Reduced-Order Models for Stochastic Partial Differential Equations

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In honor of Martin Schultz
Yale University, October 2012

Yale Numerical Analysis Group, c. 1981

Partial Differential Equations with Uncertain Coefficients

Examples:

Diffusion equation: $-\nabla \cdot (a(\mathbf{x}, \boldsymbol{\xi}) \nabla u) = f$

Navier-Stokes equations: $-\nabla \cdot (a(\mathbf{x}, \boldsymbol{\xi}) \nabla \vec{u}) + (\vec{u} \cdot \nabla)\vec{u} + \nabla p = \vec{f}$

$\nabla \cdot \vec{u} = 0$

Posed on $\mathcal{D} \subset \mathbb{R}^d$ with suitable boundary conditions

Sources: models of diffusion in media with uncertain permeabilities
multiphase flows

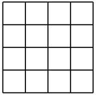
Uncertainty / randomness:

$a = a(\mathbf{x}, \boldsymbol{\xi})$ is a *random field*: for each fixed $x \in \mathcal{D}$, $a(x, \boldsymbol{\xi})$ is a random variable depending on m random parameters $\xi_1, \ldots, \xi_m$

In this study: $a(\mathbf{x}, \boldsymbol{\xi}) = a_0(\mathbf{x}) + \sum_{r=1}^{m} a_r(\mathbf{x})\, \xi_r$

Possible sources:

Karhunen-Loève expansion or Piecewise constant coefficients on $\mathcal{D}$



Monte-Carlo Simulation

Traditional approach:

Sample $a(\mathbf{x}, \xi)$ at all required $\mathbf{x} \in \mathcal{D}$, solve in usual way

Multiple realizations (samples) of $a(\mathbf{x}, \cdot)$ $\longrightarrow$
Multiple realizations of u $\longrightarrow$
Statistical properties of u obtained by averaging

Done using spatial discretization, finite elements or finite differences
$\Longrightarrow$ multiple linear(ized) discrete problems

$$A_{\boldsymbol{\xi}} u_{\boldsymbol{\xi}}^{(h)} = f_h$$

for realization of discrete solution $u_{\boldsymbol{\xi}}^{(h)}$

Problem: convergence is slow, requires many discrete PDE solves

The Stochastic Galerkin Method

Philosophy: Extend finite-element methodology to develop alternative to Monte-Carlo (Ghanem, Spanos, Babuška, Deb, Oden, Matthies, Keese, Karniadakis, Xue, Schwab, Todor)

Standard weak formulation of diffusion problem: find $u \in H^1_E(\mathcal{D})$ s.t.

$$a(u,v) = \ell(v) \quad \text{for all } v \in H^1_{E_0}(\mathcal{D}),$$

where

$$a(u,v) = \int_{\mathcal{D}} a\nabla u \cdot \nabla v dx, \quad \ell(v) = \int_{\mathcal{D}} fv dx$$

Introduce extended (*stochastic*) weak formulation

$$\langle a(u,v)\rangle = \int_{\Omega}\int_{\mathcal{D}} a\nabla u \cdot \nabla v \, dx \, dP(\Omega) = \int_{\boldsymbol{\xi}(\Omega)}\int_{\mathcal{D}} a(\mathbf{x},\boldsymbol{\xi})\,\nabla u \cdot \nabla v \, d\mathbf{x}\, \rho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$$

Bilinear form entails integral over image of random variables $\boldsymbol{\xi}$

Require joint density function associated with $\boldsymbol{\xi}$

$\boldsymbol{\xi}$ plays the role of a Cartesian coordinate

Result:

- From problem in d-dimensional physical space depending on m random parameters, get $(d+m)$-dimensional "continuous" problem
- $d = 2$ or 3, $m = 5, 50, 100, \ldots$

Discretization / Finite dimensional spaces:

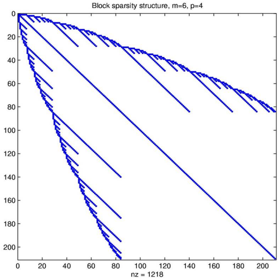
- In physical space: $\mathcal{S}_h \subset H^1_{E_0}(\mathcal{D})$, basis $\{\phi_j\}_{j=1}^N$
  Example: piecewise linear "hat functions"
- In space of random variables: $\mathcal{T}_p \subset L^2(\Gamma)$, basis $\{\psi_\ell\}_{\ell=1}^M$
  Example: m-variate polynomials in $\boldsymbol{\xi}$ of total degree p

Discrete solution:

$$u^{(hp)}(\mathbf{x}, \boldsymbol{\xi}) = \sum_{j=1}^N \sum_{\ell=1}^M u_{j\ell}\phi_j(\mathbf{x})\psi_\ell(\boldsymbol{\xi})$$

Requires solution of large coupled system (right)

Stochastic dimension: $M = \binom{m+p}{p}$



The Stochastic Collocation Method

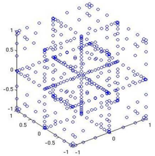
Monte-Carlo (sampling) method: find $u \in H^1_E(\mathcal{D})$ s.t.

$$\int_{\mathcal{D}} a(\mathbf{x}, \boldsymbol{\xi}^{(k)}) \nabla u \cdot \nabla v dx \quad \text{for all } v \in H^1_{E_0}(\mathcal{D})$$

for a collection of samples $\{\boldsymbol{\xi}^{(k)}\} \in L^2(\Gamma)$

Collocation (Xiu, Hesthaven, Babuška, Nobile, Tempone, Webster)

Choose $\{\boldsymbol{\xi}^{(k)}\}$ in a special way (sparse grids), then construct discrete solution $u^{(hp)}(\mathbf{x}, \boldsymbol{\xi}) \in \mathcal{S}_h^E \otimes \mathcal{T}^{(p)}$ to interpolate $\{u_h(\mathbf{x}, \boldsymbol{\xi}^{(k)})\}$



Structure of collocation solution:

$$u_p^{(hp)}(\mathbf{x}, \boldsymbol{\xi}^{(k)}) := \sum_{\boldsymbol{\xi}^{(k)} \in \Theta_p} u_c(x, \boldsymbol{\xi}^{(k)}) L_{\boldsymbol{\xi}^{(k)}}(\boldsymbol{\xi})$$

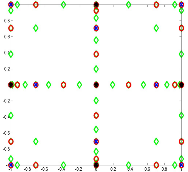
Advantages (vs. stochastic Galerkin):

- decouples algebraic system (like MC)
- applies in a straightforward way to nonlinear random terms

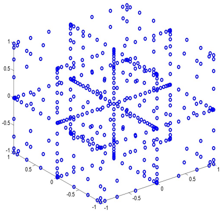
Examples of sparse grids

At right: 2D

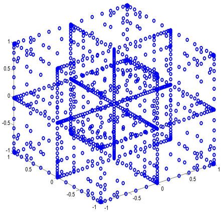
$*$ Level $p = 1$
$\times$ Level $p = 2$
$\circ$ Level $p = 3$
$\diamond$ Level $p = 4$



Below: 3D



Level $p = 5$



Level $p = 6$

Properties of These Methods

For both Galerkin and collocation

- Each computes a discrete function $u^{(hp)}$
- Moments of u estimated using moments of $u^{(hp)}$ (cheap)
- Convergence: $\|E(u) - E(u^{(hp)})\|_{H_1(\mathcal{D})} \leq c_1 h + c_2 r^p$, $r < 1$
  Exponential in polynomial degree
- Contrast with Monte Carlo:
  Perform N_{MC} (discrete) PDE solves to obtain samples $\{u_h^{(s)}\}_{s=1}^{N_{MC}}$
  Moments from averaging, e.g., $\hat{E}(u_h) = \frac{1}{N_{MC}} \sum_{s=1}^{N_{MC}} u_h^{(s)}$
  Error $\sim 1/\sqrt{N_{MC}}$

One other thing:

"p" has different meaning for Galerkin and collocation
For comparable accuracy:

$\#$ stochastic dof (Collocation) $\approx 2^p$ ($\#$ stochastic dof (Galerkin))

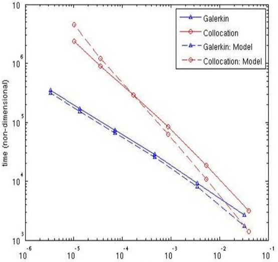
Representative Comparison

Diffusion equation: $-\nabla \cdot (a(\mathbf{x}, \xi) \nabla u) = f$

On unit square with 32×32 finite-difference discretization

Coefficient: Five-term Karhunen-Loève expansion:

$$a(\mathbf{x}, \xi) = a_0(\mathbf{x}) + \sum_{r=1}^{m} \sqrt{\lambda_r}\, a_r(\mathbf{x})\, \xi_r, \quad m = 5$$



Reduced Basis Methods for Parameter-Dependent PDEs

Starting point for these examples:

Parameter-dependent PDE $\mathcal{L}_{\boldsymbol{\xi}} u = f$

In examples given:

$\mathcal{L}_{\boldsymbol{\xi}} = -\nabla \cdot (a_0 + \sum_{r=1}^{m} a_r(\mathbf{x})\xi_r)\nabla$

Complication:

Expensive if many realizations (samples of $\boldsymbol{\xi}$) are required

Idea (Patera, Boyaval, Bris, Lelièvre, Maday, Nguyen, ...):

Solve the problem on a *reduced space*

That is: by some means, choose $\boldsymbol{\xi}^{(1)}, \boldsymbol{\xi}^{(2)}, \ldots, \boldsymbol{\xi}^{(n)}$, $n \ll N$

Solve $\mathcal{L}_{\boldsymbol{\xi}^{(i)}} u^{(i)} = f$, $u^{(i)} = u(\cdot, \boldsymbol{\xi}^{(i)})$, $i = 1, \ldots, n$

For other $\boldsymbol{\xi}$, approximate $u(\cdot, \boldsymbol{\xi})$ by $\tilde{u}(\cdot, \boldsymbol{\xi}) \in span\{u^{(1)}, \ldots, u^{(n)}\}$

Terminology: $\{u^{(1)}, \ldots, u^{(n)}\}$ called **snapshots**

Approximation at discrete level:

$$u_h(\cdot,\boldsymbol{\xi}) \approx \tilde{u}_h(\cdot,\boldsymbol{\xi}) \in span\{u_h^{(1)},\ldots,u_h^{(n)}\}$$

Matrix form:

Coefficient matrix $A_{\boldsymbol{\xi}}$, nodal coefficients $\mathbf{u}_h$, $\tilde{\mathbf{u}}_h$, $\mathbf{u}^{(1)},\ldots\mathbf{u}^{(n)}$

Q = orthogonal matrix whose columns span space spanned by $\{\mathbf{u}^{(i)}\}$

Galerkin condition: make residual orthogonal to spanning space

$r = f - A_{\boldsymbol{\xi}}\tilde{\mathbf{u}}_h(\boldsymbol{\xi}) = f - A_{\boldsymbol{\xi}} Q\mathbf{y}_{\boldsymbol{\xi}}$ orthogonal to Q

Result is reduced problem: Galerkin system of order $n \ll N$:

$$[Q^T A Q]\mathbf{y}_{\boldsymbol{\xi}} = Q^T f, \quad \tilde{\mathbf{u}}_h(\boldsymbol{\xi}) = Q\mathbf{y}_{\boldsymbol{\xi}}$$

Goal: Have reduced model capture features of the model
at significantly lower cost

How are costs reduced?

Matrix A of order N

Reduced matrix $Q^T A Q$ of order $n \ll N$

Solving reduced matrix is cheap for small n

Note: making assumption that $\mathcal{L}_{\boldsymbol{\xi}}$ is affinely dependent on $\boldsymbol{\xi}$

$$\mathcal{L}_{\boldsymbol{\xi}} = \sum_{i=1}^{k} \phi_i(\boldsymbol{\xi})\mathcal{L}_i$$
$$\Rightarrow A_{\boldsymbol{\xi}} = \sum_{i=1}^{k} \phi_i(\boldsymbol{\xi})A_i$$
$$\Rightarrow Q^T A_{\boldsymbol{\xi}} A = \sum_{i=1}^{k} \phi_i(\boldsymbol{\xi})[Q^T A_i Q]$$

Means: constructing reduced matrix for new $\boldsymbol{\xi}$ is cheap

Key question: does reduced basis capture features of model?

