

Adaptive multilevel stochastic Galerkin FEM for parametric PDE problems

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Workshop

“Interplay of discretization and algebraic solvers:
a posteriori error estimates and adaptivity”

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What is this talk about...

- * Elliptic PDE problems with random inputs
(or, more generally, [high-dimensional parametric elliptic PDEs](#))
- * Stochastic Galerkin finite element method (SGFEM)
- * [Multilevel adaptivity](#) for stochastic Galerkin FEM
- * Theoretical convergence and rate optimality analysis
- * Implementation and numerical results

Parametric model problem (1/2)

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

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

■ Domains

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

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

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

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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 $x \in D$, $\mathbf{y} = (y_m)_{m \in \mathbb{N}} \in \Gamma$

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

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

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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■ Bilinear forms on \mathbb{V}

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

▶ $B(u, v) := B_0(u, v) + \sum_{m \in \mathbb{N}} \int_\Gamma y_m \int_D a_m(x) \nabla u(x, \mathbf{y}) \cdot \nabla v(x, \mathbf{y}) \, dx \, d\pi(\mathbf{y})$

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

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

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

Stochastic Galerkin FEM (1/2)

- 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

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

- Best approximation property

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

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

Stochastic Galerkin FEM (2/2)

- $\{P_\nu : \nu \in \mathcal{J}\}$ is a countable orthonormal polynomial basis of $\mathbb{P} = L^2_\pi(\Gamma)$
- $\mathcal{J} := \{\nu \in \mathbb{N}_0^{\mathbb{N}} : \#\text{supp}(\nu) < \infty\}$ where $\text{supp}(\nu) = \{m \in \mathbb{N} : \nu_m \neq 0\}$

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- Discretisation in the **parameter** domain
 - ▶ finite index set $\mathcal{P}_\bullet \subset \mathcal{J} \implies \mathbb{P}_\bullet = \text{span}\{P_\nu : \nu \in \mathcal{P}_\bullet\} \subset \mathbb{P} = L^2_\pi(\Gamma)$

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- Discretisation in the **physical** domain (**multilevel SGFEM**)
 - ▶ a hierarchy of meshes $\rightsquigarrow \{\mathcal{T}_{\bullet, \nu}\}_{\nu \in \mathcal{P}_\bullet}$
 - ▶ $u_\bullet(x, \mathbf{y}) = \sum_{\nu \in \mathcal{P}_\bullet} u_{\bullet, \nu}(x) P_\nu(\mathbf{y})$ with $u_{\bullet, \nu} \in \mathbb{X}_{\bullet, \nu} = \mathcal{S}_0^1(\mathcal{T}_{\bullet, \nu})$ for all $\nu \in \mathcal{P}_\bullet$

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- Multilevel methods in UQ
 - ▶ Multilevel Monte Carlo
[Giles '08], [Cliffe, Giles, Scheichl, Teckentrup '11], [Giles '15]
 - ▶ Multilevel quasi-Monte Carlo
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 - optimal convergence rates for practical realisations \rightsquigarrow open problem...

Hierarchical a posteriori error estimates(1/3)

- Why hierarchical error estimates?
 - ▶ provide effective error estimation in the energy norm (eff. indices ≈ 1)
 - ▶ provide reliable and efficient estimates of the error reduction;
error reduction indicators \rightsquigarrow key to adaptivity
 - ▶ facilitate convergence analysis of adaptive algorithms

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- Main ideas

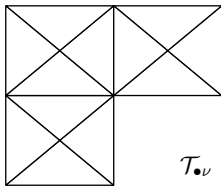
- ▶ use an enhanced approximation $\hat{u}_\bullet \in \hat{V}_\bullet \supset V_\bullet$ to estimate

$$\| \| u - u_\bullet \| \| \approx \| \| \underbrace{\hat{u}_\bullet - u_\bullet}_{\text{computable}} \| \|$$

- ▶ the enhanced approximation is based on 'uniform refinement'
- ▶ avoiding the computation of \hat{u}_\bullet via a decomposition of \hat{V}_\bullet in the spirit of [Bank, Weiser '85]

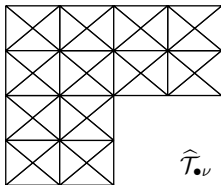
Hierarchical a posteriori error estimates (2/3)

