

Analysis of SPDEs and numerical methods for UQ Part II: Well-posed SPDEs, regularity and numerical approximations

John Burkardt[†] & Clayton Webster*

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

[†]Department of Scientific Computing Florida State University

* CEES, CASL, Computer Science and Mathematics Division Oak Ridge National Laboratory

April 2-3, 2012









- Stochastic partial differential equation (SPDE)
- 2 Finite dimensional noise approximation
- 3 Monte Carlo FEM (MCFEM)
- 4 Stochastic Regularity
- Stochastic polynomial approximation
- Stochastic Galerkin (SG) FEM
- Stochastic collocation (SC) FEM











OAK RIDGE NATIONAL LABORATORY





Consider an operator \mathcal{L} , linear or nonlinear, on a domain $D \subset \mathbb{R}^d$, which depends on some coefficients $a(\omega, x)$ with $x \in D$, $\omega \in \Omega$ and (Ω, \mathcal{F}, P) a complete probability space. The forcing $f = f(\omega, x)$ and the solution $u = u(\omega, x)$ are random fields s.t.

$$\mathcal{L}(a)(u) = f \quad \text{a.e. in } D \tag{1}$$

equipped with suitable boundary conditions.

 $A_1.$ the solution to (1) has realizations in the Banach space W(D), i.e. $u(\cdot,\omega)\in W(D)$ almost surely

 $\|u(\cdot,\omega)\|_{W(D)} \le C \|f(\cdot,\omega)\|_{W^*(D)}$

 $\begin{array}{l} A_2. \mbox{ the forcing term } f \in L^2_{\mathbb{P}}(\Omega) \otimes W^*(D) \equiv L^2_{\mathbb{P}}(\Omega; W^*(D)) \mbox{ is such that the solution } u \mbox{ is unique and bounded in } L^2_{\mathbb{P}}(\Omega) \otimes W(D) \equiv L^2_{\mathbb{P}}(\Omega; W(D)) \\ A_3. \ \mathbb{P}\left[a(\omega, x) \in (a_{min}, a_{max}) \ \forall x \in \overline{D}\right] = 1, \ a_{min} > 0, \ a_{max} < \infty \end{array}$



Consider an operator \mathcal{L} , linear or nonlinear, on a domain $D \subset \mathbb{R}^d$, which depends on some coefficients $a(\omega, x)$ with $x \in D$, $\omega \in \Omega$ and (Ω, \mathcal{F}, P) a complete probability space. The forcing $f = f(\omega, x)$ and the solution $u = u(\omega, x)$ are random fields s.t.

$$\mathcal{L}(a)(u) = f \quad \text{a.e. in } D \tag{1}$$

equipped with suitable boundary conditions.

 $A_1.$ the solution to (1) has realizations in the Banach space W(D), i.e. $u(\cdot,\omega)\in W(D)$ almost surely

$$\|u(\cdot,\omega)\|_{W(D)} \le C \|f(\cdot,\omega)\|_{W^*(D)}$$

 $\begin{array}{l} {\it A_2.} \mbox{ the forcing term } f\in L^2_{\mathbb{P}}(\Omega)\otimes W^*(D)\equiv L^2_{\mathbb{P}}(\Omega;W^*(D)) \mbox{ is such that the solution } u \mbox{ is unique and bounded in } L^2_{\mathbb{P}}(\Omega)\otimes W(D)\equiv L^2_{\mathbb{P}}(\Omega;W(D)) \\ {\it A_3.} \ \mathbb{P}\left[a(\omega,x)\in (a_{min},a_{max}) \ \forall x\in \overline{D}\right]=1, \ a_{min}>0, \ a_{max}<\infty \end{array}$





Example: The linear elliptic problem

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

with $f(\omega, \cdot)$ square integrable with respect to \mathbb{P} , satisfies assumptions A_1 , A_2 and A_3 with $W(D) = H_0^1(D)$

Example: The nonlinear elliptic problem

Similarly, for $k \in \mathbb{N}^+$,

$$\begin{aligned} & \left(-\nabla \cdot (a(\omega, \cdot)\nabla u(\omega, \cdot)) + u(\omega, \cdot)|u(\omega, \cdot)|^{k} = f(\omega, \cdot) & \text{in } \Omega \times D, \\ & u(\omega, \cdot) = 0 & \text{on } \Omega \times \partial D, \end{aligned} \end{aligned}$$

satisfies assumptions A_1 , A_2 and A_3 with $W(D) = H_0^1(D) \cap L^{k+2}(D)$



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

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

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 $\widetilde{u} = u - \overline{u}$,

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

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: to develop highly efficient, robust and scalable techniques that include uncertainty in the models, allow us to quantify uncertainty in the outputs and provide reliable and verifiable predictions. **Probability Theory** provides an effective tool to describe and propagate uncertainty.



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

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

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 $\widetilde{u} = u - \overline{u}$,

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

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: to develop highly efficient, robust and scalable techniques that include uncertainty in the models, allow us to quantify uncertainty in the outputs and provide reliable and verifiable predictions. **Probability Theory** provides an effective tool to describe and propagate uncertainty.



WLOG assume the random fields $a(\omega, x)$ and $f(\omega, x)$ depends on a finite number of random variables $\mathbf{Y}(\omega) = [Y_1(\omega), \dots, Y_N(\omega)] : \Omega \to \mathbb{R}^N$:

 $a_N(\omega, x) = a(\mathbf{Y}(\omega), x), \quad f_N(\omega, x) = f(\mathbf{Y}(\omega), x)$

- Piecewise constant material properties: Let $\{D_n\}_{n=1}^N$ be a partition of D then define $a_N(\omega, x) = \sum_{i=1}^N \sigma_i Y_i(\omega) \chi_{D_i}(x)$
- One-dimensional random field suitably truncated, e.g. lognormal permeability model in groundwater flows

• $\forall \omega \in \Omega, \ a(\omega, \cdot) \in L^{\infty}(D)$

- $\forall x_0 \in D$, $a(\cdot, x_0)$ is a random variable, e.g. $a(\cdot, x_0) \sim N(\mu, \sigma)$
- the interaction between points is described by a covariance function,

e.g. $\mathbb{C}ov[a](x_1, x_2) = \mathbb{E}\left[\widetilde{a}(\cdot, x_1)\widetilde{a}(\cdot, x_2)\right] = \sigma^2 \exp\left(-\frac{\|x_1 - x_2\|^2}{L_c^2}\right)$

Expand a in a Karhunen-Loève expansion and retain the first N terms, denoted a_N , to capture most of the variability



WLOG assume the random fields $a(\omega, x)$ and $f(\omega, x)$ depends on a finite number of random variables $\mathbf{Y}(\omega) = [Y_1(\omega), \dots, Y_N(\omega)] : \Omega \to \mathbb{R}^N$:

$$a_N(\omega, x) = a(\mathbf{Y}(\omega), x), \quad f_N(\omega, x) = f(\mathbf{Y}(\omega), x)$$

- Piecewise constant material properties: Let $\{D_n\}_{n=1}^N$ be a partition of D then define $a_N(\omega, x) = \sum_{i=1}^N \sigma_i Y_i(\omega) \chi_{D_i}(x)$
- One content of the second state of the seco
 - $\forall \omega \in \Omega, \ a(\omega, \cdot) \in L^{\infty}(D)$
 - $\forall x_0 \in D$, $a(\cdot, x_0)$ is a random variable, e.g. $a(\cdot, x_0) \sim N(\mu, \sigma)$
 - the interaction between points is described by a covariance function,

e.g.
$$\mathbb{C}ov[a](x_1, x_2) = \mathbb{E}\left[\widetilde{a}(\cdot, x_1)\widetilde{a}(\cdot, x_2)\right] = \sigma^2 \exp\left(-\frac{\|x_1 - x_2\|^2}{L_c^2}\right)$$

Expand a in a Karhunen-Loève expansion and retain the first N terms, denoted a_N , to capture most of the variability



 $\begin{array}{l} b_n: \text{ eigenfunctions of } \int_D \mathbb{C}_a(x_1,x_2)b_n(x_2)dx_2 = \lambda_n b_n(x_1), \ \|b_n\|_{L^2(D)} = 1\\ Y_n: \text{ uncorrelated RVs with } \mathbb{V}ar[Y_n] = \lambda_n \end{array}$

Example: Uniform random field

$$a(\omega, x) = a_0 + \sigma \sum_{n=1}^{\infty} b_n(x) Y_n(\omega)$$

•
$$Y_n \sim U(-\sqrt{3}, \sqrt{3}), \quad \mathbb{E}[Y_n] = 0, \quad \mathbb{V}ar[Y_n] = 1$$

• $a_{min} = a_0 - \sigma \sum_{n=1}^{\infty} \sqrt{3} \|b_n\|_{L^{\infty}(D)} > 0$ if σ is not too large

Example: Lognormal random field

$$a(\omega, x) = a_0 + \exp\left(\sum_{n=1}^{\infty} b_n(x) Y_n(\omega)\right)$$

• $Y_n \sim N(0, 1)$, $\mathbb{E}[Y_n] = 0$, $\mathbb{V}ar[Y_n] = 1$ • $a_{min} = 0$ and $a_{max} = \infty$





Approximating a Stochastic PDE Transform SBVP to Parameterized deterministic BVP



• Given $a_N(\mathbf{Y}(\omega), x)$, $f_N(\mathbf{Y}(\omega), x) \Rightarrow u_N(Y_1(\omega), \dots, Y_N(\omega), x)$ s.t.

