  - Stochastic high dimensional model representation method, HDMR, (X. Ma and N. Zabaras, 2009).
Overview of GPCE

- A second order stochastic process can be expanded as

\[ X(\omega) = \sum_{j=0}^{P} \hat{a}_j \psi_j(\zeta) \]

where \( \psi_j(\zeta) \) are orthogonal polynomials from the Wiener-Askey family. The corresponding type of polynomials are associated with the distribution of random variable \( \zeta \).

- The inner product is defined as:

\[ \langle f(\zeta)g(\zeta) \rangle = \int f(\zeta)g(\zeta)dP(\zeta) = \int f(\zeta)g(\zeta)W(\zeta)d\zeta \]

where the weighting function has the same form as the probability distribution function of \( \zeta \).

- We also have the orthogonality relation:

\[ \langle \psi_i \psi_j \rangle = \langle \psi_i^2 \rangle \delta_{ij} \]
Denote the one dimensional interpolation formula as
\[ U^i(f) = \sum_{j=1}^{m_i} f(Y^i_j) \cdot a_j^i \]

In higher dimension, a simple case is the tensor product formula
\[ (U^{i_1} \otimes \cdots \otimes U^{i_N})(f) = \sum_{j_1=1}^{m_1} \cdots \sum_{j_N=1}^{m_N} f(Y^{i_1}_{j_1}, \ldots, Y^{i_N}_{j_N}) \cdot (a^{i_1}_{j_1} \otimes \cdots \otimes a^{i_N}_{j_N}) \]

Using the 1D formula, the sparse interpolant \( A_{q,N} \), where \( q \) is the depth of sparse grid interpolation \((q \geq 0, q \in \mathbb{N}_0)\) and \( N \) is the number of stochastic dimensions, is given by the Smolyak algorithm as
\[
A_{q,N}(f) = A_{q-1,N}(f) + \Delta A_{q,N}(f) \quad \Delta^i = U^i - U^{i-1} \quad U^0 = 0 \\
A_{-1,N} = 0 \\
A_{q-1,N}(f) = \sum_{|i| \leq q-1} (\Delta^{i_1} \otimes \cdots \otimes \Delta^{i_N}) \Delta A_{q,N}(f) = \sum_{|i| = q} \sum_{j_1 \in B_i} (a^{i_1}_{j_1} \otimes \cdots \otimes a^{i_N}_{j_N}) \cdot (f(Y^{i_1}_{j_1}, \ldots, Y^{i_N}_{j_N}) - A_{q-1,N}(f)(Y^{i_1}_{j_1}, \ldots, Y^{i_N}_{j_N}))
\]

Here we define the \textbf{hierarchical surplus} as:
\[
w^i_j = f(Y^{i_1}_{j_1}, \ldots, Y^{i_N}_{j_N}) - A_{|i|-1,N}(f)(Y^{i_1}_{j_1}, \ldots, Y^{i_N}_{j_N})
\]
Decomposition of the random space – Multi-element based method
Multi-element based method

- Basic concept:
  - Decompose the space of random inputs into small elements.
  - In each element of the support space, we generate a new random vector and apply the stochastic method such as GPCE and collocation.
  - The global PDF is also simultaneously discretized. Thus, the global PC basis is not orthogonal with the local PDF in a random element. We need to reconstruct the orthogonal basis numerically in each random element. The only exception is the uniform distribution whose PDF is a constant.
  - We can potentially decompose the random space adaptively to increase its efficiency.
Decomposition of the random space

- Let $\xi: \Omega \to \mathbb{R}^d$ denote a $d$-dimensional random variable defined on $B = \times_{i=1}^d [a_i, b_i]$ where $a_i$ and $b_i$ are finite or infinite in $\mathbb{R}$ and the components of $\xi$ are independent identically-distributed (i.i.d.) random variables.

- We define a decomposition $D$ of $B$ as

$$D = \begin{cases} \begin{align*} B_k &= [a_{k,1}, b_{k,1}] \times [a_{k,2}, b_{k,2}] \times \ldots \times [a_{k,d}, b_{k,d}] \\ B &= \bigcup_{k=1}^N B_k \\ B_{k_1} \cap B_{k_2} &= \emptyset \quad \text{if} \quad k_1 \neq k_2 \end{align*} \end{cases}$$

where $k_1, k_2 = 1, 2, \ldots, N$

- Based on the decomposition $D$, we define the following indicator random variables:

$$I_{B_k} = \begin{cases} 1 & \text{if} \quad \xi \in B_k, \\ 0 & \text{otherwise} \end{cases} \quad k = 1, 2, \ldots, N$$
Decomposition of the random space

Thus, $\Omega = \bigcup_{k=1}^{N} I_{B_k}^{-1}(1)$ is a decomposition of the sample space $\Omega$, where

$$I_{B_i}^{-1}(1) \cap I_{B_j}^{-1}(1) = \emptyset \quad \text{for} \quad i \neq j$$

It is obvious that the probability for a random variable $\xi$ in random element $B_k$ is

$$\Pr(I_{B_k} = 1) = \int_{B_k} f(\xi) d\xi$$

where $f(\xi)$ is the PDF of $\xi$.

Given any point $q = (q_1, q_2, \ldots, q_d)$, we use $\xi \leq q$ to denote $\xi_i \leq q_i$ for $i = 1, 2 \ldots d$.

According to the law of total probability, we can obtain

$$\Pr(\xi \leq q) = \sum_{k=1}^{N} \Pr(\xi \leq q \mid I_{B_k} = 1) \Pr(I_{B_k} = 1)$$
Decomposition of the random space

- Then using Bayes’ rule, we can define a new random variable \( \xi_k : I_{B_k}^{-1}(1) \mapsto B_k \) in \( k \)th random element \( B_k \) on the probability space \((I_{B_k}^{-1}(1), F \cap I_{B_k}^{-1}(1), P(\cdot | I_{B_k} = 1))\) subject to a local conditional PDF

\[
\hat{f}_k(\xi_k | I_{B_k} = 1) = \frac{f(\xi_k)}{\Pr(I_{B_k} = 1)}
\]

where \( \Pr(I_{B_k} = 1) > 0 \)

- Let \( u(x, t; \xi) \in L_2(\Omega, F, P) \) denote a second-order space-time related random field. For simplicity, we may drop \( x \) and \( t \).

