An Efficient Reduced Basis Solver for SGFEM Matrix Equations.

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Joint work with: Valeria Simoncini, David Silvester.

PDEs + Random Inputs

To perform forward UQ, we can may apply Stochastic FEMs:

- ▷ Monte Carlo FEMs (inc QMC, MLMC, ...)
- ▷ **Stochastic Galerkin FEMs (SGFEMs)** (this talk)
- ▷ Stochastic collocation FEMs
- ▷ Reduced basis FEMs
- ▷ ...

SGFEMs have limitations for interesting/complex problems.

$$u(\boldsymbol{x}, \boldsymbol{\xi}(\omega)) \approx \sum_{i=1}^{n_X} \sum_{j=1}^{n_{\mathcal{P}}} u_{ij} \phi_i(\boldsymbol{x}) \psi_j(\boldsymbol{\xi}(\omega))$$

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Outline

- **Intro**: standard SGFEM approximation for

$$-\nabla \cdot a\left(\boldsymbol{x}, \boldsymbol{\xi}(\omega)\right) \nabla u(\boldsymbol{x}, \boldsymbol{\xi}(\omega)) = f(\boldsymbol{x})$$

- **Matrix equation** formulation of SGFEM systems

- **Reduced basis** iterative solver **(MultiRB)**:
  - ▷ Exploits **low rank** of solution object
  - ▷ **Memory-efficient**

1. Standard SGFEM

Find $u(\boldsymbol{x}, \boldsymbol{y}) : D \times \Gamma \to \mathbb{R}$ such that

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

(+ boundary conditions) where

$$\boxed{a(\mathbf{x}, \mathbf{y}) = a_0(\mathbf{x}) + \sum_{m=1}^{\infty} a_m(\mathbf{x}) y_m},$$

and $\mathbf{y}$ is the image of a vector of countably many **random variables** $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots,)$ taking values in some set Γ (the **parameter domain**).

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Weak Formulation

Find $u \in V_g := L^2(\Gamma, H^1_g(D))$ satisfying:

$$\int_\Gamma (a \nabla u, \nabla v)_{L^2(D)} \, d\pi(\boldsymbol{y}) = \int_\Gamma (f, v)_{L^2(D)} \, d\pi(\boldsymbol{y}) \qquad \forall v \in V_0.$$

Weak Formulation

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To construct a Galerkin approximation:

- Let $X \subset H^1_g(D)$ be a **finite element space** on D
- Let $\mathcal{P} \subset L^2(\Gamma)$ be a set of M-variate **polynomials** on Γ
  - ▷ total degree $\leq k \Rightarrow$ $\boxed{\text{dim}(\mathcal{P}) = \frac{(M+k)!}{M!k!}}$
  - ▷ tensor product $\Rightarrow$ $\boxed{\text{dim}(\mathcal{P}) = \Pi_{m=1}^{M} (k_m + 1)}$

SGFEM Linear Systems

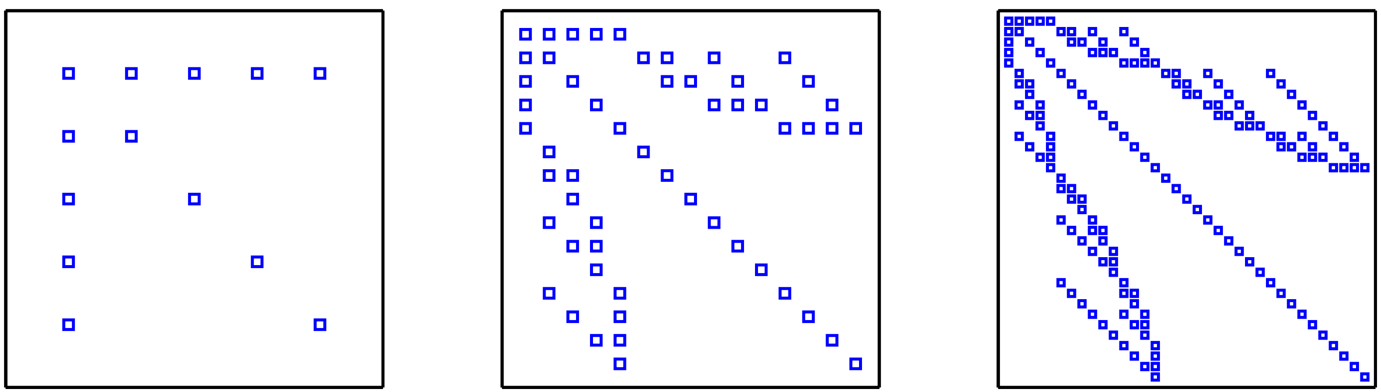
Construct $u_{X\mathcal{P}} \in X \otimes \mathcal{P}$ by solving **one** linear system, $A\mathbf{u} = \mathbf{f}$ of size