 $\mathcal{L}(a_N)(\boldsymbol{u_N}) = f_N \text{ in } D \text{ a.s.}$

- $\Gamma_n \equiv Y_n(\Omega) \subset \mathbb{R}$ and $\Gamma = \prod_{n=1}^N \Gamma_n \subset \mathbb{R}^N$ image of the random vector $\mathbf{Y}(\Omega)$ (curse of dimensionality when N is large)
- $\mathbf{Y} = (Y_1, Y_2, \dots, Y_N)$ has a joint PDF $\rho : \Gamma \to \mathbb{R}_+$, with $\rho \in L^{\infty}(\Gamma)$, i.e. for $\mathbf{y} \in \Gamma$ $\mathbb{P}\left[Z \in \gamma \subset \Gamma\right] = \int_{\Omega} \rho(\mathbf{y}) d\mathbf{y},$

i.e. transform the measure
$$\mathbb{P}$$
 to \mathbb{R}^N

Quantities of interest (Qol)

Our goal of predicting the statistical behavior of a physical system often requires the approximation of multi-dimensional statistical Qols, e.g.:

$$\mathbb{E}[u](x) = \int_{\Gamma} u(\mathbf{y}, x) \rho(\mathbf{y}) d\mathbf{y}, \quad \text{where } \mathbf{y} \in \Gamma^N \text{ and } x \in \overline{D}$$





Approximating a Stochastic PDE Transform SBVP to Parameterized deterministic BVP



• Given $a_N(\mathbf{Y}(\omega), x)$, $f_N(\mathbf{Y}(\omega), x) \Rightarrow u_N(Y_1(\omega), \dots, Y_N(\omega), x)$ s.t.

 $\mathcal{L}(a_N)(\boldsymbol{u_N}) = f_N \text{ in } D \text{ a.s.}$

- $\Gamma_n \equiv Y_n(\Omega) \subset \mathbb{R}$ and $\Gamma = \prod_{n=1}^N \Gamma_n \subset \mathbb{R}^N$ image of the random vector $\mathbf{Y}(\Omega)$ (curse of dimensionality when N is large)
- $\mathbf{Y} = (Y_1, Y_2, \dots, Y_N)$ has a joint PDF $\rho : \Gamma \to \mathbb{R}_+$, with $\rho \in L^{\infty}(\Gamma)$, i.e. for $\mathbf{y} \in \Gamma$ $\mathbb{P}\left[Z \in \gamma \subset \Gamma\right] = \int_{\Sigma} \rho(\mathbf{y}) d\mathbf{y},$

i.e. transform the measure $\mathbb P$ to $\mathbb R^N$

Quantities of interest (Qol)

Our goal of predicting the statistical behavior of a physical system often requires the approximation of multi-dimensional statistical Qols, e.g.:

$$\mathbb{E}[u](x) = \int_{\Gamma} u(\mathbf{y}, x) \rho(\mathbf{y}) d\mathbf{y}, \quad \text{where } \mathbf{y} \in \Gamma^N \text{ and } x \in \overline{D}$$



• By Lax-Milgram $\exists ! \ u \in H_P = L^2_P(\Omega; H^1_0(D))$ to the linear SPDE s.t.

$$\|u\|_{H_P} \le \frac{C_P}{a_{min}} \left(\int_D \mathbb{E}[f^2] \, dx\right)^{1/2}$$

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

$$\begin{cases} -\nabla \cdot (a(\mathbf{y}, x) \nabla u(\mathbf{y}, x)) &= f(\mathbf{y}, x) & \text{ for a.e. } x \in D, \\ u(\mathbf{y}, x) &= 0 & \text{ for a.e. } x \in \partial D, \end{cases}$$

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

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

$$\mathbb{E}\left[\int_{D} a(\mathbf{y}, x) \nabla u(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \, dx\right] = \mathbb{E}\left[\int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \, dx\right]$$
$$\int \int a(\mathbf{y}, x) \nabla u(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \, \rho(\mathbf{y}) \, dx \, d\mathbf{y} = \int \int f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \, \rho(\mathbf{y}) \, dx \, dx$$



• By Lax-Milgram $\exists ! \ u \in H_P = L^2_P(\Omega; H^1_0(D))$ to the linear SPDE s.t.

$$\|u\|_{H_P} \le \frac{C_P}{a_{min}} \left(\int_D \mathbb{E}[f^2] \, dx\right)^{1/2}$$

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

$$\begin{cases} -\nabla \cdot (a(\mathbf{y}, x) \nabla u(\mathbf{y}, x)) &= f(\mathbf{y}, x) & \text{ for a.e. } x \in D, \\ u(\mathbf{y}, x) &= 0 & \text{ for a.e. } x \in \partial D, \end{cases}$$

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

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

$$\mathbb{E}\left[\int_{D} a(\mathbf{y}, x) \nabla u(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \, dx\right] = \mathbb{E}\left[\int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \, dx\right]$$
$$\int_{\Gamma} \int_{D} a(\mathbf{y}, x) \nabla u(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \, \rho(\mathbf{y}) dx d\mathbf{y} = \int_{\Gamma} \int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \, \rho(\mathbf{y}) dx d\mathbf{y}$$

A brief taxonomy of methods For numerical soln. of PDEs with random input data



Stochastic finite element methods (SFEMs)



- methods for which spatial discretization is effected using finite element methods (FEMs)[†]
- Stochastic sampling methods (SSMs): random samples in Γ of PDE inputs are used to compute ensemble averages of statistical Qols, e.g. MCFEM - non-intrusive
- Stochastic polynomial approximation
 - Stochastic Galerkin methods (SGMs): probabilistic discretization is also effected by a spectral Galerkin projection onto e.g. an L²_p-orthogonal basis (Wiener or polynomial chaos) - intrusive
 - probabilistic discretization is effected by collocating the FE solution on a particular set of of points and then connect the realizations with suitable interpolatory basis (Lagrangian) *non-intrusive*

A brief taxonomy of methods For numerical soln. of PDEs with random input data



Stochastic finite element methods (SFEMs)



- methods for which spatial discretization is effected using finite element methods (FEMs)[†]
- Stochastic sampling methods (SSMs): random samples in Γ of PDE inputs are used to compute ensemble averages of statistical Qols, e.g. MCFEM - non-intrusive
- Stochastic polynomial approximation
 - Stochastic Galerkin methods (SGMs): probabilistic discretization is also effected by a spectral Galerkin projection onto e.g. an L²_p-orthogonal basis (Wiener or polynomial chaos) - intrusive
 - probabilistic discretization is effected by collocating the FE solution on a particular set of of points and then connect the realizations with suitable interpolatory basis (Lagrangian) *non-intrusive*

A brief taxonomy of methods For numerical soln. of PDEs with random input data



Stochastic finite element methods (SFEMs)



- methods for which spatial discretization is effected using finite element methods (FEMs)[†]
- Stochastic sampling methods (SSMs): random samples in Γ of PDE inputs are used to compute ensemble averages of statistical Qols, e.g. MCFEM - non-intrusive
- Stochastic polynomial approximation
 - Stochastic Galerkin methods (SGMs): probabilistic discretization is also effected by a spectral Galerkin projection onto e.g. an L²_ρ-orthogonal basis (Wiener or polynomial chaos) - intrusive
 - Stochastic Collocation methods (SCMs): probabilistic discretization is effected by collocating the FE solution on a particular set of of points and then connect the realizations with suitable interpolatory basis (Lagrangian) - non-intrusive



O Spatial discretization:

[†]Throughout, we assume that spatial discretization is effected using finite element methods; most of what we say also holds for other spatial discretization approaches, e.g., finite differences, finite volumes, spectral, etc.

Probabilistic discretization:

Throughout, we assume that the probabilistic discretization is effected using globally supported spectral or interpolatory basis functions. In this sense adaptive refinement refers to the anisotropic polynomial order used by the global basis.

