Multilevel adaptivity for stochastic finite element methods

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What is this talk about...

- * Computational methods for uncertainty quantification (UQ)
 - PDEs with uncertain or parameter-dependent inputs
 - forward UQ: propagation of uncertainty from the inputs/data to the output/solution
 - approximations of the input-output map
- * Numerical solution of elliptic PDE problems with parametric or uncertain inputs using
 - stochastic Galerkin FEM
 - stochastic collocation FEM
- * Design and analysis of adaptive algorithms
 - focus on multilevel adaptivity

Parametric model problem

- Domains
 - $D \subset \mathbb{R}^2 \rightsquigarrow$ physical domain
 - $\Gamma := [-1, 1]^{\mathbb{N}}$ or $\Gamma := [-1, 1]^{\mathcal{M}} \rightsquigarrow$ parameter domain

Parametric model problem

Problem formulation: find $u: D \times \Gamma \to \mathbb{R}$ satisfying

$$\begin{aligned} -\nabla_{x} \cdot (a(x, \mathbf{y}) \nabla_{x} u(x, \mathbf{y})) &= f(x) \qquad x \in D, \ \mathbf{y} \in \Gamma, \\ u(x, \mathbf{y}) &= 0 \qquad x \in \partial D, \ \mathbf{y} \in \Gamma \end{aligned}$$

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Remark: parameters $y_1, y_2, ...$ can be seen as images (observations) of independent real-valued random variables with cumulative distribution functions $\pi_1(y_1), \pi_2(y_2), ...$ Then, the joint cumulative distribution function is defined as

$$\pi(\mathbf{y}) := \prod_{m=1}^{\infty} \pi_m(y_m), \text{ and } \int_{-1}^{1} \mathrm{d}\pi_m(y_m) = \int_{\Gamma} \mathrm{d}\pi(\mathbf{y}) = 1.$$

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- Challenges for numerics (and analysis)

 - guaranteed and reliable error control in approximations (rigorous a posteriori error analysis)
 - tuning of spatial and stochastic components of approximations
 - adaptive algorithms that are provably convergent with optimal rates

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 - effective and dimension independent
 - estimating the moments of the solution

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 - $L^2_{\pi}(\Gamma) = \operatorname{span}\{\Psi_n : n \in \mathbb{N}\}$ or $\operatorname{span}\{\Psi_n : n = 1, \dots, N\} \subset L^2_{\pi}(\Gamma), N \in \mathbb{N}$

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 - if $u(x, \mathbf{y}) \in L^2_{\pi}(\Gamma; H^1_0(D))$, then

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Problem formulation: find $u: D \times \Gamma \to \mathbb{R}$ satisfying $-\nabla_x \cdot (a(x, \mathbf{y})\nabla_x u(x, \mathbf{y})) = f(x) \qquad x \in D, \ \mathbf{y} \in \Gamma,$ $u(x, \mathbf{y}) = 0 \qquad x \in \partial D, \ \mathbf{y} \in \Gamma$

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• candidates for Ψ_n : orthogonal polynomials, Lagrange basis functions, ...

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- Affine-parametric diffusion coefficient
 - $\Gamma := [-1, 1]^{\mathbb{N}} \rightsquigarrow$ parameter domain

•
$$a(x, \mathbf{y}) = a_0(x) + \sum_{m \in \mathbb{N}} y_m a_m(x)$$
 for $x \in D$, $\mathbf{y} = (y_m)_{m \in \mathbb{N}} \in \Gamma$

•
$$0 < a_0^{\min} \le a_0(x) \le a_0^{\max} < \infty$$
 for almost all $x \in D$

$$\bullet \quad \tau := \frac{1}{a_0^{\min}} \left\| \sum_{m \in \mathbb{N}} |a_m| \right\|_{L^{\infty}(D)} < 1 \quad \& \quad \sum_{m \in \mathbb{N}} \|a_m\|_{L^{\infty}(D)} < \infty$$

Remark: $a_0(x)$ typically represents the mean field, i.e., $a_0(x) = \int_{\Gamma} a(x, \mathbf{y}) d\pi(\mathbf{y})$.

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$$B_0(u, v) := \int_{\Gamma} \int_{D} a_0(x) \nabla u(x, \mathbf{y}) \cdot \nabla v(x, \mathbf{y}) \, \mathrm{d}x \, \mathrm{d}\pi(\mathbf{y})$$

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Weak formulation: given $f \in L^2(D)$, find $u \in \mathbb{V}$ such that

$$B(u, v) = F(v) := \int_{\Gamma} \int_{D} f(x) v(x, \mathbf{y}) \, \mathrm{d}x \, \mathrm{d}\pi(\mathbf{y}) \quad \text{for all } v \in \mathbb{V} \tag{(*)}$$

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[Schwab, Gittelson '11]: the assumptions on $a(x, \mathbf{y})$ ensure the wellposedness of (\star) .

Finite dimensional subspace

 $\mathbb{V}_{\bullet} \subset \mathbb{V} \,\cong\, \mathbb{X} \otimes \mathbb{P}$

Galerkin projection:

find $u_{\bullet} \in \mathbb{V}_{\bullet}$ such that $B(u_{\bullet}, v_{\bullet}) = F(v_{\bullet})$ for all $v \in \mathbb{V}_{\bullet}$

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Galerkin orthogonality

$$B(u - u_{\bullet}, v_{\bullet}) = 0$$
 for all $v_{\bullet} \in \mathbb{V}_{\bullet}$

Best approximation property

 $||| u - u_{\bullet} ||| = \min_{\mathbf{v}_{\bullet} \in \mathbb{V}_{\bullet}} ||| u - v_{\bullet} |||, \text{ where } ||| \cdot ||| := B(\cdot, \cdot)^{1/2}$

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• Main question: how to choose \mathbb{V}_{\bullet} ?