Strategy for generating a basis / choosing snapshots (Patera, et al.):

For $\tilde{u}_h(\cdot,\boldsymbol{\xi}) \approx u_h(\cdot,\boldsymbol{\xi})$ (equivalently, $\tilde{\mathbf{u}}_{\boldsymbol{\xi}} \approx \mathbf{u}_{\boldsymbol{\xi}}$), use an **error indicator** $\eta(\tilde{u}_h) \approx \|e_h\|$, $e_h = u_h - \tilde{u}_h$

Given: a set of candidate parameters $\mathcal{X} = \{\boldsymbol{\xi}\}$,
an initial choice $\boldsymbol{\xi}^{(1)} \in \mathcal{X}$, and $u^{(1)} = u(\cdot,\boldsymbol{\xi}^{(1)})$

Set $Q = \mathbf{u}^{(1)}$

`while` $max_{\boldsymbol{\xi}\in\mathcal{X}}\left(\eta(\tilde{u}_h(\cdot,\boldsymbol{\xi}))\right) > \tau$

compute $\tilde{u}_h(\cdot,\boldsymbol{\xi})$, $\eta(\tilde{u}_h(\cdot,\boldsymbol{\xi}))$, $\forall\,\boldsymbol{\xi}\in\mathcal{X}$ % use current reduced

let $\boldsymbol{\xi}^* = argmax_{\boldsymbol{\xi}\in\mathcal{X}}\left(\eta(\tilde{u}_h(\cdot,\boldsymbol{\xi}))\right)$ % basis

`if` $\eta(\tilde{u}_h(\cdot,\boldsymbol{\xi}^*)) > \tau$ `then`

augment basis with $u_h(\cdot,\boldsymbol{\xi}^*)$, update Q with $\mathbf{u}_{\boldsymbol{\xi}^*}$

`endif`

`end`

Potentially expensive, but just viewed as "offline" *preprocessing*
"*Online*" simulation done using reduced basis

Reduced Basis + Sparse Grid Collocation

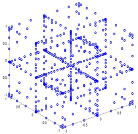
Adapt to sparse grid collocation: Recall collocation solution

$$u_q^{(hp)}(x,\boldsymbol{\xi}^{(k)}) = \sum_{\boldsymbol{\xi}^{(k)}\in\Theta_q} u_c(x,\boldsymbol{\xi}^{(k)}) L_{\boldsymbol{\xi}^{(k)}}(\boldsymbol{\xi}) \qquad (1)$$

Main ideas:

1. Use sparse grid collocation points as candidate set $\mathcal{X}$,
2. Use reduced solution as coefficient $u_c(\cdot,\boldsymbol{\xi}^{(k)})$ whenever possible

Algorithm

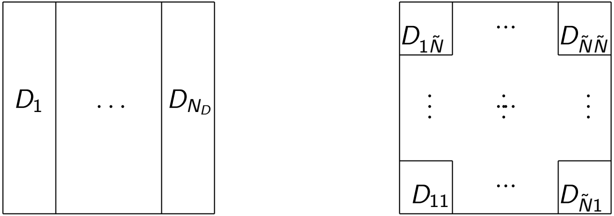


for each sparse grid level p
    for each point $\boldsymbol{\xi}^{(k)}$ at level p
        compute reduced solution $u_R(\cdot,\boldsymbol{\xi}^{(k)})$
        if $\eta(u_R(\cdot,\boldsymbol{\xi}^{(k)})) \le \tau$, then
            use $u_R(\cdot,\boldsymbol{\xi}^{(k)})$ as coefficient $u_c(\cdot,\boldsymbol{\xi}^{(k)})$ in (1)
        else
            compute snapshot $u_h(\cdot,\boldsymbol{\xi}^{(k)})$, use it as $u_c(\cdot,\boldsymbol{\xi}^{(k)})$ in (1)
            augment reduced basis with $u_h(\cdot,\boldsymbol{\xi}^{(k)})$, update Q with $\mathbf{u}_{\boldsymbol{\xi}^{(k)}}$
        endif
    end
end

