Analysis of SPDEs and numerical methods for UQ

Part IV: Convergence of the Sparse grid SCFEM and applications to stochastic inverse problems

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Thanks to Max Gunzburger & Guannan Zhang (FSU), Fabio Nobile (MOX), Raul Tempone (KAUST)

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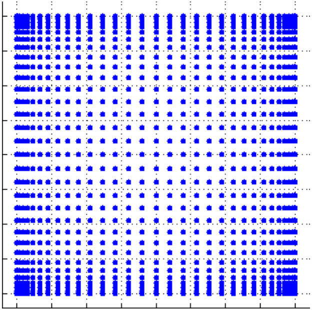
Outline

1. Sparse grid stochastic collocation FEM (sgSCFEM)
2. Theoretical convergence rates
3. To intrude or not intrude?
4. Stochastic inverse problems - control and identification
5. Lots of things we did not cover
6. Concluding remarks
7. Lots of references

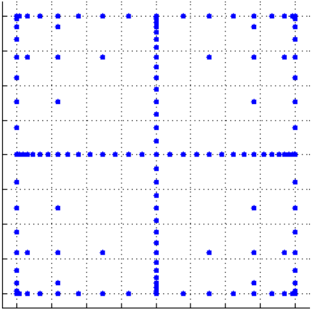
Asymptotic accuracy & convergence

What about the *curse of dimensionality*?



Tensor product grid

$\varepsilon_{TP}(M) \leq C(N) M^{-g_{min}/N}$



Sparse grid

$\varepsilon_{SG}(M) \leq \widetilde{C}(N) M^{-?}$

- The TP-SCFEM is a non-intrusive method with faster convergence than MCFEM (for smooth solutions)
- The number of samples grows exponentially fast with the number of RVs. Clearly unfeasible, even for moderate N

High-dimensional NI approximations

Sparse grid stochastic collocation FEM (sgSCFEM)

- Recall that $\mathscr{U}_n^{m(i_n)}$ be the ith level interpolant in the direction y_n using $m(i_n)$ points

$$\mathscr{U}_n^{m(i_n)} : C^0(\Gamma_n) \to \mathcal{P}_{m(i_n)-1}(\Gamma_n), \quad \mathscr{U}_n^0[u] = 0 \; \forall u \in C^0(\Gamma_n)$$

- The TP-SCFEM: $u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^{N} \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \le p$
- The nth difference operator: $\Delta_n^{m(i_n)}[u] = \mathscr{U}_n^{m(i_n)}[u] - \mathscr{U}_n^{m(i_n-1)}[u]$
- The hierarchical surplus: $\Delta_n^{m(\mathbf{i})}[u](\mathbf{y}) = \bigotimes_{n=1}^{N} \Delta_n^{m(i_n)}[u](\mathbf{y})$ where $\mathbf{i} = (i_1, \ldots, i_N) \in \mathbb{N}_+^N$ is a multi-index

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sgSCFEM
High-dimensional interpolation approach

Basic idea: linear combination of tensor product grids, with a relatively low number of points (but maintain the asymptotic accuracy)

The tensor product SCFEM interpolant is defined as:

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$$u_p^{SG}(\mathbf{y}) = \sum_{g(\mathbf{i}) \leq p} \bigotimes_{n=1}^{N} \Delta_n^{m(i_n)}[u](\mathbf{y}) = \sum_{g(\mathbf{i}) \leq p} c(\mathbf{i}) \bigotimes_{n=1}^{N} \mathscr{U}_n^{m(i_n)}[u](\mathbf{y})$$

with $c(\mathbf{i}) = \sum_{\substack{\mathbf{j} \in \{0,1\}^N \\ g(\mathbf{i}+\mathbf{j}) \leq p}} (-1)^{|\mathbf{j}|_1}$ and $g : \mathbb{N}^N \to \mathbb{N}$ a strictly increasing function

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sgSCFEM

Choice of index set $g(\mathbf{i}) \leq p$

- Can build sparse grids corresponding to any polynomial space $\mathcal{P}_{\mathcal{J}(p)}(\Gamma)$
  - Tensor product (TP): $m(i) = i$, $g(\mathbf{i}) = \max_n \alpha_n (i_n - 1) \leq p$
  - Total Degree (TD): $m(i) = i$, $g(\mathbf{i}) = \sum_n \alpha_n (i_n - 1) \leq p$
  - Hyperbolic Cross (HC): $m(i) = i$, $g(\mathbf{i}) = \prod_n (i_n)^{\alpha_n} \leq p + 1$
  - Smolyak (SM): $m(i) = 2^{i-1} + 1$, $i > 1$, $g(\mathbf{i}) = \sum_n \alpha_n (i_n - 1) \leq p$
- The corresponding anisotropic versions are straightforward
- SM is the most widely used approach and corresponds to the original Smolyak construction [Smolyak '63]

$$c(\mathbf{i}) = (-1)^{p+N-|\mathbf{i}|_1} \binom{N-1}{p+N-|\mathbf{i}|_1}, \quad \text{with } p - N + 1 \leq g(\mathbf{i}) \leq p$$

$$u_p^{SG}(\mathbf{y}) = \sum_{p-N+1 \leq g(\mathbf{i}) \leq p} c(\mathbf{i}) \bigotimes_{n=1}^{N} \mathscr{U}_n^{m(i_n)}[u](\mathbf{y})$$

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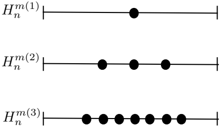
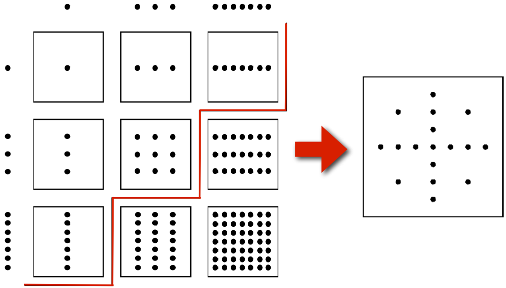
Example: $N = 2$ isotropic sparse grid

Nested rules minimize the amount of work

Nested equidistant grids with $m(i) = 1, 3$ and 7:



Grids $H_1^{m(i_1)} \otimes H_2^{m(i_1)}$ for $i_1, i_2 \leq p = 3$ and the *isotropic* sparse grid
$4 = p + 1 \leq i_1 + i_2 \leq p + 2 = 5$, e.g. $(3,1) + (1,3) + (2,2) + (2,3) + (3,2)$

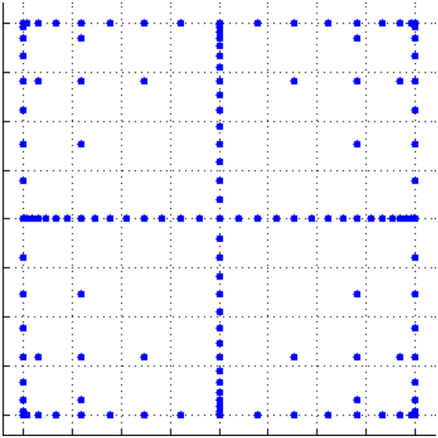


Generating Smolyak sparse grids: $N = 2$

Using Clenshaw-Curtis abscissas

$N = 2$ isotropic sparse grid: $p = 5$

$\Rightarrow |\mathbf{i}|_1 \leq p + N = 7$



$\mathscr{A}(5, 2)$

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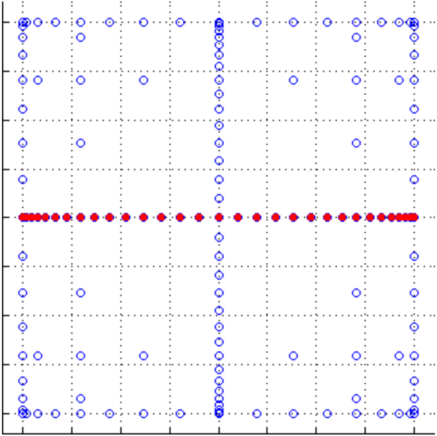

