An adaptive stochastic Galerkin FEM for parametric PDEs with singular solutions

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Joint work with **Alex Bespalov** (University of Birmingham)

Outline

1. Parametric equations and stochastic Galerkin FEM (sGFEM)
2. Hierarchical *a posteriori* error estimation
3. An adaptive algorithm using the sGFEM
4. Numerical experiments

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Parametric model problem

Consider the following parametric problem

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

where $D \subset \mathbb{R}^2$ is a polygonal domain, the *parameter domain* Γ is given by

$$\Gamma := \prod_{m=1}^{\infty} \underbrace{[-1, 1]}_{=:\Gamma_m}, \qquad \Big(\mathbf{y} = (y_m)_{m=1}^{\infty} \in \Gamma, \ y_m \in \Gamma_m \Big),$$

and the parametric coefficient $a(\mathbf{x}, \mathbf{y})$ is given by

$$a(\mathbf{x}, \mathbf{y}) = a_0(\mathbf{x}) + \sum_{m=1}^{\infty} y_m \, a_m(\mathbf{x}), \qquad \text{with} \qquad \begin{cases} 0 < \alpha_0^{\min} \leq a_0(\mathbf{x}) \leq \alpha_0^{\max} \text{ a.e. in } D, \\ \displaystyle\sum_{m=1}^{\infty} \|a_m\|_{L^\infty(D)} < \alpha_0^{\min}. \end{cases}$$

Moreover, let $\pi = \pi(\mathbf{y})$ be a product measure on $(\Gamma, \mathcal{B}(\Gamma))$ given by

$$\pi(\mathbf{y}) := \prod_{m=1}^{\infty} \pi_m(y_m), \quad \mathbf{y} \in \Gamma,$$

where each π_m is a measure on $(\Gamma_m, \mathcal{B}(\Gamma_m))$.

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Stochastic weak formulation

Let V be the tensor product space given by

$$V := H_0^1(D) \otimes L_\pi^2(\Gamma) \simeq L_\pi^2(\Gamma; H_0^1(D)),$$

where $H_0^1(D)$ is a Sobolev space over D and $L_\pi^2(\Gamma)$ denotes the Lebesgue space of square-integrable functions with respect to the measure π.

Then, find $u = u(\mathbf{x}, \mathbf{y}) \in V$ such that

$$B(u, v) := B_0(u, v) + \sum_{m=1}^{\infty} B_m(u, v) = \int_\Gamma \int_D f(\mathbf{x}) v(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \, d\pi(\mathbf{y}) =: F(v) \qquad \forall \, v \in V,$$

where

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

$$B_m(u, v) := \int_\Gamma \int_D a_m(\mathbf{x}) \nabla u(\mathbf{x}, \mathbf{y}) \cdot \nabla v(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \, y_m \, d\pi(\mathbf{y}), \quad \forall \, m \geq 1,$$

▷ The assumptions on $a(\mathbf{x}, \mathbf{y})$ ensure the well-posedness of the weak formulation[1].

▷ The bilinear forms B and B_0 induce two equivalent norms

$$\text{energy norm} \quad \rightarrow \quad \sqrt{B(\cdot, \cdot)} =: \|\cdot\|_B \simeq \|\cdot\|_{B_0} := \sqrt{B_0(\cdot, \cdot)};$$

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Discretisation: stochastic Galerkin FEM (sGFEM)

Discretisation requires a Galerkin projection onto a finite-dimensional subspace of V. Then, we look for a function $u_{X\mathfrak{P}} \in V_{X\mathfrak{P}}$ satisfying

$$B(u_{X\mathfrak{P}}, v) = F(v) \qquad \forall\, v \in V_{X\mathfrak{P}} := X \otimes \mathcal{P}_{\mathfrak{P}} \;\subset\; H^1_0(D) \otimes L^2_\pi(\Gamma) = V.$$

How to choose X and $\mathcal{P}_{\mathfrak{P}}$?

- We let $X = X(\mathcal{T})$ be a first-order finite element space, i.e., it is spanned by piecewise linear functions associated with a conforming mesh $\mathcal{T}$ of D;

- We let $\mathcal{P}_{\mathfrak{P}}$ be a polynomial space on Γ constructed as follows.
  Let $\{p^m_k\}_{k\geq 0}$ (with $p^m_0 := 1$) be an orthonormal basis of $L^2_{\pi_m}(\Gamma_m)$ and

$$\mathfrak{I} := \Big\{ \nu = (\nu_1, \nu_2, \dots) \in \mathbb{N}_0^{\mathbb{N}} \;:\; \#\mathrm{supp}(\nu) < \infty \Big\}.$$

  For a finite-dimensional subset $\mathfrak{P} \subset \mathfrak{I}$, define

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  - The set $\mathfrak{P}$ is called the "index set", each $\nu \in \mathfrak{P}$ is called "index", and $\#\mathfrak{P} = \dim(\mathcal{P}_{\mathfrak{P}})$;

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Hierarchical error estimation: enrichments

Idea: compare $u_{X\mathfrak{P}} \in V_{X\mathfrak{P}}$ with another approximation $u^*_{X\mathfrak{P}} \in V^*_{X\mathfrak{P}} \supset V_{X\mathfrak{P}}$ that is supposed to be more accurate. Therefore

$$\|e\|_B = \|u - u_{X\mathfrak{P}}\|_B \approx \|u^*_{X\mathfrak{P}} - u_{X\mathfrak{P}}\|_B =: \|e^*\|_B \quad \leftarrow \quad \text{error estimate}$$

and e^* satisfies

$$B(e^*, v) = F(v) - B(u_{X\mathfrak{P}}, v) \qquad \forall\, v \in V^*_{X\mathfrak{P}}.$$

In order to avoid the computation of $u^*_{X\mathfrak{P}}$, consider the following hierarchical enrichments.

1. Consider the "detail space" $Y \subset H^1_0(D)$ such that $X \cap Y = \{0\}$ and define:

$$X^* := X \oplus Y;$$

2. Consider the "detail index set" $\mathfrak{Q} \subset \mathfrak{I}$ such that $\mathfrak{P} \cap \mathfrak{Q} = \emptyset$ and define:

$$\mathfrak{P}^* := \mathfrak{P} \cup \mathfrak{Q}; \qquad \mathcal{P}_{\mathfrak{P}^*} := \mathcal{P}_{\mathfrak{P}} \oplus \mathcal{P}_{\mathfrak{Q}};$$

3. Define the enhanced space $V^*_{X\mathfrak{P}}$ as

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Hierarchical error estimation: error estimates

▷ By exploiting the hierarchical decomposition of $V^*_{X\mathfrak{P}}$, we define the "spatial" estimator $e_{Y\mathfrak{P}} \in V_{Y\mathfrak{P}}$ and the "parametric" estimator $e_{X\mathfrak{Q}} \in V_{X\mathfrak{Q}}$ satisfying respectively

$$B_0(e_{Y\mathfrak{P}}, v) = F(v) - B(u_{X\mathfrak{P}}, v) \qquad \forall\, v \in V_{Y\mathfrak{P}},$$
$$B_0(e_{X\mathfrak{Q}}, v) = F(v) - B(u_{X\mathfrak{P}}, v) \qquad \forall\, v \in V_{X\mathfrak{Q}},$$

and let

$$\eta := \left(\|e_{Y\mathfrak{P}}\|^2_{B_0} + \|e_{X\mathfrak{Q}}\|^2_{B_0} \right)^{1/2}.$$