 Adaptive wavelet stochastic collocation method for non-smooth solutions of SPDEs, Max Gunzburger, Clayton Webster, Guannan Zhang
 Wednesday 2:30pm: MS53 - Recent Advances in Numerical SPDEs



$$\begin{pmatrix} -\nabla \cdot (a(\mathbf{y}_k, \cdot) \nabla u^h(\mathbf{y}_k, \cdot)) = f(\mathbf{y}_k, \cdot), & \text{in } D \\ u^h(\mathbf{y}_k, \cdot) = 0, & \text{on } \partial D \end{pmatrix}$$

If desired evaluate the QoI $Q\left(u^h(\mathbf{y}_k,\cdot)
ight)$

) Approximate statistics, e.g. expectations $\mathbb{E}[u^h](x)$, by sample averages:

$$\mathbb{E}\left[u^{h}(\mathbf{y})\right](x) \approx \frac{1}{M} \sum_{k=1}^{M} u^{h}(\mathbf{y}_{k}) \rho(\mathbf{y}_{k}) := \mathscr{E}\left(u^{h}; M\right), \quad \mathbf{y}_{k} \in \Gamma$$

$$\left\|\mathbb{E}[u^{h}] - \mathscr{E}\left(u^{h}; M\right)\right\| \leq \mathsf{TOL}$$



$$\begin{cases} -\nabla \cdot (a(\mathbf{y}_k, \cdot) \nabla u^h(\mathbf{y}_k, \cdot)) = & f(\mathbf{y}_k, \cdot), & \text{in } D \\ u^h(\mathbf{y}_k, \cdot) = & 0, & \text{on } \partial D \end{cases}$$

If desired evaluate the QoI $Q\left(u^h(\mathbf{y}_k,\cdot)
ight)$

3 Approximate statistics, e.g. expectations $\mathbb{E}[u^h](x)$, by sample averages:

$$\mathbb{E}\left[u^{h}(\mathbf{y})\right](x) \approx \frac{1}{M} \sum_{k=1}^{M} u^{h}(\mathbf{y}_{k}) \rho(\mathbf{y}_{k}) := \mathscr{E}\left(u^{h}; M\right), \quad \mathbf{y}_{k} \in \Gamma$$

$$\left\|\mathbb{E}[u^h] - \mathscr{E}\left(u^h; M\right)\right\| \leq \mathsf{TOL}$$



$$\begin{cases} -\nabla \cdot (a(\mathbf{y}_k, \cdot) \nabla u^h(\mathbf{y}_k, \cdot)) = & f(\mathbf{y}_k, \cdot), & \text{in } D \\ u^h(\mathbf{y}_k, \cdot) = & 0, & \text{on } \partial D \end{cases}$$

If desired evaluate the QoI $Q\left(u^h(\mathbf{y}_k,\cdot)\right)$

3 Approximate statistics, e.g. expectations $\mathbb{E}[u^h](x)$, by sample averages:

$$\mathbb{E}\left[u^{h}(\mathbf{y})\right](x) \approx \frac{1}{M} \sum_{k=1}^{M} u^{h}(\mathbf{y}_{k}) \rho(\mathbf{y}_{k}) := \mathscr{E}\left(u^{h}; M\right), \quad \mathbf{y}_{k} \in \Gamma$$

$$\left\|\mathbb{E}[u^{h}] - \mathscr{E}\left(u^{h}; M\right)\right\| \leq \mathsf{TOL}$$



$$\begin{cases} -\nabla \cdot (a(\mathbf{y}_k, \cdot) \nabla u^h(\mathbf{y}_k, \cdot)) = & f(\mathbf{y}_k, \cdot), & \text{in } D \\ u^h(\mathbf{y}_k, \cdot) = & 0, & \text{on } \partial D \end{cases}$$

If desired evaluate the QoI $Q\left(u^h(\mathbf{y}_k,\cdot)\right)$

(3) Approximate statistics, e.g. expectations $\mathbb{E}[u^h](x)$, by sample averages:

$$\mathbb{E}\left[u^{h}(\mathbf{y})\right](x) \approx \frac{1}{M} \sum_{k=1}^{M} u^{h}(\mathbf{y}_{k}) \rho(\mathbf{y}_{k}) := \mathscr{E}\left(u^{h}; M\right), \quad \mathbf{y}_{k} \in \Gamma$$

$$\left\|\mathbb{E}[u^h] - \mathscr{E}\left(u^h; M\right)\right\| \leq \mathsf{TOL}$$

SPDEs Input noise MCFEM Regularity Polynomial approx. SCFEM SCFEM Summary
Convergence of the MCFEM
Error splitting
$$\mathbb{E}[u] - \mathscr{E}(u^h; M) = \underbrace{\left(\mathbb{E}[u - u^h]\right)}_{\text{Spatial Discret.}} + \underbrace{\left(\mathbb{E}[u^h] - \frac{1}{M}\sum_{k=1}^{M} u^h(\mathbf{y}_k)\rho(\mathbf{y}_k)\right)}_{\text{Statistical Error}}$$

• Spatial discretization error:

$$\left\| \mathbb{E}[u-u^{h}] \right\|_{L^{2}(D)} + h \left\| \mathbb{E}[u-u^{h}] \right\|_{H^{1}_{0}(D)} \le Ch^{2} \sqrt{\mathbb{E}\left[\|f\|_{L^{2}(D)}^{2} \right]}$$

• **Statistical Error**: Within confidence level $\alpha \in (0, 1)$, $\exists \delta(\alpha) > 0$ s.t.

$$\begin{split} \mathbb{P}\left[\left\|\mathbb{E}[u^{h}] - \frac{1}{M}\sum_{k=1}^{M} u^{h}(\mathbf{y}_{k})\rho(\mathbf{y}_{k})\right\|_{H_{0}^{1}(D)} \leq \delta \frac{C_{u}}{\sqrt{M}}\right] \geq \alpha \\ (M_{n})^{\beta} \left\|\mathbb{E}[u^{h}] - \mathscr{E}\left(u^{h}; M\right)\right\|_{H_{0}^{1}(D)} \to 0 , n \to \infty \text{ a.s.} \\ \text{all } \beta \in (0, 1/2) \text{ with } M_{n} = 2^{n} \end{split}$$

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary
Convergence of the MCFEM
Error splitting
$$\mathbb{E}[u] - \mathscr{E}(u^h; M) = \underbrace{\left(\mathbb{E}[u-u^h]\right)}_{\text{Spatial Discret.}} + \underbrace{\left(\mathbb{E}[u^h] - \frac{1}{M}\sum_{k=1}^{M} u^h(\mathbf{y}_k)\rho(\mathbf{y}_k)\right)}_{\text{Statistical Error}}$$

• Spatial discretization error:

for

$$\left\| \mathbb{E}[u-u^{h}] \right\|_{L^{2}(D)} + h \left\| \mathbb{E}[u-u^{h}] \right\|_{H^{1}_{0}(D)} \leq Ch^{2} \sqrt{\mathbb{E}\left[\|f\|_{L^{2}(D)}^{2} \right]}$$

• Statistical Error: Within confidence level $\alpha \in (0,1)$, $\exists \delta(\alpha) > 0$ s.t.

$$\begin{split} \mathbb{P}\left[\left\|\mathbb{E}[u^h] - \frac{1}{M}\sum_{k=1}^M u^h(\mathbf{y}_k)\rho(\mathbf{y}_k)\right\|_{H_0^1(D)} \leq \delta \frac{C_u}{\sqrt{M}}\right] \geq \alpha \\ (M_n)^{\beta} \left\|\mathbb{E}[u^h] - \mathscr{E}\left(u^h; M\right)\right\|_{H_0^1(D)} \to 0 \ , n \to \infty \text{ a.s.} \\ \text{all } \beta \in (0, 1/2) \text{ with } M_n = 2^n \end{split}$$

Other sampling-based methods Attempting to cope with the *curse of dimensionality*

Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of Qols by sample averages: $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{k=1}^M Q(u(\mathbf{y}_k))\rho(\mathbf{y}_k), \quad \mathbf{y}_k \in \Gamma$

- **4** Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods**: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences
- **O** Latin Hypercube Sampling: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^N\right)$ abscissas are chosen to ensure "good" spacing in each 1-D component
- **O** Lattice rules: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^{(N+1)/2})$ abscissas are "good" lattice points



National Laboratory

Other sampling-based methods Attempting to cope with the curse of dimensionality

Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of Qols by sample $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{k=1}^{M} Q(u(\mathbf{y}_{k}))\rho(\mathbf{y}_{k}), \quad \mathbf{y}_{k} \in \Gamma$ averages:

- **()** Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods:** $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences



National Laboratory

Other sampling-based methods Attempting to cope with the *curse of dimensionality*

nsionality

Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of Qols by sample averages: $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{i=1}^M Q(u(\mathbf{y}_k))\rho(\mathbf{y}_k), \quad \mathbf{y}_k \in \Gamma$

- Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods**: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences
- Solution Hypercube Sampling: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^N\right)$ abscissas are chosen to ensure "good" spacing in each 1-D component
- Lattice rules: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^{(N+1)/2})$ abscissas are "good" lattice points



Other sampling-based methods Attempting to cope with the *curse of dimensionality*

Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of Qols by sample averages: $\mathbb{F}[Q(u(\mathbf{x}))] \simeq \frac{1}{2} \sum_{k=1}^M Q(u(\mathbf{x}_k)) Q(\mathbf{x}_k) = \mathbf{x}_k \in \Gamma$

- $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{k=1}^{M} Q(u(\mathbf{y}_k)) \rho(\mathbf{y}_k), \quad \mathbf{y}_k \in \Gamma$
- Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods**: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences
- Solution Latin Hypercube Sampling: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^N\right)$ abscissas are chosen to ensure "good" spacing in each 1-D component
- Lattice rules: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^{(N+1)/2}\right)$ abscissas are "good" lattice points





Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of QoIs by sample averages: $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{k=1}^M Q(u(\mathbf{y}_k))\rho(\mathbf{y}_k), \quad \mathbf{y}_k \in \Gamma$

- Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods**: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences
- **3** Latin Hypercube Sampling: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^N\right)$ abscissas are chosen to ensure "good" spacing in each 1-D component
- $\label{eq:Lattice rules: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^{(N+1)/2}\right)$ abscissas are "good" lattice points }$