$\mathbf{i} = (6, 1) \Rightarrow (33 \times 1)$

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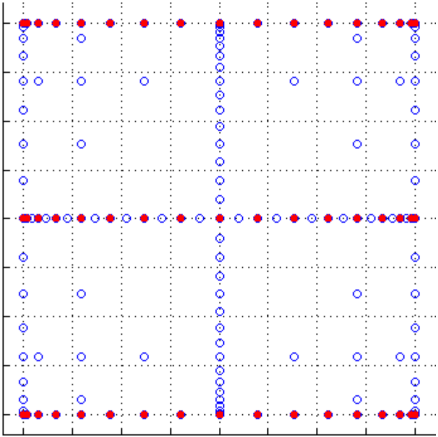

$\mathbf{i} = (5, 2) \Rightarrow (17 \times 3)$

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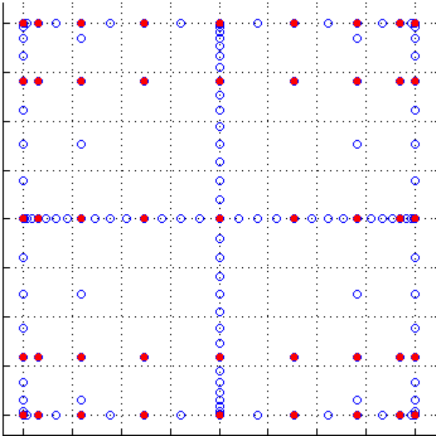

$\mathbf{i} = (4, 3) \Rightarrow (9 \times 5)$

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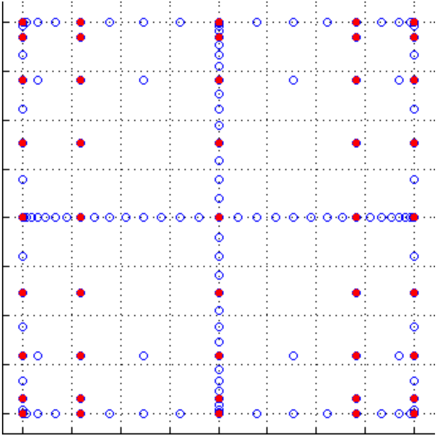

$\mathbf{i} = (3, 4) \Rightarrow (5 \times 9)$

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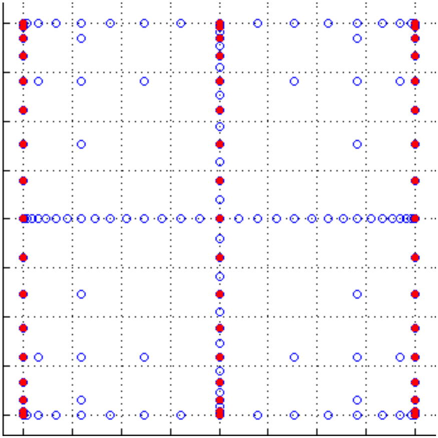

$\mathbf{i} = (2, 5) \Rightarrow (3 \times 17)$

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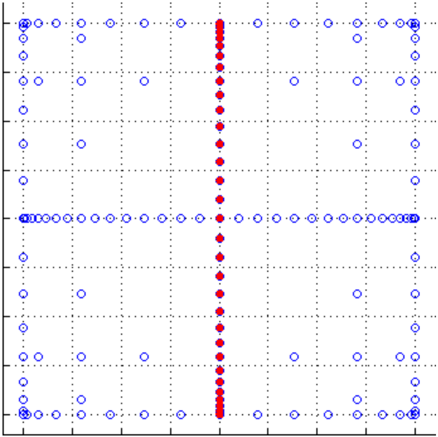

$\mathbf{i} = (1, 6) \Rightarrow (1 \times 33)$

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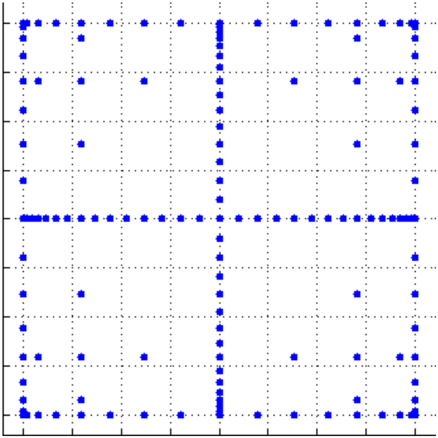

$\mathscr{A}(5, 2)$

Error Analysis

The ultimate goal is to give a priori estimates for the total error (in terms of the # of samples M:

$$\epsilon = u - u_p = u - \mathscr{I}_p^{(N)} \pi_h u_N$$

- $\mathscr{I}_p^{(N)}$ is the N-dimensional sparse grid interpolant
- π_h is the finite element projection operator
- u_N is the truncated representation of the solution
- u_p is the fully discrete (in $\Omega \times D$) approximation

$$\|\mathbb{E}[u-u_p]\|_{W(D)} \le \mathbb{E}\left[\|u-u_p\|_{W(D)}\right] \le \|u-u_p\|_{L^2_P(\Omega;W(D))}$$

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Convergence of C-C sparse grids:

Asymptotic accuracy: sgSCFEM vs TP-SCFEM

Recall: convergence of the *isotropic* FTP: $\varepsilon_{TP}(M) \approx \mathcal{O}\left(M^{-g_{min}/N}\right)$

Theorem [Nobile-Tempone-CW, 2008a]:

For functions $u \in C^0(\Gamma^N; W(D))$, the *isotropic sparse grid* method satisfies

$$\varepsilon(M) = \|u - u_p\|_{L^2_\rho} \leq C(N) M^{\frac{-g_{min}}{\log(2N)}},$$

- An analogous result holds for the Gaussian abscissas
- $C \leq 1$ for highly isotropic problems (sub-exponential convergence)
- Exploits the smoothness of the function (as opposed to MC, QMC, LHS, etc.) while reducing the *curse of dimensionality*
- $g_{min} \sim r$ when $u \in \mathcal{W}_r^{(N)}$ (bdd mixed derivatives of order r)
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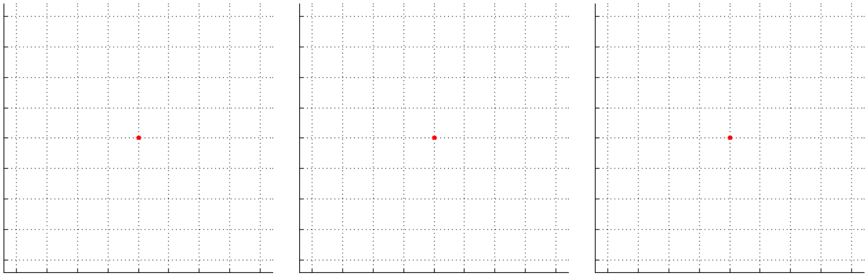
Dimension-adaptive sparse grids

Anisotropic sgSCFEM [Nobile-Tempone-Webster]

Let $g(\mathbf{i}) = \sum_{n=1}^{N} \alpha_n (i_n - 1)$, $\alpha_n = g_n$ and $m(i) = \begin{cases} 1, & i = 1 \\ 2^{i+1} - 1, & i > 1 \end{cases}$

$N = 2$ anisotropic sparse grid: $g(\mathbf{i}) \leq p = 0$



$\alpha_2/\alpha_1 = 1$ $\alpha_2/\alpha_1 = 1.5$ $\alpha_2/\alpha_1 = 2$

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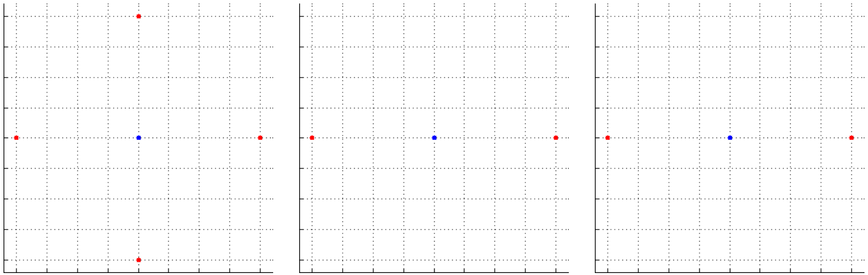