▷ The error estimate η is both *reliable* and *efficient*[2], i.e.,

$$\eta \;\simeq\; \|u - u_{X\mathfrak{P}}\|_B = \|e\|_B;$$

▷ The quantities $\|e_{Y\mathfrak{P}}\|_{B_0}$ and $\|e_{X\mathfrak{Q}}\|_{B_0}$ provide an estimate of the error reduction[3] achieved if either the enhanced approximation $u_{X^*\mathfrak{P}} \in V_{X\mathfrak{P}} \oplus V_{Y\mathfrak{P}}$ or $u_{X\mathfrak{P}^*} \in V_{X\mathfrak{P}} \oplus V_{X\mathfrak{Q}}$ is going to be computed, i.e.,

$$\|e_{Y\mathfrak{P}}\|_{B_0} \;\simeq\; \|u_{X^*\mathfrak{P}} - u_{X\mathfrak{P}}\|_B, \qquad \|e_{X\mathfrak{Q}}\|_{B_0} \;\simeq\; \|u_{X\mathfrak{P}^*} - u_{X\mathfrak{P}}\|_B.$$

[2] **Bespalov, Silvester**, SIAM J. Sci. Comput., 38 (2016), pp. A2118–A2140;
[3] **Bespalov, Powell, Silvester**, SIAM, J. Sci. Comput., 36 (2014), pp. A339–A363;

Hierarchical error estimation: error estimates

▷ By exploiting the hierarchical decomposition of $V^*_{X\mathfrak{P}}$, we define the "spatial" estimator $e_{Y\mathfrak{P}} \in V_{Y\mathfrak{P}}$ and the "parametric" estimator $e_{X\mathfrak{Q}} \in V_{X\mathfrak{Q}}$ satisfying respectively

$$B_0(e_{Y\mathfrak{P}}, v) = F(v) - B(u_{X\mathfrak{P}}, v) \qquad \forall\, v \in V_{Y\mathfrak{P}},$$
$$B_0(e_{X\mathfrak{Q}}, v) = F(v) - B(u_{X\mathfrak{P}}, v) \qquad \forall\, v \in V_{X\mathfrak{Q}},$$

and let

$$\eta := \left(\|e_{Y\mathfrak{P}}\|^2_{B_0} + \|e_{X\mathfrak{Q}}\|^2_{B_0} \right)^{1/2}.$$

▷ The error estimate η is both *reliable* and *efficient*[2], i.e.,

$$\eta \;\simeq\; \|u - u_{X\mathfrak{P}}\|_B = \|e\|_B;$$

▷ The quantities $\|e_{Y\mathfrak{P}}\|_{B_0}$ and $\|e_{X\mathfrak{Q}}\|_{B_0}$ provide an estimate of the error reduction[3] achieved if either the enhanced approximation $u_{X^*\mathfrak{P}} \in V_{X\mathfrak{P}} \oplus V_{Y\mathfrak{P}}$ or $u_{X\mathfrak{P}^*} \in V_{X\mathfrak{P}} \oplus V_{X\mathfrak{Q}}$ is going to be computed, i.e.,

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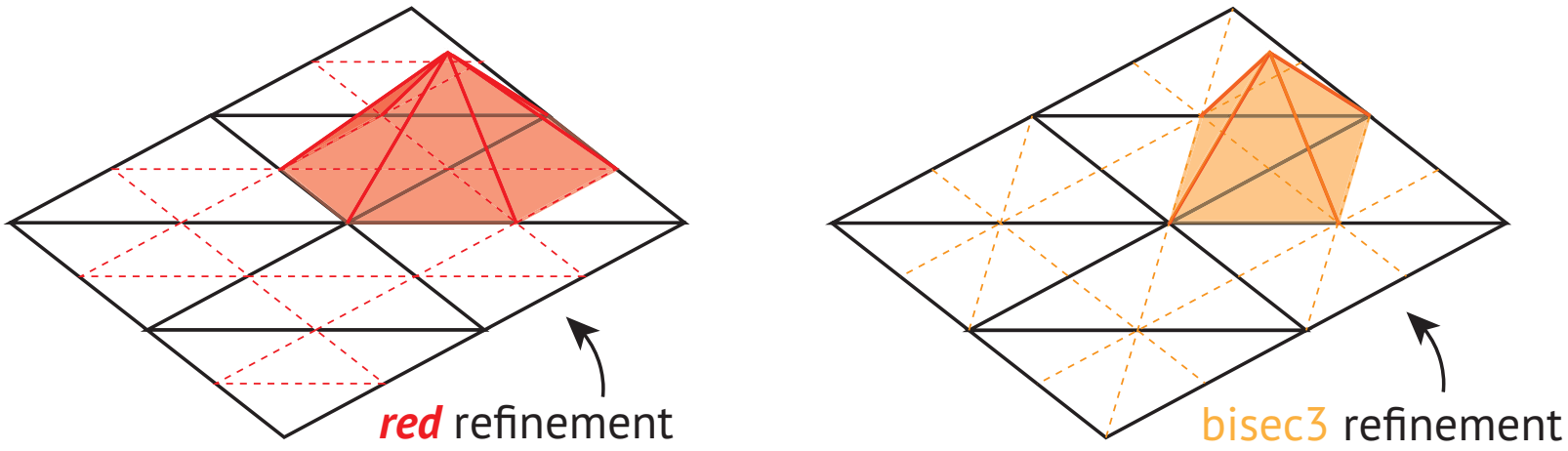
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Hierarchical error estimation: detail space and detail index set

▷ **The choice of** Y: finite element space spanned by the piecewise linear functions associated with the edge midpoints of $\mathcal{T}$. For example:

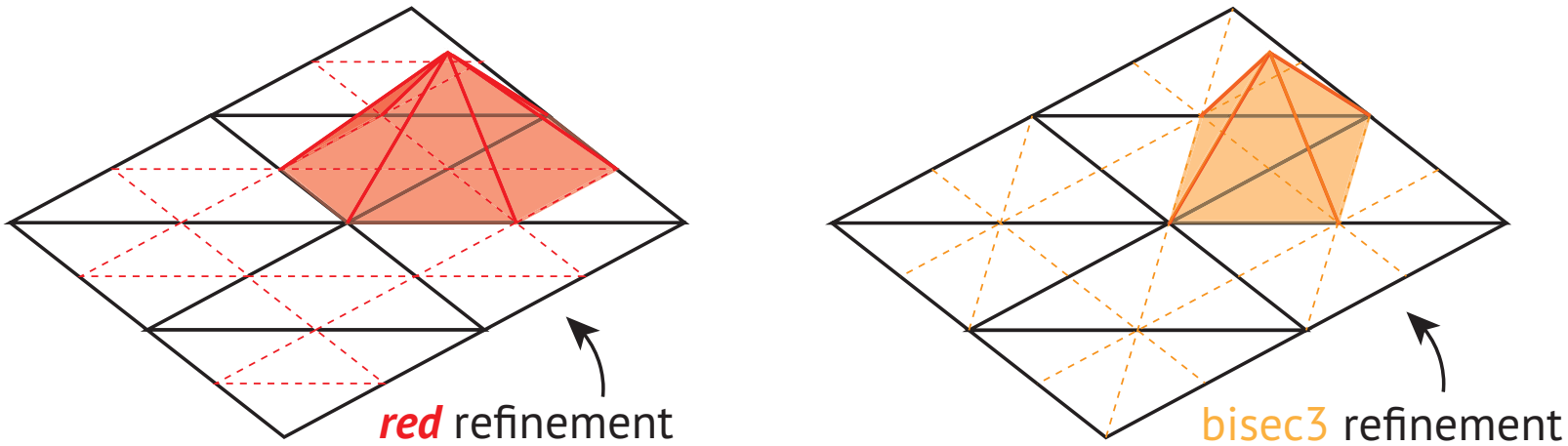


▷ **The choice of** $\mathfrak{Q}$: we construct $\mathfrak{Q}$ from $\mathfrak{P}$ by activating 1 parameter more and by increasing the total polynomial degree in the active parameters by 1. For example:

$$\text{if} \qquad \mathfrak{P} = \left\{ \begin{matrix} (0,0,0,\dots) \\ (1,0,0,\dots) \end{matrix} \right\} \qquad \text{then} \qquad \mathfrak{Q} = \left\{ \begin{matrix} (0,1,0,\dots) \\ (1,1,0,\dots) \\ (2,0,0,\dots) \end{matrix} \right\}.$$

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Outline

1. Parametric equations and stochastic Galerkin FEM (sGFEM)
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3. An adaptive algorithm using the sGFEM
4. Numerical experiments

Adaptive algorithm

The adaptive loop involves the four modules

SOLVE, ESTIMATE, MARK, and REFINE

also employed in deterministic (non-parametric) FEM.