- **Proposition 1** (X. Wan and G. Karniadakis, 2006) Let \( P_M u(\xi) \) denote the Galerkin projection of \( u(\xi) \) onto the polynomial chaos basis \( \{\psi_i(\xi)\} \) up to polynomial order \( M, \ i = 1, 2, \ldots, M \). If \( P_M u(\xi) \) converges to \( u(\xi) \) in the \( L_2 \) sense with respect to the PDF \( f(\xi) \), then \( P_M u(\xi_k) \) converges to \( u(\xi_k) \) in the \( L_2 \) sense with respect to the conditional PDF \( \hat{f}_k(\xi_k | I_{B_k} = 1) \) \( k = 1, 2, \ldots, N \)
**Decomposition of the random space**

**Proof.** According to the assumption, we know that (Wan & Karniadakis, 2006)

\[
E[(u(\xi) - P_M u(\xi))^2] = \int_B (u(\xi) - P_M u(\xi))^2 f(\xi) d\xi \to 0 \quad \text{as} \quad M \to \infty
\]

On the other hand

\[
E[(u(\xi) - P_M u(\xi))^2] = \sum_{k=1}^N \Pr(I_{B_k} = 1) \int_{B_k} (u(\xi_k) - P_M u(\xi_k))^2 \hat{f}_k(\xi_k \mid I_{B_k} = 1) d\xi_k \quad (\ast)
\]

We obtain

\[
\int_{B_k} (u(\xi_k) - P_M u(\xi_k))^2 \hat{f}_k(\xi_k \mid I_{B_k} = 1) d\xi_k \to 0 \quad \text{as} \quad M \to \infty
\]

since both \( \Pr(I_{B_k} = 1) \) and the integrand on the right-hand side of (\ast) are positive for \( k = 1, 2\ldots, N \)
So there exists a local polynomial approximation for each random element \( B_k \), which converges in \( L_2 \) sense with respect to the local conditional PDF.

For the orthogonal basis \( \{ \psi_i(\xi) \} \) on the entire random space, \( u(\xi) - P_M u(\xi) \) is orthogonal to the space \( V(M, \xi) := \text{span} \{ \psi_i(\xi) : i \leq M \} \).

However, \( u(\xi_k) - P_M u(\xi_k) \) is not orthogonal to the space \( V(M, \xi_k) \) with respect to the conditional PDF \( \hat{f}_k(\xi_k | I_{B_k} = 1) \), since the orthogonality \( \langle \psi_i \psi_j \rangle = \langle \psi_i^2 \rangle \delta_{ij} \) is valid only on the entire random space of \( \xi \) with respect to the PDF \( f(\xi) \).

Thus, we will reconstruct the local polynomial chaos modes numerically to make them mutually orthogonal with respect to the local conditional PDF.

Since in each random element we perform a spectral expansion as in gPC, this method is referred to as “multi-element generalized polynomial chaos” (ME-gPC).
Decomposition of the random space

To approximate a random field $u(\xi)$ using Me-gPC, we expand the random field spectrally in each element $B_k$, then reconstruct the entire random field.

Let $\hat{u}_k(\xi_k)$ be the local polynomial chaos expansion in element $B_k$. The approximation on the entire random support space can be defined as

$$u^r(\xi) = \sum_{k=1}^{N} \hat{u}_k(\xi_k) I_{B_k} = \sum_{k=1}^{N} \sum_{j=0}^{M} \hat{u}_{k,j} \psi_{k,j}(\xi) I_{B_k}$$

It is easy to see that

$$\int_B (u^r(\xi) - u(\xi))^2 f(\xi) d\xi$$

$$= \sum_{k=1}^{N} \Pr(I_{B_k} = 1) \int_{B_k} (u^r(\xi_k) - u(\xi_k))^2 \hat{f}_k(\xi_k \mid I_{B_k} = 1) d\xi_k$$

where $u^r(\xi_k) = \sum_{k=1}^{N} \hat{u}_k(\xi_k) I_{B_k} (\xi_k \in B_k) = \hat{u}_k(\xi_k)$
And we just showed that $\hat{u}_k(\xi_k)$ converges locally in the $L_2$ sense with respect to $\hat{f}_k(\xi_k | I_{B_k} = 1)$.

Thus

$$\int_B (u^r(\xi) - u(\xi))^2 f(\xi) d\xi$$

$$= \sum_{k=1}^{N} \Pr(I_{B_k} = 1) \int_{B_k} (\hat{u}_k(\xi_k) - u(\xi_k))^2 \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k \to 0 \quad \text{as} \quad M \to \infty$$

This means, the approximation $u^r(\xi)$ converges to $u(\xi)$ in the $L_2$ sense.

It is easy to see that by law of total probability, any $m^{th}$ moment on the entire domain can be obtained as

$$\int_B u^m(\xi) f(\xi) d\xi \approx \sum_{k=1}^{N} \Pr(I_{B_k} = 1) \int_{B_k} \hat{u}^m(\xi_k) \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k$$
Here, we discuss only the construction of one-dimensional orthogonal polynomials, since the high dimensional basis can be constructed from the one-dimensional basis.

It is a distinctive feature of orthogonal polynomial that they satisfy a three-term recurrence relation, (W. Gautschi, 1982)

\[ \pi_{i+1}(\tau) = (\tau - \alpha_i)\pi_i(\tau) - \beta_i\pi_{i-1}(\tau), \quad i = 0,1,\ldots \]

\[ \pi_0(\tau) = 1, \quad \pi_{-1}(\tau) = 0, \]

where \{\pi_i(\tau)\} is a set of (monic) orthogonal polynomials,

\[ \pi_i(\tau) = \tau^i + \text{lower - degree terms}, \quad i = 0,1,\ldots, \]

The coefficients \( \alpha_i \) and \( \beta_i \) are uniquely determined by a positive measure \( m(\tau) \). In our case, it is the local conditional PDF \( f_k(\xi_k \mid I_{B_k} = 1) \)
For a continuous measure $m(\tau)$, there are two classical methods to compute the recurrence coefficients $\alpha_i$ and $\beta_i$: the Stieltjes procedure and the modified Chebyshev algorithm (W. Gautschi, 1982).

