Efficient Techniques for Quantifying Uncertainty

Jasmine Foo
Sloan-Kettering Institute, NYC
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*Brown University, Division of Applied Mathematics

Goals of Uncertainty Quantification

- Estimate moments of solutions to systems with stochastic or uncertain parameters
- Calculate probability of certain events (e.g. catastrophic failure, cell death)
- Understand propagation of uncertainty in time
- Parameter sensitivity analysis
- ...

Outline

- Model problem and notation
- Introduction to stochastic spectral methods
- Multi-Element Probabilistic Collocation Method
- Numerical Examples
- Extension of MEPCM (future work)
- Acknowledgements

Model Problem

$$(\Omega, \mathcal{F}, P)$$

Probability space

$$L(\mathbf{x}, t, \omega; u) = f(\mathbf{x}, t, \omega)$$

$$\omega \in \Omega$$

differential operator

random dependence

$u(\mathbf{x}, t; \omega)$ = ?

Examples:

Simple ODE

$$\frac{\partial u}{\partial x} = \xi(\omega) u$$

$$\xi : \Omega \to \Gamma \subset \mathbb{R}$$

random variable

parameter space

Diffusion problem with stochastic permeability:

$a(x;\omega)$ a spatial random process

$$\begin{cases} -\nabla \cdot (a(x;\omega)\nabla u) &= \quad f(x,\omega) \quad \text{in } D, \\ u &= \quad 0 \quad \text{on } \partial D, \end{cases}$$

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Stochastic spectral methods

Stochastic spectral methods utilize a polynomial spanning basis on the RANDOM space Γ .

Wiener 1938

$$T(\mathbf{x},t;\omega) = \sum_{i=0}^{\infty} T_i(\mathbf{x},t)\Psi_i(\xi(\omega))$$

$\Psi_i(\xi(\omega))$: ***Generalized*** Polynomial Chaos

Basis choice is problem dependent

- Computationally efficient moment estimation in problems with stochastic parameters *(orders of magnitude faster than Monte Carlo, high order accuracy)*

- Recently adapted for sensitivity analysis and correlation analysis in biological applications (Kim et al, 2007; F. et al, 2008-preprint)

- Limitations: “curse of dimensionality”

Generalized Polynomial Chaos (GPC) Basis

Assume: one random input variable ξ with probability density function (PDF) ρ

GPC basis made up of polynomial functionals of random variables, e.g:

$$\Psi_0(\xi) = 1$$

$$\Psi_1(\xi) = \xi$$

$$\Psi_2(\xi) = \xi^2 - 1$$

$$\Psi_3(\xi) = \xi^3 - 3\xi$$

$$\Psi_4(\xi) = \xi^4 - 6\xi^2 + 3.$$

One-dimensional Hermite family.

Generalized Polynomial Chaos (GPC) Basis

- Orthogonality: $\langle \Psi_i \Psi_j \rangle = \langle \Psi_i^2 \rangle \delta_{ij}$ $\quad w = \rho$

where the inner product $\langle f(\xi) g(\xi) \rangle = \int f(\xi) g(\xi) w(\xi) \mathrm{d}\xi$

- Weight function determined by PDF of ξ : $\quad w = \rho$

Polynomial		PDF ρ
Hermite	⟺	Gaussian
Jacobi	⟺	Beta

Xiu & Karniadakis, 02; Ghanem & Spanos, 91; Cameron & Martin 47

Stochastic Spectral Methods

1. Expand the unknown solution into combination of polynomial chaos basis functions

Unknown coefficients called “gPC coefficients”

Number of basis functions used

$$u(\mathbf{x}, t; \omega) = \sum_{i=1}^{P} u_i(\mathbf{x}, t)\Psi_i(\xi)$$

Polynomial chaos basis functions

2. Expand the random parameters in L , f into combinations of polynomial chaos basis functions , e.g.:

$$f(\mathbf{x}, t; \omega) = \sum_{i=1}^{P} f_i(\mathbf{x}, t)\Psi_i(\xi)$$

Known coefficients

3. Solve for the unknown coefficients $u_i(\mathbf{x}, t)$ via galerkin/collocation projection

Moments

Question: Knowing the coefficients u_i , how can we find the moments of $u(\mathbf{x},t;\omega)$?