$$\boxed{n_X n_{\mathcal{P}} = \text{dim}(X) \times \text{dim}(\mathcal{P})}$$

where

$$A \;=\; G_0 \otimes K_0 + \sum_{m=1}^{M} G_\ell \otimes K_\ell .$$

Matrix structure (total degree case) $M = 4$ and $k = 1, 2, 3$.



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SGFEM Linear Systems

$$A = G_0 \otimes K_0 + \sum_{m=1}^{M} G_m \otimes K_m$$

G_0, G_m are associated with $\mathcal{P}$ (the polynomial space) and K_0, K_m are associated with X (the FEM space). All are **sparse**.

Can solve $A\mathbf{u} = \mathbf{f}$ using **standard Krylov methods**. Need:

- ▷ multiplications with A
- ▷ application of P^{-1} (preconditioner) to vectors
- ▷ **memory** to store 4 vectors of length $n_X n_{\mathcal{P}}$!

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Example

Choose $D = [-1,1] \times [1,1]$ and $X = \mathbb{Q}_1$ with $\boxed{n_X = 65,025}$ and

$$a(\boldsymbol{x},\boldsymbol{y}) = 1 + \sigma \sum_{m=1}^{20} \sqrt{\lambda_m}\varphi_m(\boldsymbol{x})y_m, \qquad y_m \in \left[-\sqrt{3},\sqrt{3}\right],$$

where $\sigma = 0.1$ and (λ_m, φ_m) are eigenpairs associated with

$$C_a(\boldsymbol{x},\boldsymbol{x}') = \sigma^2 \exp\left(-\frac{1}{2}\|\boldsymbol{x}-\boldsymbol{x}'\|_1\right)$$

M	k	n_P	Preconditioned CG
20	2	231	7.4e1 (6)
	3	1,771	5.6e2 (6)
	4	$\mathbf{10,626}$	**Out of Memory**

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Adaptive SGFEM (1)

- start with **low-dimensional** spaces $X^{(0)}, \mathcal{P}^{(0)}$ and compute $u_{X\mathcal{P}}^{(0)}$

- estimate the (e.g, energy) error using **a posterior estimators**

$$\eta \approx \mathbb{E}\left[\| a^{1/2} \nabla \left(u - u_{X\mathcal{P}}^{(0)} \right) \|_{L^2(D)}^2 \right]^{1/2}$$

- learn if **enrichment** is needed for $X^{(0)}$ **or** $\mathcal{P}^{(0)}$ (or both)

- compute $u_{X\mathcal{P}}^{(\ell)} \in X^{(\ell)} \otimes \mathcal{P}^{(\ell)}, \ell = 1, 2, \ldots$

See work by: Bespalov, Powell, Silvester, Crowder **(S-IFISS MATLAB Software)** and Schwab, Eigel, Gittelson, Zander etc.

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Adaptive SGFEM (2)

- start with standard **(probably too large)** spaces $X, \mathcal{P}$

- convert linear system $A\mathbf{u} = \mathbf{f}$ into a matrix equation, with solution U

- apply an iterative method to generate $U_k \approx U$, $k = 0, 1, 2, \ldots$ where

$$U_k = V_k Y_k, \qquad V_k \in \mathbb{R}^{n_X \times n_R},\ Y_k \in \mathbb{R}^{n_R \times n_{\mathcal{P}}}$$

with $\boxed{n_R << n_X}$

Note: the product $V_k Y_k$ is **never** formed!

2. Matrix Equation Formulation

Define the $\boxed{n_X \times n_P}$ **solution matrix**

$$U = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{n_P}], \qquad \mathbf{u} = \text{vec}(U).$$

Rewrite $A\mathbf{u} = \mathrm{f}$ as a **multi-term matrix equation**

$$\boxed{K_0 U G_0 + \sum_{m=1}^{M} K_m U G_m = F.}$$

Key fact: U is often a **low-rank matrix**. Standard Krylov iterative methods like CG do not take advantage of this.