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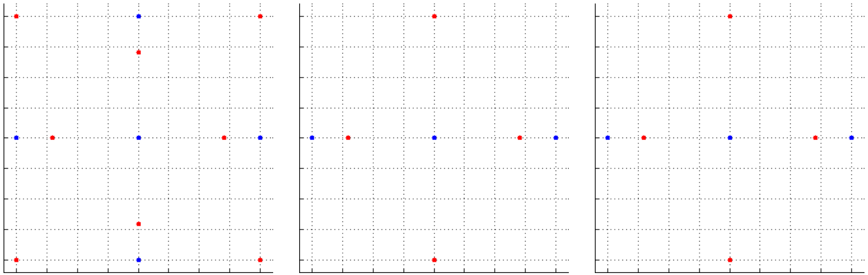

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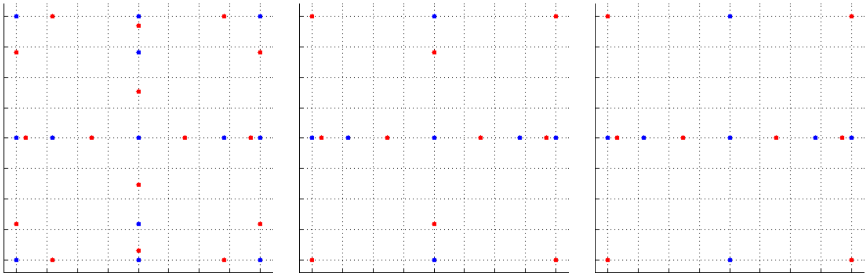
$N = 2$ anisotropic sparse grid: $g(\mathbf{i}) \leq p = 3$



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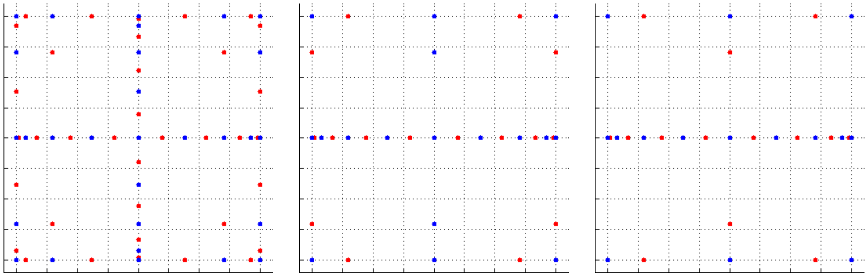

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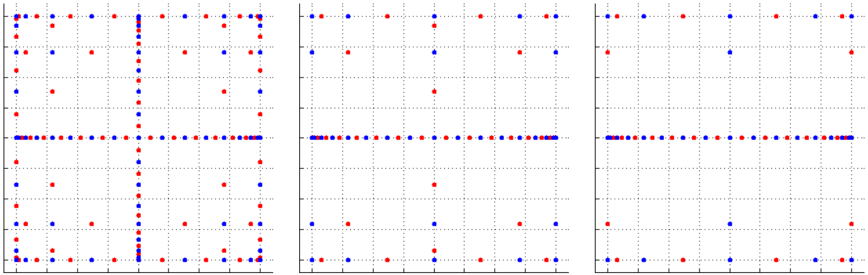

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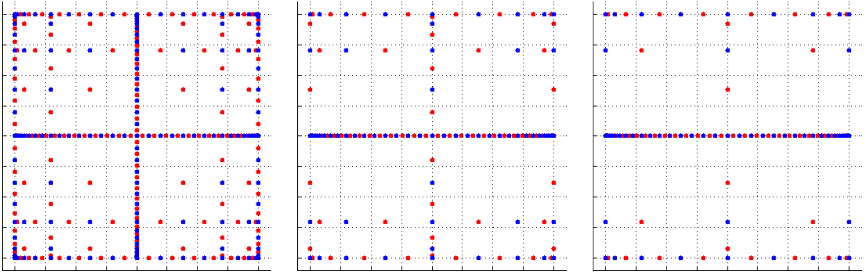

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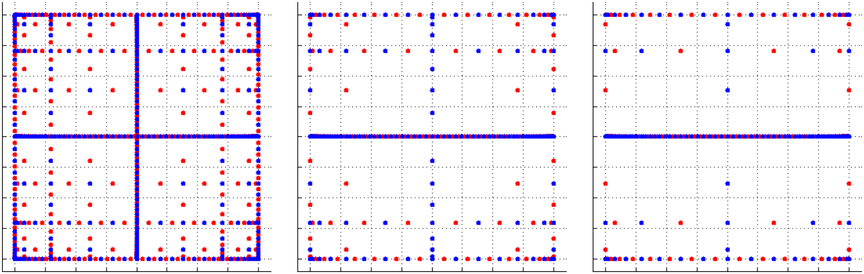

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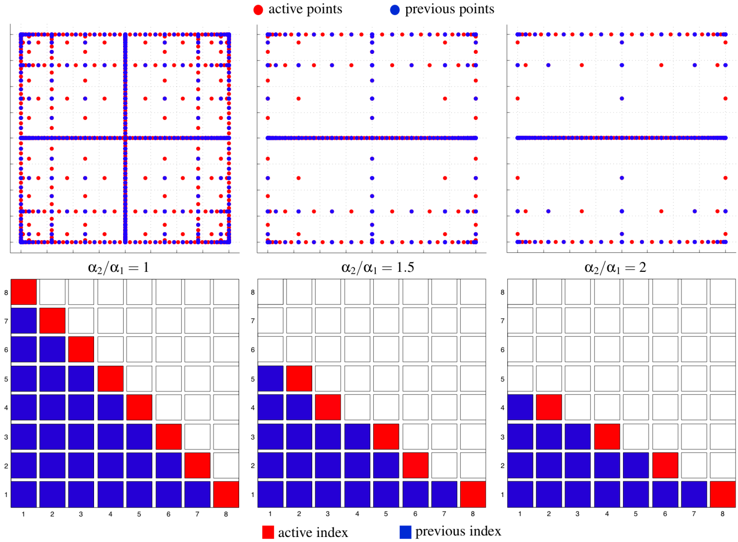
Generated C-C anisotropic sgSCFEM

Correspondng indices (i_1, i_2) s.t. $\alpha_1 i_1 + \alpha_2 i_2 \leq 7$



How to construct anisotropic weights?

Example: Γ_n bounded

1-dimensional analysis: polynomial approximation (L^2 projection or interpolation using Gauss points) in y_n (only) yields exponential convergence

$$\varepsilon_n = \|u - u_p\|_{L^2_\rho} \leq C e^{-g_n p_n}$$

Optimal choice for anisotropic weights: $\alpha_n = g_n$

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$$g_n = \log\left(\frac{2\tau_n}{|\Gamma_n|} + \sqrt{1 + \frac{4{\tau_n}^2}{|\Gamma_n|^2}}\right)$$

  and numerically (*a posteriori*), $\log_{10}(\varepsilon_n) \approx \log_{10}(d_n) - p_n \log_{10}(e)\alpha_n$
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Convergence Anisotropic sgSCFEM

Clenshaw-Curtis points

Recall: convergence of sparse isotropic SC: $\varepsilon_{SG}(M) \approx \mathcal{O}\left(M^{-g_{min}/(log(2N))}\right)$

Theorem [Nobile-Tempone-CW, 2008b]

For functions $u \in C^0(\Gamma^N; W(D))$ and $\alpha_n = g_n$, the **dimension-adaptive** sparse approximation approach satisfies:

$$\varepsilon(M) = \|u - u_p\|_{L^2_{\rho,N}} \leq C(\boldsymbol{\alpha}, N) M^{\frac{-g_{min}}{\mathscr{G}(g_{min}, N)}},$$

where $\mathscr{G}(g_{min}, N) = \log(2) + \sum_{n=1}^{N} \frac{g_{min}}{g_n}$

- An analogous result holds for the Gaussian abscissas
- $g_{min} = r$ when $u \in \mathcal{W}_r^{(N)}$ (bdd mixed derivatives of order r)
- For highly isotropic problems $\mathscr{G}(g_{min}, N) \approx \log(2N)$
- For highly anisotropic problems, i.e. the larger the ratio $\alpha_{max}/\alpha_{min}$ becomes, the smaller the constant and $\mathscr{G}(g_{min}, N) << \log(2N)$
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On "infinite dimensional noise"