The Stieltjes procedure uses the fact that the coefficients $\alpha_i$ and $\beta_i$ can be expressed by the following simple formulas:

$$\alpha_i = \frac{\langle \pi_i, \pi_i \rangle}{\langle \pi_i, \pi_i \rangle}, \quad i = 0, 1, 2, \ldots$$

$$\beta_0 = \langle \pi_0, \pi_0 \rangle, \quad \beta_i = \frac{\langle \pi_i, \pi_i \rangle}{\langle \pi_{i-1}, \pi_{i-1} \rangle}, \quad i = 1, 2, \ldots,$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in terms of the measure $m(\tau)$

$$\langle f, g \rangle = \int f(\tau)g(\tau)m(\tau)d\tau$$

we use an interpolatory quadrature to evaluate the integral (Notaris, 2001).

The above two formulas together with the recurrence relation can be used to calculate recursively as many coefficients $\alpha_i$ and $\beta_i$ as desired.
Using the Stieltjes procedure, the recurrence coefficients $\alpha_i$ and $\beta_i$ are computed iteratively using the following stopping criterion: (W. Gautschi, 1994)

$$|\beta_i^s - \beta_i^{s-1}| \leq \varepsilon \beta_i^s, \quad i = 0, 1, \ldots, n-1$$

where $s$ is the number of quadrature points and $\varepsilon$ is the relative error.

For other methods, refer to (W. Gautschi, 1982)

If a measure $m(\tau)$ is given and orthogonal polynomials up to $p$th order are needed, we first compute the recurrence coefficients $\alpha_i$ and $\beta_i, \quad i = 0, 1, \ldots, n-1$

Once the recurrence coefficients are obtained, the orthogonal polynomials are uniquely determined. From the recurrence coefficients, the Gauss-type quadrature points and the corresponding integration weights can be effectively derived (W. Gautschi, 1994)

Then we can compute the expectation value $\langle \psi_k^2 \rangle$ and $\langle \psi_i \psi_j \psi_k \rangle$, which are needed in the SSFEM formulation.
An adaptive procedure

- Let us assume that the gPC expansion of random field in element $k$ is

$$\hat{u}_k (\xi_k) = \sum_{i=0}^{N_p} \hat{u}_{k,i} \psi_{k,i}(\xi_k)$$

where $p$ is the highest order of PC and $N_p$ denotes the total number of basis modes given by

$$N_p = \frac{(p+d)!}{p!d!} - 1$$

where $d$ is the dimension of $\xi_k$ and $\hat{u}_{k,i}$ is the $i^{th}$ projection coefficient in the element $k$

- From the orthogonality of gPC, the local variance approximated by PC with order $p$ is given by

$$\sigma_{k,p}^2 = \sum_{i=1}^{N_p} \hat{u}_{k,i}^2 \langle \psi_i^2 \rangle$$
An adaptive procedure

- The approximate global mean $\bar{u}$ and variance $\bar{\sigma}^2$ can be expressed by

  $$\bar{u} = \sum_{k=1}^{N} \hat{u}_{k,0} \Pr(I_{B_k} = 1), \quad \bar{\sigma}^2 = \sum_{k=1}^{N} \left[ \sigma_{k,p}^2 + (\hat{u}_{k,0} - \bar{u})^2 \right] \Pr(I_{B_k} = 1)$$

- Let $\gamma_k$ denote the error of local variance. We can write the exact global variance as

  $$\sigma^2 = \bar{\sigma}^2 + \sum_{k=1}^{N} \gamma_k \Pr(I_{B_k} = 1)$$

- We define the local decay rate of relative error of the gPC approximation in each element as follows:

  $$\eta_k = \frac{\sigma_{k,p}^2 - \sigma_{k,p-1}^2}{\sigma_{k,p}^2} = \frac{\sum_{i=N_{p-1}+1}^{N_p} \hat{u}_{k,i}^2 \langle \psi_i^2 \rangle}{\sigma_{k,p}^2}$$
Some derivations

Global mean:

\[ \bar{u} = \int_B u(\xi) f(\xi) d\xi \approx \sum_{k=1}^N \Pr(I_{B_k} = 1) \int_{B_k} \hat{u}_k(\xi_k) \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k \]

As we have seen before, the first term is 1, i.e. \( \psi_0(\xi_k) = 1 \)

So

\[ \int_{B_k} \hat{u}_k(\xi_k) \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k = \int_{B_k} \sum_{i=0}^P \hat{u}_{k,i} \psi_i(\xi_k) \psi_0(\xi_k) \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k \]

\[ = \hat{u}_{k,0} \]

\[ \bar{u} = \sum_{k=1}^N \hat{u}_{k,0} \Pr(I_{B_k} = 1) \]
Some derivations

Global variance:

$$\sigma^2 = \int_B (u(\xi) - \bar{u})^2 f(\xi) d\xi \approx \sum_{k=1}^{N} \Pr(I_{B_k} = 1) \int_{B_k} (\hat{u}_k(\xi_k) - \bar{u})^2 f_k(\xi_k | I_{B_k} = 1) d\xi_k$$

Using again that $$\psi_0(\xi_k) = 1$$, we can show that:

$$\int_{B_k} (\hat{u}_k(\xi_k) - \bar{u})^2 f_k(\xi_k | I_{B_k} = 1) d\xi_k$$

$$= \int_{B_k} \left( \sum_{i=0}^{P} \hat{u}_{k,i} \psi_i(\xi_k) - \bar{u} \right)^2 \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k$$

$$= \int_{B_k} \left[ \sum_{i=1}^{P} \hat{u}_{k,i} \psi_i(\xi_k) + (\hat{u}_{k,0} - \bar{u})\psi_0(\xi_k) \right]^2 \hat{f}_k(\xi_k | I_{B_k} = 1) d\xi_k$$

$$= \sum_{i=1}^{P} \hat{u}_{k,i}^2 \left< \psi_i^2(\xi_k) \right> + (\hat{u}_{k,0} - \bar{u})^2 \left< \psi_0^2(\xi_k) \right>$$
Some derivations

Global variance:

Define

\[ \sigma_{k,p}^2 = \sum_{i=1}^{P} \hat{u}_{k,i}^2 \langle \psi_i^2 \rangle \]

as local variance, and \( \langle \psi_0^2(\xi_k) \rangle = 1 \)

So

\[ \int_{B_k} (\hat{u}_k(\xi_k) - \bar{u})^2 \hat{f}_k(\xi_k \mid I_{B_k} = 1) \, d\xi_k \]

\[ = \sum_{i=1}^{P} \hat{u}_{k,i}^2 \langle \psi_i^2(\xi_k) \rangle + (\hat{u}_{k,0} - \bar{u})^2 \langle \psi_0^2(\xi_k) \rangle \]

\[ = \sigma_{k,p}^2 + (\hat{u}_{k,0} - \bar{u})^2 \]

\[ \overline{\sigma}^2 = \sum_{k=1}^{N} \left[ \sigma_{k,p}^2 + (\hat{u}_{k,0} - \bar{u})^2 \right] \Pr(I_{B_k} = 1) \]
An adaptive procedure

- Based on $\eta_k$ and the scaled parameter $\Pr(I_{B_k} = 1)$, a random element will be selected for potential refinement when the following condition is satisfied

$$\eta_k^\alpha \Pr(I_{B_k} = 1) \geq \theta_1, \quad 0 < \alpha < 1$$

where $\alpha$ and $\theta_1$ are prescribed constants.