To Assess Effectiveness

Benchmark problems: Diffusion equation $-\nabla \cdot (a(\mathbf{x}, \boldsymbol{\xi})\nabla u) = f$ in $\mathbb{R}^2$

Piecewise constant diffusion coefficient parameterized as a random variable $\boldsymbol{\xi} = [\xi_1, \cdots, \xi_{N_D}]^T$ independently and uniformly distributed in $\Gamma = [0.01, 1]^{N_D}$



(a) Case 1: N_D subdomains (b) Case 2: $N_D = \tilde{N} \times \tilde{N}$ subdomains

To assess effectiveness: consider

Full snapshot set, set of snapshots for all possible parameter values:

$$\mathcal{S}_\Gamma := \{u_h(\cdot, \boldsymbol{\xi}), \boldsymbol{\xi} \in \Gamma\}$$

Finite snapshot set, for finite $\Theta \subset \Gamma$:

$$\mathcal{S}_\Theta := \{u_h(\cdot, \boldsymbol{\xi}), \boldsymbol{\xi} \in \Theta\}$$

Question:

How many samples $\{\boldsymbol{\xi}\}$ / $\{u_h(\cdot, \boldsymbol{\xi})\}$ are needed to accurately represent the features of $\mathcal{S}_\Gamma$?

Experiment: to gain insight into this, estimate "rank" of $\mathcal{S}_\Gamma$

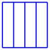
Generate a large set Θ of samples of $\boldsymbol{\xi}$
Generate the finite snapshot set $\mathcal{S}_\Theta$ associated with Θ
Construct the matrix S_Θ of coefficient vectors $\mathbf{u}_{\boldsymbol{\xi}}$ from $\mathcal{S}_\Theta$
Compute the rank of S_Θ

Results follow. Used 3000 samples

Experiment was repeated ten times with similar results

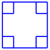
Estimated ranks of $\mathcal{S}_\Gamma$ for two classes of benchmark problems

Case 1



Grid \ N_D	2	3	4	5	6	7	8	9	10
$33^2 = 1089$	3	12	18	30	40	53	55	76	84
$65^2 = 4225$	3	12	18	30	40	48	55	70	87
$129^2 = 16641$	3	12	18	28	39	48	55	72	81

Case 2



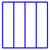
Grid \ N_D	4	9	16	25	36	49	64
$33^2 = 1089$	27	121	193	257	321	385	449
$65^2 = 4225$	28	148	290	465	621	769	897
$129^2 = 16641$	28	153	311	497	746	1016	1298

Trends:

- Rank is dramatically smaller than problem dimension N
- Rank is independent of problem dimension ($\sim$ (mesh size)$^{-2}$)
- In most cases, cost of treating reduced problem of given rank is low

Comparison with algorithm performance

Case 1



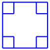
Case 1, 5 × 1 subdomains, 65 × 65 grid, rank=30

q	6	7	8	9	10	11	12	13	16
tol \ $\lvert\Theta_q\rvert$	11	61	241	801	2433	7K	19K	52K	870K
10^{-3}	10	9	0	0	0	0	0	0	0
10^{-4}	10	11	1	0	0	0	0	0	0
10^{-5}	10	13	0	0	0	0	0	0	0

Case 1, 9 × 1 subdomains, 65 × 65 grid, rank=70, $tol = 10^{-4}$

q	10	11	12	13	14	15	16	17
$\lvert\Theta_q\rvert$	19	181	1177	6001	26017	100897	361249	1218049
$N_{full\ solve}$	18	34	2	1	1	0	0	0