- Observe that if $g_n \approx g_{min} n^\gamma$, with $\gamma > 1$, the series $\sum_{n=1}^{\infty} \frac{g_{min}}{g_n} < \infty$ and there is a limit rate of convergence:

$$M^{-\mu_N} \leq M^{-\mu_\infty}, \quad \mu_\infty > 0$$

- An estimate for the constant can be found in [NTW08b]:

$$C(\mathrm{g}, N) = \frac{1}{2} \sum_{d=1}^{N} \left(\frac{16}{\frac{\mathscr{G}(d)}{d} e} \right)^d \exp\left(\sum_{n=1}^{N} \left\{ k_1 \frac{1}{g(n)} + k_2 \frac{1}{\sqrt{g(n)}} - \log(\sinh(g(n))) \right\} \right), \quad \mathscr{G}(d) = \sum_{i=1}^{d} g(i)$$

- Given a monotone sequence g_n that goes to infinity (for instance $g_n \approx g_{min} n^\gamma$, $\gamma > 0$), we have

$$\lim_{N\to\infty} C(\alpha, N) = C^* < \infty \qquad \textbf{NO curse of dimensionality!}$$

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Numerical example

SG-SCFEM

We let $\mathbf{x} = (x_1, x_2)$ and consider the following nonlinear elliptic SPDE:

$$\begin{cases} -\nabla \cdot (a(\omega, x_1)\nabla u(\omega, \mathbf{x})) &= \cos(x_1)\sin(x_2) \quad \mathbf{x} \in [0,1]^2 \\ u(\omega, \mathbf{x}) &= 0 \quad \text{on } \partial D \end{cases}$$

The diffusion coefficient is a 1d random field (varies only in x_1) and is $a(\omega, x_1) = 0.5 + \exp\{\gamma(\omega, x_1)\}$, where γ is a truncated 1d random field with correlation length L and covariance

$$Cov[\gamma](x_1, \tilde{x}_1) = \exp\left(-\frac{(x_1 - \tilde{x}_1)^2}{L^2}\right), \quad \forall (x_1, \tilde{x}_1) \in [0,1]$$

$$\gamma(\omega, x_1) = 1 + Y_1(\omega)\left(\frac{\sqrt{\pi}L}{2}\right)^{1/2} + \sum_{n=2}^{N} \beta_n \varphi_n(x_1) Y_n(\omega)$$

$$\beta_n := \left(\sqrt{\pi}L\right)^{1/2} e^{\frac{-\left(\lfloor \frac{n}{2} \rfloor \pi L\right)^2}{8}}, \quad \varphi_n(x_1) := \begin{cases} \sin\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ even,} \\ \cos\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ odd} \end{cases}$$

- $\mathbb{E}[Y_n] = 0$ and $\mathbb{E}[Y_n Y_m] = \delta_{nm}$ for $n, m \in \mathbb{N}_+$ and iid in $U(-\sqrt{3}, \sqrt{3})$

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Calculating the weighting parameters

A priori selection: $N = 11$

A priori of the dimension weights $\alpha_n = g_n$:

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For this problem we have

$$g_n = \begin{cases} \log\left(1 + c/\sqrt{L}\right), & \text{for } n << L^{-2} \\ n^2 L^2, & \text{for } n > L^{-2} \end{cases}$$

	α_1	α_2, α_3	α_4, α_5	α_6, α_7	α_8, α_9	α_{10}, α_{11}
$L = 1/2$	0.20	0.19	0.42	1.24	3.1	5.8
$L = 1/64$	0.79	0.62	0.62	0.62	0.62	0.62

Goal: $\|\mathbb{E}[\epsilon]\|_{L^2(D)} \approx \|\mathbb{E}\left[u_p^{SG}(\mathbf{y},x) - u_{p_{max}+1}^{SG}(\mathbf{y},x)\right]\|_{L^2(D)}$

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$$\|\mathbb{E}[\epsilon_n]\|_{L^2(D)} \approx \|\mathbb{E}\left[u_p(y_n,x) - u_{p_{max}+1}(y_n,x)\right]\|_{L^2(D)}$$

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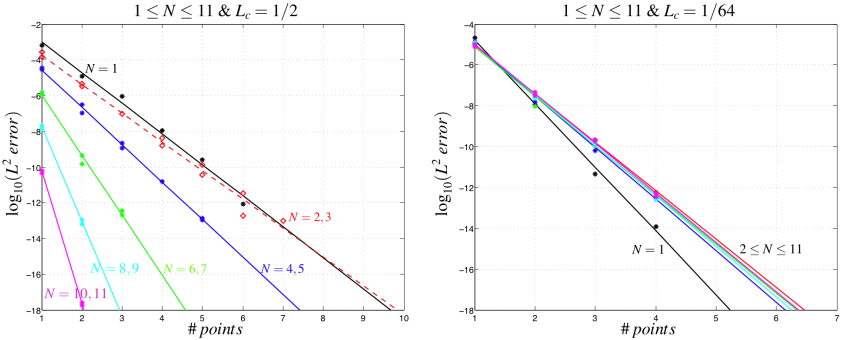
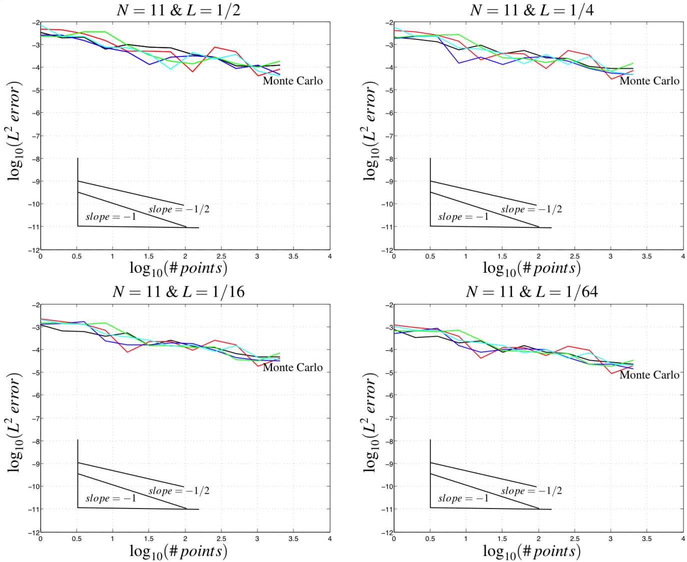


A linear least square approximation to fit $\log_{10}(\|E[\varepsilon_n]\|_{L^2(D)})$ versus p_n. For $n = 1, 2, \ldots, N = 11$ we plot: on the left, the highly anisotropic case $L_c = 1/2$ and on the right, the isotropic case $L_c = 1/64$

Convergence Comparisons

$N = 11$ random variables



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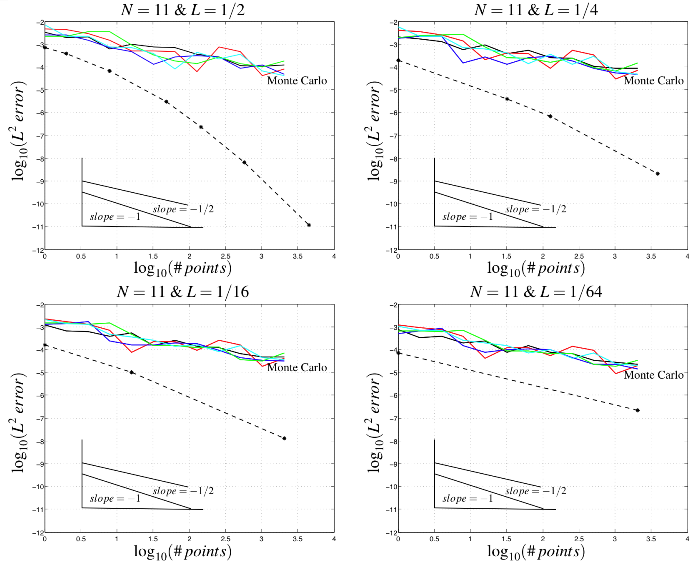