- Furthermore, in the selected random element $k$, we use another threshold parameter $\theta_2$ to choose the most sensitive random dimension. We define the sensitivity of each random dimension as

$$r_i = \frac{(\hat{u}_{i,p})^2 \langle \psi_{i,p}^2 \rangle}{\sum_{j=N_{p-1}+1}^{N_p} \hat{u}_j \langle \psi_j^2 \rangle}, \quad i = 1, 2, \ldots, d,$$

where we drop the subscript $k$ for clarity and the subscript $i,p$ denotes the mode consisting only of random dimension $\xi_i$ with polynomial order $p$. 


An adaptive procedure

- All random dimensions which satisfy

\[ r_i \geq \theta_2 \cdot \max_{j=1,\ldots,d} r_j, \quad 0 < \theta_2 < 1, \quad i = 1, 2, \ldots, d, \]

will be split into two equal random elements in the next time step while all other random dimensions will remain unchanged.

- If \( \xi_k \) corresponds to element \( [a, b] \) in the original random space \([-1,1]\), the element \( [a, \frac{a+b}{2}] \) and \( [\frac{a+b}{2}, b] \) will be generated in the next level if the two criteria are both satisfied.

- Through this adaptive procedure, we can reduce the total element number while gaining the same accuracy and efficiency.
Numerical implementation

- In (X. Wan, G. Karniadakis, 2006), it is proved that for any orthogonal polynomials defined on $[a, b]$, where $a$ and $b$ are positive, we have

$$\langle \pi_{i+1}, \pi_{i+1} \rangle \leq (b-a)^2 \langle \pi_i, \pi_i \rangle$$

- Thus, if the element is small, the $L_2$ norm of $\pi_i$ will lead to underflow quickly, i.e. become very small.

- In practice, we rescale the random elements with finite boundaries by the following linear transformation:

$$\xi_{k,i} = \frac{b_{k,i} - a_{k,i}}{2} Y_{k,i} + \frac{b_{k,i} + a_{k,i}}{2} \quad i = 1, 2 \ldots d.$$  

where we map the random variable $\xi_k$ defined in element $k$ to a random variable $Y_k$ defined in $[-1,1]^d$.

- The PDF of $Y_k$ can be obtained as

$$\bar{f}(Y_k) = \det \left| \frac{\partial \xi_k}{\partial Y_k} \right| \hat{f}(\xi_k(Y_k)) = \frac{f(\xi_k(Y_k))}{\Pr(I_{B_k} = 1)} \prod_{i=1}^d \frac{b_{k,i} - a_{k,i}}{2}$$
We now summarize the overall ME-gPC algorithm:

- Step 1: build a stochastic ODE system by gPC
- Step 2: perform the decomposition of random space adaptively
  - time step $i$: from 1 to $M$
  - loop over all the random elements
  - if $\eta_k \Pr(I_{B_k} = 1) \geq \theta_1$ in element $k$, then
    - if $r_n \geq \theta_2 \cdot \max_{j=1,...,d} r_j$, then
      - split random dimension $\xi_n$ into two equal ones $\xi_{n,1}$ and $\xi_{n,2}$
      - map $\xi_{n,1}$ and $\xi_{n,2}$ to $Y_{n,1}$ and $Y_{n,2}$ defined on $[-1,1]$
      - construct one-dimensional orthogonal polynomials for $Y_{n,1}$ and $Y_{n,2}$
    - end if
    - construct one-dimensional orthogonal polynomials using tensor products
  - end if
  - update the information by gPC method
  - end element loop
  - end time step
- Step 3: postprocessing stage

(X. Wan, G. Karniadakis, 2006)
Numerical implementation

- The continuity relation:

\[ u_{B_1}(\xi) = u_{B_2}(\xi), \quad \xi \in \overline{B}_1 \cap \overline{B}_2 \]

where \( \overline{B}_1 \) and \( \overline{B}_2 \) indicate the closure of two adjacent random elements, respectively, is \textit{not} required as in the deterministic problems since the measure of the interface is zero.

- Complexity of ME-gPC: We decompose a stochastic problem into \( N \) independent ones, since continuity is unnecessary in random space. Thus, if polynomials of the same order are used in both gPC and ME-gPC, the cost of ME-gPC will increase linearly by a factor \( N \) compared to the cost of gPC.

- However, ME-gPC loses efficiency for problems with strong discontinuity and high-dimensional random inputs, because the number of random elements has to increase fast to maintain a desired accuracy.
We can also apply conventional/adaptive sparse grid collocation method to solve the stochastic problem in each sub domain.

As shown in earlier lecture, the local mean and variance is very easy to compute through integration of the basis function or applying the sparse grid quadrature method directly and thus we can get the global mean and variance through the formula discussed earlier.

However, in order to apply the adaptive criterion developed for GPCE, we need to find the local gPC basis in each element.

To do this, we can project the collocation solution onto each basis to obtain its expansion coefficient using the numerical quadrature rule associated with the collocation points since there exists a unique correspondence between gPC basis and Lagrange basis defined by grid points used in ME-PCM.
Let us assume that the gPC expansion of random field in element $k$ is

$$\hat{u}_k(\xi_k) = \sum_{i=0}^{N_p} \hat{u}_{k,i} \psi_{k,i}(\xi_k)$$

where $p$ is the highest order of PC and $N_p$ denotes the total number of basis modes given by

$$N_p = \frac{(p + d)!}{p!d!} - 1$$

where $d$ is the dimension of $\xi_k$ and $\hat{u}_{k,i}$ is the $i^{th}$ projection coefficient in the element $k$.