Pros: Allow for reusability of deterministic codes and the convergence rate is independent of the regularity of $u(\mathbf{y})$ (and dimension with MC methods)



Let $\{\mathbf{y}_k\}_{k=1}^M$ be iid samples. Approximate expectations of QoIs by sample averages: $\mathbb{E}[Q(u(\mathbf{y}))] \approx \frac{1}{M} \sum_{k=1}^M Q(u(\mathbf{y}_k))\rho(\mathbf{y}_k), \quad \mathbf{y}_k \in \Gamma$

- Monte Carlo methods: $\varepsilon(M) \approx \mathcal{O}(M^{-1/2})$ abscissas are (pseudo) random numbers
- **Quasi-Monte Carlo methods**: $\varepsilon(M) \approx \mathcal{O}(M^{-1}(\log(M))^N)$ abscissas are low discrepancy sequences
- Solution Hypercube Sampling: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^N\right)$ abscissas are chosen to ensure "good" spacing in each 1-D component
- Lattice rules: $\varepsilon(M) \approx \mathcal{O}\left(M^{-1}(\log(M))^{(N+1)/2}\right)$ abscissas are "good" lattice points

Cons: The sampling methods do not yield fully discrete approximations and slow convergence rates do not exploit the possible regularity of the functional



• Let $\Gamma_n^* = \prod_{\substack{j=1\\j\neq n}}^N \Gamma_j$, and let \mathbf{y}_n^* denote an arbitrary element of Γ_n^*

Theorem: Regularity [Linear: BNT07], [Nonlinear: W07, GW11]

For each $y_n \in \Gamma_n$, there exists $\tau_n > 0$ such that the function $u(y_n, \mathbf{y}_n^*, x)$ as a function of y_n , $u : \Gamma_n \to C^0(\Gamma_n^*; W(D))$ admits an analytic extension $u(z, \mathbf{y}_n^*, x)$, $z \in \mathbb{C}$, in the region of the complex plane

$$\Sigma(\Gamma_n;\tau_n) \equiv \{z \in \mathbb{C}, \ \operatorname{dist}(z,\Gamma_n) \leq \tau_n\}.$$

Moreover, $\forall z \in \Sigma(\Gamma_n; \tau_n)$,

$$\|u(z)\|_{C^0(\Gamma_n^*;W(D))} \le \lambda$$

with λ a constant independent of n.

Remark: The analyticity of the solution $u(\mathbf{y}, x)$ w.r.t. each random direction y_n suggests the use of (multivariate) polynomial approximation





- The analyticity of the solution $u(\mathbf{y}, x)$ w.r.t. each random direction y_n suggests the use of (multivariate) polynomial approximation
 - what is the correct polynomial approximation subspace?
- The solution must be approximated w.r.t. all RV's $Y_1(\omega), \ldots, Y_N(\omega) \Rightarrow$ Possible high-dimensional problem!
 - how do we compute numerical approximations within those subspaces?
- The numerical method must convergence using as few d.o.f.'s as possible
 what is the resulting complexity of my polynomial approximation?

E.g. Curse of dimensionality: (Isotropic) TP's of degree p in N dimensions

#d.o.f.
$$M = (p+1)^{1}$$

ror $\leq C e^{-gM\, {ar n} \over N}$

mpractical in higher dimensions



- The analyticity of the solution $u(\mathbf{y}, x)$ w.r.t. each random direction y_n suggests the use of (multivariate) polynomial approximation
 - what is the correct polynomial approximation subspace?
- The solution must be approximated w.r.t. all RV's $Y_1(\omega), \ldots, Y_N(\omega) \Rightarrow$ Possible high-dimensional problem!
 - how do we compute numerical approximations within those subspaces?
- The numerical method must convergence using as few d.o.f.'s as possible
 what is the resulting complexity of my polynomial approximation?

E.g. Curse of dimensionality: (Isotropic) TP's of degree p in N dimensions error $\leq Ce^{-gp}$, #d.o.f. $M = (p+1)^N$ \Leftrightarrow error $\leq Ce^{-gM^{\frac{1}{N}}}$ Impractical in higher dimensions



Multivariate polynomial approximation Fully discrete *stochastic* solutions



Basic idea: approximate the response $u(\mathbf{y}, \cdot)$ by multi-variate global polynomials. The numerical solution should convergence quickly since the solution is analytic in \mathbf{y} .

Approximating spaces:

- Let \mathcal{T}_h be a triangulation of D and $W^h(D) \subset W(D)$ contains cont. piecewise polynomials defined in \mathcal{T}_h
 - Assume $J = \dim[W^h(D)]$ and $\{\phi_j(x)\}_{j=1}^J \subset W_h(D)$ is a FE basis for the deterministic domain
- ② Let $\mathbf{p} = (p_1, \dots, p_N)$ be a multi-index, $\mathcal{J}(p) \subset \mathbb{N}^N$ a multi-index set, with $p \in \mathbb{N}_+$, and define:

Multivariate polynomial space

$$\mathcal{P}_{\mathcal{J}(p)}(\Gamma) = \operatorname{span}\left\{\prod_{n=1}^{N} y_n^{p_n}, \text{ with } \mathbf{p} \in \mathcal{J}(p)\right\} \subset L^2_{\rho}(\Gamma)$$

• Assume $M = \dim \left[\mathcal{P}_{\mathcal{J}(p)}(\Gamma) \right]$ and $\{\psi_k\}_{k=1}^M$ form a basis for $\mathcal{P}_{\mathcal{J}(p)}(\Gamma)$, e.g. multivariate Legendre, Hermite, Lagrange, etc.



Multivariate polynomial approximation Fully discrete *stochastic* solutions



Basic idea: approximate the response $u(\mathbf{y}, \cdot)$ by multi-variate global polynomials. The numerical solution should convergence quickly since the solution is analytic in \mathbf{y} .

Approximating spaces:

- Let \mathcal{T}_h be a triangulation of D and $W^h(D) \subset W(D)$ contains cont. piecewise polynomials defined in \mathcal{T}_h
 - Assume $J = \dim[W^h(D)]$ and $\{\phi_j(x)\}_{j=1}^J \subset W_h(D)$ is a FE basis for the deterministic domain
- ② Let $\mathbf{p} = (p_1, ..., p_N)$ be a multi-index, $\mathcal{J}(p) \subset \mathbb{N}^N$ a multi-index set, with $p \in \mathbb{N}_+$, and define:

Multivariate polynomial space

$$\mathcal{P}_{\mathcal{J}(p)}(\Gamma) = \operatorname{span}\left\{\prod_{n=1}^N y_n^{p_n}, \quad \text{with } \mathbf{p} \in \mathcal{J}(p)\right\} \subset L^2_\rho(\Gamma)$$

• Assume $M = \dim \left[\mathcal{P}_{\mathcal{J}(p)}(\Gamma) \right]$ and $\{\psi_k\}_{k=1}^M$ form a basis for $\mathcal{P}_{\mathcal{J}(p)}(\Gamma)$, e.g. multivariate Legendre, Hermite, Lagrange, etc.


Multivariate polynomial approximation Fully discrete *stochastic* solutions II

Multivariate polynomial space

$$\mathcal{P}_{\mathcal{J}(p)}(\Gamma) = \operatorname{span}\left\{\prod_{n=1}^{N} y_n^{p_n}, \quad \text{with } \mathbf{p} \in \mathcal{J}(p)\right\} \subset L^2_{\rho}(\Gamma)$$

Fully discrete approximations: $u_p \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$ s.t.

$$u_p(\mathbf{y}, x) = \sum_{j=1}^{J} \sum_{k=1}^{M} c_{jk} \phi_j(x) \psi_k(\mathbf{y}) = \sum_{k=1}^{M} u_k(x) \psi_k(\mathbf{y}), \quad \text{with } u_k(x) \in W^h(D)$$

- To compute the fully discrete approximation using SFEMs requires the resolution of the coefficients u_k which can be accomplished via:
 - intrusive methods by solving the fully coupled $JM\times JM$ system (i.e. JM equations and JM degrees of freedom
 - $\bullet\,$ non-intrusive methods by de-coupling the above expression and solving a M system's of size J
- Our goal is to estimate the error $||u u_p||_{L^2_o(\Gamma)}$

National Laboratory

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary



Multivariate polynomial approximation Fully discrete *stochastic* solutions II

Multivariate polynomial space

$$\mathcal{P}_{\mathcal{J}(p)}(\Gamma) = \operatorname{span}\left\{\prod_{n=1}^{N} y_n^{p_n}, \quad \text{with } \mathbf{p} \in \mathcal{J}(p)\right\} \subset L^2_{\rho}(\Gamma)$$

Fully discrete approximations: $u_p \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$ s.t.

$$u_p(\mathbf{y}, x) = \sum_{j=1}^J \sum_{k=1}^M c_{jk} \phi_j(x) \psi_k(\mathbf{y}) = \sum_{k=1}^M u_k(x) \psi_k(\mathbf{y}), \quad \text{with } u_k(x) \in W^h(D)$$