known

Mean: $\langle u(\mathbf{x},t)\rangle$ = $\left\langle \sum_{i=1}^{P} u_i(\mathbf{x},t)\Psi_i(\omega) \right\rangle = u_0(\mathbf{x},t)$

orthogonality of basis functions wrt PDF

Variance: $\langle u^2(\mathbf{x},t)\rangle - \langle u(\mathbf{x},t)\rangle^2$

$\langle u^2(\mathbf{x},t)\rangle$= $\left\langle \left(\sum_{i=1}^{P} u_i(\mathbf{x},t)\Psi_i(\omega) \right)^2 \right\rangle = \sum_{i=1}^{P} u_i^2(\mathbf{x},t) < \Psi_i^2 >$

known known

Well-chosen basis functions make calculating moments easy

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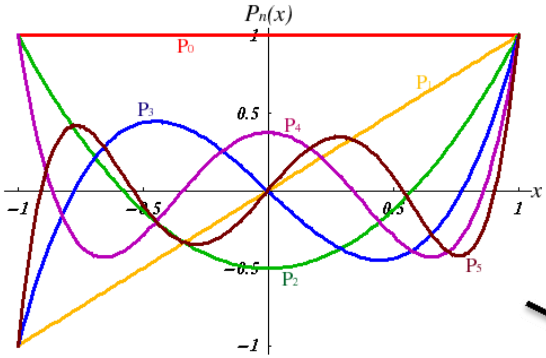
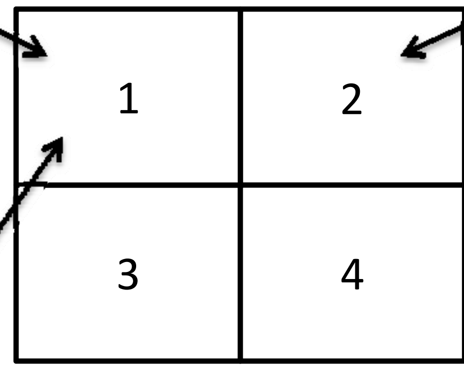
Multi-Element Probabilistic Collocation Method (ME-PCM)



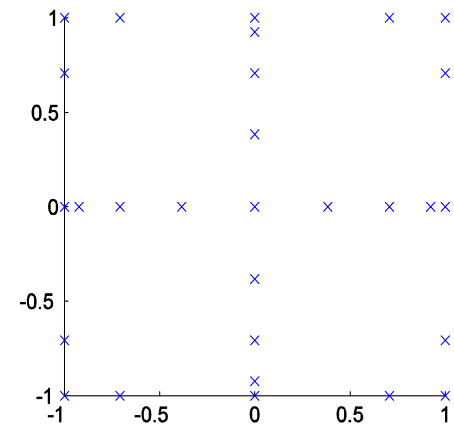
local GPC basis in each element, orthogonal wrt local conditional PDF

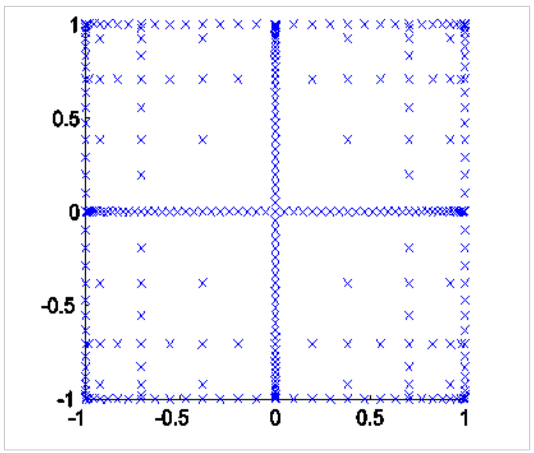
Domain decomposition of random space into elements



(example 2D random space)