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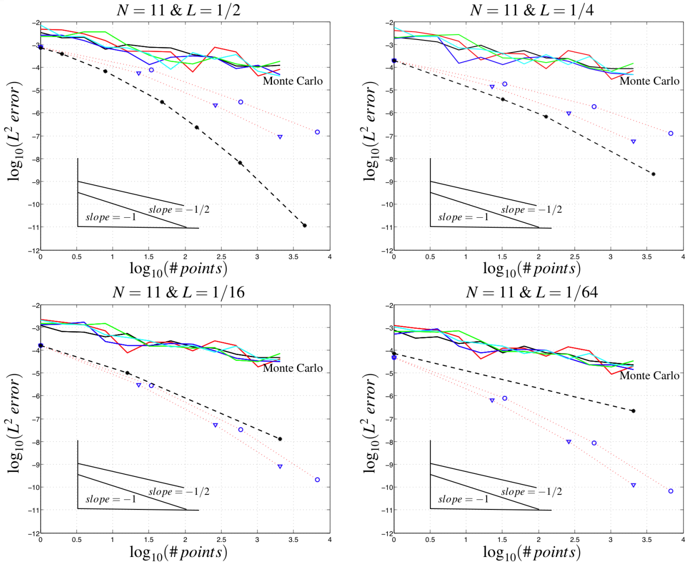

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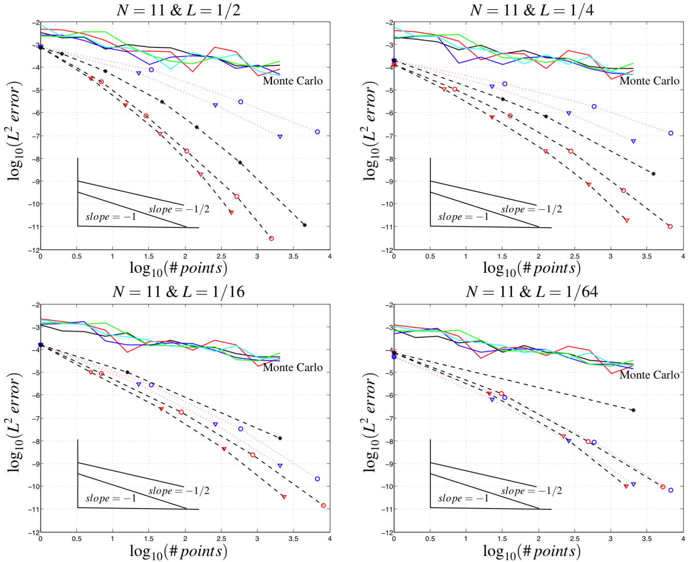


Convergence Comparisons II

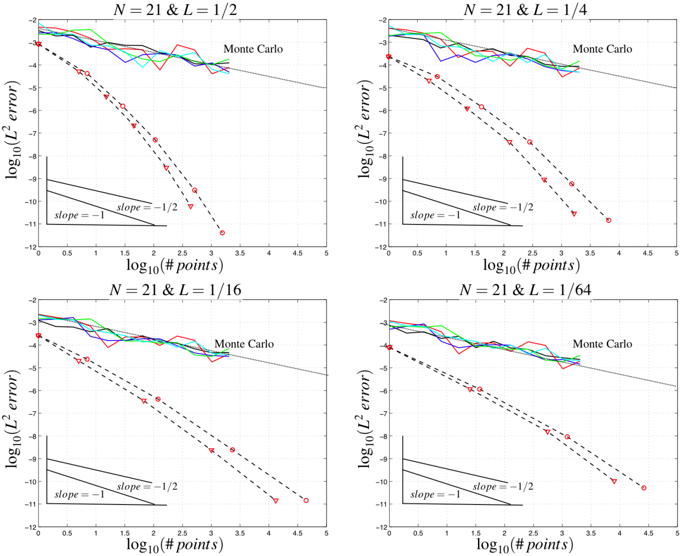
$N = 11$ random variables

L	AS	AF	IS	MC
1/2	50	252	2512	$5.0e + 09$
1/4	158	1259	3981	$2.0e + 09$
1/16	199	1958	501	$1.6e + 09$
1/64	316	199530	360	$1.3e + 09$

Table: For Γ^N, with $N = 11$, we compare the number of deterministic solutions required by the Anisotropic Smolyak (AS) using Clenshaw-Curtis abscissas, Anisotropic Full Tensor product method (AF) using Gaussian abscissas, Isotropic Smolyak (IS) using Clenshaw-Curtis abscissas and the Monte Carlo (MC) method using random abscissas, to reduce the original error by a factor of 10^4.

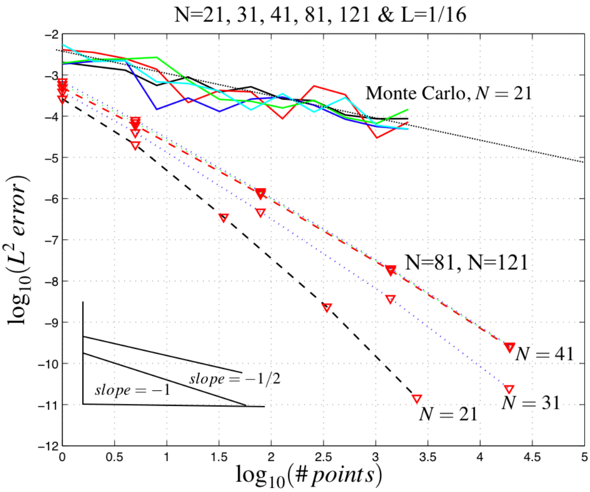
Convergence Comparisons III

$N = 21$ random variables



Convergence Comparisons IV:

$N = 21, \dots, 121, \dots \infty$ random variables (*A posteriori approach*)



SGFEM vs. SCFEM

OAK RIDGE National Laboratory

We have already pointed out that both the SGFEM and SCFEM approaches can be tuned to the same polynomial space $\mathcal{P}_{\mathcal{J}(p)}(\Gamma)$

- In general $M_{SC} \geq \dim\left(\mathcal{P}_{\mathcal{J}(p)}(\Gamma)\right) \equiv M_{SG}$ (L^2 optimality of the Galerkin projection)
    - However, since the SGFEM results in large coupled systems, pre-conditioners and iterative solvers become necessary. Therefore:

$$\text{Cost}_{\text{SG}} = \dim\left(\mathcal{P}_{\mathcal{J}(p)}(\Gamma)\right) \times (\#\text{ iterative solves})$$

    - The cost of the deterministic FEM remains fixed between SG and SC. As such

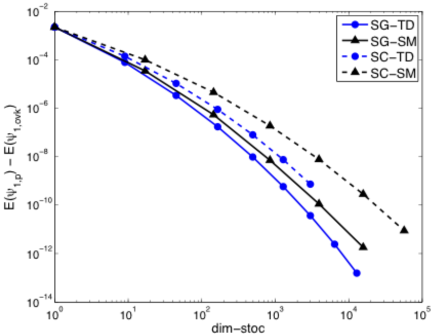
$$\text{Cost}_{\text{SC}} = \text{card}\left(H^{M_{SC}}\right) = \#\text{collocation points in } \Gamma$$

- Numerical Comparison: J. Bäck, F. Nobile, L. Tamellini, and R. Tempone. Stochastic spectral Galerkin and collocation methods for PDEs with random coefficients: a numerical comparison, *Lecture Notes in Computational Science and Engineering, pages 43-62. Springer, 2011*

SGFEM vs. SCFEM

Numerical comparison [Bäck et. al, 2011]: Error vs. dim

piecewise material properties, i.e. $a(\omega, x) = b_0 + \sum_{n=1}^{8} Y_n(\omega)\chi_{D_n}(x)$, $a|_{D_n} \sim U(0.01, 0.8)$ with deterministic forcing term $f = 100$ and zero BC's

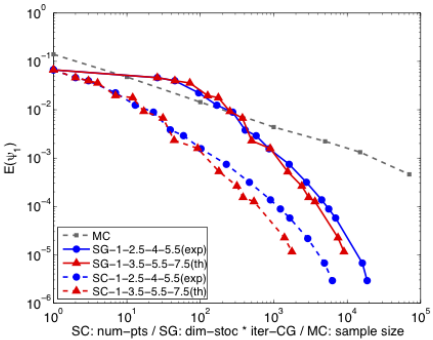


The Galerkin method is solved with a conjugate gradient method with block diagonal pre-conditioner: $\text{Cost}_{\text{SG}} = \dim\left(\mathcal{P}_{\mathcal{J}(p)}(\Gamma)\right) \times (\#\ \text{PCG iterations})$

aSGFEM vs. aSCFEM

Numerical comparison [Bäck et. al, 2011]: Error vs Cost

piecewise material properties, i.e. $a(\omega, x) = b_0 + \sum_{n=1}^{4} Y_n(\omega)\chi_{D_n}(x)$, $a|_{D_n} \sim U(0.01, 0.8)$ with deterministic forcing term $f = 100$ and zero BC's