Case 2



Comparison with algorithm performance

Case 2, 2×2 subdomains, 65×65 grid, rank=28

q	5	6	7	8	9	10	11	12	15
$\lvert\Theta_q\rvert$ / tol	9	41	137	401	1105	2.9K	7.5K	18.9K	272K
10^{-3}	7	11	3	0	0	0	0	0	0
10^{-4}	7	12	3	0	0	0	0	0	0
10^{-5}	7	13	2	3	0	0	0	0	0

Case 2, 4×4 subdomains, 65×65 grid, rank=290, $tol = 10^{-4}$

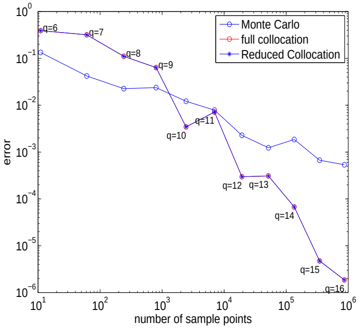
q	17	18	19	20	21
$\lvert\Theta_q\rvert$	33	545	6049	51137	353729
$N_{full\ solve}$	32	168	27	3	4

To assess accuracy: Examine error (vs. reference solution) in expected values of full or reduced collocation solution:

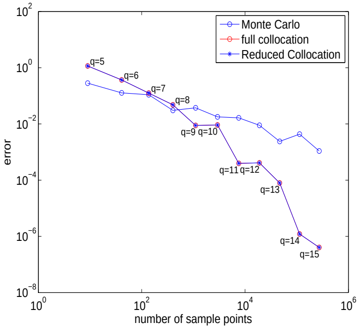
Full collocation $$\epsilon_h := \left\| \tilde{\mathbb{E}}\left(u_q^{hsc}\right) - \tilde{\mathbb{E}}\left(u_r^{hsc}\right) \right\|_0 \Big/ \left\| \tilde{\mathbb{E}}\left(u_r^{hsc}\right) \right\|_0$$

Reduced collocation $$\epsilon_R := \left\| \tilde{\mathbb{E}}\left(u_q^{rsc}\right) - \tilde{\mathbb{E}}\left(u_r^{hsc}\right) \right\|_0 \Big/ \left\| \tilde{\mathbb{E}}\left(u_r^{hsc}\right) \right\|_0$$

Case 1: vertical subdomains



Case 2: square subdomains



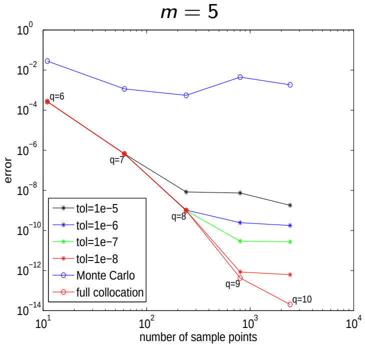
Different example: diffusion coefficient with KL expansion:

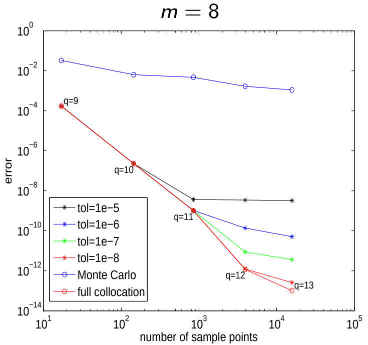
Diffusion coefficient $a_0 + \sigma \sum_{r=1}^{m} \sqrt{\lambda_r} a_r(\mathbf{x}) \xi_r)$

From covariance function $c(\mathbf{x}, \mathbf{y}) = \sigma \exp\left(-\frac{|x_1 - y_1|}{c} - \frac{|x_2 - y_2|}{c} \right)$

Smaller correlation length $c \sim$ more terms m

Examine $c = 4$, $m = 4$ and $c = 2.5$, $m = 8$.





Concluding Remarks

For PDEs with uncertain, parameter-dependent coefficients:

- *Spectral methods*: stochastic Galerkin, stochastic collocation, offer prospects for fast solution
- They suffer from "the curse of dimensionality"
- Costs of collocation can be reduced using reduced basis methodology