• $\{P_{\nu} : \nu \in \mathcal{J}\}$ is a countable orthonormal polynomial basis of $\mathbb{P} = L^2_{\pi}(\Gamma)$

• gPC expansion: $\mathbb{V} \ni u(x, \mathbf{y}) = \sum_{\nu \in \mathbb{J}} u_{\nu}(x) P_{\nu}(\mathbf{y})$ with unique $u_{\nu} \in \mathbb{X} = H_0^1(D)$

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• $\mathfrak{I} := \{\nu \in \mathbb{N}_0^{\mathbb{N}} : \# \operatorname{supp}(\nu) < \infty\}$ where $\operatorname{supp}(\nu) = \{m \in \mathbb{N} : \nu_m \neq 0\}$

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Example

$$\nu = (2, 5, 0, 3, 0, 0, 0, \dots) \rightsquigarrow \operatorname{supp}(\nu) = \{1, 2, 4\}$$

$$\Rightarrow P_{\nu}(\mathbf{y}) = P_2(y_1) P_5(y_2) P_3(y_4)$$

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- Discretisation in the parameter domain
 - finite index set $\mathcal{P}_{\bullet} \subset \mathcal{I} \implies \mathbb{P}_{\bullet} = \operatorname{span}\{P_{\nu} : \nu \in \mathcal{P}_{\bullet}\} \subset \mathbb{P} = L^{2}_{\pi}(\Gamma)$
 - semidiscrete approximation via truncation of gPC expansion

$$u(x, \mathbf{y}) \approx \sum_{\nu \in \mathfrak{P}_{\bullet}} u_{\nu}(x) P_{\nu}(\mathbf{y}) \in \mathbb{X} \otimes \mathbb{P}_{\bullet} \text{ with coefficients } u_{\nu} \in \mathbb{X} = H^{1}_{0}(D)$$

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- Discretisations in the physical domain
 - A sequence of meshes $\rightsquigarrow \{\mathcal{T}_{\bullet\nu}\}_{\nu\in\mathcal{P}_{\bullet}}$

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Pythagoras theorem: $u \in \mathbb{V}$, $u_{\bullet} \in \mathbb{V}_{\bullet} \subset \mathbb{V}$, $\hat{u}_{\bullet} \in \widehat{\mathbb{V}}_{\bullet} \supset \mathbb{V}_{\bullet}$ (enhanced approx.)

$$||| u - u_{\bullet} |||^{2} = ||| (u - \hat{u}_{\bullet}) + (\hat{u}_{\bullet} - u_{\bullet}) |||^{2} = ||| u - \hat{u}_{\bullet} |||^{2} + \underbrace{||| \hat{u}_{\bullet} - u_{\bullet} |||^{2}}_{\text{computable}}$$

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- Pythagoras theorem & saturation assumption imply that

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Bank, Weiser '85]: decomposition $\widehat{\mathbb{V}}_{\bullet} = \mathbb{V}_{\bullet} \oplus \mathbb{W}_{\bullet}$

 \implies hierarchical error estimation without computing enhanced approximations \widehat{u}_{\bullet}

Enhancement of SGFEM approximations (1/2)

- Enhancement of approximations in physical domain
 - initial mesh \mathcal{T}_0
 - \blacktriangleright add new vertices to $\mathcal{T}_{\bullet} \rightsquigarrow$ mesh refinement
 - mesh refinement by newest vertex bisection (NVB)
 - $\widehat{\mathcal{T}}_{\bullet} \rightsquigarrow$ uniform refinement of \mathcal{T}_{\bullet}



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- Enhancement of approximations in the parameter domain
 - add new indices to \mathcal{P}_{\bullet}
 - ▶ finite set $Q_{\bullet} \subset \mathcal{I} \setminus \mathcal{P}_{\bullet} \rightsquigarrow$ detail index set ('boundary' of \mathcal{P}_{\bullet})

•
$$\widehat{\mathcal{P}}_{\bullet} = \mathcal{P}_{\bullet} \cup \mathcal{Q}_{\bullet} \rightsquigarrow$$
 uniform enrichment of \mathcal{P}_{\bullet}

$$\widehat{\mathbb{P}}_{\bullet} = \operatorname{span}\{P_{\nu} : \nu \in \widehat{\mathbb{P}}_{\bullet}\} \supset \mathbb{P}_{\bullet}$$

Example

▶
$$\mathcal{P}_{\bullet} = \{(0, 0, ...); (1, 0, ...); (0, 1, 0, ...)\}$$

 $\implies \Omega_{\bullet} = \{(2, 0, ...); (1, 1, 0, ...); (0, 2, 0, ...); (0, 0, 1, 0, ...)\}$

Enhancement of SGFEM approximation (2/2)

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[B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]

$$\widehat{\mathbb{V}}_{\bullet} = \bigoplus_{\substack{\nu \in \mathcal{P}_{\bullet} \\ \text{spatial enhancement}}} \left[\widehat{\mathbb{X}}_{\bullet\nu} \otimes \operatorname{span}\{P_{\nu}\} \right] \oplus \bigoplus_{\substack{\nu \in \mathcal{Q}_{\bullet} \\ \text{parametric enhancement}}} \left[\mathbb{X}_{0} \otimes \operatorname{span}\{P_{\nu}\} \right]$$
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[B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]



Recap: $||| u - u_{\bullet} ||| \simeq ||| \hat{u}_{\bullet} - u_{\bullet} |||$, but we want to avoid computing $\hat{u}_{\bullet} \in \hat{V}_{\bullet}$!