Low Rank Example

Let $D = [0,1] \times [0,1]$ with $a_0 = 1$, $y_m \in [-1,1]$ and

$$a_m(\mathbf{x}) = \gamma_m \cos(2\pi\beta_1 x_1) \cos(2\pi\beta_2 x_2), \qquad \gamma_m = O(m^{-4})$$

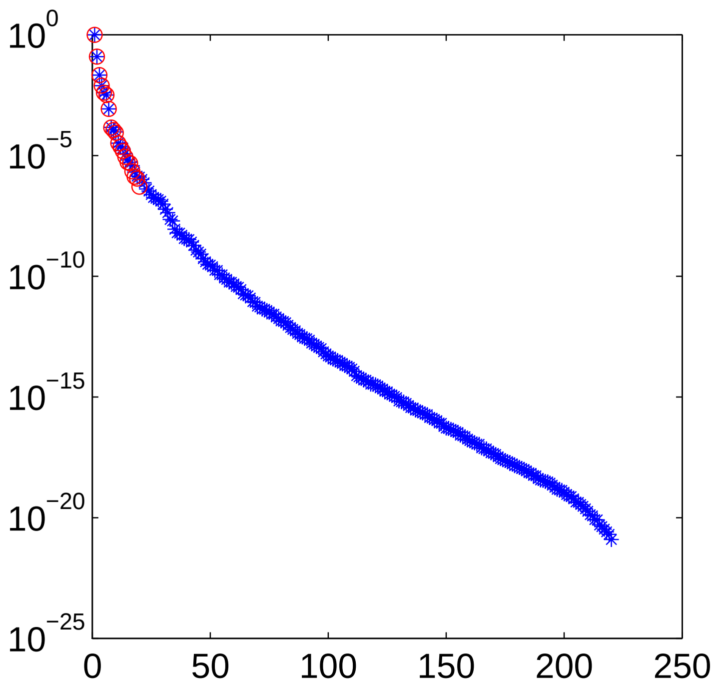
(**fast decay** coefficients).

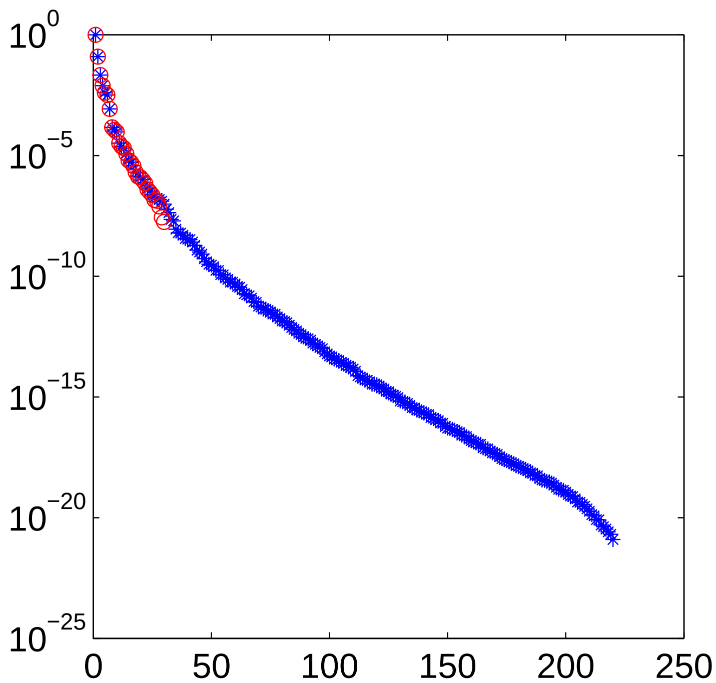
			Tol=10^{-6}	Tol=10^{-7}	Tol=10^{-8}
M	k	n_P	rank	rank	rank
5	3	56	19	24	30
	4	126	23	29	37
9	3	220	21	29	34
	4	715	23	32	41

Approximate ranks of the SGFEM solution matrix U ($n_X = 4,096$).

Singular Values ($n_X = 4,096$, $n_{\mathcal{P}} = 220$)

Singular values of U (blue), and a **reduced solution matrix** (red) of size $n_R \times n_P$ for $n_R = 20$ (left) and $n_R = 30$ (right).