- To compute the fully discrete approximation using SFEMs requires the resolution of the coefficients u_k which can be accomplished via:
 - intrusive methods by solving the fully coupled $JM \times JM$ system (i.e. JM equations and JM degrees of freedom
 - non-intrusive methods by de-coupling the above expression and solving a ${\cal M}$ system's of size J
- *Our goal* is to estimate the error $||u u_p||_{L^2_{\rho}(\Gamma)}$

National Laboratory

Polynomial spaces Anisotropic representations



Rewrite the fully discrete approximation using the multi-index notation:

$$u_p = \sum_{\mathbf{p} \in \mathcal{J}(p)} u_{\mathbf{p}}(x) \psi_{\mathbf{p}}(\mathbf{y}), \quad \mathbf{p} = (p_1, \dots, p_N)$$

where, if $\mathbf{y} = (y_1, \dots, y_N)$ independent then

$$\psi_{\mathbf{p}}(\mathbf{y}) = \prod_{n=1}^{N} \psi_{p_n}^{(n)}(y_n), \quad \psi_{p_n}^{(n)} \in L^2_{\rho_n}(\Gamma_n)$$

Several choices for polynomial multi-index $\mathbf{p} \in \mathcal{J}(p)$ [BNTT11]:

- Tensor products (TP): $\max_n \alpha_n p_n \leq p$ (Intractable for large N),
- Total degree (TD): $\sum_{n=1}^{N} \alpha_n p_n \leq p$,
- Hyperbolic cross (HC): $\prod_{n=1}^{N} (p_n+1)^{\alpha_n} \leq p+1$,
- Smolyak method (SM): $\sum_{n=1}^{N} \alpha_n f(p_n) \leq f(p)$ with $_{f(p)} = \begin{cases} 0, p=0\\ 1, p=1\\ \lceil \log_2(p) \rceil, p \geq 2 \end{cases}$

Anisotropic: introduce weight vector $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_N) \in \mathbb{R}^N_+$, with $\alpha_{min} = 1$ TD, HC & SM all reduce the *curse of dimensionality* w.r.t. TP methods Polynomial spaces Anisotropic representations



Rewrite the fully discrete approximation using the multi-index notation:

$$u_p = \sum_{\mathbf{p} \in \mathcal{J}(p)} u_{\mathbf{p}}(x) \psi_{\mathbf{p}}(\mathbf{y}), \quad \mathbf{p} = (p_1, \dots, p_N)$$

where, if $\mathbf{y} = (y_1, \dots, y_N)$ independent then

$$\psi_{\mathbf{p}}(\mathbf{y}) = \prod_{n=1}^{N} \psi_{p_n}^{(n)}(y_n), \quad \psi_{p_n}^{(n)} \in L^2_{\rho_n}(\Gamma_n)$$

Several choices for polynomial multi-index $\mathbf{p} \in \mathcal{J}(p)$ [BNTT11]:

- Tensor products (TP): $\max_n \alpha_n p_n \leq p$ (Intractable for large N),
- Total degree (TD): $\sum_{n=1}^{N} \alpha_n p_n \leq p$,
- Hyperbolic cross (HC): $\prod_{n=1}^{N} (p_n + 1)^{\alpha_n} \le p + 1$,
- Smolyak method (SM): $\sum_{n=1}^{N} \alpha_n f(p_n) \leq f(p)$ with $f(p) = \begin{cases} 0, p=0\\ 1, p=1\\ \lceil \log_2(p) \rceil, p \geq 2 \end{cases}$

Anisotropic: introduce weight vector $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_N) \in \mathbb{R}^N_+$, with $\alpha_{min} = 1$ TD, HC & SM all reduce the *curse of dimensionality* w.r.t. TP methods SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

Example (anisotropic) polynomial spaces N = 2, p = 8 with $\alpha = (1, 2)$







National Laboratory



J. Burkardt, http://www.sc.fsu.edu/~burkardt, C. Webster, http://www.csm.ornl.gov/~cgwebster — April 2-3, 2012



Monomials up to 4th degree. Those below the line are the useless monomials we capture (using tensor products) and are not needed (and not possible) in higher dimensions - they don't add the asymptotic accuracy and the cost increases exponential as the dimensions increase

 $\max(p_1, p_2) < 4$



Monomials up to 4th degree. Those below the line are the useless monomials we capture (using tensor products) and are not needed (and not possible) in higher dimensions - they don't add the asymptotic accuracy and the cost increases exponential as the dimensions increase

Recall
$$M = \dim \left[\mathcal{P}_{\mathcal{J}(p)}(\Gamma) \right] \Longrightarrow M_{TD} = \frac{(N+p)!}{N!p!} \ll M_{TP} = (p+1)^N$$

 $\max(p_1, p_2) \le 4$

 $y_1^2 y_2^4$



General basis in N dimensions Total degree vs. Tensor products



N =	p =	K = total $#$ of probabilistic	
∦ RVs,	maximal degree	degrees of freedom	
$\dim(\Gamma)$	of polynomials	using total	using tensor
		degree basis	product basis
3	3	20	64
	5	56	216
5	3	56	1,024
	5	252	7,776
10	3	286	1,048,576
	5	3,003	60,046,176
20	3	1,771	$> 1 \times 10^{12}$
	5	53,130	$> 3 imes 10^{15}$
100	3	176,851	$> 1 \times 10^{60}$
	5	96,560,646	$> 6 imes 10^{77}$

• tensor products become computational infeasible in higher dimensions



Stochastic Galerkin approximation

Find
$$u_p^{SG} \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$$
 s.t.

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

Stochsatic Galerkin (SG) FEM Galerkin projection onto the subspace $\mathcal{P}_{\mathcal{T}(p)}(\Gamma) \otimes W^{h}(D)$

$$\mathbb{E}\left[\int_{D} a(\mathbf{y}, x) \nabla u_{p}^{SG}(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \ dx\right] = \mathbb{E}\left[\int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \ dx\right]$$

for all $v \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$

- Typically u_p^{SG} is defined using an L_{ρ}^2 -orthogonal basis $\{\psi_k\}_{k=1}^{M_{SG}}$ constructed from univariate $L_{\rho_n}^2$ -orthogonal polynomials i.e. assuming independent RVs, e.g. $\rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n)$ -Wiener (polynomial) chaos
- Optimal index set of cardinality M_{TD} corresponds to the TD subspace

[Ghanem-Spanos], [Karniadakis-Xiu], [Matthies-Keese], [Schwab-Todor et. al], [Knio-Le Maître et. al], [Babuška et. al], etc.

Stochsatic Galerkin (SG) FEM Galerkin projection onto the subspace $\mathcal{P}_{\mathcal{T}(p)}(\Gamma) \otimes W^{h}(D)$

Stochastic Galerkin approximation

Find $u_p^{SG} \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$ s.t.

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

$$\mathbb{E}\left[\int_{D} a(\mathbf{y}, x) \nabla u_{p}^{SG}(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \ dx\right] = \mathbb{E}\left[\int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \ dx\right]$$

for all $v \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$

- Typically u_p^{SG} is defined using an L_{ρ}^2 -orthogonal basis $\{\psi_k\}_{k=1}^{M_{SG}}$ constructed from univariate $L_{\rho_n}^2$ -orthogonal polynomials i.e. assuming independent RVs, e.g. $\rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n)$ -Wiener (polynomial) chaos
- Optimal index set of cardinality M_{TD} corresponds to the TD subspace

Pros: Guaranteed L^2 optimality of the projection and spectral convergence for smooth stochastic solutions

[Ghanem-Spanos], [Karniadakis-Xiu], [Matthies-Keese], [Schwab-Todor et. al], [Knio-Le Maître et. al], [Babuška et. al], etc.

National Laboratory



Stochastic Galerkin approximation

Find $u_p^{SG} \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$ s.t.

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

Stochsatic Galerkin (SG) FEM Galerkin projection onto the subspace $\mathcal{P}_{\mathcal{T}(p)}(\Gamma) \otimes W^{h}(D)$

$$\mathbb{E}\left[\int_{D} a(\mathbf{y}, x) \nabla u_{p}^{SG}(\mathbf{y}, x) \cdot \nabla v(\mathbf{y}, x) \ dx\right] = \mathbb{E}\left[\int_{D} f(\mathbf{y}, x) \cdot v(\mathbf{y}, x) \ dx\right]$$

for all $v \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$

- Typically u_p^{SG} is defined using an L_{ρ}^2 -orthogonal basis $\{\psi_k\}_{k=1}^{M_{SG}}$ constructed from univariate $L_{\rho_n}^2$ -orthogonal polynomials i.e. assuming independent RVs, e.g. $\rho(\mathbf{y}) = \prod_{n=1}^N \rho_n(y_n)$ -Wiener (polynomial) chaos
- Optimal index set of cardinality M_{TD} corresponds to the TD subspace
- **Cons**: Inherently a fully coupled *intrusive* approximation that requires the resolution of **large** systems (integrals and residuals) as well as novel (problem specific) pre-conditioning techniques

[Ghanem-Spanos], [Karniadakis-Xiu], [Matthies-Keese], [Schwab-Todor et. al], [Knio-Le Maître et. al], [Babuška et. al], etc.