A posteriori error estimation: spatial and parametric estimators

- Two-level spatial error estimator [Mund, Stephan, Weiße '98], [Mund, Stephan '99]
 - Fix a multiindex $\nu \in \mathcal{P}_{\bullet}$
 - $\mathcal{N}_{\bullet,\nu}^+ \rightsquigarrow$ set of interior midpoints in $\mathcal{T}_{\bullet,\nu}$

• $\widehat{\varphi}_{\bullet,\nu,z} \in \widehat{\mathbb{X}}_{\bullet,\nu} \rightsquigarrow$ hat function associated with $z \in \mathcal{N}_{\bullet,\nu}^+$

•
$$(\mathbb{X}\text{-errors})^2 \approx \sum_{\nu \in \mathcal{P}_{\bullet}} \sum_{z \in \mathcal{N}_{\bullet,\nu}^+} \eta_{\bullet}^2(\nu, z)$$



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Hierarchical parametric error estimator
 [B., Silvester '16], [B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]

•
$$(\mathbb{P}\text{-error})^2 \approx \sum_{\nu \in \mathbf{Q}_{\bullet}} \eta_{\bullet}^2(\nu)$$



A posteriori error estimation: main results

[B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]

•
$$\eta_{\bullet}^2 = (\text{estim. } \mathbb{X}\text{-errors})^2 + (\text{estim. } \mathbb{P}\text{-error})^2 = \sum_{\nu \in \mathcal{P}_{\bullet}} \sum_{z \in \mathcal{N}_{\bullet,\nu}^+} \eta_{\bullet}^2(\nu, z) + \sum_{\nu \in \mathfrak{Q}_{\bullet}} \eta_{\bullet}^2(\nu)$$

Theorem 1 (equivalence of total error estimate and error reduction) There exists $C = C(a_0, \tau, T_0) \ge 1$ such that

$$C^{-1} \eta_{\bullet}^{2} \leq ||| \, \widehat{u}_{\bullet} - u_{\bullet} \, |||^{2} \leq C \, \eta_{\bullet}^{2}$$

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Corollary (efficiency & reliability)

•
$$||| u - u_{\bullet} |||^2 \ge C^{-1} \eta_{\bullet}^2$$
 (efficiency)

saturation assumption
$$\implies ||| u - u_{\bullet} |||^2 \le \frac{C}{1 - q_{\text{sat}}^2} \eta_{\bullet}^2$$
 (reliability)

A posteriori error estimation: main results

[B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]

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$$\eta_{\bullet}^2 = (\text{estim. } \mathbb{X}\text{-errors})^2 + (\text{estim. } \mathbb{P}\text{-error})^2 = \sum_{\nu \in \mathcal{P}_{\bullet}} \sum_{z \in \mathcal{N}_{\bullet,\nu}^+} \eta_{\bullet}^2(\nu, z) + \sum_{\nu \in \mathfrak{Q}_{\bullet}} \eta_{\bullet}^2(\nu)$$

Theorem 1 (equivalence of total error estimate and error reduction) There exists $C = C(a_0, \tau, T_0) \ge 1$ such that

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Remark

- $\eta_{\bullet}(\nu, z)$ is associated with an interior edge midpoint $z \in \mathcal{N}_{\bullet,\nu}^+$ for each $\nu \in \mathcal{P}_{\bullet}$
- $\eta_{\bullet}(\nu)$ is associated with a new index $\nu \in \Omega_{\bullet}$

These are local *error reduction indicators* for spatial refinement / parametric enrichment \implies key to adaptivity

INPUT: initial mesh \mathcal{T}_0 , initial index set $\mathcal{P}_0 = \{(0, 0, \dots)\}$, tolerance tol FOR $\ell = 0, 1, 2, 3, \dots$ DO:

- SOLVE: compute $u_{\ell} \in \mathbb{V}_{\ell}$ for index set \mathcal{P}_{ℓ} and meshes $\mathcal{T}_{\ell,\nu}$ $(\nu \in \mathcal{P}_{\ell})$
- ESTIMATE: compute *local* error indicators and the *total* error estimate
 - ► spatial & parametric indicators $\{\eta_{\ell}(\nu, z); z \in \mathcal{N}_{\ell,\nu}^+, \nu \in \mathcal{P}_{\ell}\}$ & $\{\eta_{\ell}(\nu); \nu \in \mathcal{Q}_{\ell}\}$
 - energy error estimate η_{ℓ}
 - ▶ IF $\eta_\ell < ext{tol THEN STOP}$

MARK: mark certain vertices $\mathcal{M}_{\ell,\nu} \subseteq \mathcal{N}^+_{\ell,\nu}$ ($\nu \in \mathcal{P}_{\ell}$) and indices $\mathcal{R}_{\ell} \subseteq \mathcal{Q}_{\ell}$