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



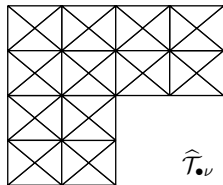
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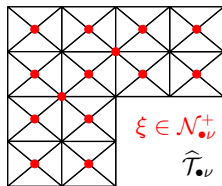
- Enhancement of approximations in the **parameter** domain
 - ▶ add new indices to \mathcal{P}_{\bullet}
 - ▶ finite set $\mathcal{Q}_{\bullet} \subset \mathcal{J} \setminus \mathcal{P}_{\bullet} \rightsquigarrow$ detail index set ('boundary' of \mathcal{P}_{\bullet})
 - ▶ $\widehat{\mathcal{P}}_{\bullet} = \mathcal{P}_{\bullet} \cup \mathcal{Q}_{\bullet} \rightsquigarrow$ uniform enrichment of \mathcal{P}_{\bullet}
 - ▶ $\widehat{\mathbb{P}}_{\bullet} = \text{span}\{P_{\nu} : \nu \in \widehat{\mathcal{P}}_{\bullet}\} \supset \mathbb{P}_{\bullet}$

Example

- ▶ $\mathcal{P}_{\bullet} = \{(0, 0, \dots); (1, 0, \dots); (0, 1, 0, \dots)\}$
 $\implies \mathcal{Q}_{\bullet} = \{(2, 0, \dots); (1, 1, 0, \dots); (0, 2, 0, \dots); (0, 0, 1, 0, \dots)\}$

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- Local error indicators
 - ▶ local **spatial** indicators $\eta_{\bullet}(\nu, \xi)$ for each $\nu \in \mathcal{P}_{\bullet}$ and for each $\xi \in \mathcal{N}_{\bullet,\nu}^+$
 - ▶ individual **parametric** indicators $\eta_{\bullet}(\nu)$ for each $\nu \in \mathcal{Q}_{\bullet}$

Hierarchical a posteriori error estimates (3/3)

- Total error estimate (for multilevel SGFEM)

$$\eta_{\bullet}^2 = (\text{estim. X-error})^2 + (\text{estim. P-error})^2 = \sum_{\nu \in \mathcal{P}_{\bullet}} \sum_{\xi \in \mathcal{N}_{\bullet, \nu}^+} \eta_{\bullet}^2(\nu, \xi) + \sum_{\nu \in \Omega_{\bullet}} \eta_{\bullet}^2(\nu)$$

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Theorem 1 [B., Praetorius, Ruggeri; SIAM/ASA JUQ '21]

- ▶ $\eta_{\bullet} \simeq \|\hat{u}_{\bullet} - u_{\bullet}\|$
- ▶ $\|u - u_{\bullet}\| \gtrsim \eta_{\bullet}$ (efficiency)
- ▶ saturation assumption $\implies \|u - u_{\bullet}\| \lesssim \eta_{\bullet}$ (reliability)

Adaptive SGFEM algorithm

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
 $\{\eta_\ell(\nu, \xi); \xi \in \mathcal{N}_{\ell,\nu}^+, \nu \in \mathcal{P}_\ell\}$ & $\{\eta_\ell(\nu); \nu \in \mathcal{Q}_\ell\}$
 - ▶ energy error estimate η_ℓ
 - ▶ IF $\eta_\ell < \text{tol}$ 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 $\rightsquigarrow \mathcal{P}_{\ell+1} = \mathcal{P}_\ell \cup \mathcal{R}_\ell, \quad \mathcal{T}_{\ell,\nu} = \mathcal{T}_0 \quad \forall \nu \in \mathcal{R}_\ell$

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

Marking strategy

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$$\eta_\ell^2 = \sum_{\nu \in \mathcal{P}_\ell} \sum_{\xi \in \mathcal{N}_{\ell,\nu}^+} \eta_\ell^2(\nu, \xi) + \sum_{\nu \in \mathcal{Q}_\ell} \eta_\ell^2(\nu)$$
- **Separate** marking/enrichment of spatial and parametric components
 - ▶ two independent marking thresholds $\theta_{\mathbb{X}} \in (0, 1]$ and $\theta_{\mathbb{P}} \in (0, 1]$