SGFEM Spectral orthogonal basis



The L_{ρ}^2 -orthogonal basis was originally developed to approximate white noise processes with Gaussian measure [Wiener, 1938].

• the univariate Hermite polynomials H(y) serve as the foundation for the construction of the multi-dimensional Hermite polynomials - orthogonal with respect to the Gaussian measure





Hermite polynomials

Generalized Multi-dimensional orthonormal polynomials

Let $\left\{H_{p_n}^{(n)}\right\}_{p_n=0}^p$ denote the set of univariate Hermite polynomials (of degree $\leq p$) defined in $L^2_{\rho_n}(\Gamma_n)$, that are orthonormal w.r.t. the Gaussian PDF $\rho_n(y_n)$, for each $n = 1, \ldots, N$:

$$\int_{\Gamma_n} H_{p_n}^{(n)}(y_n) H_{r_n}^{(n)}(y_n) \rho_n(y_n) \, dy_n = \delta_{p_n r_n}, \quad p_n, r_n \in \{0, \dots, p\}$$

The multi-variate $L^2_{\rho}(\Gamma)$ -orthogonal Hermite basis is defined as a tensor-product of the univariate polynomials with $\mathbf{p} \in \mathcal{J}(p)$:

$$H_{\mathbf{p}}(\mathbf{y}) = \prod_{n=1}^{N} H_{p_n}^{(n)}(y_n), \quad \text{s.t. } \rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n),$$

where $ho(\mathbf{y})$ is the Gaussian joint-PDF

identical construction for other orthonormal bases (generalized PC)
 e.g. Y uniform RVs → Legendre polynomial basis, etc.

National Laborator



Hermite polynomials

Generalized Multi-dimensional orthonormal polynomials

Let $\left\{H_{p_n}^{(n)}\right\}_{p_n=0}^p$ denote the set of univariate Hermite polynomials (of degree $\leq p$) defined in $L^2_{\rho_n}(\Gamma_n)$, that are orthonormal w.r.t. the Gaussian PDF $\rho_n(y_n)$, for each $n = 1, \ldots, N$:

$$\int_{\Gamma_n} H_{p_n}^{(n)}(y_n) H_{r_n}^{(n)}(y_n) \rho_n(y_n) \, dy_n = \delta_{p_n r_n}, \quad p_n, r_n \in \{0, \dots, p\}$$

The multi-variate $L^2_{\rho}(\Gamma)$ -orthogonal Hermite basis is defined as a tensor-product of the univariate polynomials with $\mathbf{p} \in \mathcal{J}(p)$:

$$H_{\mathbf{p}}(\mathbf{y}) = \prod_{n=1}^{N} H_{p_n}^{(n)}(y_n), \quad \text{s.t. } \rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n),$$

where $\rho(\mathbf{y})$ is the Gaussian joint-PDF

identical construction for other orthonormal bases (generalized PC)
 e.g. Y uniform RVs → Legendre polynomial basis, etc.

National Laborato



J. Burkardt, http://www.sc.fsu.edu/~burkardt, C. Webster, http://www.csm.ornl.gov/~cgwebster — April 2-3, 2012



The Askey scheme

Connections between PDF and the orthogonal polynomials



Distribution	Density function	Polynomial	Support
Normal	$\frac{1}{\sqrt{2\pi}}e^{\frac{-y^2}{2}}$	Hermite $H_n(y)$	$[-\infty,\infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(y)$	[-1, 1]
Beta	$\frac{(1-y)^{\alpha}(1+y)^{\beta}}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi $P_n^{(lpha,eta)}(y)$	[-1, 1]
Exponential	e^{-y}	Laguerre $L_n(y)$	$[0,\infty]$
Gamma	$rac{y^lpha e^{-y}}{\Gamma(lpha+1)}$	Generalized Laguerre $L_n^{(lpha)}(y)$	$[0,\infty]$







- Leads to a single large coupled system (of size $JM \times JM$ typically $M = M_{TD}$) which requires preconditioning methods, e.g. CG [Ghanem-Pellisetti], [Helman-Powell et.al], [Ullman et.al] etc.
 - most preconditioning methods are very problem specific
- terms in the coupled matrix will require computations of the form:

$$A_{kl}(x) = \mathbb{E}\left[a(\cdot, x)\psi_k\psi_l\right] = \int_{\Gamma} a(\mathbf{y}, x)\psi_k(\mathbf{y})\psi_l(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y}$$

- could be High-Dimensional integration problem! If $a(\mathbf{y}, x)$ is nonlinear in \mathbf{y} or if $\mathbf{Y}(\omega)$ is not independent then this is certainly possible
- For linear problems and independent RV's, i.e. $\rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n)$, using the multivariate orthonormal basis computations simplify significantly
 - sparse matrix approaches can be exploited







- Leads to a single large coupled system (of size $JM \times JM$ typically $M = M_{TD}$) which requires preconditioning methods, e.g. CG [Ghanem-Pellisetti], [Helman-Powell et.al], [Ullman et.al] etc.
 - most preconditioning methods are very problem specific
- terms in the coupled matrix will require computations of the form:

$$A_{kl}(x) = \mathbb{E}\left[a(\cdot, x)\psi_k\psi_l\right] = \int_{\Gamma} a(\mathbf{y}, x)\psi_k(\mathbf{y})\psi_l(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y}$$

- could be High-Dimensional integration problem! If $a(\mathbf{y}, x)$ is nonlinear in \mathbf{y} or if $\mathbf{Y}(\omega)$ is not independent then this is certainly possible
- For linear problems and independent RV's, i.e. $\rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n)$, using the multivariate orthonormal basis computations simplify significantly
 - sparse matrix approaches can be exploited







- Leads to a single large coupled system (of size $JM \times JM$ typically $M = M_{TD}$) which requires preconditioning methods, e.g. CG [Ghanem-Pellisetti], [Helman-Powell et.al], [Ullman et.al] etc.
 - most preconditioning methods are very problem specific
- terms in the coupled matrix will require computations of the form:

$$A_{kl}(x) = \mathbb{E}\left[a(\cdot, x)\psi_k\psi_l\right] = \int_{\Gamma} a(\mathbf{y}, x)\psi_k(\mathbf{y})\psi_l(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y}$$

• could be High-Dimensional integration problem!

If $a(\mathbf{y},x)$ is nonlinear in \mathbf{y} or if $\mathbf{Y}(\omega)$ is not independent then this is certainly possible

- For linear problems and independent RV's, i.e. $\rho(\mathbf{y}) = \prod_{n=1}^{N} \rho_n(y_n)$, using the multivariate orthonormal basis computations simplify significantly
 - sparse matrix approaches can be exploited

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

SGFEM Linear problems with independent RVs



Recall from above:

A

$$\begin{split} \mathbf{A}_{kl}(x) &= \int_{\Gamma} a(\mathbf{y}, x) \psi_k(\mathbf{y}) \psi_l(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} \\ &= \mathbb{E}[a](x) \int_{\Gamma} \psi_k \psi_l \rho(\mathbf{y}) d\mathbf{y} + \sum_{n=1}^N b_n(x) \int_{\Gamma} y_n \psi_k \psi_l \rho(\mathbf{y}) d\mathbf{y} \\ &= \mathbb{E}[a](x) \delta_{kl} + \sum_{n=1}^N b_n(x) \prod_{m=1}^N \int_{\Gamma_m} y_n^{\delta_{nm}} \psi_{k_m}^{(m)} \psi_{l_m}^{(m)} \rho_m(y_m) dy_m \end{split}$$

- matrix becomes dense when the coefficient and/or PDE is nonlinear
- condition number deteriorates when approximating using non-uniform RVs





J. Burkardt, http://www.sc.fsu.edu/~burkardt, C. Webster, http://www.csm.ornl.gov/~cgwebster — April 2-3, 2012



We can use the orthogonality of the basis to yield an expression for the unknown coefficients - that is non-intrusive

$$\int_{\Gamma} u(\mathbf{y}, \cdot) \psi_{k'}(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} = \sum_{k}^{M_{SG}} u_k(x) \int_{\Gamma} \psi_k(\mathbf{y}) \psi_{k'}(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} = u_{k'},$$

 $k'=1,\ldots M_{SG}.$

- ${f \circ}$ the integrals could be high dimensional for each of the M_{SG} coefficients
- \bullet the convergence of $u_p \to u$ is dictated by the accurate calculation of the coefficients which becomes dominated by the "error" in the integration scheme

Instead we will consider a powerful *non-intrusive* alternative approach whose polynomial coefficients are the nodal values of the deterministic FEM, i.e. a sampling-based approach with the added benefit of remaining a polynomial approximation



We can use the orthogonality of the basis to yield an expression for the unknown coefficients - that is non-intrusive

$$\int_{\Gamma} u(\mathbf{y}, \cdot) \psi_{k'}(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} = \sum_{k}^{M_{SG}} u_k(x) \int_{\Gamma} \psi_k(\mathbf{y}) \psi_{k'}(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} = u_{k'},$$

 $k'=1,\ldots M_{SG}.$

- ${\, \bullet \,}$ the integrals could be high dimensional for each of the M_{SG} coefficients
- the convergence of $u_p\to u$ is dictated by the accurate calculation of the coefficients which becomes dominated by the "error" in the integration scheme