▷ **Input**: data a, f; coarse $\mathcal{T}_0$; initial $\mathfrak{P}_0$; parameters $\theta_X, \theta_{\mathfrak{P}} \in (0,1)$; tolerance ε;
▷ **Output**: final Galerkin solution u_k; final energy error estimate η_k;

1. SOLVE: compute the approximation u_k s.t. $B(u_k, v) = F(v), \forall\, v \in V^k_{X\mathfrak{P}} = X(\mathcal{T}_k) \otimes \mathcal{P}_{\mathfrak{P}_k}$;

2. ESTIMATE: let $e_{Y\mathfrak{P}}|_K$ and $e^{(\mu)}_{X\mathfrak{Q}}$ be the error contributions from each element $K \in \mathcal{T}_k$ and each single index $\mu \in \mathfrak{Q}_k$, respectively. Then compute

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If $\eta_k < \varepsilon$ then end loop; otherwise:

3. MARK[4]: create a set of marked elements $\mathcal{M}_k \subset \mathcal{T}_k$ and marked indices $\mathfrak{M}_k \subset \mathfrak{Q}_k$ s.t.

$$\sum_{K \in \mathcal{M}_k} \|e_{Y\mathfrak{P}}|_K\|^2_{B_0} \geq \theta_X \|e_{Y\mathfrak{P}}\|^2_{B_0}, \qquad \eta^2_{\mathfrak{M}} := \sum_{\mu \in \mathfrak{M}_k} \|e^{(\mu)}_{X\mathfrak{Q}}\|^2_{B_0} \geq \theta_{\mathfrak{P}} \|e_{X\mathfrak{Q}}\|^2_{B_0};$$

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Adaptive algorithm (cont.)

3.1 MARK (NEIGHBOURS ELEMENTS): create the set $\mathcal{R}_k \supset \mathcal{M}_k$ of the overall elements that (eventually) have to be refined, and let

$$\eta_{\mathcal{R}}^2 := \sum_{K \in \mathcal{R}_k} \|e_{Y\mathfrak{P}}|_K\|_{B_0}^2 .$$

4. REFINE: **If** $\eta_{\mathfrak{M}} > \eta_{\mathcal{R}}$ **then**

Polynomial enrichment: $\mathfrak{P}_{k+1} = \mathfrak{P}_k \cup \mathfrak{M}_k$ and $\mathcal{T}_{k+1} = \mathcal{T}_k$;

else

Mesh refinement: $\mathcal{T}_{k+1} = \text{longest–edge–bisection}(\mathcal{T}_k)$ and $\mathfrak{P}_{k+1} = \mathfrak{P}_k$;

end

Initialisation:

▷ Parameters $y_m \sim U(-1, 1)$ i.i.d: this corresponds to $\pi_m(y_m) = 1/2$, $m \geq 1$;

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Model Problem 1

Consider the problem on the L-shaped domain $D := (-1,1)^2 \setminus (-1,0]^2$

$$\begin{aligned} -\nabla \cdot (a(\mathbf{x},\mathbf{y})\nabla u(\mathbf{x},\mathbf{y})) &= 1 \quad \mathbf{x} = (x_1,x_2) \in D, \quad \mathbf{y} \in \Gamma, \\ u(\mathbf{x},\mathbf{y}) &= 0 \quad \mathbf{x} = (x_1,x_2) \in \partial D, \ \mathbf{y} \in \Gamma. \end{aligned}$$

where the random coefficient[5] is given by

$$a(\mathbf{x},\mathbf{y}) = 1 + \sum_{m=1}^{\infty} y_m \left[\frac{\bar{\alpha}}{m^2} \cos(2\pi\beta_1(m)x_1)\cos(2\pi\beta_2(m)x_2) \right], \qquad \bar{\alpha} = 0.547,$$

with

$$\begin{aligned} \beta_1(m) &:= m - k(m)(k(m)+1)/2, \\ \beta_2(m) &:= k(m) - \beta_1(m), \end{aligned} \qquad k(m) := \left\lfloor -1/2 + \sqrt{1/4 + 2m} \right\rfloor$$

Algorithm's input parameters:

$$\theta_X = 0.2, \qquad \theta_{\mathfrak{B}} = 0.9, \qquad \varepsilon = 5 \cdot 10^{-3}.$$

[5] **Eigel, Gittelson, Schwab, Zander**, Comput. Methods. Appl. Mech. Engrg., 2014