- REFINE: enhance approximation space
 - ▶ mesh refinement (NVB) $\rightsquigarrow \mathcal{T}_{\ell+1,\nu} = \text{refine}(\mathcal{T}_{\ell,\nu}, \mathcal{M}_{\ell,\nu}) \quad \forall \nu \in \mathcal{P}_{\ell}$
 - ▶ parametric enrichment $\rightsquigarrow \mathcal{P}_{\ell+1} = \mathcal{P}_{\ell} \cup \mathcal{R}_{\ell}, \ \mathcal{T}_{\ell,\nu} = \mathcal{T}_0 \ \forall \nu \in \mathcal{R}_{\ell}$

OUTPUT: stochastic Galerkin approximations $\{u_\ell\}$ and error estimates $\{\eta_\ell\}$

Convergence results

[B., Praetorius, Rocchi, Ruggeri; SINUM '19]

[B., Praetorius, Ruggeri; arXiv preprint '22]

Theorem 2 (plain convergence)

For any marking threshold $\theta \in (0, 1]$ (in Dörfler marking), adaptive multilevel SGFEM algorithm yields a convergent sequence of error estimates, i.e., $\eta_{\ell} \to 0$ as $\ell \to \infty$.

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Theorem 3 (linear convergence)

For any marking threshold $\theta \in (0, 1]$, saturation assumption \implies linear convergence

 $\exists q \in (0,1) \text{ such that } ||| u - u_{\ell+1} ||| \le q ||| u - u_{\ell} ||| \text{ for all } \ell \in \mathbb{N}_0$

Experiment 1: cookie problem

•
$$-\nabla \cdot (a\nabla u) = f$$
 in $D \times \Gamma$, $u = 0$ on $\partial D \times \Gamma$

•
$$a(x, \mathbf{y}) = a_0(x) + \sum_{m \in \mathbb{N}} y_m a_m(x)$$

•
$$D = (0, 1)^2 \rightsquigarrow$$
 square domain

- nine circular inclusions $D_m \subset D$ (m = 1, ..., 9)
- Expansion coefficients $\{a_m\}_{m \in \mathbb{N}_0}$
 - $\blacktriangleright a_0 \equiv 1$
 - $a_m = 0.5 \chi_{D_m}$ for m = 1, 3, 7, 9
 - $a_m = 0.7 \chi_{D_m}$ for m = 2, 4, 6, 8
 - $a_m = 0.9 \chi_{D_m}$ for m = 5
 - $a_m \equiv 0$ for m > 9

f
$$\equiv 1$$

• $d\pi_m(y_m) = \frac{1}{2} dy_m \rightsquigarrow$ uniform probability measure on [-1, 1]





Experiment 1: rate optimality of adaptive ML-SGFEM



Experiment 1: locally refined meshes in ML-SGFEM



Optimal convergence of adaptive multilevel SGFEM

[B., Praetorius, Ruggeri; IMA J. Numer. Anal. '22]

- Concept of 'multilevel structure' $\rightsquigarrow \mathbb{P}_{\bullet} = [\mathcal{P}_{\bullet}, (\mathcal{T}_{\bullet\nu})_{\nu \in \mathcal{P}_{\bullet}}], \ \#\mathbb{P}_{\bullet} \simeq \dim \mathbb{V}_{\bullet}$
- Concept of 'multilevel refinement' $\rightarrow \mathbb{P}_{\circ} = \mathbb{REFINE}(\mathbb{P}_{\bullet}, \mathbb{M}_{\bullet})$
- Concept of optimality \rightsquigarrow approximation class \mathbb{A}_s (s > 0)

 $u \in \mathbb{A}_s \quad \Longleftrightarrow \quad \exists \left\{ \mathbf{P}_{\ell}^{\star} \right\}_{\ell \in \mathbb{N}_0} \text{ such that } ||| u - u_{\ell}^{\star} ||| = \mathcal{O}\left(\left(\dim \mathbb{V}_{\ell}^{\star} \right)^{-s} \right)$

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Theorem 4 (rate optimality of adaptive multilevel SGFEM) For sufficiently small marking threshold θ , strong saturation assumption \implies optimal convergence

If
$$s > 0$$
 and $u \in \mathbb{A}_s$, then $\sup_{\ell \in \mathbb{N}_0} (\# \mathbb{P}_{\ell} - \# \mathbb{P}_0 + 1)^s ||| u - u_{\ell} ||| \le C ||u||_{\mathbb{A}_s}$

Saturation assumption vs. strong saturation assumption

- Saturation assumption
 - ▶ SGFEM solution $u_{\bullet} \in \mathbb{V}_{\bullet}$
 - Enhanced ('uniformly refined') SGFEM solution $\widehat{u}_{\bullet} \in \widehat{\mathbb{V}}_{\bullet}$
 - There exist a constant $q_{\text{sat}} \in (0, 1)$ s.t. $||| u \hat{u}_{\bullet} ||| \le q_{\text{sat}} ||| u u_{\bullet} |||$