Γ





sparse collocation grids

unknowns

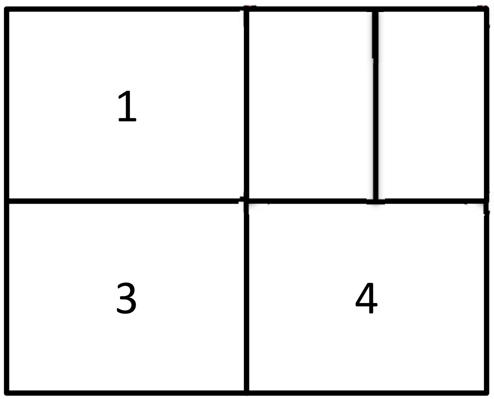
$$\sum_{i=1}^{P} u_i(\mathbf{x}, t)\, \Psi_i(\xi)$$

local solution expansion in each element

sampling method

Multi-Element Probabilistic Collocation Method (ME-PCM)

Adaptivity:



- In each element, calculate relative variance due to highest modes of basis

$$\eta_k = \frac{\sigma_{k,p} - \sigma_{k,p-1}}{\sigma_{k,p-1}},$$

$\sigma_{k,p}$ is the local variance from p-th order polynomial chaos.

- If exceeds a certain tolerance, FLAG

- Calculate the variance in each dimension

- Split element in dimension of highest variance and construct new bases on new elements

Convergence rates of the ME-PCM

Using the **degree of exactness** m of the quadrature rule, the moments error of ME-PCM using a uniform mesh can be expressed as:

$$\left|\mathbb{E}\|u\|_{H_0^1(D)} - \hat{u}_{mean}\right| \leq$$

physical space norm

MEPCM mean solution

$$\epsilon + C\|E_\Gamma\|_{m+1,\infty,\Gamma}|u_k|_{W^{m+1,\infty}(\Gamma;H_0^1(D))}h^{m+1}$$

spatial discretization error

stochastic discretization error

where h is the size of the elements.

Remark: norm of error functional $\|E_\Gamma\|_{m+1,\infty,\Gamma}$ usually exhibits p-type convergence in polynomial interpolation order, obtaining h/p-type convergence of the moments error. Similar hp-type results obtained for L2 error.

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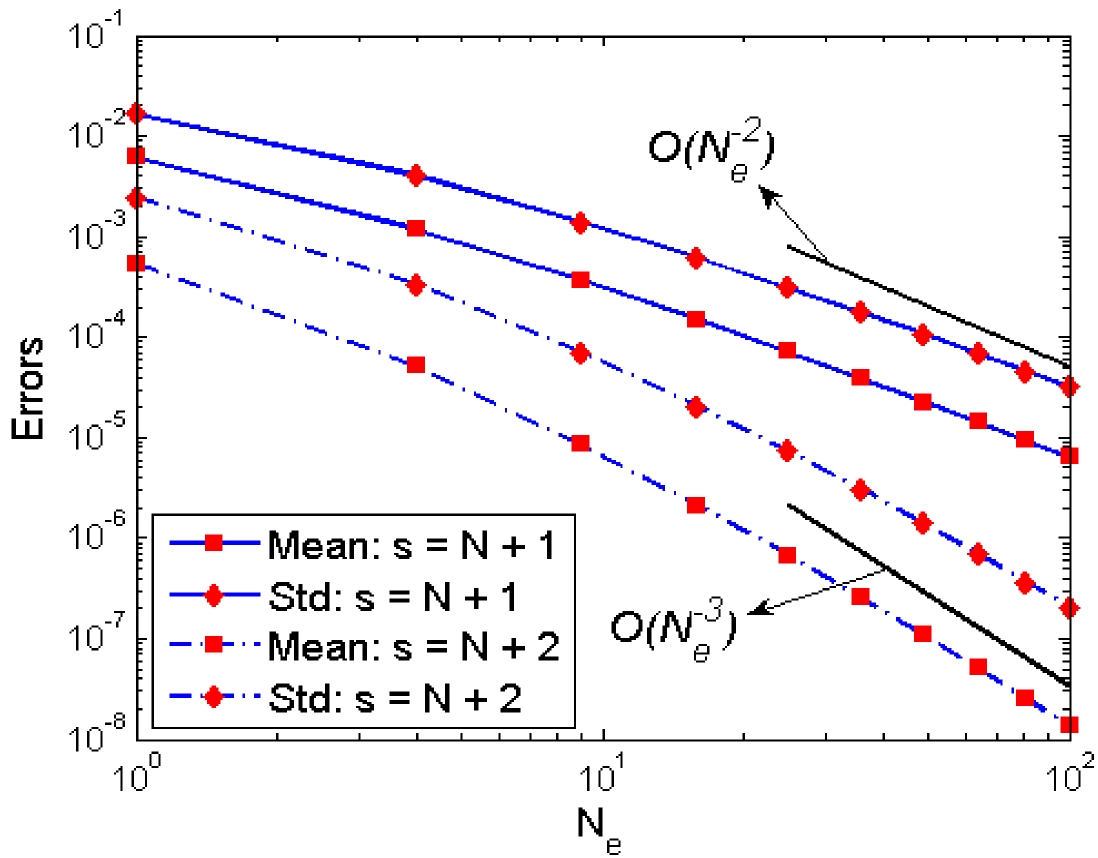
ME-PCM study of stochastic elliptic problem