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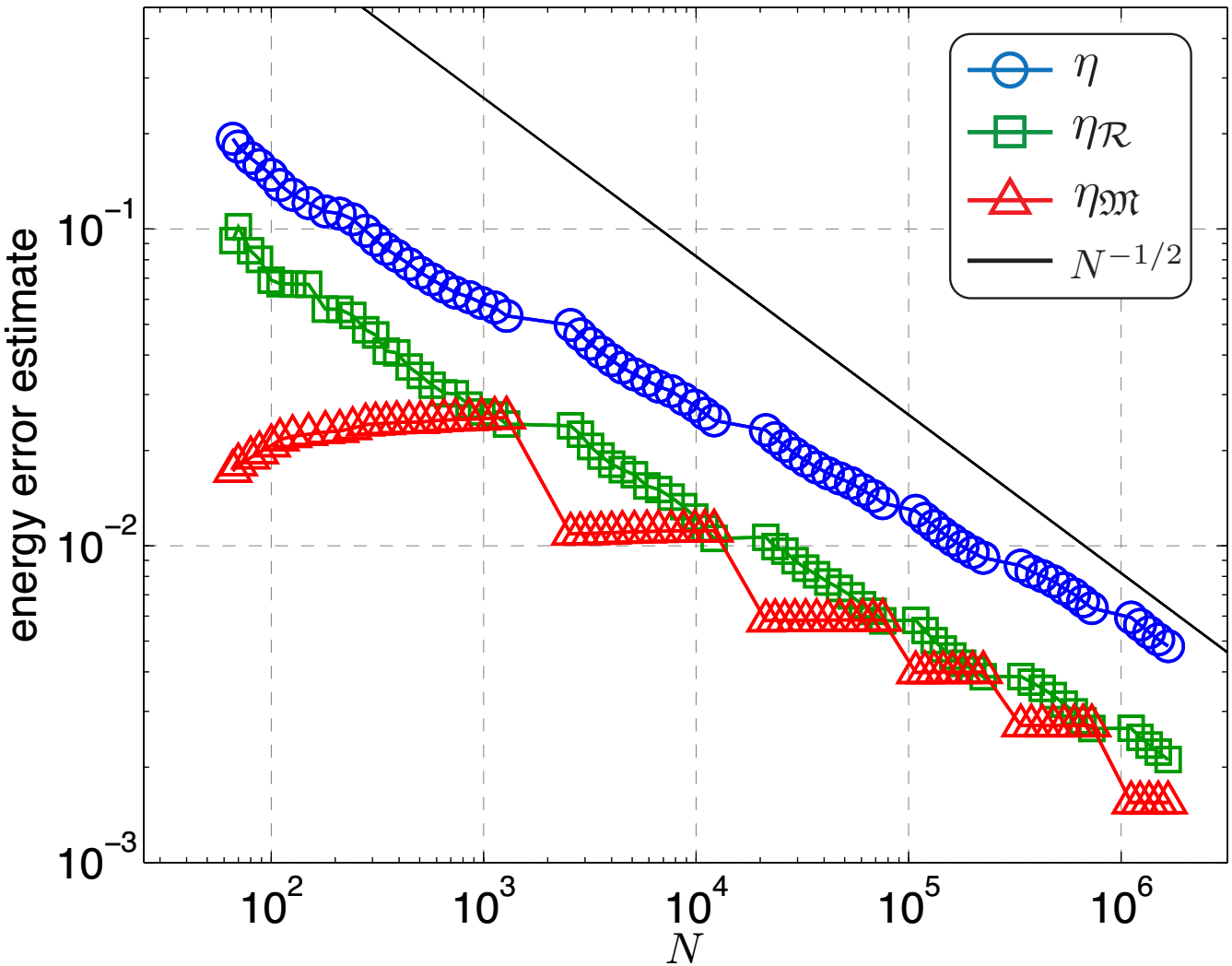
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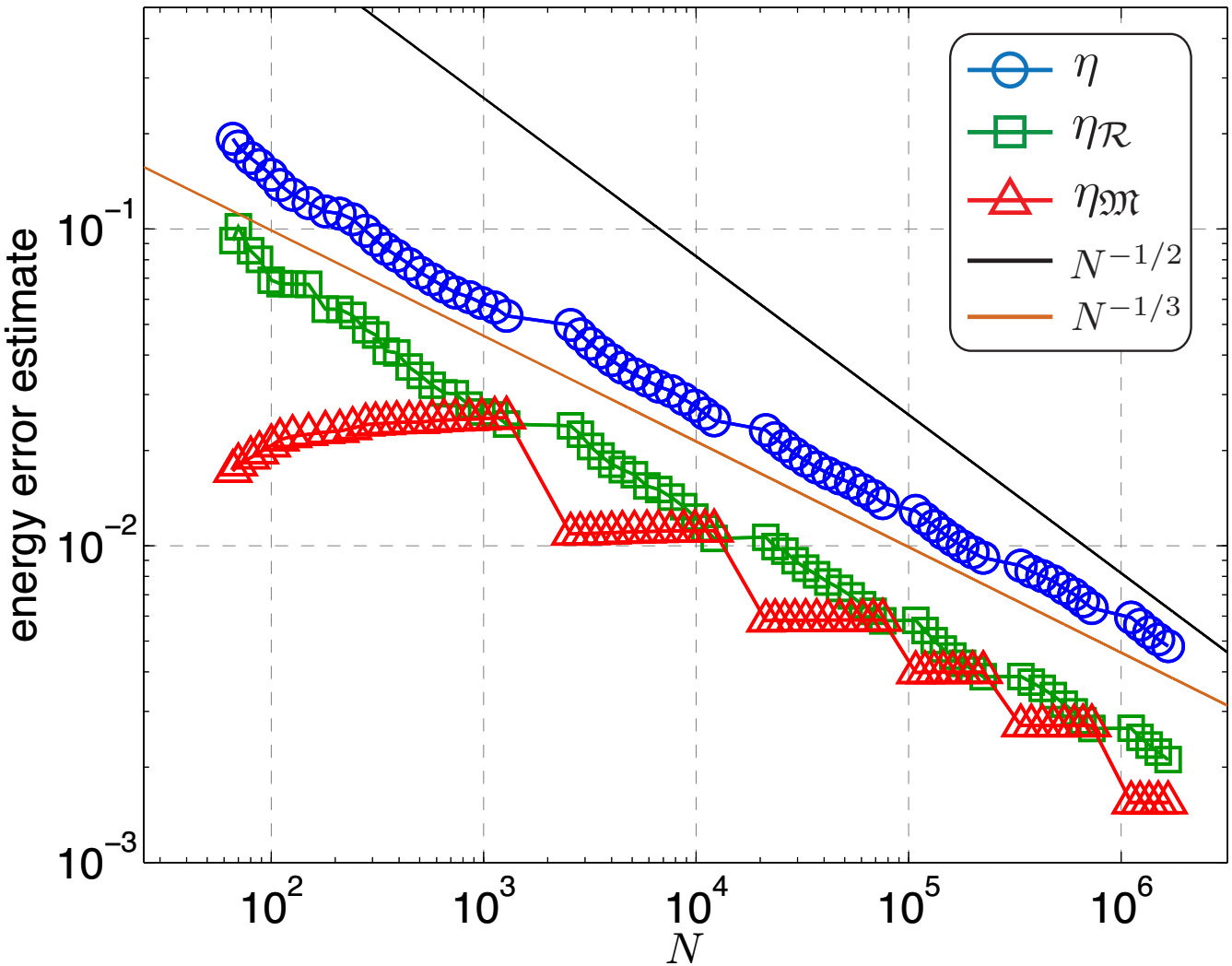
Model Problem 1: decay of the estimated energy error

▷ Iterations (K): 71; ▷ Vertices ($\#\mathcal{V}_K$): 72‘322; ▷ Elements ($\#\mathcal{T}_K$): 145‘595;
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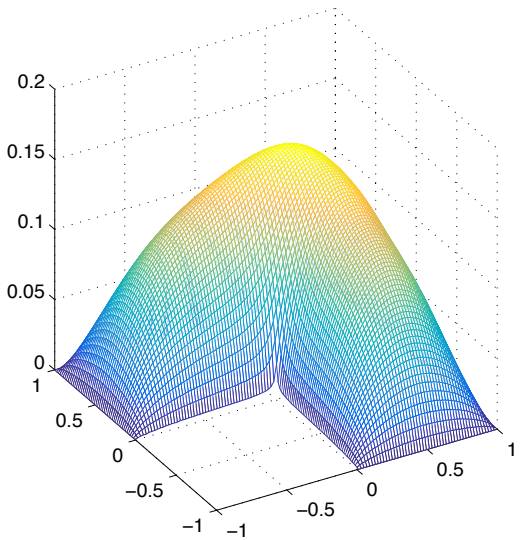
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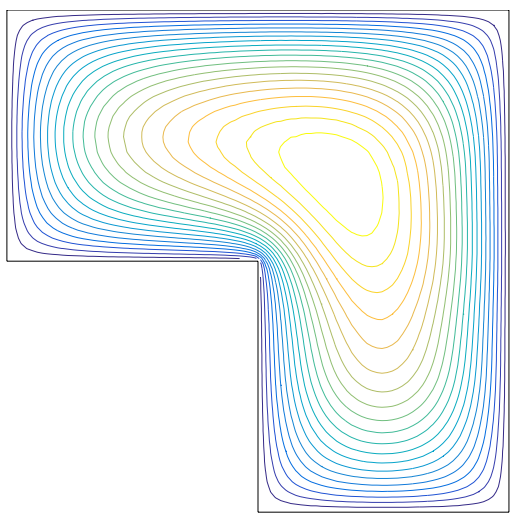
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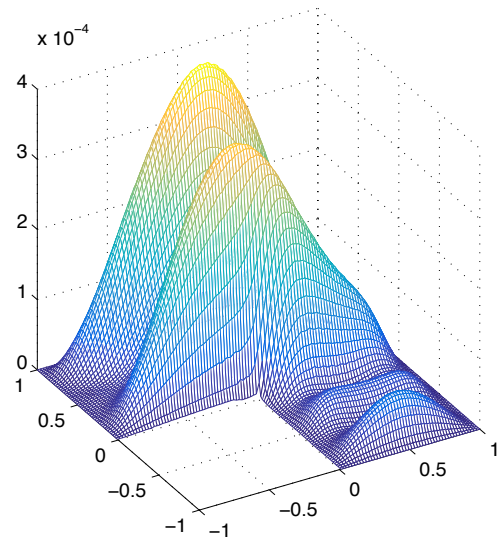
Model Problem 1: mean value, variance and mesh