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- Strong saturation assumption
 - ▶ $\mathbb{P}_{\bullet} \in \mathbb{REFINE}(\mathbb{P}_{0}) \rightsquigarrow$ any multilevel structure obtained from \mathbb{P}_{0}
 - ▶ $\mathbb{P}_{\star} \in \mathbb{REFINE}(\mathbb{P}_{\bullet}) \rightsquigarrow$ a refined multilevel structure obtained from \mathbb{P}_{\bullet}
 - ▶ $\mathbb{P}_{\circ} := \mathbb{REFINE}(\mathbb{P}_{\bullet}, \mathbb{M}_{\bullet}) \implies$ a multilevel structure obtained from \mathbb{P}_{\bullet} by one step of multilevel refinement towards \mathbb{P}_{\star}
 - ▶ There exist constants $\exists \, 0 < \kappa_{
 m sat} \leq q_{
 m sat} < 1$ such that

$$||| u - u_{\star} ||| \le \kappa_{\mathrm{sat}} ||| u - u_{\bullet} ||| \implies || u - u_{\circ} ||| \le q_{\mathrm{sat}} ||| u - u_{\bullet} |||$$

Parametric model problem revisited

Problem formulation: find $u: D \times \Gamma \to \mathbb{R}$ satisfying $-\nabla_x \cdot (a(x, \mathbf{y})\nabla_x u(x, \mathbf{y})) = f(x, \mathbf{y}) \qquad x \in D, \ \mathbf{y} \in \Gamma,$ $u(x, \mathbf{y}) = 0 \qquad x \in \partial D, \ \mathbf{y} \in \Gamma$

- Parametric diffusion coefficient
 - $\Gamma := [-1, 1]^M \rightsquigarrow$ parameter domain, $M \in \mathbb{N}$
 - ► $0 < a_{\min} \leq \underset{x \in D}{\operatorname{ess inf}} a(x, \mathbf{y}) \leq \underset{x \in D}{\operatorname{ess sup}} a(x, \mathbf{y}) \leq a_{\max} < \infty$ π -a.e. on Γ

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• Weak formulation: given $f \in L^2_{\pi}(\Gamma, L^2(D))$, find $u : \Gamma \to \mathbb{X} := H^1_0(D)$ s.t.

$$\int_{D} a(x, \mathbf{y}) \nabla u(x, \mathbf{y}) \cdot \nabla v(x) \, \mathrm{d}x = \int_{D} f(x, \mathbf{y}) v(x) \, \mathrm{d}x \quad \forall v \in \mathbb{X}, \ \pi\text{-a.e. on } \Gamma.$$

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■ [Babuška, Nobile, Tempone '07]: $\exists ! u \in \mathbb{V} := L^2_{\pi}(\Gamma; \mathbb{X}).$

Sampling the PDE inputs at a sparse grid $\mathcal{Y}_{\bullet} = \mathcal{Y}_{\Lambda_{\bullet}}$ of collocation points in Γ

- Sampling the PDE inputs at a sparse grid $\mathcal{Y}_{\bullet} = \mathcal{Y}_{\Lambda_{\bullet}}$ of collocation points in Γ
- Solving decoupled discrete problems: for each $z \in \mathcal{Y}_{\bullet}$, find $u_{\bullet z} \in \mathbb{X}_{\bullet z}$ satisfying

$$\int_{D} a(x, \mathbf{Z}) \nabla u_{\bullet \mathbf{Z}}(x) \cdot \nabla v(x) dx = \int_{D} f(x, \mathbf{Z}) v(x) dx \ \forall v \in \mathbb{X}_{\bullet \mathbf{Z}} := \mathcal{S}_{0}^{1}(\mathcal{T}_{\bullet \mathbf{Z}}) \subset H_{0}^{1}(D)$$

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- Building a multivariable interpolant

$$u^{\mathrm{SC}}_{\bullet}(\mathbf{x},\mathbf{y}) = \sum_{\mathbf{z}\in\mathcal{Y}_{\bullet}} u_{\bullet\mathbf{z}}(\mathbf{x})L_{\bullet\mathbf{z}}(\mathbf{y}),$$

 $\left\{ \mathit{L}_{\bullet z}(y): z \in \mathcal{Y}_{\bullet} \right\} - \text{multivariable Lagrange basis functions associated with } \mathcal{Y}_{\bullet}$

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- Main features of the stochastic collocation FEM (SC-FEM)
 - a sampling method that generates 'surrogate approximations'
 - ▶ single-level $(X_{\bullet z} = X_{\bullet} \forall z \in \mathcal{Y}_{\bullet})$ vs. multilevel $(X_{\bullet z} \neq X_{\bullet z'}$ for $z \neq z')$
 - ▶ not a projection method → no (global) Galerkin orthogonality

Hierarchical a posteriori error estimation in SC-FEM (1/2)

[B., Silvester, Xu '22], [B., Silvester '23]

•
$$\mathbb{V} := L^2_{\pi}(\Gamma; H^1_0(D)), \|\cdot\| := \|\cdot\|_{\mathbb{V}}$$

An enhanced SC-FEM approximation $\widehat{u}^{SC}_{\bullet}$ satisfying the saturation property

$$\|u - \widehat{u}^{ ext{SC}}_{ullet}\| \le q_{ ext{sat}} \|u - u^{ ext{SC}}_{ullet}\|$$
 with $q_{ ext{sat}} \in (0, 1)$

This gives a reliable error estimate

$$\|u - u_{\bullet}^{\mathrm{SC}}\| \le \left(1 - q_{\mathrm{sat}}\right)^{-1} \|\widehat{u}_{\bullet}^{\mathrm{SC}} - u_{\bullet}^{\mathrm{SC}}\|$$

• How to choose the enhanced approximation \hat{u}_{\bullet}^{SC} ?