Then the coefficients can be computed as follows:

$$\hat{u}_{k,i} = \frac{\langle \hat{u}_k(\xi_k), \psi_{k,i}(\xi_k) \rangle}{\langle \psi_{k,i}^2(\xi_k) \rangle}$$

where the numerator is known and the denominator is a high dimensional integral which can be computed using sparse grid quadrature.
From the definition of the two error estimators:

\[
\eta_k = \frac{\sigma_{k,p}^2 - \sigma_{k,p-1}^2}{\sigma_{k,p}^2} = \sum_{i=N_{p-1}+1}^{N_p} \hat{u}_{k,i}^2 \langle \psi_i^2 \rangle, \quad i = 1, 2, \ldots, d,
\]

we note that not all gPC coefficients are utilized in the adaptivity criterion. In fact, from above we can see that it is only necessary to project the collocation solution onto the highest modes of the basis in order to evaluate this criterion. The order \( p \) of the polynomial chaos basis used can be determined by the following proposition

**Proposition:** To maintain an accurate transformation between collocation solutions and the gPC spectral expansion, the polynomial order of the gPC basis can be taken up to \( \lceil m/2 \rceil \), where \( \lceil \cdot \rceil \) indicates the integer not larger than * and \( m \) indicated the degree of exactness of the quadrature rule.
Numerical Example
The Kraichnan-Orszag three-mode problem

- The governing equations are (X.Wan, G. Karniadakis, 2005),

\[
\begin{align*}
\frac{dx_1}{dt} &= x_2 x_3 \\
\frac{dx_2}{dt} &= x_1 x_3 \\
\frac{dx_3}{dt} &= -2x_1 x_2
\end{align*}
\]

subject to stochastic initial conditions:

\[x_1(0) = x_1(0; \omega), \quad x_2(0) = x_2(0; \omega), \quad x_3(0) = x_3(0; \omega)\]

- There is a discontinuity when the random initial condition approaches \(x_1 = x_2\). So let us first look at the discontinuity in the deterministic solution.
The Kraichnan-Orszag three-mode problem

Singularity at plane \( x_2 = 1 \)
The Kraichnan-Orszag three-mode problem

- For computational convenience and clarity, we first perform the following transformation

\[
\begin{bmatrix}
    y_1 \\
    y_2 \\
    y_3
\end{bmatrix} = \begin{bmatrix}
    \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\
    \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\
    0 & 0 & 1
\end{bmatrix} \begin{bmatrix}
    x_1 \\
    x_2 \\
    x_3
\end{bmatrix}
\]

(X.Wan, G. Karniadakis, 2005)

- The resulting governing equations become:

\[
\frac{dy_1}{dt} = y_1y_3, \quad \frac{dy_2}{dt} = -y_2y_3, \quad \frac{dy_3}{dt} = -y_1^2 + y_2^2
\]

- The discontinuity then occurs at the planes \( y_1 = 0 \) and \( y_2 = 0 \).

- Thus, we study the stochastic response subject to the following random initial input:

\[
y_1(0; \omega) = 1, \quad y_2(0; \omega) = 0.1\xi(\omega), \quad y_3(0; \omega) = 0
\]

where \( \xi \sim U(-1,1) \). Since the random initial data \( y_2(0; \omega) \) can cross the plane \( y_2 = 0 \) we know that gPC will fail for this case.
The Kraichnan-Orszag three-mode problem

Singularity at plane $y_1 = 0$
In the earlier two figures, we showed the evolution of the mean and variance of $y_1$ within the time interval [0,30].

The gPC results were obtained with polynomial order $p=15$.

It can be seen that comparing to the results given by Monte Carlo with 1,000,000 realizations, gPC with polynomial order $p=15$ begins to lose accuracy at and fails beyond this point.
Adaptive ME - gPC

Mean of y₁

MC : 1,000,000
ME-gPC : N = 28, p = 3, theta = 0.01
ME-gPC : N = 76, p = 3, theta = 0.001

Variance of y₁

MC : 1,000,000
ME-gPC : N = 28, p = 3, theta = 0.01
ME-gPC : N = 76, p = 3, theta = 0.001
Adaptive mesh with $\alpha = \frac{1}{2}$, $p = 3$, $\theta_1 = 0.01$

Adaptive mesh with $\alpha = \frac{1}{2}$, $p = 3$, $\theta_1 = 0.001$
Adaptive ME - PCM

Variance of $y_1$

Length of Elements

MC-SOBOL: 1,000,000
ME-PCM: $\theta = 10^{-3}$
Adaptive ME – PCM : 2D input

- MC-SOBOL: 1,000,000
- ME-PCM: $\theta_1=10^{-3}$, $\theta_2=10^{-2}$
Decomposition of random dimension -
- High Dimensional Model Representation (HDMR)
Motivation

- Previously developed conventional and adaptive collocation methods are not suitable for high-dimensional problems due to their weakly dependence on the dimensionality (logarithmic) in the error estimate. Although ASGC can alleviate the problem to some extent, it depends on the regularity of the problem and it is only effective when some random dimensions are more important than others.

- As is well known, in realistic random heterogeneous media often we deal with a very small correlation length and this results in a rather high-dimensional stochastic space with nearly the same weights along each dimension. In this case, all the previously developed stochastic methods are obviously not applicable.

- These modeling issues for high-dimensional stochastic problems motivate the use of the so called High dimensional model representation (HDMR) technique.
Let \( f(Y) \) be a real-value multivariate stochastic function: \( \mathbb{R}^N \rightarrow \mathbb{R} \), which depends on a \( N \)-dimensional random vector \( Y = (Y_1, Y_2, \ldots, Y_N) \in [0,1]^N \). A HDMR of \( f(Y) \) can be described by

\[
f(Y) = f_0 + \sum_{s=1}^{N} \sum_{i_1 < \cdots < i_s} f_{i_1 \cdots i_s} (Y_{i_1}, \ldots, Y_{i_s})
\]

where the interior sum is over all sets of \( s \) integers \( i_1, \ldots, i_s \), that satisfy \( 1 \leq i_1 < \cdots < i_s \leq N \). This relation means that

\[
f(Y) = f_0 + \sum_{i=1}^{N} f_i (Y_i) + \sum_{i_1 < i_2} f_{i_1 i_2} (Y_{i_1}, Y_{i_2}) + \sum_{i_1 < i_2 < i_3} f_{i_1 i_2 i_3} (Y_{i_1}, Y_{i_2}, Y_{i_3}) + \cdots + \sum_{i_1 < \cdots < i_s} f_{i_1 \cdots i_s} (Y_{i_1}, \ldots, Y_{i_s}) + \cdots + f_{12 \ldots N} (Y_1, \ldots, Y_N)
\]

can be viewed as a finite hierarchical correlated function expansion in terms of the input random variables with increasing dimensions.