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- **Separate** marking/enrichment of spatial and parametric components
 - ▶ two independent marking thresholds $\theta_{\mathbb{X}} \in (0, 1]$ and $\theta_{\mathbb{P}} \in (0, 1]$
- **Combined** marking/enrichment of spatial and parametric components
 - ▶ use Dörfler marking for

$$\{\eta_\ell(\nu, \xi); \nu \in \mathcal{P}_\ell, \xi \in \mathcal{N}_{\ell,\nu}^+\} \cup \{\eta_\ell(\nu); \nu \in \mathcal{Q}_\ell\}$$

with $\theta \in (0, 1]$ yields $\mathcal{M}_{\ell,\nu} \subseteq \mathcal{N}_{\ell,\nu}^+$ ($\nu \in \mathcal{P}_\ell$) and $\mathcal{R}_\ell \subseteq \mathcal{Q}_\ell$ satisfying

$$\theta \eta_\ell^2 \leq \sum_{\nu \in \mathcal{P}_\ell} \sum_{\xi \in \mathcal{M}_{\ell,\nu}} \eta_\ell^2(\nu, \xi) + \sum_{\nu \in \mathcal{R}_\ell} \eta_\ell^2(\nu)$$

- ▶ too costly for the single-level SGFEM

Convergence of adaptive algorithm (1/2)

Single-level SGFEM: [B., Praetorius, Rocchi, Ruggeri; SINUM '19]

Multilevel SGFEM: [B., Praetorius, Ruggeri; IMANUM (appeared online)]

Theorem 2 (plain convergence)

For any $\theta_{\mathbb{X}}, \theta_{\mathbb{P}} \in (0, 1]$ (resp., $\theta \in (0, 1]$) $\implies \lim_{\ell \rightarrow \infty} \eta_{\ell} = 0$.

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Remarks

- ▶ Theorem 2 provides a theoretical guarantee that the adaptive algorithm terminates after a finite number of iterations
- ▶ No assumptions on the Galerkin approximations generated by the algorithm
- ▶ The result extends to more general marking criteria and to $D \subset \mathbb{R}^3$

Proof of Theorem 2

Energy error estimate: $\eta_\ell^2 = \sum_{\nu \in \mathcal{P}_\ell} \sum_{\xi \in \mathcal{N}_{\ell, \nu}^+} \eta_\ell^2(\nu, \xi) + \sum_{\nu \in \mathcal{Q}_\ell} \eta_\ell^2(\nu)$

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Proposition 1 (Extension of the results in [Morin, Siebert, Veerer '08])

The multilevel spatial refinement that follows Dörfler marking strategy *along a subsequence* $(\ell_k)_{k \in \mathcal{N}_0}$ guarantees convergence of spatial error estimates *along this subsequence*, i.e., $\sum_{\nu \in \mathcal{P}_{\ell_k}} \sum_{\xi \in \mathcal{N}_{\ell_k}^+} \eta_{\ell_k}(\nu, \xi)^2 \rightarrow 0$ as $k \rightarrow \infty$.

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Proposition 2

The parametric enrichment that follows the Dörfler marking strategy *along a subsequence* $(\mathcal{P}_{\ell_k})_{k \in \mathcal{N}_0} \subset (\mathcal{P}_\ell)_{\ell \in \mathcal{N}_0}$ guarantees convergence of the *whole sequence* of parametric error estimates, i.e., $\sum_{\nu \in \mathcal{Q}_\ell} \eta_\ell(\nu)^2 \rightarrow 0$ as $\ell \rightarrow \infty$.

Convergence of adaptive algorithm (2/2)

Single-level SGFEM: [B., Praetorius, Rocchi, Ruggeri; SINUM '19]

Multilevel SGFEM: [B., Praetorius, Ruggeri; IMANUM (appeared online)]

Theorem 3 (linear convergence)

Saturation assumption \implies linear converg. for any $\theta_{\mathbb{X}}, \theta_{\mathbb{P}} \in (0, 1]$ (resp., $\theta \in (0, 1]$):

$$\exists q_{\text{lin}} \in (0, 1) \text{ s.t. } \| \| u - u_{\ell+1} \| \| \leq q_{\text{lin}} \| \| u - u_{\ell} \| \| \quad \forall \ell \in \mathbb{N}_0$$

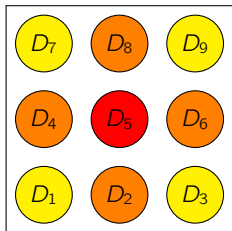
Numerical results: cookie problem

[B., Praetorius, Ruggeri; IMANUM (appeared online)]

- $-\nabla \cdot (a \nabla u) = f$ 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 $D_m \subset D$ ($m = 1, \dots, 9$)