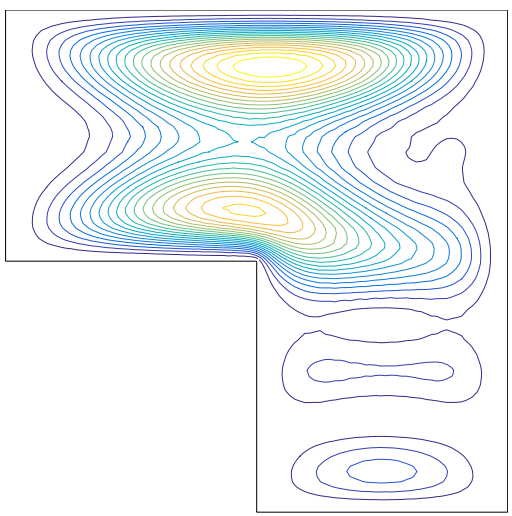
$\mathbb{E}[u_{X\mathfrak{P}}]$



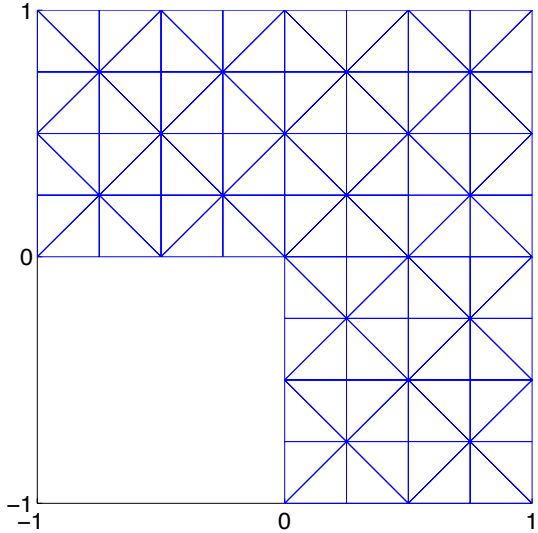


$\mathrm{Var}(u_{X\mathfrak{P}})$

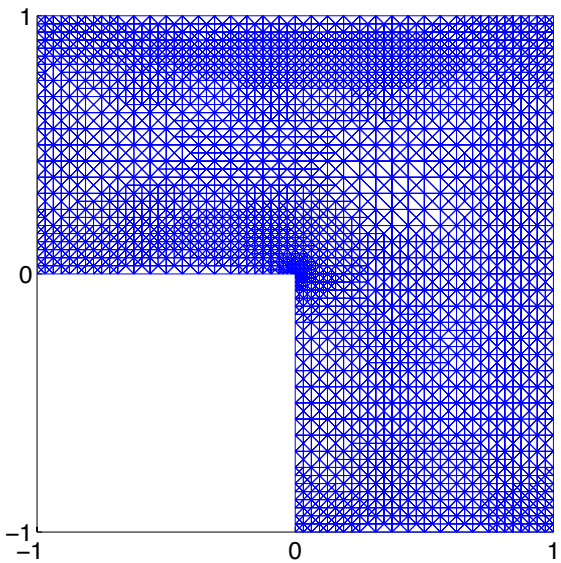




Initial mesh



Final mesh



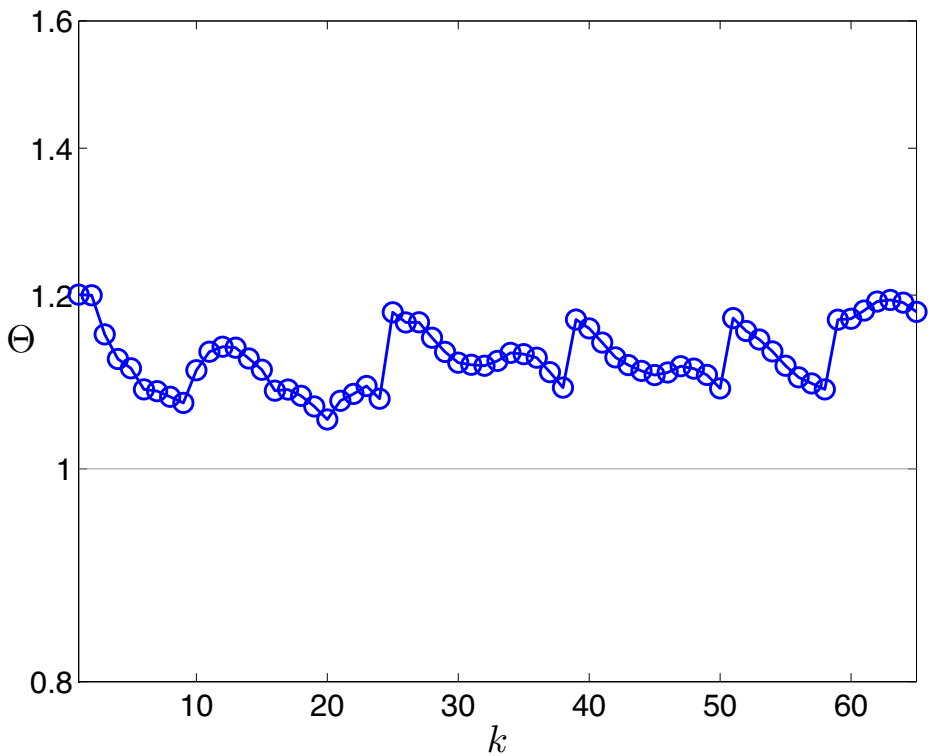
Model Problem 1: effectivity indices and final index set

Reference solution u_{ref} computed with P_2 approximation over a fine mesh with the final index set (on the right). Total *dof*: 26'745'665. Since

$$\|e_k\|_B \approx (\|u_{\text{ref}}\|_B^2 - \|u_k\|_B^2)^{1/2} =: \|e_k^{\text{ref}}\|_B,$$

effectivity indices:

$$\Theta_k := \eta_k / \|e_k^{\text{ref}}\|_B$$



Final index set ($\mathfrak{P}_{71}$)

$k = 0$	(0 0)
	(1 0)
$k = 25$	(0 1)
	(2 0)
$k = 39$	(0 0 1)
	(1 1 0)
	(3 0 0)
$k = 51$	(0 0 0 1)
	(1 0 1 0)
	(2 1 0 0)
$k = 59$	(0 0 0 0 1)
	(0 2 0 0 0)
	(1 0 0 1 0)
	(2 0 1 0 0)
	(4 0 0 0 0)
$k = 67$	(0 0 0 0 0 1)
	(0 1 1 0 0 0)
	(1 0 0 0 0 1)
	(1 0 0 0 1 0)
	(1 2 0 0 0 0)
	(2 0 0 1 0 0)
	(3 0 1 0 0 0)
	(3 1 0 0 0 0)