▷

Reformulated Matrix Equation

$$K_0 U G_0 + \sum_{m=1}^{M} K_m U G_m = \mathbf{f}_0 \mathbf{g}_0^\top$$

Reformulated Matrix Equation

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- Using $G_0 = I$ and Cholesky factorisation $K_0 = LL^\top$:

$$X + \sum_{m=1}^{M} \hat{K}_m X G_m = \hat{\mathbf{f}}_0 \mathbf{g}_0^\top$$

where $X := L^\top U$, $\hat{K}_m = L^{-1} K_m L^{-\top}$ **(preconditioning)**.

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- ▷ Introduce **shifts** so FEM matrices are **positive definite**:

$$X \left(I - \sum_{m=1}^{M} \alpha_m G_m \right) + \sum_{m=1}^{M} \left(\hat{K}_m + \alpha_m I \right) X G_m = \hat{\mathbf{f}}_0 \mathbf{g}_0^\top$$

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Reformulated Matrix Equation

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  where $X := L^\top U$, $\hat{K}_m = L^{-1} K_m L^{-\top}$ **(preconditioning)**.

- Introduce **shifts** so FEM matrices are **positive definite**:

$$\boxed{X B_0 + \sum_{m=1}^{M} A_m X B_m = \hat{\mathbf{f}}_0 \mathbf{g}_0^\top}$$

3. Reduced Basis Approximation

Given $\mathcal{K}_R \subset \mathbb{R}^{n_R}$ with $\boxed{n_R \ll n_X}$ and an orthonormal basis

$$V_R = [\mathbf{v}_1, \ldots, \mathbf{v}_{n_R}],$$

$X \approx X_R := V_R Y_R$, where the $\boxed{n_R \times n_P}$ **reduced solution** Y_R satisfies

$$V_R^\top R_R = 0$$

where R_R is the residual.

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where R_R is the residual. Equivalently,

$$\underbrace{\left(V_R^\top V_R\right)}_{n_R \times n_R} Y_R B_0 + \sum_{m=1}^{M} \underbrace{\left(V_R^\top A_m V_R\right)}_{n_R \times n_R} Y_R B_m = \underbrace{\left(V_R^\top \hat{\mathbf{f}}_0^\top\right)}_{n_R \times 1} \mathbf{g}_0.$$

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MultiRB Iterative Method

- ▷ Start with $V_0 = \text{span}\{\mathbf{v}_0\}$

- ▷ For $j = 1, 2, \ldots$ (until convergence)

  - Augment V_{j-1} with at most M new vectors

$$(A_m + s_j I)^{-1} \mathbf{v}_{j-1} \in \mathbb{R}^{n_X}, \qquad m = 1, \ldots, M$$

  - Truncate SVD & orthonormalise to obtain V_j

  - Solve reduced problem to find Y_j

Requires $\boxed{O((n_X + n_P) \cdot M)}$ **memory** rather than $O(n_X \cdot n_P)$

(Motivated by **rational Krylov methods** for Sylvester equations $(M = 1)$).

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Krylov subspaces

Recall, the **standard Krylov space** of dimension k associated with a vector $\mathbf{v}_0$ and matrix A is

$$\mathbb{K}_k(A, \mathbf{v}_0) = \text{span}\left\{\mathbf{v}_0, A\mathbf{v}_0, A^2\mathbf{v}_0, \ldots, A^{k-1}\mathbf{v}_0\right\}.$$

Krylov subspaces

Recall, the **standard Krylov space** of dimension k associated with a vector $\mathbf{v}_0$ and matrix A is

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For Sylvester equations (M=1), we use **rational Krylov spaces**

$$\begin{aligned}\overline{\mathbb{K}}_k(A, \mathbf{v}_0, \mathbf{s}) = \quad & \text{span}\left\{\mathbf{v}_0, (A + s_1 I)^{-1}\mathbf{v}_0, (A + s_2 I)^{-1}(A + s_1 I)^{-1}\mathbf{v}_0,\right. \\ & \left.\ldots\ldots, \Pi_{j=1}^{k}(A + s_j I)^{-1}\mathbf{v}_0 \right\}.\end{aligned}$$

where $\mathbf{s} = (s_1, s_2, \ldots)$ are **parameters**.

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MultiRB Spaces

Suppose $M = 3$. Initialise $V_0 = \text{span}\{\mathbf{v}_0\}$, e.g. $\mathbf{v}_0 = K_0^{-1}\mathbf{f}$.