Instead we will consider a powerful *non-intrusive* alternative approach whose polynomial coefficients are the nodal values of the deterministic FEM, i.e. a sampling-based approach with the added benefit of remaining a polynomial approximation



- **()** Choose a set of points $H_M = {\mathbf{y}_k \in \Gamma}_{k=1}^M$
- ② For each k solve the FE solution $u_k(x) = u(\mathbf{y}_k, x)$, given $a_k(x) = a(\mathbf{y}_k, x)$ and $f_k(x) = f(\mathbf{y}_k, x)$
- **③** Interpolate the sampled values: $u_p(\mathbf{y}, x) = \sum_{k=1}^M u_k(x) L_k(\mathbf{y})$, yielding the fully discrete SC approximation $u_p \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma) \otimes W^h(D)$, where $L_k \in \mathcal{P}_{\mathcal{J}(p)}(\Gamma)$ are suitable combinations of Lagrange interpolants

Quantity of interest, e.g. $\mathbb{E}[u](x)$ $\mathbb{E}[u](x) \approx \int_{\Gamma} u_p(\mathbf{y}, x) \rho(\mathbf{y}) d\mathbf{y} = \sum_{k=1}^M u_k(x) \underbrace{\int_{\Gamma} L_k(y) \rho(\mathbf{y}) dy}_{\text{precomputed weights}} = \sum_{k=1}^M u_k(x) w_k$

[Tatang], [Mathelin-Hussani], [Hesthaven-Xiu], [Babuška et. al], [Zabaras et.al], [Nobile-Tempone-CW], etc.













Selected function values









The interpolant



Determine the approximate polynomial u_p









The QoI = Integrating the approximating polynomial **EXACTLY**

Stochastic Collocation (SC) FEM

OAK RIDGE

- preserves the convergence rate to the stochastic Galerkin FEM (SGFEM)
- **Pros:** there are several advantages wrt the SGFEM approach:
 - completely decouples computations as Monte Carlo does,
 - efficiently treats the case of non-independent RVs by introducing an auxiliary density
 - No difficulty in treating nonlinear problems, exponential expansions of RFs, unbounded RVs (e.g. Gaussian), etc.,
 - effectively handle problems that depend on random input data described by a moderately large number of RVs with the use of sparse gird collocation ([Smolyak '63], [Griebel et al '98-'03-'04], [Hesthaven-Xiu '05], [Barthelmann-Novak-Ritter '00], [Zabaras et al '07], [Nobile-Tempone-W. '08])

Cons:

- can use more DoFs then the SGFEM to represent the same polynomial subspace
- the (interpolation) Lebesgue constant can impact the rate of convergence

Stochastic Collocation (SC) FEM



preserves the convergence rate to the stochastic Galerkin FEM (SGFEM)

Pros: there are several advantages wrt the SGFEM approach:

- completely decouples computations as Monte Carlo does,
- efficiently treats the case of non-independent RVs by introducing an auxiliary density
- No difficulty in treating nonlinear problems, exponential expansions of RFs, unbounded RVs (e.g. Gaussian), etc.,
- effectively handle problems that depend on random input data described by a moderately large number of RVs with the use of sparse gird collocation ([Smolyak '63], [Griebel et al '98-'03-'04], [Hesthaven-Xiu '05], [Barthelmann-Novak-Ritter '00], [Zabaras et al '07], [Nobile-Tempone-W. '08])

Cons:

- can use more DoFs then the SGFEM to represent the same polynomial subspace
- the (interpolation) Lebesgue constant can impact the rate of convergence

Stochastic Collocation (SC) FEM



preserves the convergence rate to the stochastic Galerkin FEM (SGFEM)

Pros: there are several advantages wrt the SGFEM approach:

- completely decouples computations as Monte Carlo does,
- efficiently treats the case of non-independent RVs by introducing an auxiliary density
- No difficulty in treating nonlinear problems, exponential expansions of RFs, unbounded RVs (e.g. Gaussian), etc.,
- effectively handle problems that depend on random input data described by a moderately large number of RVs with the use of sparse gird collocation ([Smolyak '63], [Griebel et al '98-'03-'04], [Hesthaven-Xiu '05], [Barthelmann-Novak-Ritter '00], [Zabaras et al '07], [Nobile-Tempone-W. '08])

Cons:

- can use more DoFs then the SGFEM to represent the same polynomial subspace
- the (interpolation) Lebesgue constant can impact the rate of convergence





Tensor product SCFEM

The simplest multi-dimensional interpolant



Basic idea is to construct the point set H^M for each variable y_n : $H_n^{m(i_n)}$

- choose the level i_n of interpolation in the nth direction
- set the number of points used by the i_n th interpolant, denoted $m(i_n)$
- define the set $H_n^{m(i_n)} = \left\{y_n^1, y_n^2, \dots, y_n^{m(i_n)}\right\}$ of 1d interpolating points:
 - according to the measure $\rho(y_n)dy_n$, e.g. Gauss-Hermite (Normal), Gauss-Legendre, Clenshaw-Curtis (Uniform), etc.

•
$$H^M = H_1^{m(i_1)} \times \cdots \times H_N^{m(i_N)}$$
 where $M_{TP} = m(i_1)m(i_2)\dots m(i_N)$
• $\mathbf{y}_{\mathbf{k}} = \left(y_1^{k_1}, y_2^{k_2}, \dots, y_N^{k_N}\right)$, where $\mathbf{k} \in \mathsf{TP} \equiv \left\{\mathbf{k} \in \mathbb{N}_+^N : k_n < m(i_n)\right\}$

The tensor product (TP) Lagrange-interpolant is defined by

$$u_p^{TP}(\mathbf{y}, x) = \sum_{\mathbf{k}\in\mathsf{TP}}^{M_{TP}} u_{\mathbf{k}}(x) L_{\mathbf{k}}(\mathbf{y}), \quad \text{with } L_{\mathbf{k}}(\mathbf{y}) = \prod_{n=1}^{N} \prod_{s=1, s\neq k_n}^{m(i_n)} \frac{y_n - y_n^s}{y_n^{k_n} - y_n^s}$$



Tensor product SCFEM

The simplest multi-dimensional interpolant



Basic idea is to construct the point set H^M for each variable y_n : $H_n^{m(i_n)}$

- $\bullet\,$ choose the level i_n of interpolation in the $n{\rm th}\,$ direction
- set the number of points used by the i_n th interpolant, denoted $m(i_n)$
- define the set $H_n^{m(i_n)} = \left\{y_n^1, y_n^2, \dots, y_n^{m(i_n)}\right\}$ of 1d interpolating points:
 - according to the measure $\rho(y_n)dy_n$, e.g. Gauss-Hermite (Normal), Gauss-Legendre, Clenshaw-Curtis (Uniform), etc.

•
$$H^M = H_1^{m(i_1)} \times \cdots \times H_N^{m(i_N)}$$
 where $M_{TP} = m(i_1)m(i_2)\dots m(i_N)$
• $\mathbf{y}_{\mathbf{k}} = \left(y_1^{k_1}, y_2^{k_2}, \dots, y_N^{k_N}\right)$, where $\mathbf{k} \in \mathsf{TP} \equiv \left\{\mathbf{k} \in \mathbb{N}_+^N : k_n < m(i_n)\right\}$

The tensor product (TP) Lagrange-interpolant is defined by:

$$u_p^{TP}(\mathbf{y}, x) = \sum_{\mathbf{k}\in\mathsf{TP}}^{M_{TP}} u_{\mathbf{k}}(x) L_{\mathbf{k}}(\mathbf{y}), \quad \text{with } L_{\mathbf{k}}(\mathbf{y}) = \prod_{n=1}^N \prod_{s=1, s\neq k_n}^{m(i_n)} \frac{y_n - y_n^s}{y_n^{k_n} - y_n^s}$$



Let $\mathscr{U}_n^{m(i_n)}$ be the *i*th level interpolant in the direction y_n using $m(i_n)$ points:

$$\mathscr{U}_{n}^{m(i_{n})}[u](y_{n}) = \sum_{k=1}^{m(i_{n})} u(y_{n}^{k}) l_{n}^{k}(y_{n}), \quad \{y_{n}^{1}, \dots, y_{n}^{m(i_{n})}\} \in \Gamma_{n}$$

- $\mathscr{U}_n^{m(i_n)}: C^0(\Gamma_n) \to \mathcal{P}_{m(i_n)-1}(\Gamma_n), \quad \mathscr{U}_n^0[u] = 0 \ \forall u \in C^0(\Gamma_n)$
- The degree in the y_n direction is $p_n = m(i_n) 1$

The TP-SC approximation is given by

$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \le p$$

• the interpolation requires $M_{TP} = \prod_{n=1}^{N} m(i_n)$ function evaluations (In this case, solutions of the PDE)



Let $\mathscr{U}_n^{m(i_n)}$ be the *i*th level interpolant in the direction y_n using $m(i_n)$ points:

$$\mathscr{U}_{n}^{m(i_{n})}[u](y_{n}) = \sum_{k=1}^{m(i_{n})} u(y_{n}^{k}) l_{n}^{k}(y_{n}), \quad \{y_{n}^{1}, \dots, y_{n}^{m(i_{n})}\} \in \Gamma_{n}$$