Active parameters: 6

Model Problem 2

Let $D := (-1,1)^2 \setminus \{(x_1, x_2) \ : \ -1 \leq x_1 < 0, x_2 = 0\}$ be a crack domain and consider

$$\begin{aligned} -\nabla \cdot \big(a(\mathbf{x},\mathbf{y})\nabla u(\mathbf{x},\mathbf{y})\big) &= e^{-(x_1+0.5)^2-(x_2-0.5)^2} && \mathbf{x} = (x_1,x_2) \in D, \quad \mathbf{y} \in \Gamma, \\ u(\mathbf{x},\mathbf{y}) &= 0 && \mathbf{x} = (x_1,x_2) \in \partial D, \ \mathbf{y} \in \Gamma. \end{aligned}$$

where the random coefficient[6] is given by

$$a(\mathbf{x},\mathbf{y}) = 1 + \frac{1}{\sqrt{3}} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} y_{ij} \sqrt{\nu_{ij}}\, \phi_{ij}(\mathbf{x}), \qquad y_{ij} \sim U(-1,1),$$

with $\phi_{00}(\mathbf{x}) := 1$, and

$$\phi_{ij}(\mathbf{x}) := 2\cos(i\pi x_1)\cos(j\pi x_2), \qquad \nu_{ij} := (1/4)e^{-\pi(i^2+j^2)}, \qquad \forall\ i,j \geq 1.$$

Reordering in terms of a single index m so that the quantities ν_m appear in descending order:

$$a(\mathbf{x},\mathbf{y}) = 1 + \frac{1}{\sqrt{3}} \sum_{m=1}^{\infty} y_m \sqrt{\nu_m}\, \phi_m(\mathbf{x}), \qquad y_m \sim U(-1,1).$$

Algorithm's input parameters:

$$\theta_X = 0.5, \qquad \theta_{\mathfrak{B}} = 0.5, \qquad \varepsilon = 3 \cdot 10^{-3}.$$

[6] **Lord, Powell, Shardlow**, Cambridge University Press, 2014

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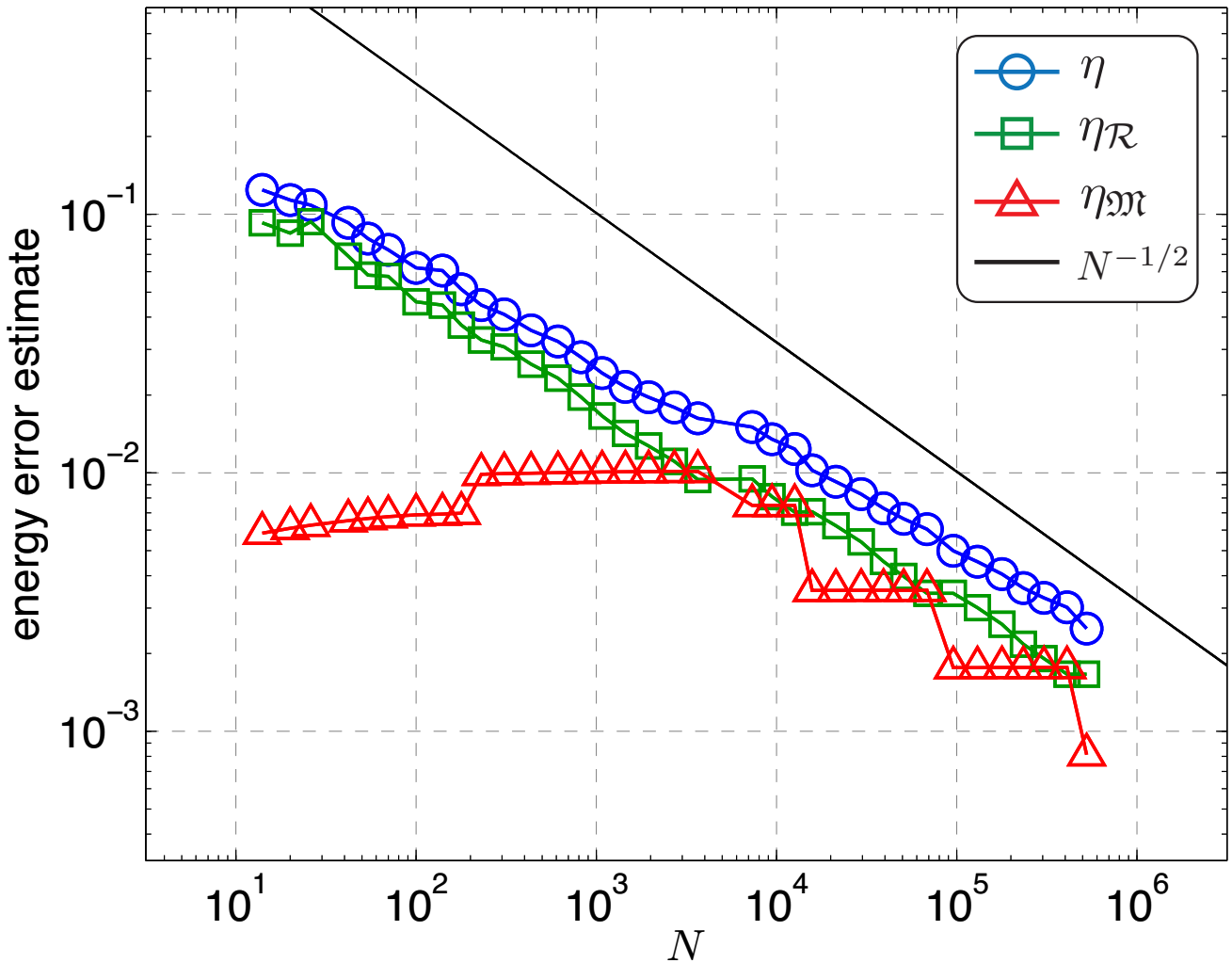
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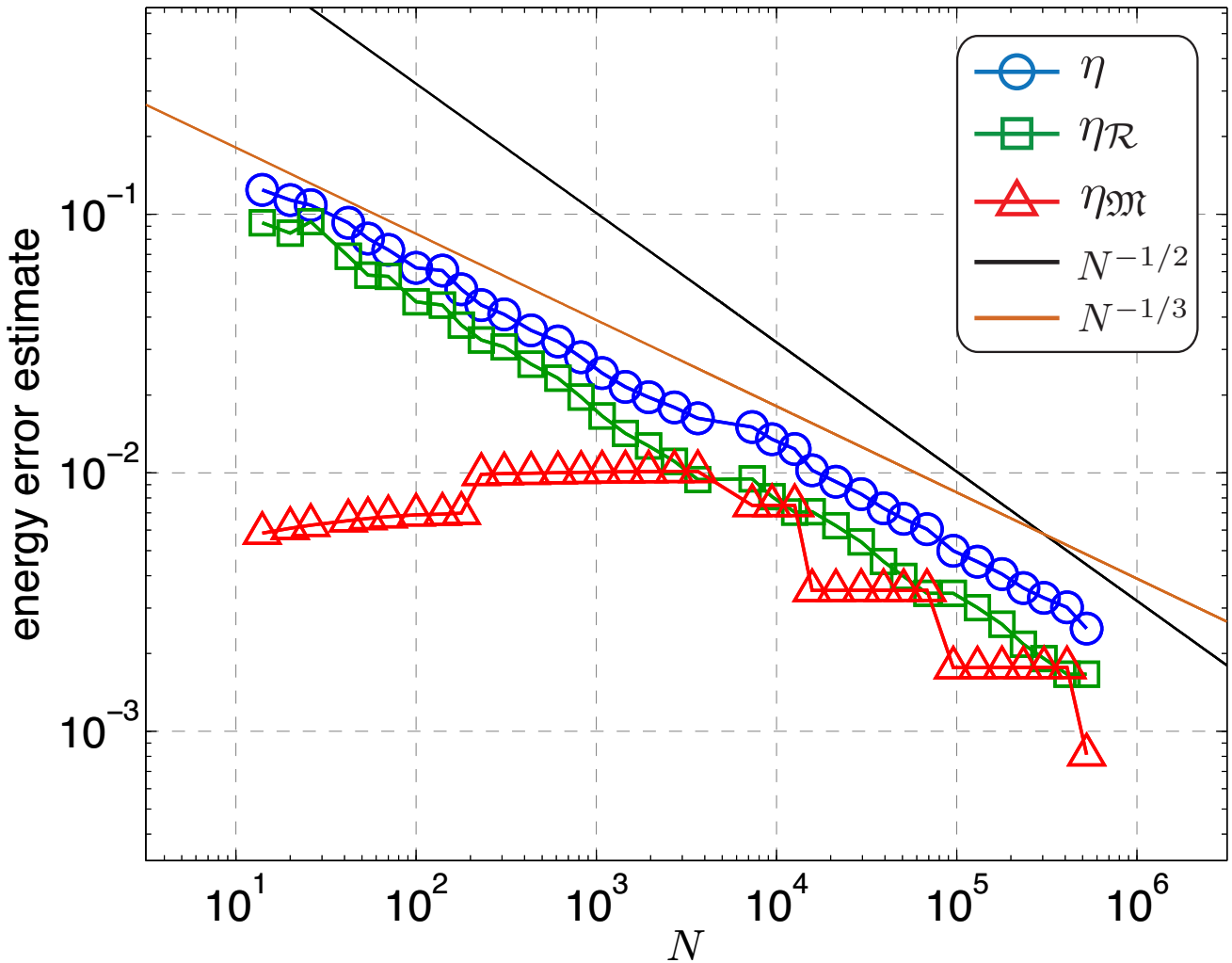
Model Problem 2: decay of the estimated energy error