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x};\omega)\nabla u(\boldsymbol{x};\omega)) = \sin(x)\cos(y) & \text{in } D, \\ u(\boldsymbol{x};\omega) = 0 \quad \text{on } \partial D, & D = [0,1]^2 \end{cases}$$

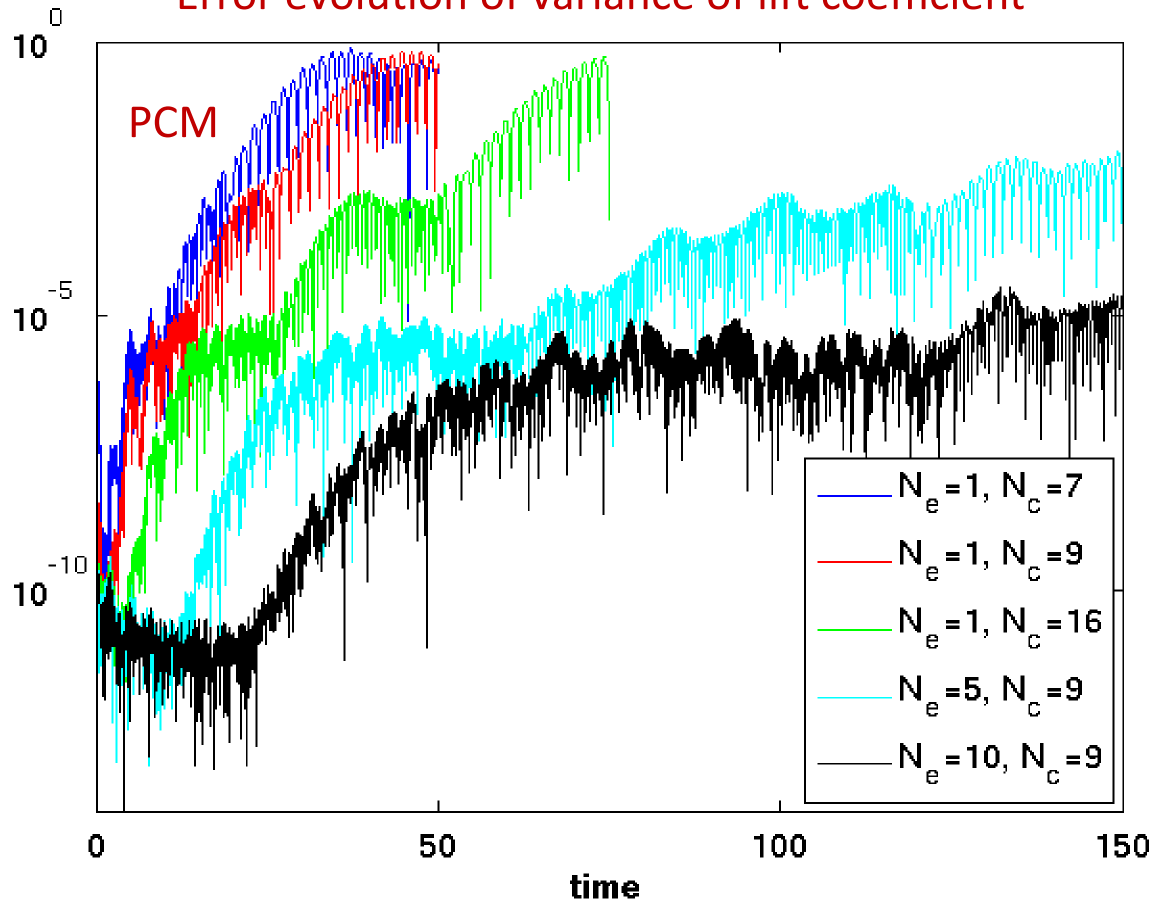


- $a(x;\omega)$ is a two-dimensional random input (N=2)
- Y_n are B(1,1) -distributed on [-1,1]
- MEPCM: uniform mesh on $[-1,1]^2$, Gauss sparse grids
- *h*-convergence asymptotically reaches: $O(N_e^{\frac{-(m+1)}{N}})$