Approximation using anisotropic total degree polynomial spaces for both the Galerkin and Collocation methods (weights both theoretically and numerically)

Stochastic inverse problems

Applications of sgSCFEM to control and identification

Forward Problem: to approximate u or some statistical QoI depending on u:

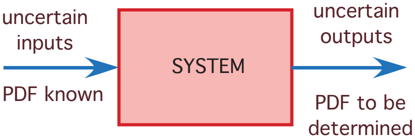
$$\mathbf{\Phi}_u = \langle \mathbf{\Phi}(u) \rangle := \mathbb{E}\left[\mathbf{\Phi}(u)\right] = \int_{\Omega} \int_{D} \Phi(u(\omega, x), \omega, x) dx \, d\mathbb{P}(\omega)$$

e.g. $\overline{u}(x_0) = \mathbb{E}[u](x_0)$, OR $\mathbb{V}ar[u](x_0) = \mathbb{E}[(\widetilde{u})^2](x_0)$, where $\widetilde{u} = u - \overline{u}$,

OR $\mathbb{P}\left[u \geq u_0\right] = \mathbb{P}\left[\{\omega \in \Omega \,:\, u(\omega, x_0) \geq u_0\}\right] = \mathbb{E}\left[\chi_{\{u \geq u_0\}}\right]$,

OR even statistics of functionals of u, i.e. $\phi(u) = \int_{\Sigma \subset D} u(\cdot, x) dx$

where Σ is a subdomain of interest.



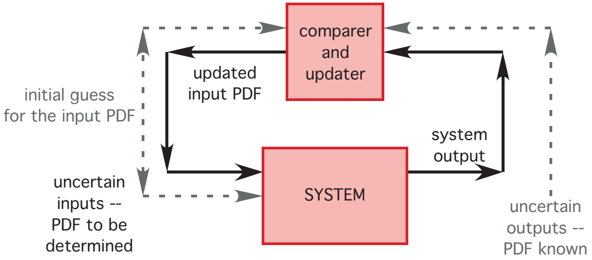
Goal of the computations

Stochastic QoI

Inverse Problem: Given a set of measurements $\{\eta(\omega, x, t)\}$ corresponding to some statistical QoI $\mathbb{Q}[u]$ (e.g. moments, inverse CDF, etc) depending on the solution u to the SPDE, minimize the functional

$$\mathbb{Q}\big(\|u(\omega,\cdot)|_{a,f} - \eta(\omega,\cdot)\|^2_{L^2(D)} \big) \quad \text{OR} \quad \|\mathbb{Q}\big(u(\cdot,x)|_{a,f}\big) - \mathbb{Q}\left(\eta(\cdot,x)\right)\|^2_{L^2(D)}$$

s.t. the random u and the optimal stochastic coefficients satisfy the state



- accomplished via Bayesian methods or by **optimization** approaches

Stochastic optimal control

Part 1. Theory for applications to linear SPDEs

- Let $a_{\min}, a_{\max} > 0$ and denote $\mathcal{U}_{ad}$ the set of admissible coefficients s.t.

$$\mathcal{U}_{ad} = \{a \in L^\infty(\Gamma; L^\infty(D)) : \mathbb{P}(a_{\min} \leq a(\omega, x) \leq a_{\max}, \text{ a.e. } x \in D) = 1\}$$

- Let $\overline{u}(\mathbf{y}, x)$ and $a(\mathbf{y}, x)$ be given target and coefficient random fields

The stochastic optimal control problems: minimize the functionals

$$J_{C_1}(f, u) = \mathbb{E}\left[\frac{1}{2}\|u(\mathbf{y}, x) - \overline{u}(\mathbf{y}, x)\|^2_{L^2(D)} + \frac{\alpha}{2}\|f(\mathbf{y}, x)\|^2_{L^2(D)}\right] \qquad (C_1)$$

$$J_{C_2}(f, u) = \frac{1}{2}\left\|\mathbb{E}[u](x) - \mathbb{E}[\overline{u}](x)\right\|^2_{L^2(D)} + \frac{\alpha}{2}\left\|\mathbb{E}[f](x)\right\|^2_{L^2(D)} \qquad (C_2)$$

over all $u \in L^2_\rho(\Gamma; H^1_0(D) \cap H^2(D))$ and $f \in L^2_\rho(\Gamma, L^2(D))$, subject to

$$-\nabla \cdot (a(\mathbf{y}, x)\nabla u(\mathbf{y}, x)) = f(\mathbf{y}, x) \quad \text{in } \Gamma \times D$$

Remark: Using (C_2) we can easily replace $\mathbb{E}[\cdot]$ with higher order statistics or even $\Phi^{-1}[\cdot]$, the inverse CDF

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Stochastic optimal control

Part 2. Theory for applications to linear SPDEs

Theorem [GTW12]

$(\widetilde{u}, \widetilde{f})$ is the unique optimal pair in problem (C_1) or (C_2) *if and only if* there exists an adjoint or co-state stochastic process $\xi \in L^2_\rho(\Gamma; H^1_0(D))$ such that

$$\begin{cases} -\nabla \cdot (a(\mathbf{y},x)\nabla \xi(\mathbf{y},x)) = \mathbb{F}\big(\widetilde{u}(\mathbf{y},x) - \overline{u}(\mathbf{y},x)\big) & \text{in } \Gamma \times D, \\ \widetilde{f}(\mathbf{y},x) = -\frac{1}{\alpha}\,\xi(\mathbf{y},x) & \text{a.e. in } \Gamma \times D, \\ \xi(\mathbf{y},x) = 0 & \text{on } \Gamma \times \partial D, \end{cases}$$

where $\mathbb{F}[\cdot] = \mathcal{I}_d[\cdot]$ for problem (C_1) and $\mathbb{F}[\cdot] = \mathbb{E}[\cdot]$ for problem (C_2)

- The optimal control $\widetilde{f}$, the optimal state $\widetilde{u}$ and the optimal adjoint state $\xi(\mathbf{y},x)$ can be determined from solving the minimization problems (C_1) or (C_2) directly or by solving the system of *couple stochastic PDEs*:

$$\begin{cases} -\nabla \cdot (a(\mathbf{y},x)\nabla \widetilde{u}(\mathbf{y},x)) = -\frac{1}{\alpha}\,\xi(\mathbf{y},x) \\ -\nabla \cdot (a(\mathbf{y},x)\nabla \xi(\mathbf{y},x)) = \mathbb{F}\big(\widetilde{u}(\mathbf{y},x) - \overline{u}(\mathbf{y},x)\big) \end{cases}$$

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Stochastic parameter identification

Part 1. Theory for applications to linear SPDEs

- Given a perturbed stochastic observation $\overline{u}(\mathbf{y}, x)$ of the state, determine the coefficient $a(\mathbf{y}, x)$ such that $u|_a = \overline{u}$ (or even $\mathbb{Q}[u|_a)] = \mathbb{Q}[\overline{u}]$)
- $\mathcal{A}_{ad} = \{(u, a) \mid u \in L^2_\rho(\Gamma; H^1_0(D) \cap H^2(D))$ and $a \in L^\infty(\Gamma; L^\infty(D))\}$

The stochastic iD problems: Given $f(\mathbf{y}, x)$, Minimize the functionals

$$J_{P_1}(a, u) = \mathbb{E}\left[\frac{1}{2}\|u(\mathbf{y}, x) - \overline{u}(\mathbf{y}, x)\|^2_{L^2(D)} + \frac{\beta}{2}\|a(\mathbf{y}, x)\|^2_{L^2(D)}\right] \qquad (P_1)$$

$$J_{P_2}(a, u) = \frac{1}{2}\left\|\mathbb{E}[u](x) - \mathbb{E}[\overline{u}](x)\right\|^2_{L^2(D)} + \frac{\beta}{2}\left\|\mathbb{E}[a](x)\right\|^2_{L^2(D)} \qquad (P_2)$$