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Suppose $M = 3$. Initialise $V_0 = \text{span}\{\mathbf{v}_0\}$, e.g. $\mathbf{v}_0 = K_0^{-1}\mathbf{f}$.

▷ Iteration 1

$$V_1 = \text{span}\left\{\mathbf{v}_0, (A_1 + s_1 I)^{-1}\,\mathbf{v}_0, (A_2 + s_1 I)^{-1}\,\mathbf{v}_0, (A_3 + s_1 I)^{-1}\,\mathbf{v}_0\right\}$$

- Truncate (SVD) and orthonormalise
- $V_1 = \text{span}\{\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$

MultiRB Spaces

Suppose $M = 3$. Initialise $V_0 = \text{span}\,\{\mathbf{v}_0\}$, e.g. $\mathbf{v}_0 = K_0^{-1}\mathbf{f}$.

- Iteration 1

  $V_1 = \text{span}\left\{\mathbf{v}_0, (A_1 + s_1 I)^{-1}\,\mathbf{v}_0, (A_2 + s_1 I)^{-1}\,\mathbf{v}_0, (A_3 + s_1 I)^{-1}\,\mathbf{v}_0\right\}$

  - Truncate (SVD) and orthonormalise

  - $V_1 = \text{span}\,\{\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$

- Iteration 2

$$V_2 = \text{span}\,\{\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$$
$$(A_1 + s_2 I)^{-1}\,\mathbf{v}_1, (A_2 + s_2 I)^{-1}\,\mathbf{v}_1, (A_3 + s_2 I)^{-1}\,\mathbf{v}_1\Big\}$$
$$= \text{span}\Big\{\mathbf{v}_0, (A_1 + s_1 I)^{-1}\,\mathbf{v}_0, (A_2 + s_1 I)^{-1}\,\mathbf{v}_0, (A_3 + s_1 I)^{-1}\,\mathbf{v}_0$$
$$(A_1 + s_2 I)^{-1}\,(A_1 + s_1 I)^{-1}\,\mathbf{v}_0, (A_2 + s_2 I)^{-1}\,(A_1 + s_1 I)^{-1}\,\mathbf{v}_0,$$
$$(A_3 + s_2 I)^{-1}\,(A_1 + s_1 I)^{-1}\,\mathbf{v}_0\Big\}$$

Numerical Results: Case 1

Let $D = [0,1]^2$ and $X = \mathbb{Q}_1$ with $\boxed{n_X = 65,025}$. Let $y_m \in [-1,1]$ and