For most well-defined physical systems, the first- and second-order expansion terms are expected to have most of the impact upon the output and the contribution of higher-order terms would be insignificant.

High dimensional model representation (HDMR)

\[ f(Y) = f_0 + \sum_{i=1}^{N} f_i(Y_i) + \sum_{i_1 < i_2}^{N} f_{i_1i_2}(Y_{i_1},Y_{i_2}) + \sum_{i_1 < i_2 < i_3}^{N} f_{i_1i_2i_3}(Y_{i_1},Y_{i_2},Y_{i_3}) + \ldots + \sum_{i_1 < \ldots < i_s}^{N} f_{i_1 \ldots i_s}(Y_{i_1},\ldots,Y_{i_s}) + \ldots + f_{12\ldots N}(Y_1,\ldots,Y_N) \]

In this expansion:

- \( f_0 \) denotes the zeroth-order effect which is a constant.

- The component function \( f_i(Y_i) \) gives the effect of the variable \( Y_i \) acting independently of the other input variables.

- The component function \( f_{i_1i_2}(Y_{i_1},Y_{i_2}) \) describes the interactive effects of the variables \( Y_{i_1} \) and \( Y_{i_2} \). Higher-order terms reflect the cooperative effects of increasing numbers of variables acting together to impact upon \( Y \).

- The last term \( f_{12\ldots N}(Y_1,\ldots,Y_N) \) gives any residual dependence of all the variables locked together in a cooperative way to influence the output \( f(Y) \).
HDMR: Compact notation

- This equation is often written in a more compact notation:

\[ f(Y) = \sum_{u \subseteq D} f_u(Y_u) \]

for a given set \( u \subseteq D \) where \( D := \{1, \ldots, N\} \) denotes the set of coordinate indices and \( f_\emptyset(Y_\emptyset) = f_0 \). Here, \( Y_u \) denotes the \( |u| \)-dimensional vector containing those components of \( Y \) whose indices belong to the set \( u \), where \( |u| \) is the cardinality of the corresponding set \( u \), i.e. \( Y_u = (Y_i)_{i \in u} \).

- For example, if \( u = \{1, 3, 5\} \) then \( |u| = 3 \) and \( f_u(Y_u) \) implies \( f_{135}(Y_1, Y_3, Y_5) \).

- The component functions \( f_u(Y_u) \) can be derived by minimizing the error functional

\[
\int_G \left[ f(Y) - f_0 - \sum_{i=1}^{N} f_i(Y_i) - \cdots - \sum_{i_1 < \cdots < i_s} f_{i_1 \cdots i_s}(Y_{i_1}, \ldots, Y_{i_s}) \right]^2 d\mu(Y) \quad 0 \leq s \leq N
\]

subject to the orthogonal constraint

\[
\int_{G^N} f_u(Y_u) f_v(Y_v) d\mu(Y) = 0, \quad \text{for} \quad u \neq v
\]
HDMR: Component functions

- The measure $d \mu$ determines the particular form of the error functional and of the component functions.

- By the variational principal, the component functions $f_u(Y_u)$ can be explicitly given as

$$f_u(Y_u) := \sum_{v \subseteq u} (-1)^{|u|-|v|} P_v f(Y_v)$$

where the measure $\mu$ induces the projection operator $P_u : \Gamma^N \rightarrow \Gamma^{|u|}$

$$P_u f(Y_u) := \int_{\Gamma^{N-|u|}} f(Y) d\mu_{\mathcal{D}\setminus u}(Y)$$

where

$$d\mu_{\mathcal{D}\setminus u}(Y) := \prod_{i \notin u} d\mu_i(Y_i)$$

- There are two different forms of HDMD induced by different measure: ANOVA-HDMR and CUT-HDMR.
**HDMR**

Lebesgue measure \( d\mu(\mathbf{Y}) = d(\mathbf{Y}) = \prod_{i=1}^{N} Y_i \)

\[
P_{u} f(\mathbf{Y}_{u}) := \int_{\Gamma_{N-|u|}} f(\mathbf{Y}) d\mathbf{Y}_{D\setminus u}
\]

\(|N-|u|| \text{ dimensional integration} \)

\[
f_{0} = \int_{\Gamma_{N}} f(\mathbf{Y}) d\mathbf{Y}, \quad f_{i}(Y_{i}) = \int_{\Gamma_{N-1}} f(\mathbf{Y}) \prod_{j\neq i} dY_{j} - f_{0}
\]

\[
f_{ij}(Y_{i}, Y_{j}) = \int_{\Gamma_{N-2}} f(\mathbf{Y}) \prod_{k\neq i,j} dY_{k} - f_{i}(Y_{i}) - f_{j}(Y_{j}) - f_{0}, \quad \ldots
\]

Computational expensive

Dirac measure \( d\mu(\mathbf{Y}) = \prod_{i=1}^{N} \delta(Y_{i} - \bar{Y}_{i}) dY_{i} \)

at a reference point \( \mathbf{Y} = (\bar{Y}_{1}, \ldots, \bar{Y}_{N}) \)

\[
P_{u} f(\mathbf{Y}_{u}) := f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus \mathbf{Y}_{u}}
\]

\(|u| \text{ dimensional function} \)

\[
f_{0} = f(\bar{\mathbf{Y}}), \quad f_{i}(Y_{i}) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus Y_{i}} - f_{0}
\]

\[
f_{ij}(Y_{i}, Y_{j}) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus (Y_{i}, Y_{j})} - f_{i}(Y_{i}) - f_{j}(Y_{j}) - f_{0}, \quad \ldots
\]

Computational efficient

---

**Materials Process Design and Control Laboratory**

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Within the framework of CUT-HDMR, we can write
\[
f(Y) = \sum_{u \subseteq D} f_u(Y_u) = \sum_{u \subseteq D} \sum_{v \subseteq u} (-1)^{|u|-|v|} f(Y_v)_{Y=Y_v \setminus Y_v}
\]
where the notation $Y=Y_v \setminus Y_v$ means that the components of $Y$ other than those indices that belong to the set equal to those of the reference point.