Hierarchical a posteriori error estimation in SC-FEM (2/2)

Recall that
$$u_{\bullet}^{SC}(x, \mathbf{y}) = \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} u_{\bullet \mathbf{z}}(x) \mathcal{L}_{\bullet \mathbf{z}}(\mathbf{y})$$

$$\widehat{u}_{\bullet}^{SC}(x, \mathbf{y}) := \sum_{\substack{\mathbf{z} \in \mathcal{Y}_{\bullet} \\ \text{spatial enhancement}}} \widehat{u}_{\bullet \mathbf{z}}(x) \mathcal{L}_{\bullet \mathbf{z}}(\mathbf{y}) + \left(\sum_{\substack{\mathbf{z}' \in \widehat{\mathcal{Y}}_{\bullet} \\ \mathbf{z}' \in \widehat{\mathcal{Y}}_{\bullet}}} u_{0\mathbf{z}'}(x) \widehat{\mathcal{L}}_{\bullet \mathbf{z}'}(\mathbf{y}) - \sum_{\substack{\mathbf{z} \in \mathcal{Y}_{\bullet} \\ \mathbf{z} \in \mathcal{Y}_{\bullet}}} u_{0\mathbf{z}}(x) \mathcal{L}_{\bullet \mathbf{z}}(\mathbf{y})\right)$$
parametric enhancement

$$\widehat{u}_{\bullet \mathbf{z}} \in \widehat{\mathbb{X}}_{\bullet \mathbf{z}} \text{ (uniform mesh-refinement) } \forall \mathbf{z} \in \mathcal{Y}_{\bullet} = \mathcal{Y}_{\Lambda_{\bullet}}$$

$$\widehat{\mathcal{Y}}_{\bullet} = \mathcal{Y}_{\widehat{\Lambda}_{\bullet}} \text{ with } \widehat{\Lambda}_{\bullet} := \Lambda_{\bullet} \cup \mathbb{R}(\Lambda_{\bullet}) \quad \rightsquigarrow \quad \widehat{\Lambda}_{\bullet} \text{ is monotone!}$$

$$u_{0\mathbf{z}}(x) \quad u_{0\mathbf{y}}(x) \in \mathbb{X}_{0} := S_{0}^{1}(\mathcal{T}_{0}) \quad \forall \mathbf{z} \in \mathcal{Y}_{\bullet} \text{ and } \forall \mathbf{z}' \in \widehat{\mathcal{Y}}_{\bullet}$$

Hierarchical a posteriori error estimation in SC-FEM (2/2)

Recall that
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$$\widehat{u}_{\bullet}^{SC}(x, \mathbf{y}) := \underbrace{\sum_{z \in \mathcal{Y}_{\bullet}} \widehat{u}_{\bullet z}(x) L_{\bullet z}(\mathbf{y})}_{\text{spatial enhancement}} + \underbrace{\left(\sum_{z' \in \widehat{\mathcal{Y}_{\bullet}}} u_{0z'}(x) \widehat{L}_{\bullet z'}(\mathbf{y}) - \sum_{z \in \mathcal{Y}_{\bullet}} u_{0z}(x) L_{\bullet z}(\mathbf{y})\right)}_{\text{parametric enhancement}}$$

$$A \text{ posteriori error estimate}$$

$$\|u - u_{\bullet}^{SC}\| \leq \frac{1}{1 - q_{\text{sat}}} \|\widehat{u}_{\bullet}^{SC} - u_{\bullet}^{SC}\|$$

$$\leq \frac{1}{1-q_{\text{sat}}} \left(\underbrace{\left\| \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} (\hat{u}_{\bullet \mathbf{z}} - u_{\bullet \mathbf{z}}) L_{\bullet \mathbf{z}} \right\|}_{\text{spatial estimate}} + \underbrace{\left\| \sum_{\mathbf{z}' \in \hat{\mathcal{Y}}_{\bullet} \setminus \mathcal{Y}_{\bullet}} \left(u_{0\mathbf{z}'} - \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} u_{0\mathbf{z}} L_{\bullet \mathbf{z}}(\mathbf{z}') \right) \hat{L}_{\bullet \mathbf{z}'} \right\|}_{\text{parametric estimate}} \right)$$

Hierarchical a posteriori error estimation in SC-FEM (2/2)

Recall that
$$u_{\bullet}^{SC}(x, \mathbf{y}) = \sum_{z \in \mathcal{Y}_{\bullet}} u_{\bullet z}(x) L_{\bullet z}(\mathbf{y})$$