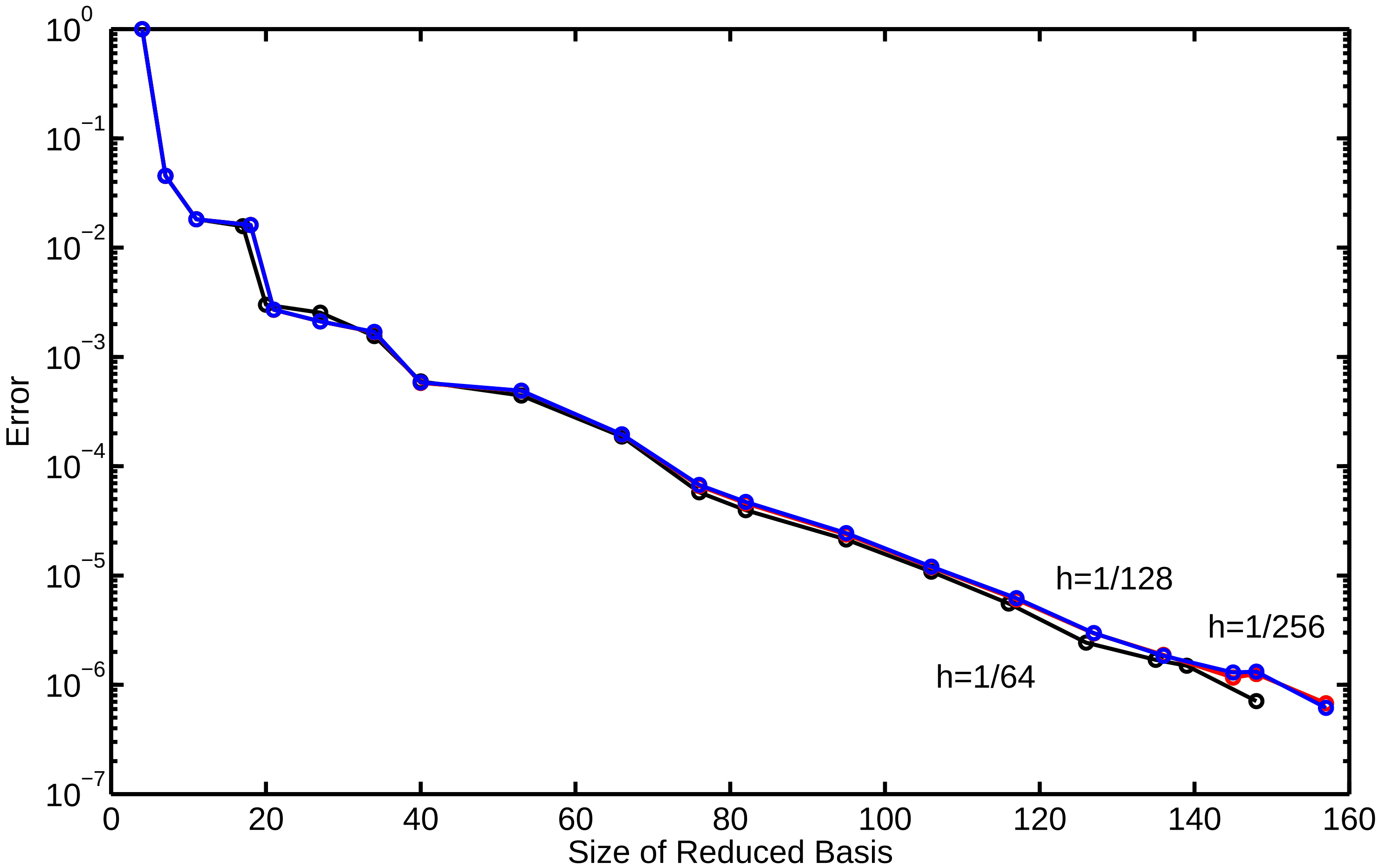
$$a(\boldsymbol{x}, \boldsymbol{y}) = 1 + \sum_{m=1}^{\infty} \gamma_m \cos(2\pi\beta_1 x_1) \cos(2\pi\beta_2 x_2)\, y_m,$$

with $\gamma_m = O(m^{-4})$ **(fast decay)**.

M	k	n_P	$iter$	n_R	time	Standard PCG
5	3	56	19	77	2.65e1	2.17e1 (12)
	4	126	19	77	2.52e1	5.31e1 (14)
	5	252	23	94	3.23e1	1.03e2 (14)
16	3	969	14	106	6.19e1	4.90e2 (12)
	4	4,845	15	117	8.47e1	2.81e3 (14)
	5	$\mathbf{20,349^*}$	15	117	$\mathbf{2.15e2}$	**Out of Memory**

Mesh-independent Convergence

Stop when $\|X_j - X_{j-1}\|_F / \|X_{j-1}\|_F \leq TOL$.



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Numerical Results: Case 2

Choose $D = [-1,1]^2$ and $X = \mathbb{Q}_1$ with $\boxed{n_X = 65{,}025}$ and

$$a(\boldsymbol{x},\boldsymbol{y}) = 1 + \sigma \sum_{m=1}^{20} \sqrt{\lambda_m}\varphi_m(\boldsymbol{x}) y_m, \qquad y_m \in \left[-\sqrt{3}, \sqrt{3}\right],$$

where $\sigma = 0.1$ and (λ_m, φ_m) are eigenpairs associated with

$$C_a(\boldsymbol{x},\boldsymbol{x}') = \sigma^2 \exp\left(-\frac{1}{2}\|\boldsymbol{x}-\boldsymbol{x}'\|_1\right)$$

M	k	n_P	$iter$	n_R	time	Standard PCG
20	2	231	10	171	6.1e1	7.4e1 (6)
	3	1,771	10	171	6.6e1	5.6e2 (6)
	4	**10,629**	10	171	**1.1e2**	**Out of Memory**

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References

▷ An efficient reduced basis solver for stochastic Galerkin matrix equations, **SIAM Journal Sci. Comp., 39(1), (2017).** **[PSS,2017]**

- Valeria Simoncini (Bologna), David Silvester (Manchester)

▷ Other work on SGFEMs (linear algebra + approximation theory) at:

`http://www.maths.manchester.ac.uk/~cp/`

or email me at `c.powell@manchester.ac.uk`.