Noisy flow past 2D stationary cylinder

- Noisy inflow boundary condition $u = 1 + \delta\xi, \quad v = 0$
- Performance in long time-integration considered.
- Spectrum of solution in parametric (random) space increases with time.

Error evolution of variance of lift coefficient



- δ = 0.1, ξ uniformly distributed on $[-\sqrt{3}, \sqrt{3}]$
- Gauss-Legendre tensor product grid in each element.
- Time integration for 25 vortex-shedding cycles

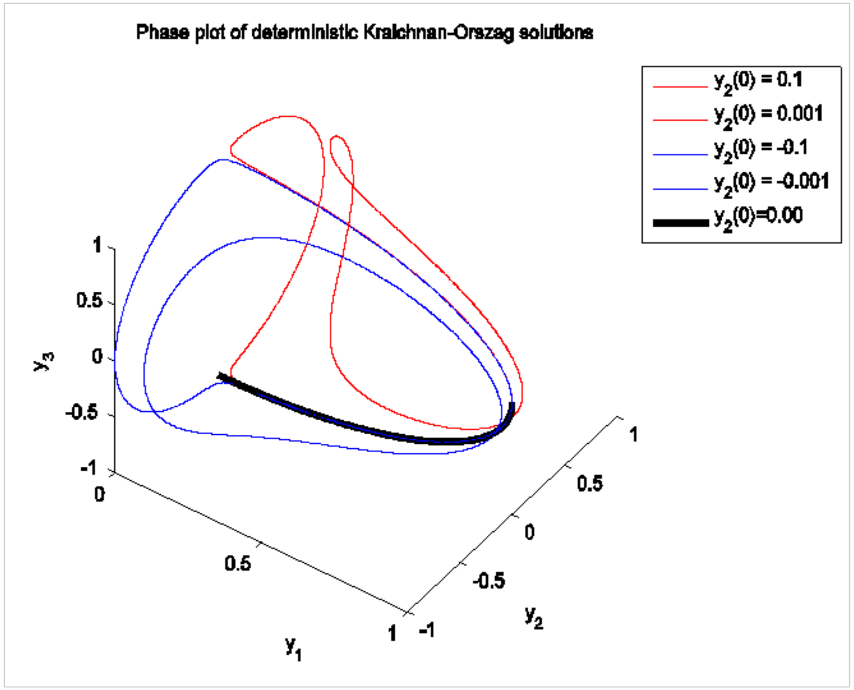
ME-PCM and discontinuities in random space:

Kraichnan-Orszag problem with 2D random input:

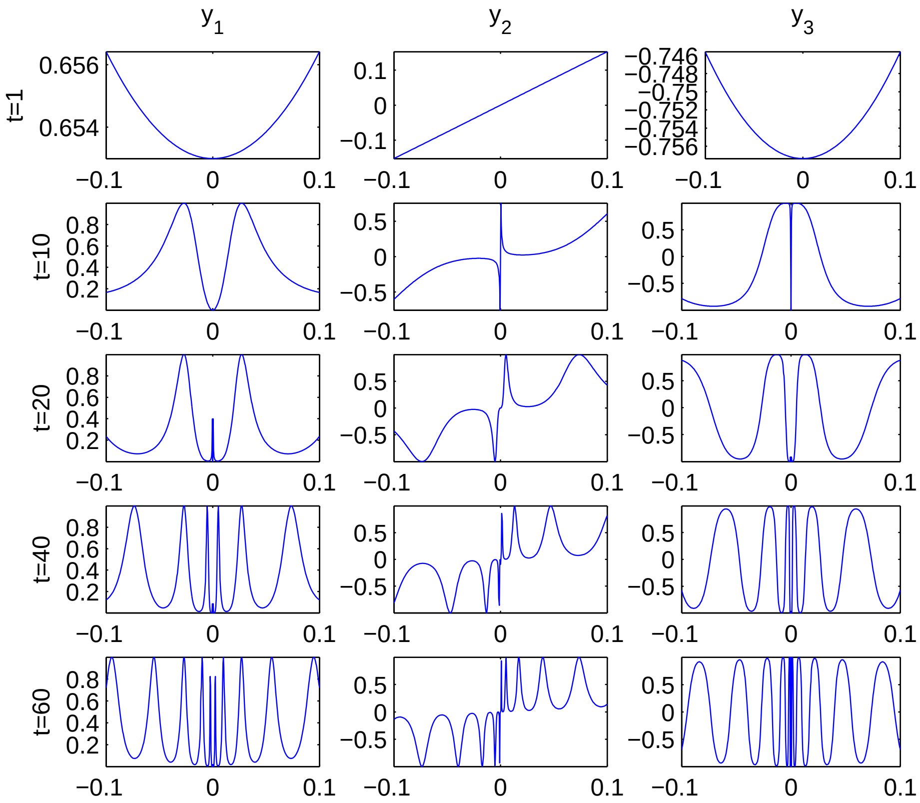
$$\frac{dy_1}{dt} = y_1 y_3 \quad \frac{dy_2}{dt} = -y_2 y_3 \quad \frac{dy_3}{dt} = -{y_1}^2 + {y_3}^2$$

$$y_1(0) = 1.0 \quad y_2(0) = 0.1\xi_1 \quad y_3 = \xi_2$$

$\xi_1, \quad \xi_2$ iid, uniform rvs on [-1,1]



Response curves on [-0.1,0.1]

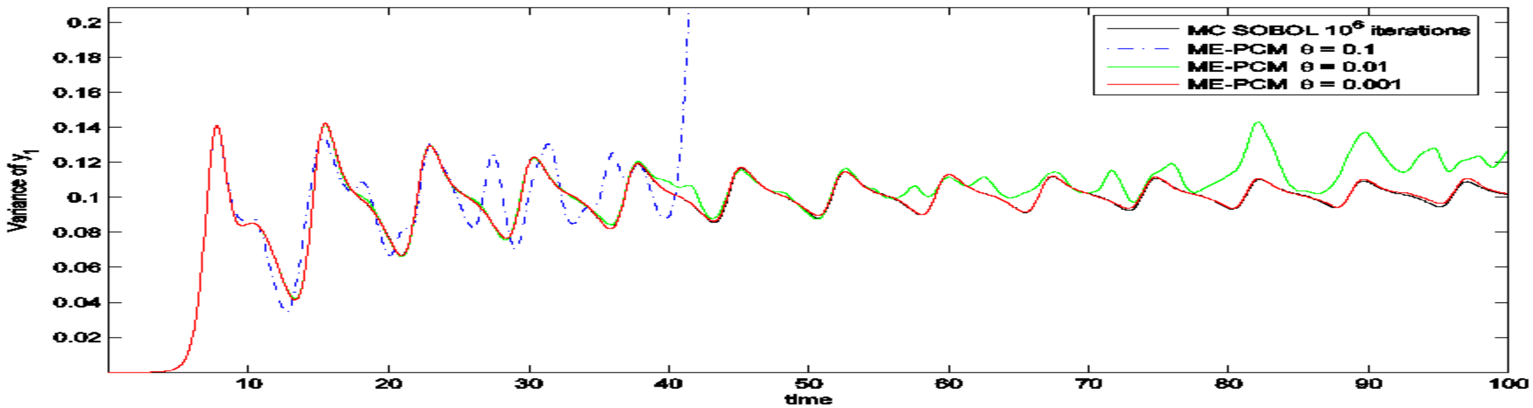


Solution exhibits discontinuous dependence on $y_2(0)$ at the origin.

h-Adaptive ME-PCM: Kraichnan-Orszag problem

h-Adaptive ME-PCM at varying θ levels for long time integration:

1D random input: $y_1(0) = 1.0 \quad y_2(0) = 0.1\xi_1 \quad y_3 = 0$



Computational cost (seconds) of h-Adaptive ME-PCM vs h-Adaptive ME-GPC:

2D random input: $y_1(0) = 1.0 \quad y_2(0) = 0.1\xi_1 \quad y_3 = \xi_2$

Error level ϵ_{L^2}	h-Adaptive ME-PCM	h-Adaptive ME-gPC
10^{-2}	0.5	11.95
10^{-3}	3.43	29.31
10^{-4}	38.8	337.7

h-Adaptive ME-PCM is faster even with two extra projection steps

- ME-gPC: Legendre chaos p=2
- MEPCM: Gauss-Legendre tensor grid
- Decrease θ (adaptivity tolerance) to achieve desired accuracy

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- ❑ Multi-element probabilistic collocation method (ME-PCM)
- ❑ ME-PCM Numerical examples
- ➢ Future work: Extension for higher-dimensional problems (MEPCM-A)

Future work: MEPCM-A for higher-dimensional problems

Using ANOVA-type decompositions: based on the hierarchical decomposition of a multidimensional function into combinations of functions of subgroups of its dimensions (Hoeffding 1948):

demonstrated to be effective in problems with over 100 random dimensions

$$\mathcal{I}_\mu f(x_1, x_2, \ldots, x_N) \quad =$$

$$\mathcal{I}_\mu f_0 + \sum_{j_1,(\nu=1)}^{N} \mathcal{I}_\mu f_{j_1}(x_{j_1}) + \sum_{j_1<j_2,(\nu=2)}^{N} \mathcal{I}_\mu f_{j_1,j_2}(x_{j_1}, x_{j_2}) +$$

$$\sum_{j_1<j_2<j_3(\nu=3)}^{N} \mathcal{I}_\mu f_{j_1,j_2,j_3}(x_{j_1}, x_{j_2}, x_{j_3}) + \cdots \mathcal{I}_\mu f_{j_1,\ldots,j_N}(x_{j_1}, \cdots, x_{j_N})$$

μ : order of approximation in each dimension

ν : dimension of each sub-problem

Use of ANOVA-type decompositions for standard PCM - Griebel, Schwab (2005, 2007).

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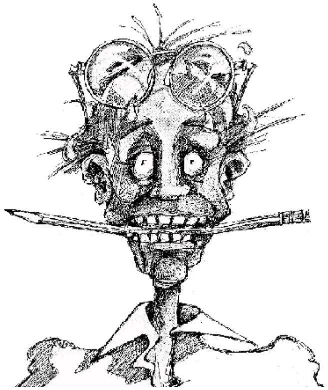

L2 error for stochastic elliptic problem

We consider the $L^2(\Gamma; H_0^1(D))$ error of MEPCM interpolant for the stochastic elliptic problem. Input assumed to be uniform random vector.

$$\|\tilde{u} - u\|_{L^2(\Gamma;H_0^1(D))} \leq \|\tilde{u} - u_k\|_{L^2(\Gamma;H_0^1(D))} + \|u_k - u\|_{L^2(\Gamma;H_0^1(D))}$$

stochastic discretization error deterministic discretization error

For MEPCM using a uniform mesh of size h and Gauss-Legendre abscissas on each element, the stochastic discretization error is bounded as:

$$\|\tilde{u} - u\|_{L^2(\Gamma;H_0^1(D))} \leq C \sum_{j=1}^{N} \exp\{-r_j(h)p_j\}.$$

$$where \quad r_j(h) = \log\left[\frac{\alpha_j}{2h}\left(1 + \sqrt{1 + \frac{h^2}{\alpha_j^2}}\right)\right]$$

(related to stochastic regularity of solution in each random dimension, Babuska 2007)

L2 error of ME-PCM interpolant

Remarks:

- Rewriting $r_j(h)$ as:

$$r_j(h) = \log \frac{1}{h} + \log \left[\frac{\alpha_j}{2} \left(1 + \sqrt{1 + \frac{h^2}{\alpha_j^2}} \right) \right]$$

we obtain the factor in the error estimate:

$$\exp(-p_j \log \frac{1}{h}) = h^{p_j}$$

demonstrating h-type convergence for this problem.

- Alternatively, fixing h we obtain p-type convergence through the term:

$$\exp(-r_j(h)p_j)$$

- Result generalizable to non-uniform random inputs, other types of interpolation (e.g. sparse grids, etc).