• $\widehat{u}_{\bullet}^{SC}(x, \mathbf{y}) := \sum_{\substack{z \in \mathcal{Y}_{\bullet} \\ \text{spatial enhancement}}} \widehat{u}_{\bullet z}(x) L_{\bullet z}(\mathbf{y}) + \underbrace{\left(\sum_{z' \in \widehat{\mathcal{Y}}_{\bullet}} u_{0z'}(x) \widehat{L}_{\bullet z'}(\mathbf{y}) - \sum_{z \in \mathcal{Y}_{\bullet}} u_{0z}(x) L_{\bullet z}(\mathbf{y})\right)}_{\text{parametric enhancement}}$
• A posteriori error estimate
 $\|u - u_{\bullet}^{SC}\| \leq \frac{1}{1 - q_{\text{sat}}} \|\widehat{u}_{\bullet}^{SC} - u_{\bullet}^{SC}\|$
 $\leq \frac{1}{1 - q_{\text{sat}}} \left(\underbrace{\left\|\sum_{z \in \mathcal{Y}_{\bullet}} (\widehat{u}_{\bullet z} - u_{\bullet z}) L_{\bullet z}\right\|}_{\text{spatial estimate}} + \underbrace{\left\|\sum_{z' \in \widehat{\mathcal{Y}}_{\bullet} \setminus \mathcal{Y}_{\bullet}} (u_{0z'} - \sum_{z \in \mathcal{Y}_{\bullet}} u_{0z} L_{\bullet z}(z')) \widehat{L}_{\bullet z'}\right\|}_{\text{parametric estimate}} \right)$

• Error indicators (e.g., spatial error indicators $\mu_{\bullet z}$)

$$\mu_{\bullet} := \left\| \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} (\widehat{u}_{\bullet \mathbf{z}} - u_{\bullet \mathbf{z}}) L_{\bullet \mathbf{z}} \right\| \leq \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} \|\widehat{u}_{\bullet \mathbf{z}} - u_{\bullet \mathbf{z}}\|_{\mathbb{X}} \|L_{\bullet \mathbf{z}}\|_{L^{2}_{\pi}(\Gamma)} \lesssim \sum_{\mathbf{z} \in \mathcal{Y}_{\bullet}} \mu_{\bullet \mathbf{z}} \|L_{\bullet \mathbf{z}}\|_{L^{2}_{\pi}(\Gamma)}$$

INPUT: $\Lambda_0 = \{\mathbf{1}\}; \ \mathcal{T}_{0z} := \mathcal{T}_0 \ \forall \mathbf{z} \in \widehat{\mathcal{Y}}_0 = \mathcal{Y}_{\Lambda_0 \cup \mathrm{R}(\Lambda_0)};$ output counter k; tolerance tol FOR $\ell = 0, 1, 2, 3, \ldots$ DO:

- SOLVE: compute $u_{\ell z} \in \mathbb{X}_{\ell z}$ for all $z \in \widehat{\mathcal{Y}}_{\ell} = \mathcal{Y}_{\widehat{\Lambda}_{\ell}} = \mathcal{Y}_{\Lambda_{\ell} \cup \mathrm{R}(\Lambda_{\ell})}$
- ESTIMATE: compute error indicators
 - spatial indicators $\mu_{\ell z}$ for all $z \in \mathcal{Y}_{\ell}$
 - parametric indicators $\tau_{\ell\nu}$ for all $\nu \in \mathrm{R}(\Lambda_{\ell})$
 - ▶ If $l = jk, j \in \mathbb{N}$, compute the total error estimate η_l and exit if $\eta_l < \text{tol}$
- MARK: mark certain edges/elements $\mathcal{M}_{\ell z}$ $(z \in \mathcal{Y}_{\ell})$ and indices $\Upsilon_{\ell} \subseteq \mathrm{R}(\Lambda_{\ell})$
- REFINE: enhance approximations
 - ▶ mesh refinement (NVB) $\rightsquigarrow \mathcal{T}_{(\ell+1)z} := \mathsf{refine}(\mathcal{T}_{\ell z}, \mathcal{M}_{\ell z})$ for all $z \in \mathcal{Y}_{\ell}$
 - ▶ parametric enrichment $\rightsquigarrow \Lambda_{\ell+1} := \Lambda_{\ell} \cup \Upsilon_{\ell}$ and construct meshes $\mathcal{T}_{(\ell+1)z'}$ for each new collocation point z'

DUTPUT: SC-FEM approximation $u_{\ell^*}^{SC}$ and the error estimate η_{ℓ^*} for some $\ell^* = jk$

Parametric enrichment

• Parametric enrichment $\rightsquigarrow \Lambda_{\ell+1} := \Lambda_{\ell} \cup \Upsilon_{\ell}$

Key issue: allocation of meshes $\mathcal{T}_{(\ell+1)z'}$ for each new collocation point z'

Parametric enrichment

- Parametric enrichment → Λ_{ℓ+1} := Λ_ℓ ∪ Υ_ℓ
 Key issue: allocation of meshes T_{(ℓ+1)z'} for each new collocation point z'
- Set $\widetilde{\text{tol}} := (\#\mathcal{Y}_{\ell})^{-1} \sum_{\mathbf{z} \in \mathcal{Y}_{\ell}} \mu_{\ell \mathbf{z}} \|L_{(\ell+1)\mathbf{z}}\|_{L^{2}_{\pi}(\Gamma)}$

Parametric enrichment

- $\label{eq:rescaled} \begin{array}{l} \mbox{Parametric enrichment} \rightsquigarrow \Lambda_{\ell+1} := \Lambda_\ell \cup \Upsilon_\ell \\ \mbox{Key issue: allocation of meshes } \mathcal{T}_{(\ell+1)z'} \mbox{ for each new collocation point } z' \end{array}$
- Set $\widetilde{\text{tol}} := (\#\mathcal{Y}_{\ell})^{-1} \sum_{\mathbf{z} \in \mathcal{Y}_{\ell}} \mu_{\ell \mathbf{z}} \|L_{(\ell+1)\mathbf{z}}\|_{L^{2}_{\pi}(\Gamma)}$
- For each new collocation point \mathbf{z}'
 - Initialise the mesh $\mathcal{T}_{(\ell+1)\mathbf{z}'} := \mathcal{T}_0$
 - Iterate the standard adaptive loop