- Expansion coefficients $\{a_m\}_{m \in \mathbb{N}_0}$

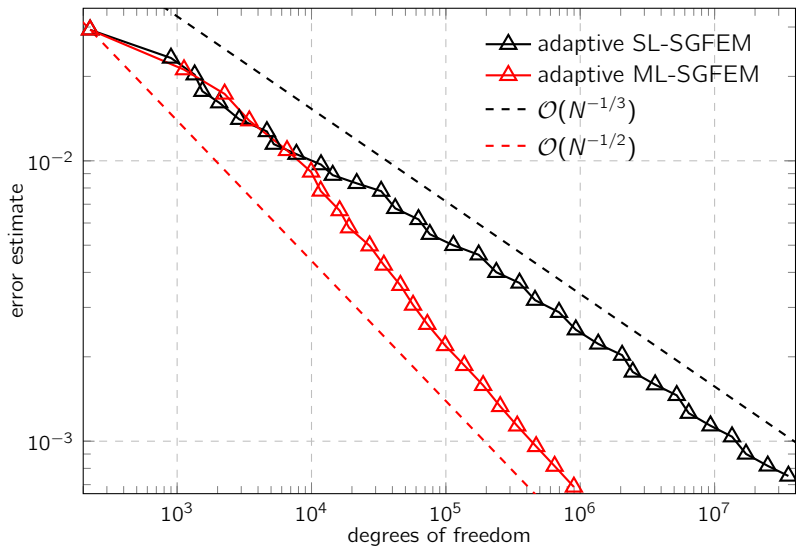
- ▶ $a_0 \equiv 1$
- ▶ $a_m = 0.5 \chi_{D_m}$ for $m = 1, 3, 7, 9$
- ▶ $a_m = 0.7 \chi_{D_m}$ for $m = 2, 4, 6, 8$
- ▶ $a_m = 0.9 \chi_{D_m}$ for $m = 5$
- ▶ $a_m \equiv 0$ for $m > 9$



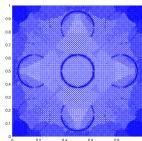
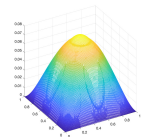
D

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

Numerical results: single-level vs. multilevel adaptive SGFEM

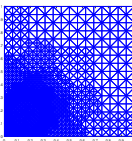
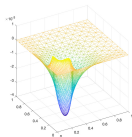


Numerical results: locally refined meshes in multilevel SGFEM



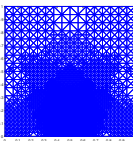
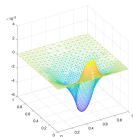
$$\nu = \mathbf{0}$$

$$\#\mathcal{T}_{\ell,\nu} = 84050$$



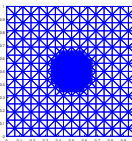
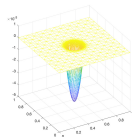
$$\nu = (1 \ 0)$$

$$\#\mathcal{T}_{\ell,\nu} = 10994$$



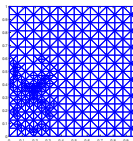
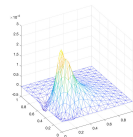
$$\nu = (0 \ 1)$$

$$\#\mathcal{T}_{\ell,\nu} = 16420$$



$$\nu = (0 \ 0 \ 0 \ 0 \ 1)$$

$$\#\mathcal{T}_{\ell,\nu} = 9528$$



$$\nu = (1 \ 0 \ 0 \ 1)$$

$$\#\mathcal{T}_{\ell,\nu} = 839$$

Optimal convergence of adaptive multilevel SGFEM

[B., Praetorius, Ruggeri; IMANUM (appeared online)]

- Concept of 'multilevel structure' $\rightsquigarrow \mathbb{P}_\bullet = [\mathcal{P}_\bullet, (\mathcal{T}_{\bullet,\nu})_{\nu \in \mathcal{P}_\bullet}]$, $\#\mathbb{P}_\bullet \simeq \dim \mathbb{V}_\bullet$

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- Concept of optimality \rightsquigarrow approximation class \mathbb{A}_s ($s > 0$)

$$w \in \mathbb{A}_s \iff \exists \{\mathbf{P}_\ell^*\}_{\ell \in \mathbb{N}_0} \text{ such that } \|w - w_\ell^*\| = \mathcal{O}((\dim \mathbb{V}_\ell^*)^{-s})$$

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Theorem 4 (rate optimality)