▷ Iterations (K): 35; ▷ Vertices ($\#\mathcal{V}_K$): 58‘526; ▷ Elements ($\#\mathcal{T}_K$): 118‘110;
▷ Indices ($\#\mathfrak{P}_K$): 9; ▷ **Final dof (N): 526‘734**;



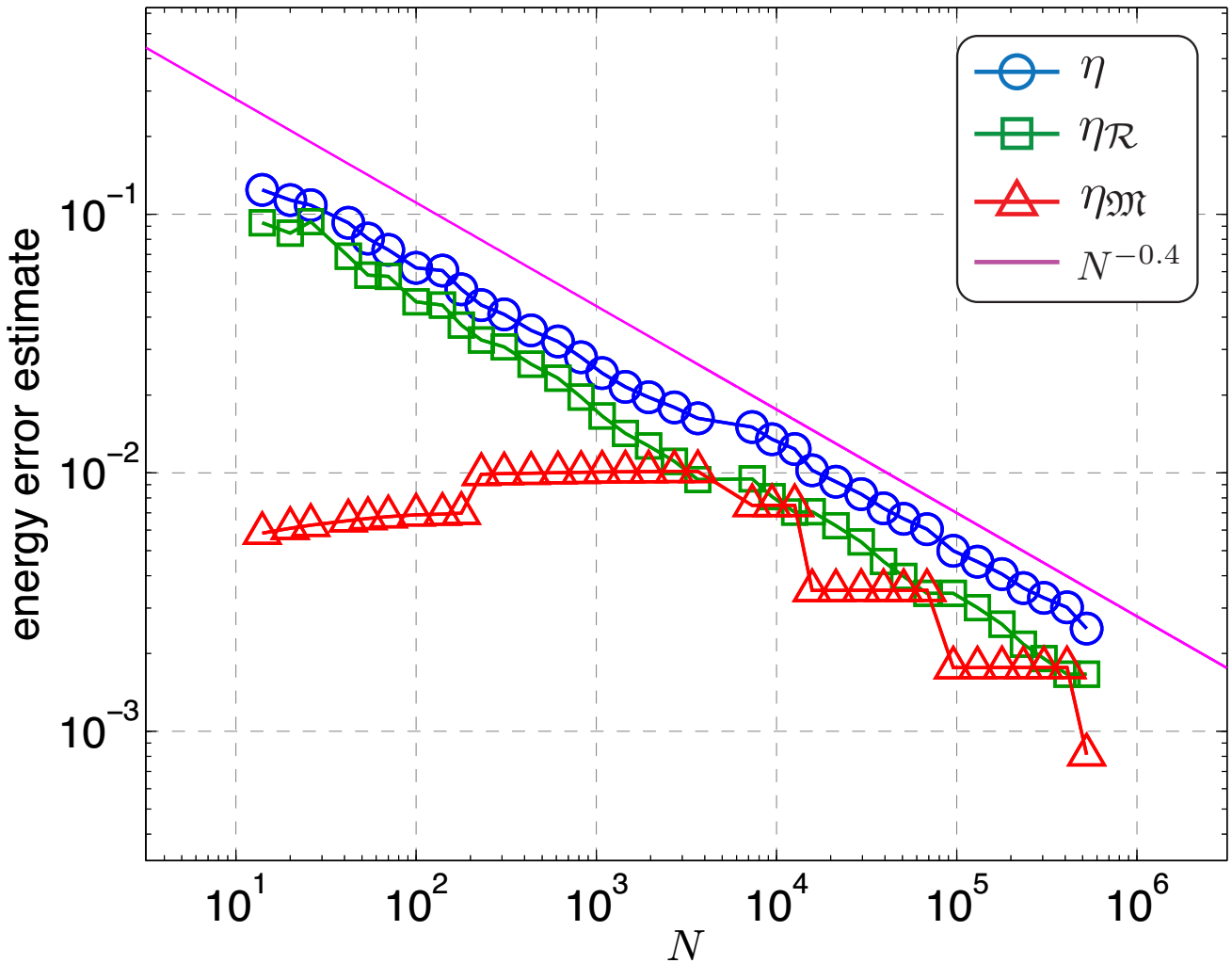
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▷ Indices ($\#\mathfrak{P}_K$): 9; ▷ **Final dof (N): 526‘734**;



Model Problem 2: final index set

Final index set ($\mathfrak{P}_{35}$)

$k = 0$ (0 0)
(1 0)

$k = 20$ (0 1)
(2 0)

$k = 23$ (0 0 1)

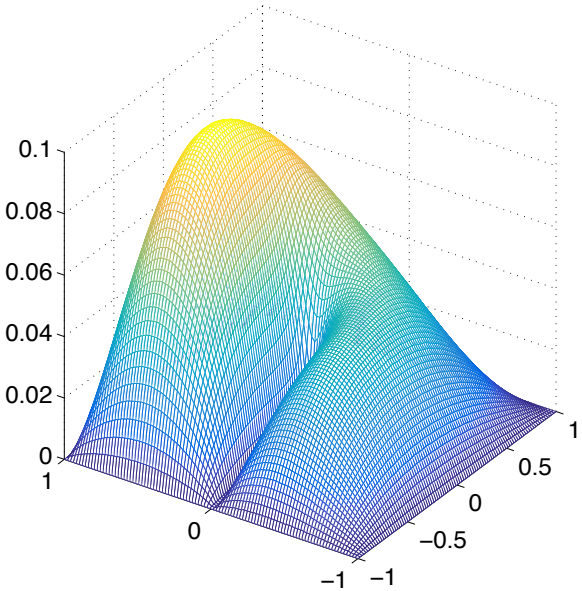
$k = 29$ (1 0 1)
(1 1 0)