 $\mathsf{SOLVE} \to \mathsf{ESTIMATE} \to \mathsf{MARK} \to \mathsf{REFINE}$

until the resolution of the mesh $\mathcal{T}_{(\ell+1)z'}$ is such that

 $\mu_{(\ell+1)\mathbf{z}'}\|L_{(\ell+1)\mathbf{z}'}\|_{L^2_\pi(\Gamma)} < \widetilde{\mathrm{tol}}$

Experiment 2: nonaffine parametric coefficient

- $-\nabla \cdot (a\nabla u) = 1$ in $D \times \Gamma$, u = 0 on $\partial D \times \Gamma$
- $D := (-1, 1)^2 \setminus (-1, 0]^2 \rightsquigarrow L$ -shaped domain



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 L-shaped domain

Diffusion coefficient $a(x, \mathbf{y}) = exp(h(x, \mathbf{y}))$

•
$$h(x, \mathbf{y}) = 1 + \sum_{m=1}^{m} \sqrt{\lambda_m} \varphi_m(x) y_m$$

- $\{(\lambda_m, \varphi_m(x))\}_{m=1}^{\infty}$ are the eigenpairs of $\int_{D \cup (-1,0]^2} \operatorname{Cov}[h](x, x') \varphi(x') dx'$
- $\operatorname{Cov}[h](x, x') = \sigma^2 \exp(-|x_1 x_1'| |x_2 x_2'|)$
- ► $\{y_m\}_{m \in \{1,...,M\}}$ are images of U(-1,1) iid mean-zero r.v., $d\pi_m(y_m) = \frac{1}{2} dy_m$

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- Adaptive stochastic collocation FEM (Clenshaw–Curtis collocation points)

D

Experiment 2: effectivity and robustness of error estimates (1/2)



Experiment 2: effectivity and robustness of error estimates (2/2)


Experiment 2: single-level vs. multilevel refinement



[Kornhuber, Youett '18], [Lang, Scheichl, Silvester '20]

•
$$-\nabla^2 u = f(x, \mathbf{y})$$
 in $D \times \Gamma$, $u = g$ on $\partial D \times \Gamma$

•
$$D := (-4, 4)^2$$
, $\Gamma = [-1, 1]^2$, $\mathbf{y} = (y_1, y_2)$, $y_1, y_2 \sim U[-1, 1]$

 $u(x, \mathbf{y}) = \exp\left(-\frac{50}{16}\{\alpha(y_1)(x_1 - y_1)^2 + (x_2 - y_2)^2\}\right) \text{ with } \alpha(y_1) = (9y_1 + 11)/2$

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- Dirichlet b.c. for sampled FEM approximations: $u_{\bullet z} = 0 \quad \forall z \in \mathcal{Y}_{\bullet}$
- Reference Qol

$$Q := \int_{\Gamma} \int_{D} \left(u(x, \mathbf{y}) \right)^2 \mathrm{d}x \, \mathrm{d}\pi(\mathbf{y}) = 0.24152872 \dots$$

- $-\nabla^2 u = f(x, \mathbf{y})$ in $D \times \Gamma$, u = g on $\partial D \times \Gamma$
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- Adaptive stochastic collocation FEM (Clenshaw–Curtis collocation points)
 - single-level vs. multilevel refinement



Experiment 3: single-level vs. multilevel refinement (2/2)

	single-level SC-FEM	multilevel SC-FEM
# iterations	38	34
# collocation points	169	153
final #dof	42'961'659	2'620'343
$\left Q(u)-Q(u^{\mathrm{SC}})\right $	4.736e-5	1.381e-4

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single-level	mesh $\mathcal{T}_{\ell z}$	mesh $\mathcal{T}_{\ell z}$
mesh \mathcal{T}_{ℓ}	z = (0, 0)	z = (1, 1)

Conclusions, extensions and outlook

- For multilevel stochastic Galerkin FEM
 - exploiting Galerkin orthogonality & properties of orthogonal polynomials
 - novel reliable and efficient a posteriori error estimates
 - rate optimal adaptive algorithms for PDEs with affine-parametric inputs
 - extensions: goal-oriented adaptivity; parameter-dependent linear elasticity

Conclusions, extensions and outlook

- For multilevel stochastic Galerkin FEM
 - exploiting Galerkin orthogonality & properties of orthogonal polynomials
 - novel reliable and efficient a posteriori error estimates
 - rate optimal adaptive algorithms for PDEs with *affine-parametric* inputs
 - extensions: goal-oriented adaptivity; parameter-dependent linear elasticity
- For multilevel stochastic collocation FEM
 - reliable, effective and robust a posteriori error estimation strategy
 - applicable to problems with *affine and nonaffine* parametric inputs
 - practical error indicators for multilevel adaptivity
 - optimal convergence rates do not seem to be feasible in general
 - optimal rates can be recovered for problems with parameter-dependent local spatial features
 - outlook: convergence analysis, goal-oriented adaptivity, ...

References & Software

- Key references
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- Software
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 - Adaptive ML-SCFEM, https://github.com/albespalov/Adaptive_ML-SCFEM