If the HDMR is a converged expansion, the choice of this point does not affect the approximation. In this work, the mean of the random input vector is chosen as the reference point.

Therefore, the $N$-dimensional stochastic problem is transformed to several lower-order $|v|$-dimensional problems $f(Y_v)_{Y=Y_v \setminus Y_v}$, which can easily solved by ASGC:
\[
f(Y) = \sum_{u \subseteq D} \sum_{v \subseteq u} (-1)^{|u|-|v|} \sum_{|i| \leq N+q} \sum_{j \in B_i} w^{ij}_v(\mathbf{x}) \cdot a^i_j(Y_v)
\]
where $w^{ij}_v(\mathbf{x})$ are the hierarchical surpluses for different sub-problems indexed by $v$ and $a^i_j(Y_v)$ is only a function of the coordinates belong to set $v$.
Let us denote

\[ J_u = \sum_{v \subseteq u} (-1)^{|u| - |v|} \sum_{|i| \leq N+q} \sum_{j \in B_i} w_v^{ij}(x) \cdot I_j^i \]

as the mean of the component function \( f_u \). Then the mean of the HDMR expansion is simply \( \mathbb{E}[f(Y)] = \sum_{u \subseteq D} J_u \).

The basic conjecture underlying HDMR is that the component functions arising in typical well-defined physical problems will not likely exhibit high-order cooperativity among the input variables such that the first- and second-order expansion terms are expected to have most of the impact upon the output and the contribution of higher-order terms would be insignificant.

In other words, instead of solving the \( N \)-dimensional problem directly using ASGC, which is impractical for extremely high dimensional problem, we only need to solve several 1- or 2- dimensional problems, which can be solved efficiently via ASGC.
Effective dimension of a stochastic function

- Let $\hat{f} := \sum_{u \subseteq D} |J_u|$ be the sum of all contributions to the mean value.

- Then, for the proportion $\alpha \in (0, 1]$, the truncation dimension is defined as the smallest integer $N_t$, such that
  $$\sum_{u \subseteq \{1, \ldots, N_t\}} |J_u| \geq \alpha \hat{f},$$

  whereas, the superposition dimension is defined as the smallest integer $N_s$, such that
  $$\sum_{|u| \leq N_s} |J_u| \geq \alpha \hat{f}$$

- The superposition dimension is also called the order of the HDMR expansion.

- With the definition of effective dimensions, we can thus truncate the expansion and take only a subset of all indices $u \subseteq D$. Here we assume that the set $S$ satisfies the following admissible condition:
  $$u \in S \text{ and } v \subset u \Rightarrow v \in S$$

  This is to guarantee that all the terms can be calculated via the expression of the component functions.
Effective dimension of a stochastic function

- In practice, we always truncate the expansion by taking only a subset of all indices $u \subseteq D$. We can define an interpolation formula $A_S f$ for the $S$ approximation of $f$ as

$$A_S f := \sum_{u \in S} A(f_u)$$

- It is common to refer to the terms $\{f_u : |u| = l\}$ collectively as the “order-terms”. Then the expansion order is the maximum of $l$. The number of collocation points in this expansion is defined as the sum of the number of points for each sub-problem, i.e. $M = \sum_{v \in S} M_v$

- However, the number of order-$l$ component function is $\sum_{i=1}^{l} \frac{N!}{i!(N-i)!}$, which increases quickly with the number of dimensions. Therefore, we developed an adaptive version of HDMR.
Approximation error

- We fix $\alpha \in (0, 1]$ and assume that $N_s$ and $N_t$, the corresponding superposition and truncation dimensions, are known. With the definition of the index set $S_{N_t, N_s} := \{u \subseteq \{1, \ldots, N_t\}, |u| \leq N_s\}$, we have the following theorem:

**Theorem 1.** Let $S = S_{N_t, N_s}$, and let $A$ be the ASGC interpolant with the same error threshold $\varepsilon$ for all the sub-problems. Then:

$$|f - A_S f| \leq c(N_s, N_t)\varepsilon + \varepsilon_t,$$

for all $f \in F_N$. Here, the constant $c(N_t, N_s)$ depends on the effective dimensions, but does not depend on the nominal dimension $N$. $\varepsilon_t$ is the truncation error of according to the definition of effective dimensions.

- Therefore, it is expected that the expansion converges to the true value with decreasing error threshold and increasing number of component functions.
As discussed before, for extremely high dimensional problem, even a second order expansion is impractical due to the increasing of the number of component functions. Therefore, we would like to develop an adaptive version of HDMR for automatically and simultaneously detecting the truncation and superposition dimensions.

We assume each component function $f_{\mathbf{u}}$ is associated with a weight which describes the contribution of the term $f_{\mathbf{u}}$ to the HDMR.

First, we try to find the important dimensions. To this end, we always construct the zeroth- and first-order HDMR expansion. This is because each first-order component function is only a one-dimensional function and contains the information from only one particular dimension. We define a weight:

$$\eta_i = \frac{\|J_{\{i\}}\|_{L_2}}{\|f_0(\mathbf{Y})\|_{L_2}} \quad J_{\{i\}} = \int f_i(Y_i) dY_i$$

Then we define the important dimensions as those whose weights are larger than a predefined error threshold $\theta_1$. Only higher order terms which consist of only these important dimensions are considered.
Adaptive HDMR

- For example, if the important dimensions are 1, 3 and 5, then only the higher order terms \{13\}, \{15\}, \{35\} and \{135\} are considered.

- However, not all the possible terms are computed. For higher-order term, a weight is also defined as

\[
\eta_u = \frac{\| J_u \|_{L^2}}{\| \sum_{v \in \mathcal{S}, |v| \leq |u|-1} J_v \|_{L^2}}
\]

We also define the important terms in a similar way. We put all the important dimensions and higher-order terms in to a set \( \mathcal{T} \). When adaptively constructing HDMR for each new order, we then only calculate the terms whose indices satisfy the admissibility relation

\[
u \in \mathcal{D} \text{ and } v \subset u \Rightarrow v \in \mathcal{T}
\]
Continued with the example, now if we want to construct the second order expansion, only \{13\}, \{15\} and \{35\} are calculated.

Then we compute the weights for each term. Assume \{13\} is the important term, the important index set is \(S_0 = \{0, 1, 3, 5, 13\}\).