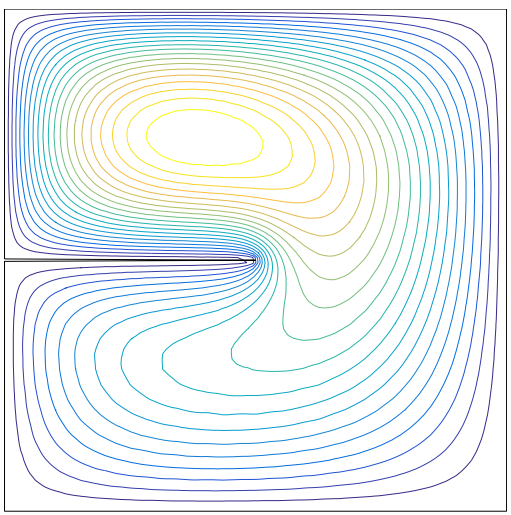
$k = 35$ (0 0 0 1)
(3 0 0 0)

Active parameters: 4

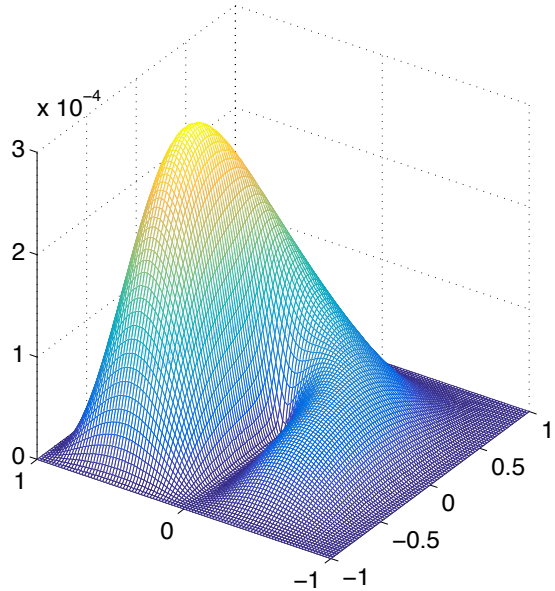
Model Problem 2: mean value, variance and mesh

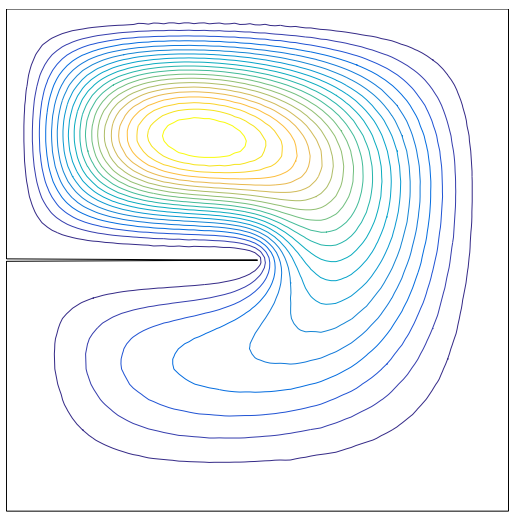
$\mathbb{E}[u_{X\mathfrak{P}}]$



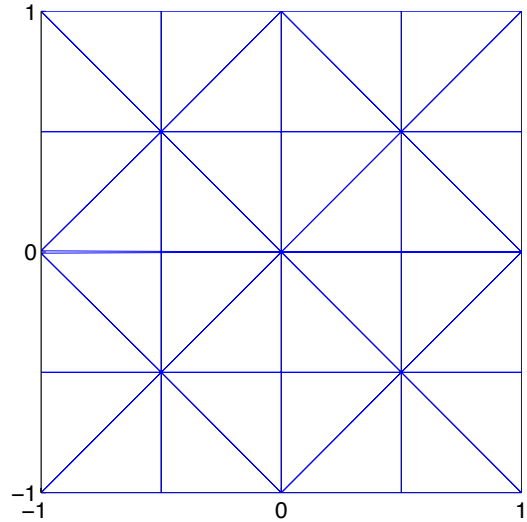


$\mathrm{Var}(u_{X\mathfrak{P}})$

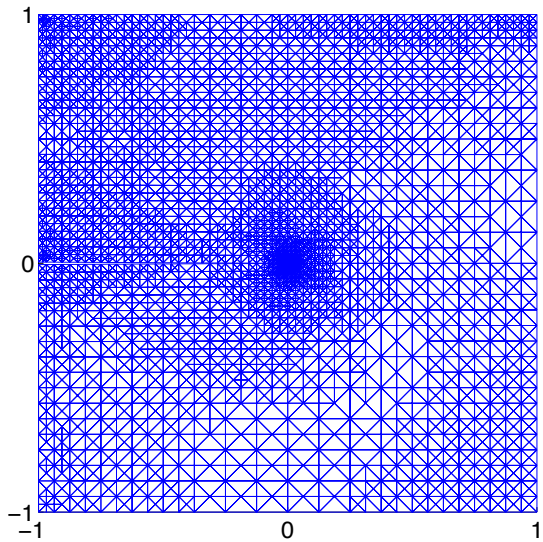




Initial mesh



Final mesh



Concluding remarks:

- ▷ Adaptive algorithm based on the comparison of separate error reduction estimates in both spatial and parametric approximations;
- ▷ Efficient and convergent (numerically!) algorithm for parametric problem with singular solutions up to small tolerances;
- ▷ Spatial features of both mean value and variance of the solution captured by appropriate mesh refinements;
- ▷ Implementation developed under the stochastic–IFISS (S–IFISS) framework: maths.manchester.ac.uk/∼djs/ifiss/sifiss.html.

Main reference:

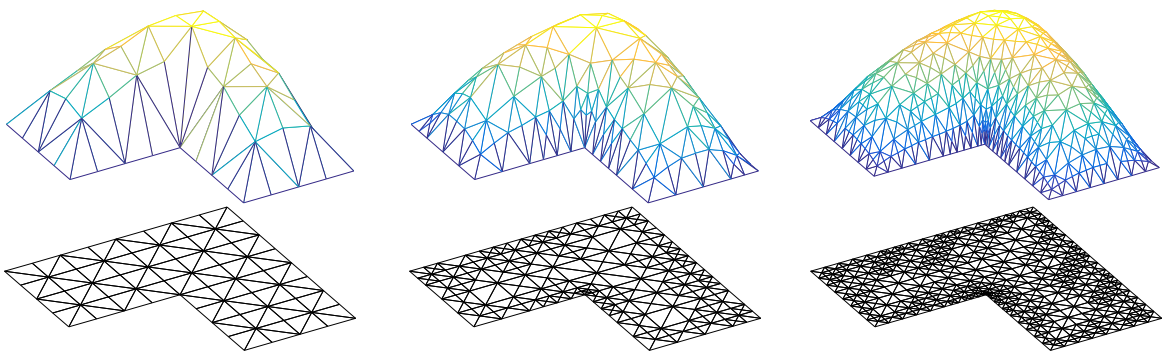
- ▷ **A. Bespalov, L. R.**, *Efficient adaptive algorithms for parametric PDEs with spatial singularities, 2017, (in preparation);*

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Thank you for your attention!