Strong saturation assumption \implies optimal convergence for sufficiently small θ , i.e., if $s > 0$ and $u \in \mathbb{A}_s$, then

$$\sup_{\ell \in \mathbb{N}_0} (\#\mathbf{P}_\ell - \#\mathbf{P}_0 + 1)^s \|u - u_\ell\| \leq C \|u\|_{\mathbb{A}_s},$$

$$\text{where } \|u\|_{\mathbb{A}_s} := \sup_{N \in \mathbb{N}_0} (N + 1)^s \min_{\substack{\mathbf{P}_{\text{opt}} \in \text{REFINE}(\mathbf{P}_0) \\ \#\mathbf{P}_{\text{opt}} - \#\mathbf{P}_0 \leq N}} \min_{v_{\text{opt}} \in \mathbb{V}_{\text{opt}}} \|u - v_{\text{opt}}\|$$

Saturation assumption vs. strong saturation assumption

- Saturation assumption
 - ▶ SGFEM solution $u_{\bullet} \in \mathbb{V}_{\bullet}$
 - ▶ Enhanced (**uniformly refined**) SGFEM solution $\hat{u}_{\bullet} \in \hat{\mathbb{V}}_{\bullet}$
 - ▶ There exist a constant $q_{\text{sat}} \in (0, 1)$ s.t. $\| \| u - \hat{u}_{\bullet} \| \| \leq q_{\text{sat}} \| \| u - u_{\bullet} \| \|$
 - ▶ $\hat{\mathbb{V}}_{\bullet} = \hat{\mathbb{X}}_{\bullet} \otimes \hat{\mathbb{P}}_{\bullet} \implies q_{\text{sat}} = q_{\text{sat},\mathbb{X}} \cdot q_{\text{sat},\mathbb{P}} \in (0, 1)$ if $q_{\text{sat},\mathbb{X}} < 1$ or $q_{\text{sat},\mathbb{P}} < 1$

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■ Strong saturation assumption

- ▶ $\mathbf{P}_{\bullet} \in \text{REFINE}(\mathbf{P}_0) \rightsquigarrow$ any multilevel structure obtained from \mathbf{P}_0
- ▶ $\mathbf{P}_{\star} \in \text{REFINE}(\mathbf{P}_{\bullet}) \rightsquigarrow$ a refined multilevel structure obtained from \mathbf{P}_{\bullet}
- ▶ $\mathbf{P}_{\circ} := \text{REFINE}(\mathbf{P}_{\bullet}, \mathbf{M}_{\bullet}) \rightsquigarrow$ a multilevel structure obtained from \mathbf{P}_{\bullet} by **one step of multilevel refinement** towards \mathbf{P}_{\star}
- ▶ There exist constants $0 < \kappa_{\text{sat}} \leq q_{\text{sat}} < 1$ such that

$$\| \| u - u_{\star} \| \| \leq \kappa_{\text{sat}} \| \| u - u_{\bullet} \| \| \implies \| \| u - u_{\circ} \| \| \leq q_{\text{sat}} \| \| u - u_{\bullet} \| \|$$

Multilevel SGFEM: implementation challenges

- linear algebra

$$\mathbf{A} = (\mathbf{A}_{\nu\mu})_{\nu,\mu \in \mathcal{P}_\bullet}, \quad \mathbf{A}_{\nu\mu} = \sum_{m=0}^{\infty} [G_m]_{\nu\mu} K_m^{\nu\mu} = \sum_{m=0}^M [G_m]_{\nu\mu} K_m^{\nu\mu}$$

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$$[K_m^{\nu\mu}]_{ij} = \int_D a_m(x) \nabla \varphi_{\bullet,\mu,z_j}(x) \cdot \nabla \varphi_{\bullet,\nu,z_i}(x) dx$$

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- computation of non-square stiffness matrices

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$$[K_m^{\nu\mu}]_{ij} = \int_D a_m(x) \nabla \varphi_{\bullet,\mu,z_j}(x) \cdot \nabla \varphi_{\bullet,\nu,z_i}(x) dx$$

- solver: preconditioned MINRES or CG
- preconditioner: mean-based preconditioner with diagonal blocks $K_0^{\nu\nu}$

What have we achieved?

- Design of adaptive algorithms for single-level and multilevel SGFEM
- Theoretical analysis
 - ▶ convergence of the adaptive algorithm
 - ▶ linear convergence (under the saturation assumption)
 - ▶ rate-optimality of adaptive multilevel SGFEM (under the strong saturation assumption)
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