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Theorem [GTW12]

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$$\widehat{a}(\mathbf{y}, x) = \max\{a_{\min}, \min\{-\frac{1}{\beta}\nabla\widehat{u}(\mathbf{y}, x)\nabla\xi(\mathbf{y}, x), a_{\max}\}\} \text{ a.e. in } \Gamma\times D,$$

where the adjoint $\xi \in L^2_P(\Gamma; H^1_0(D))$ is the solution of the nonlinear SPDE

$$-\nabla\cdot(\widehat{a}(\mathbf{y}, x)\nabla\xi(\mathbf{y}, x)) = \mathbb{F}\left(\widehat{u}(\mathbf{y}, x) - \overline{u}(\mathbf{y}, x)\right) \text{ in } \Gamma\times D$$

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Applications to stochastic parameter iD

SCFEM approximation of the coupled system

- $\widehat{a}(\omega,x) = \max\{a_{\min}, \min\{-\frac{1}{\beta}\nabla\widehat{u}(\omega,x)\nabla\xi(\omega,x), a_{\max}\}\}$ a.e. in $\Omega \times D$

Strong formulation: find $u(\mathbf{y},x), \xi(\mathbf{y},x) \in H_\rho = L^2_\rho(\Gamma^N; H^1_0(D))$ s.t.

$$\begin{cases} -\nabla\cdot(\widehat{a}(\mathbf{y},x)\nabla u(\mathbf{y},x)) = f(\mathbf{y},x) & \text{for a.e. } x \in D, \\ -\nabla\cdot(\widehat{a}(\mathbf{y},x)\nabla \xi(\mathbf{y},x)) = \mathbb{E}\big(u(\mathbf{y},x) - \overline{u}(\mathbf{y},x)\big) & \text{for a.e. } x \in D, \end{cases}$$

where $\mathbf{y} \in \Gamma^N \subset \mathbb{R}^N$ and $x \in \overline{D}$

Weak formulation: find $u, \xi \in H_\rho$ s.t., $\forall v \in H_\rho$

$$\begin{cases} \int_{\Gamma^N} (\widehat{a}\,\nabla u, \nabla v)_{L^2(D)}\rho(\mathbf{y})\,d\mathbf{y} = \int_{\Gamma^N} (f, v)_{L^2(D)}\rho(\mathbf{y})\,d\mathbf{y} \\ \int_{\Gamma^N} (\widehat{a}\,\nabla \xi, \nabla v)_{L^2(D)}\rho(\mathbf{y})\,d\mathbf{y} = \int_{\Gamma^N} ((u-\overline{u}), v)_{L^2(D)}\rho(\mathbf{y})\,d\mathbf{y} \end{cases}$$

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Strong formulation: find $u(\mathbf{y},x),\xi(\mathbf{y},x) \in H_\rho = L^2_\rho(\Gamma^N; H^1_0(D))$ s.t.

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Error estimates for (P_2)

Fully discrete stochastic identification approximation

- Recast nonlinear optimality system related to problem (P_2) by utilizing the *Brezzi-Rappaz-Raviart Theory* for approximations of nonlinear PDEs
- $\{(\lambda = \beta, \varphi(\lambda) = (u(\lambda), \kappa(\lambda)); \lambda \in \Lambda\}$ be a nonsingular branch of solns

Theorem [GTW12]

There exists a neighborhood $\mathcal{O}$ of the origin in X and, for $h \leq h_0$ small enough and M sufficiently large,a unique C^2 branch of solutions s.t.

$$\varphi_p(\lambda) \in \varphi(\lambda) + \mathcal{O}.$$

Moreover, let $H_P^6 = L_P^6(\Omega; W_0^{1,6}(D))$, then we get the estimate

$$\|u - u_p\|_{H_P^6} + \|\xi - \xi_p\|_{H_P^6} \leq C(h + M^{\frac{-g_{min}}{\mathscr{G}(g_{min}, N)}})\mathcal{E}(u, \eta, f, \overline{u}),$$

where $\mathcal{E}(u, \eta, f, \overline{u}) = \left(\|\nabla u\|_{H_P^{6*}} + \|\nabla \eta\|_{H_P^{6*}} + \|f\|_{H_P^{6*}} + \|\mathbb{E}(u - \overline{u})\|_{H_P^{6*}}\right).$

- $(u_p, \xi_p) \to (u, \xi)$ as $h \to 0$, $M \to \infty$. Similarly $a_p \to a$ through optimality condition.

Numerical Example

Stochastic parameter identification

OAK RIDGE National Laboratory

An adjoint-based gradient descent algorithm ($tol = 10^{-6}$) using sgSCFEM to compute the optimal pair $(\widehat{u}, \widehat{\kappa})$ s.t. $J_{P_1,P_2}(\widehat{\kappa}, \widehat{u}) = \inf_{(a,u)\in\mathcal{A}_{ad}} J_{P_1,P_2}(a,u)$

$$J_{P_1}(a,u) = \mathbb{E}\left[\frac{1}{2}\|u(\omega,x) - \overline{u}(\omega,x)\|^2_{L^2(D)} + \frac{\beta}{2}\|a(\omega,x)\|^2_{L^2(D)}\right] \qquad (P_1)$$

$$J_{P_2}(a,u) = \frac{1}{2}\Big\|\mathbb{E}[u](x) - \mathbb{E}[\overline{u}](x)\Big\|^2_{L^2(D)} + \frac{\beta}{2}\Big\|\mathbb{E}[a](x)\Big\|^2_{L^2(D)} \qquad (P_2)$$

Stochastic target: $\overline{u} = x(1-x^2) + \sum_{n=1}^{N} \sin\left(\frac{n\pi x}{L}\right) Y_n(\omega)$

Exact random coeff.: $\overline{a} = (1+x^3) + \sum_{n=1}^{N} \cos\left(\frac{m\pi x}{L}\right) Y_n(\omega)$

Deterministic initial guess: $a = 1 + x$

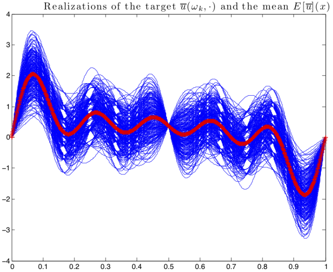
Exact given RHS: $f = \nabla\cdot(\overline{a}(\omega,x)\nabla\overline{u}(\omega,x))$

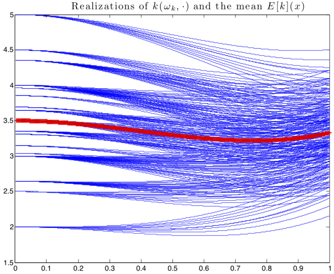
- $\mathbb{E}[Y_i] = 0$ and $\mathbb{E}[Y_iY_j] = \delta_{ij}$ for $i,j \in \mathbb{N}_+$, are taken uniform in the interval $[0,1]$, and $x \in \mathbb{R}^1$

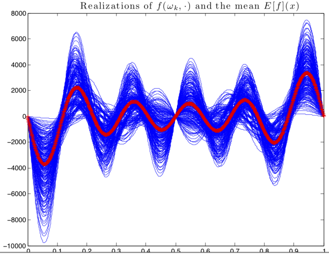
GOAL: given the random f, identify the expectation of both the parameter $a(\omega,x)$ and the state $u(\omega,x)$ and compare with the exact statistics.