- $\mathscr{U}_n^{m(i_n)}: C^0(\Gamma_n) \to \mathcal{P}_{m(i_n)-1}(\Gamma_n), \quad \mathscr{U}_n^0[u] = 0 \ \forall u \in C^0(\Gamma_n)$
- The degree in the y_n direction is $p_n = m(i_n) 1$

The TP-SC approximation is given by

$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \le p$$

• the interpolation requires $M_{TP} = \prod_{n=1}^{N} m(i_n)$ function evaluations (In this case, solutions of the PDE)






Isotropic TP SC grid constructed from C-C points for $(y_1, y_2) \in U(-1, 1)$



Choices for interpolation Based on 1-d interpolation formulas



Clenshaw-Curtis abscissas (Γ_n bounded):

- $\{y_n^k\}_{k=1}^{m(i_n)}$: extrema of Chebyshev polynomials
- ${\, \bullet \,}$ optimal for uniform convergence in Γ_n
- if $m(i_n)=2^{i_n-1}+1$ lead to nested sets, i.e. $H_n^{m(i_n)}\subset H_n^{m(i_n+1)}$

Gaussian abscissas (Γ_n bounded or unbounded): Assume, either

- Y_n independent, i.e. $\rho(\mathbf{y}) = \prod_{n=1}^N \rho_n(y_n)$, or
- construct an auxiliary joint PDF $\hat{\rho}(\mathbf{y}) = \prod_{n=1}^{N} \hat{\rho}_n(y_n)$ such that $\|\rho/\hat{\rho}\|_{L^{\infty}(\Gamma)} < \infty$ and small enough.
- $\left\{y_n^k\right\}_{k=1}^{m(i_n)}$: zeros of orthogonal polynomials with respect to $\hat{\rho}$ e.g. abscissas become roots of Gauss-Legendre, -Hermite, -Jacobi, -Laguerre polynomials corresponding to uniform, normal, beta, exponential distributions, respectively
- optimal for L^2_{ρ} convergence



Recall the $\mathbf{p}=(p_1,\ldots,p_N)$ is the polynomial degree used in each direction \mathbf{y}_n

Theorem [Babuška-Nobile-Tempone, 2007]:

Let $L^2_{\rho} \equiv L^2_{\rho}(\Gamma; H^1_0(D))$ then since u is analytic in y you get: • Γ_n bounded:

$$\left\|u-u_p^{TP}\right\|_{L^2_\rho} \le C \sum_{n=1}^N e^{-g_n p_n}, \quad \text{with } g_n = \log\left[\frac{2\tau_n}{|\Gamma_n|} + \sqrt{1 + \frac{4\tau_n^2}{|\Gamma_n|^2}}\right]$$

• Γ_n unbounded, $\hat{\rho}_n \approx e^{-\left(\delta_n y_n\right)^2}$ at infinity:

$$\left\|u - u_p^{TP}\right\|_{L^2_{\rho}} \le C \sum_{n=1}^N \sqrt{p_n} e^{-g_n \sqrt{p_n}}, \quad g_n = \frac{\sqrt{2}\tau_n}{\delta_n}$$

Error in # of samples M: $\varepsilon_{TP}(M) = \left\| u - u_p^{TP} \right\|_{L^2_{\rho}} \leq C(N) M^{-g_{min}/N}$

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

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

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

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

• The decay rates g_n can be estimated theoretically (a priori),

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

and numerically (a posteriori), $\log_{10}(arepsilon_n) pprox \log_{10}(d_n) - p_n \log_{10}(e) lpha_n$

- Theoretical estimates for linear and several nonlinear PDEs available [BNT07, W07, NTW08a, NTW08b, GW11]
- Dimension-adaptivity without paying the cost of searching and evaluating the multi-indices $\{\mathbf{p} + e_j, 1 \le j \le N\}$ using an heuristic error estimator [Gerstner-Griebel '03]

SPDEs Input noise MCFEM Regularity Polynomial approx. SGFEM SCFEM Summary

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

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

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

• The decay rates g_n can be estimated theoretically (a priori),

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

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

- Theoretical estimates for linear and several nonlinear PDEs available [BNT07, W07, NTW08a, NTW08b, GW11]
- Dimension-adaptivity without paying the cost of searching and evaluating the multi-indices $\{\mathbf{p} + e_j, 1 \leq j \leq N\}$ using an heuristic error estimator [Gerstner-Griebel '03]







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

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

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 $U(-\sqrt{3}, \sqrt{3})$







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

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

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

$$\begin{aligned} Cov[\gamma](x_1, \tilde{x}_1) &= \exp\left(-\frac{(x_1 - \tilde{x}_1)^2}{L^2}\right), \quad \forall (x_1, \tilde{x}_1) \in [0, 1] \\ \gamma(\omega, x_1) &= 1 + Y_1(\omega) \left(\frac{\sqrt{\pi L}}{2}\right)^{1/2} + \sum_{n=2}^N \beta_n \,\varphi_n(x_1) \,Y_n(\omega) \\ \beta_n &:= \left(\sqrt{\pi L}\right)^{1/2} \, e^{\frac{-\left(\lfloor \frac{n}{2} \rfloor \pi L\right)^2}{8}}, \quad \varphi_n(x_1) := \left\{ \begin{array}{c} \sin\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ even,} \\ \cos\left(\lfloor \frac{n}{2} \rfloor \pi x_1\right), & \text{if } n \text{ odd} \end{array} \right. \end{aligned}$$

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



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

$$g_n = \log\left(\frac{2\tau_n}{|\Gamma_n|} + \sqrt{1 + \frac{4{\tau_n}^2}{|\Gamma_n|^2}}\right) \quad \text{ and } \tau_n = \frac{1}{12\sqrt{\lambda_n}\|b_n\|_{L^{\infty}(D)}}$$

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	$lpha_8$, $lpha_9$	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

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

• $p = 0, 1, \dots, p_{max}$ and $u_{p_{max}+1}$ is an overkilled solution



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

$$g_n = \log\left(\frac{2\tau_n}{|\Gamma_n|} + \sqrt{1 + \frac{4{\tau_n}^2}{|\Gamma_n|^2}}\right) \quad \text{ and } \tau_n = \frac{1}{12\sqrt{\lambda_n}\|b_n\|_{L^{\infty}(D)}}$$

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

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

• $p = 0, 1, \ldots, p_{max}$ and $u_{p_{max}+1}$ is an overkilled solution



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 $L_c = 1/64$



J. Burkardt, http://www.sc.fsu.edu/~burkardt, C. Webster, http://www.csm.ornl.gov/~cgwebster — April 2-3, 2012



J. Burkardt, http://www.sc.fsu.edu/~burkardt, C. Webster, http://www.csm.ornl.gov/~cgwebster — April 2-3, 2012



- Proper input data representation/truncation is important to reduce the computational work
- Discussed the various intrusive and non-intrusive stochastic techniques for the for forward propagation of uncertainty, in particular Monte Carlo and Stochastic Galerkin/Collocation
- Global stochastic polynomial approximation is extremely effective for problems that smooth (analytic) dependence on the random variables
- Properly chosen Anisotropic polynomial spaces can improve considerably the convergence, when the input random variables have different influence on the output
- $\bullet\,$ Can we construct a polynomial approximation that maintains the fast convergence even when N becomes large?
 - sparse grid SCFEM with anisotropic refinement
 - what about stochastic inverse problems and calibration?



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

• The TP-SCFEM:
$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^{N} \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \leq p$$

• The *n*th 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: $\Delta_n^{m(\mathbf{i})}[u](\mathbf{y}) = \bigotimes_{n=1}^{\infty} \Delta_n^{m(i_n)}[u](\mathbf{y})$ where $\mathbf{i} = (i_1, \dots, i_N) \in \mathbb{N}_+^N$ is a multi-index



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

• The TP-SCFEM:
$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \leq p$$

• The *n*th 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: $\Delta_n^{m(\mathbf{i})}[u](\mathbf{y}) = \bigotimes_{n=1}^{\infty} \Delta_n^{m(i_n)}[u](\mathbf{y})$ where $\mathbf{i} = (i_1, \dots, i_N) \in \mathbb{N}_+^N$ is a multi-index



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

• The TP-SCFEM:
$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \leq p$$

 \bullet The $n{\rm th}$ 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: $\Delta_n^{m(\mathbf{i})}[u](\mathbf{y}) = \bigotimes_{n=1}^{\infty} \Delta_n^{m(i_n)}[u](\mathbf{y})$ where $\mathbf{i} = (i_1, \dots, i_N) \in \mathbb{N}_+^N$ is a multi-index



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

• The TP-SCFEM:
$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \leq p$$

• 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 $\mathbf{i} = (i_1, \dots, i_N) \in \mathbb{N}^N_+$ is a multi-index



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:

$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \le p$$

The sparse grid SCFEM is defined as

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

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



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:

$$u_p^{TP}(\mathbf{y}) = \bigotimes_{n=1}^N \mathscr{U}_n^{m(i_n)}[u](\mathbf{y}), \quad \max_n \alpha_n p_n \le p$$

The sparse grid SCFEM is defined as

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

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



- 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 ${\cal N}$