Now, we go to 3\(^{rd}\) order expansion. The only possible term is \{135\}. Its subset \{13\} and \{15\} do not belong to the important index set, i.e. does not satisfy the admissible condition. Therefore, the construction stops.

In other words, among all the possible indices, we only want to find the terms which can be computed using the previous known important component functions and find those terms which may have significant contributions to the overall expansion while ignoring other trivial terms in order to reduce the computational cost for extremely high-dimensional problem.
Let us denote the order of expansion as $p$. Furthermore, we also define a relative error $\rho$ of the integral value between two consecutive expansion orders $p$ and $p-1$ as

$$\rho = \frac{\left\| \sum_{|u| \leq p} J_u - \sum_{|u| \leq p-1} J_u \right\|_{L^2}}{\left\| \sum_{|u| \leq p-1} J_u \right\|_{L^2}}$$

If $\rho$ is smaller than another predefined error threshold $\theta_2$, the HDMR is regarded as converged and the construction stops.

In this way, the construction will automatically stop and then the obtained HDMR expansion can be used as a stochastic surrogate model (response surface) for the solution. Any statistics can be easily computed through this expansion.
**Algorithm 2** Adaptive construction of the index set $S$

Initialize: Let $S = \{\emptyset\}$, $R = \{\emptyset\}$ and $T = \{\emptyset\}$. Set $p = 1$.

Construct the zeroth and first-order component functions:
- Solve each sub-problem using the ASGC method with error threshold $\varepsilon$ and add all the indices to $S$.
- Compute the weights of each first-order term. Add those dimensions which satisfy $\eta \geq \theta_1$ to set $T$.

repeat
- $p \leftarrow p + 1$. Construct the set $R$ whose indices satisfy the admissibility relation for $|u| = p$.
- If $R \neq \{\emptyset\}$, for each index $u \in R$, solve the corresponding sub-problem using ASGC with error threshold $\varepsilon$ and add all the indices to $S$.
- Compute the weight of component functions. Add those indices which satisfy $\eta \geq \theta_1$ to set $T$ and clear set $R$.
- Compute the relative error $\rho$.

until $R = \{\emptyset\}$ or $\rho < \theta_2$;
Numerical Example
Numerical example: Flow through random media

Basic equation for pressure and velocity in a domain

\[ \nabla \cdot \mathbf{u} = f \quad \text{in} \quad D \]
\[ \mathbf{u} = -k \nabla p \quad \text{in} \quad D \]

where \( f(x) \) denotes the source/sink term. A mixed finite element method is utilized to solve the forward problem.

To impose the non-negativity of the permeability, we will treat the permeability as a log random field obtained from the K-L expansion

\[ Y(\omega) = \log(K(\omega)) = \sum_{i=1}^{N} \sqrt{\lambda_i} \phi_i(\mathbf{x})Y_i \]

where \( Y \) is a zero mean random field with a covariance function

\[ \text{Cov}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp \left( -\frac{|x_1 - y_1|}{L} - \frac{|x_2 - y_2|}{L} \right) \]

where \( L \) is the correlation length and \( \sigma \) is the standard deviation.
Numerical example: K-L Expansion

- The eigenvalues and their corresponding eigenfunctions can be determined analytically. The \( \xi_i \) are assumed as i.i.d uniform random variables on \([-1,1]\).

- According to the decay rate of eigenvalues, the number of stochastic dimensions is \( N = 33,108 \) and \( 500 \), respectively for \( L = 1.0, 0.5 \) and \( 0.25 \).

- Monte Carlo simulations are conducted for the purpose of comparison. For each case, the reference solution is taken from \( 10^6 \) samples and all errors are defined as normalized \( L_2 \) errors. In all cases, \( \theta_2 = 10^{-4} \).
Standard deviation of the \( v \) velocity-component along the cross section \( y = 0.5 \) for different correlation lengths

Number of component functions is 2271 while for the full second order expansion it is 125251. Thus, the advantage of using adaptive HDMR is obvious.
PDF at (0,0.5) for different correlation lengths

PDF of the $v$ velocity-component at point (0,0.5) for different correlation lengths

$N = 33$  
$L = 1.0$

$N = 108$  
$L = 0.5$

$N = 500$  
$L = 0.25$

$\sigma^2 = 1.0, \varepsilon = 10^{-6}$
Each PDF is generated by plotting the kernel density estimate of 10000 output samples through sampling the input space and computing the output value through the HDMR approximation.

The spatial variability determines the total input variability, which further determines the interactive effects between the input variables. The larger the input variability is, the stronger the interactive effects are. The role of HDMR component functions is to capture these input effects upon the output.

The higher the input variability is, the more component functions are needed. In our case, $\sigma^2 = 1.0$ represents a rather high input variability. Higher order terms are therefore needed to capture these effects whereas only first-order terms are not enough.

The accuracy of the PDFs indicate that the corresponding HDMR approximations are indeed very accurate. Therefore, we can obtain any statistics from this stochastic reduced-order model, which is an advantage of the current method over the naïve MC method.
Convergence of the normalized errors of the standard deviation of the $v$ velocity-component for different correlation lengths

\[ \sigma^2 = 1.0, \theta = 10^{-4} \]

$N = 33, 108, 500$

Algebraic convergence rate better than MC

Nearly the same for three cases, does not depend on the smoothness of the random space

Convergence of the normalized errors of the standard deviation of the $v$ velocity-component for different correlation lengths
Standard deviations for different $\sigma^2$ with $N = 500$

$$e = 8.08 \times 10^{-4}$$

$$e = 7.37 \times 10^{-4}$$

Standard deviation of the $v$ velocity-component along the cross section $y = 0.5$ for different $\sigma^2$. 

$L = 0.25, N = 500$
PDF at $(0,0.5)$ for different $\sigma^2$ with $N = 500$

For low input variability, even first order expansion is accurate.

For high input variability, first order expansion deviates from MC. More component terms are needed to improve the accuracy.

For moderate input variability, first order does not deviate significantly from MC. However, a few second order terms are still needed.

$\sigma^2 = 0.01$

$\sigma^2 = 0.25$

$\sigma^2 = 2.0$

PDF of the $v$ velocity-component at point $(0,0.5)$ for different $\sigma^2$
Direct solution of the 500 dimensional problem using ASGC is impractical due to the huge computational cost. convergence rate deteriorates with the increasing of the input variability. However, it is still better than that of MC

Convergence of the normalized errors of the standard deviation of the $v$ velocity-component for different $\sigma^2$