Realizations of the exact a, u and f

$N = 5$ using $M = 241$ C-C samples



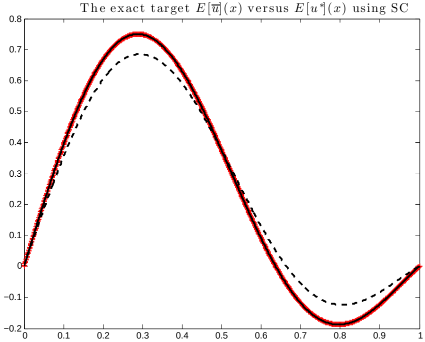


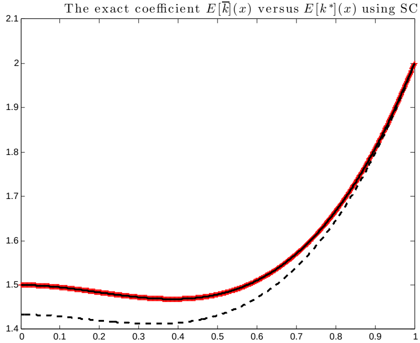


$N = 1$ example: $\inf J_{P_1,P_2}(a,u)$

Tracking the expectation of the parameter $\mathbb{E}[a]$ and the state $\mathbb{E}[u]$

$$M = 5$$

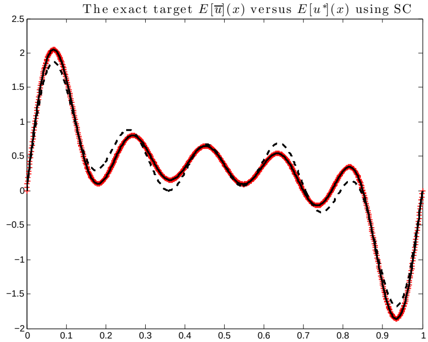


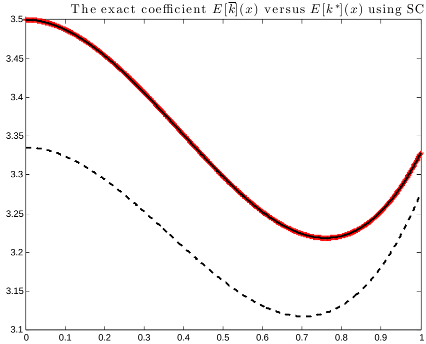


$N = 5$ example: $\inf J_{P_1,P_2}(a,u)$

Tracking the expectation of the parameter $\mathbb{E}[a]$ and the state $\mathbb{E}[u]$

$$M = 61$$

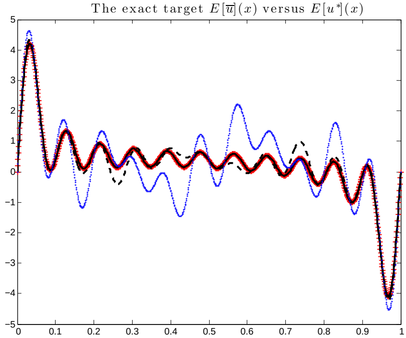


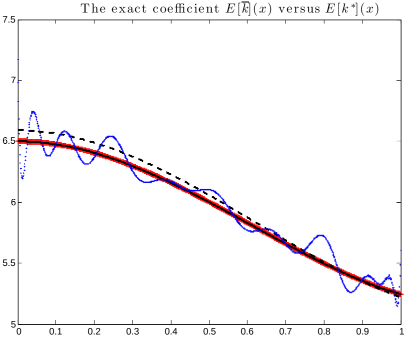


$N = 11$ example: $\inf J_{P_1,P_2}(\kappa, u)$

MCFEM vs. sgSCFEM

$$M_{gSC} = 265, \qquad M_{MC} \sim 10^6$$





$N = 11, 51$ and 121 examples: MC vs. SC

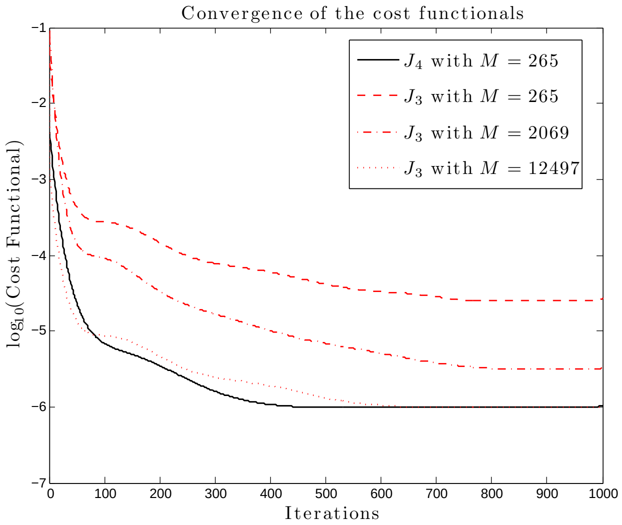
Tracking the expectation of the state $\mathbb{E}[u]$ and control $\mathbb{E}[a]$

N	sgSCFEM	MCFEM
11	360	$7e+09$
51	1581	$9e+10$
121	4801	$8e+12$

Table: For Γ^N, with $N = 11, 51$ and 121, we compare the number of deterministic solutions required by the sparse grid Stochastic Collocation FEM (sgSCFEM) using Chebyshev abscissas and the Monte Carlo FEM (MCFEM) method using random abscissas, to reduce the original error in both $\|\mathbb{E}[u] - \mathbb{E}[\overline{u}]\|_{L^2(D)}$ and $\|\mathbb{E}[a] - \mathbb{E}[\overline{a}]\|_{L^2(D)}$ by a factor of 10^6.

Convergence of the cost functionals

Gradient-based sgSCFEM: $N = 11$, $\beta = 10^{-6}$



What didn't we cover

Other polynomial space approximations

- ANOVA-type approximation: activate at most $\nu << N$ stochastic dimensions at the same time ([Todor-Schwab], [Bieri-Schwab], [Karniadakis et al]):

$$\mathbb{P}_{\mathbf{p},\nu}(\Gamma^N) = \text{span}\left\{ \prod_{n=1}^{N} y_n^{i_n}, \;\; i_n \le p_n, \;\; \sum_{n=1}^{N} \{i_n > 0\} \le \nu \right\}$$

- Best N-term approximation: approximate u with the N largest Fourier-Legendre coefficients ([Cohen-DeVore-Schwab], [Bieri-Andreev-Schwab])
- Discontinuous piecewise polynomials: "hp"-type discretization ([Karniadakis-Wan-et al], [Babuška-Tempone-Zouraris], [Ma-Zabaras], [Griebel et al], [Jakeman-Archibald-Xiu]), [Gunzburger-CW]
- Wavelet basis approaches: Wiener-Haar Galerkin basis [LeMaitre-Najim-Ghanem-Knio], generalized sparse wavelet basis [Guannan-Gunzburger-CW]
- Generalized spectral decomposition [Nouy, LeMaitre]

Concluding remarks

- PDEs with random input data arise in the context of uncertainty quantification in many engineering areas
- High-dimensional problems are a characteristic of modern forward and inverse UQ. Accurate Monte Carlo-type results take too long and tensor product methods suffer from the *curse of dimensionality*
- Properly chosen anisotropic polynomial spaces can improve considerably the convergence of both SCFEM and SGFEM, when the input random variables have different influence on the output
- Real-world applications are typically highly nonlinear which can easily be solved using *non-intrusive* approaches whereas *intrusive* approaches require large dense coupled solvers
- Global sgSCFEM is very effective for problems that feature **smooth** dependence on the random variables - even in high-dimensional spaces
    - Non-smooth or even discontinuous solutions are not well represented by global polynomials - strong oscillations (Gibbs phenomenon)
    - Explosion in computational effort with most locally adaptive methods

(Very Incomplete) List of references

Formulation of PDEs with random coefficients, i.e. SPDEs:
Babuška et al; Holden & Øksendal; Karniadakis & Xiu; Keese & Matties; Schwab & Todor; etc....

Spatial/temporal expansion of stochastic processes/random fields:
Adler; Fourier; Karhunen & Loève ; Krée & Soize; Wiener; etc...

White noise analysis / polynomial chaos (PC) / multiple Itô integrals:
Cameron & Martin; Burkardt & Webster; Hida & Potthoff; Holden & Øksendal; Itô; Malliavin; etc...

Galerkin methods for SPDEs:
Babuška & Tempone; Benth & Gjerde; Cao; Ghanem & Spanos; Karniadakis & Xiu; Keese & Matties; Schwab & Todor; etc...

Collocation methods for SPDEs:
Babuškaet al; Hesthaven & Xiu; Matelin et al; Nobile, Tempone & Webster; Tatang; etc...

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A generalized methodology for the solution of stochastic identification problems, ORNL Technical Report, 2012.

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[BGW07] J. Burkardt, M. Gunzburger and **C. Webster**
Reduced Order Modeling of some Nonlinear Stochastic Partial Differential Equations, Int. J. Num. Anal., 2007.