

Iterative solvers for stochastic Galerkin method

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Outline

- 1 Problems with parametric/uncertain data
- 2 Working with such problems
- 3 Solution methods
- 4 Stochastic Galerkin method (SGM)
- 5 Discretization
- 6 Solution methods for SGM and preconditioning
- 7 Numerical examples
- 8 Our contribution
- 9 Conclusion

Problems with parametric (uncertain) data

As an example,

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

with $u(\mathbf{x}, \boldsymbol{\xi}) = 0$ on $\partial D \times \Gamma$, data $0 < \alpha_1 \leq \mathbf{a}(\mathbf{x}, \boldsymbol{\xi}) \leq \alpha_2 < \infty$.

Parametric data/random field $\mathbf{a}(\mathbf{x}, \boldsymbol{\xi})$

a) Left:

well separated domains
with different characteristics

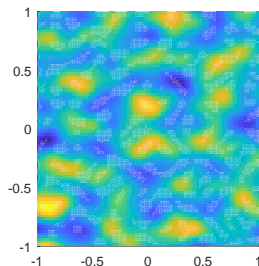
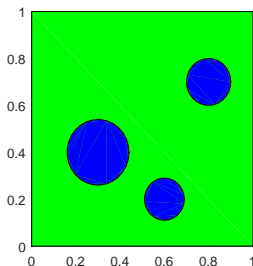
$\mathbf{a}(\mathbf{x}, \boldsymbol{\xi})$

$$= a_0(\mathbf{x}) + \chi_1(\mathbf{x})\xi_1 + \chi_2(\mathbf{x})\xi_2$$

b) Right:

Karhunen-Loève expansion,
truncated

(covariance, eigenvectors)



Karhunen-Loève expansion

Numerical computation needs discrete finite random field $\mathbf{a}(\mathbf{x}, \omega)$.

Covariance operator c ,

$$C(g)(\mathbf{x}) = \int_D c(\mathbf{x}, \mathbf{y})g(\mathbf{y})d\mathbf{y}, \quad c(\mathbf{x}, \mathbf{y}) = \text{cov}(a(\mathbf{x}, \omega), a(\mathbf{y}, \omega))$$

with eigenvalues λ_k and eigenfunctions $a_k(\mathbf{x})$, then

$$\mathbf{a}(\mathbf{x}, \omega) = a_0(\mathbf{x}) + \sum_{k=1}^{\infty} \xi_k(\omega) \sqrt{\lambda_k} a_k(\mathbf{x}),$$

where ξ_k are uncorelated random variables with zero mean and unit variance.

Truncation, check $\mathbf{a}_{\text{trunc}}(\mathbf{x}, \omega) > 0$.

Measure space $L^2_\rho(\Gamma)$

Doob-Dynkin lemma: measure space $L^2_\rho(\Gamma)$, $\rho(\xi) = dP/d\xi$ (instead of (Ω, Σ, P))

$$\mathbf{a}(\mathbf{x}, \omega) := \mathbf{a}(\mathbf{x}, \xi(\omega)), \quad \xi(\omega) = (\xi_1(\omega), \dots, \xi_{N_\xi}(\omega)),$$

where the random variables $\xi_j(\omega)$ are iid with the joint probability density

$$\rho(\xi) = \prod_{i=1}^{N_\xi} \rho_i(\xi_i) \quad \text{and} \quad \Gamma = \prod_{i=1}^{N_\xi} \Gamma_i = \prod_{i=1}^{N_\xi} \text{Im}(\xi_i).$$

Data $a(\mathbf{x}, \boldsymbol{\xi})$

a) linear w.r.t. stochastic part

$$a(\mathbf{x}, \boldsymbol{\xi}) = a_0(\mathbf{x}) + \sum_{i=1}^{N_\xi} a_i(\mathbf{x}) \xi_i, \quad \text{or} \quad a(\mathbf{x}, \boldsymbol{\xi}) = a_0(\mathbf{x}) + \sum_{i=1}^{N_\xi} \chi_i(\mathbf{x}) \xi_i$$

b) non-linear w.r.t. stochastic part

$$a(\mathbf{x}, \boldsymbol{\xi}) = \exp \left(\tilde{a}_0(\mathbf{x}) + \sum_{i=1}^{N_\xi} \tilde{a}_i(\mathbf{x}) \xi_i \right) = \sum_{j=0}^{N_a} a_j(\mathbf{x}) p_j(\boldsymbol{\xi}),$$

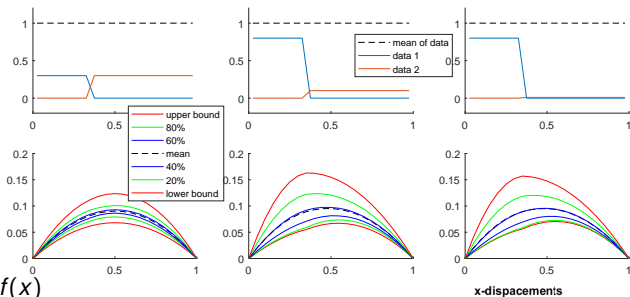
Stochastic variables / parameters $\boldsymbol{\xi} = (\xi_1, \dots, \xi_{N_\xi}) \in \Gamma$

Probability distribution $N(0, 1)$, $U(-1, 1)$, etc.

Probability density / weight function ρ

Where we can meet parametric problems

a) Studying dependency of u on the data



iso-lines

$$-(a(x, \xi)u(x, \xi))' = f(x)$$

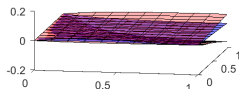
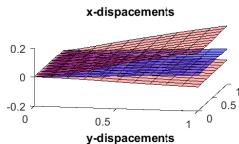
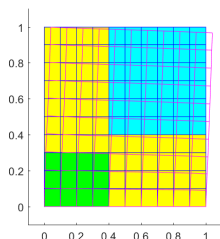
$$\xi = (\xi_1, \xi_2)$$

iso-surfaces

linear elasticity

stiffness in three domains 2 : 3 : 1

$$\xi = (\xi_1, \xi_2, \xi_3)$$



Where we meet parametric problems (cont.)

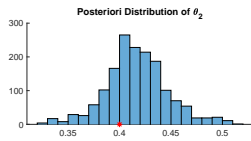
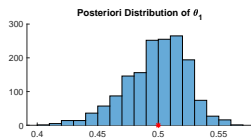
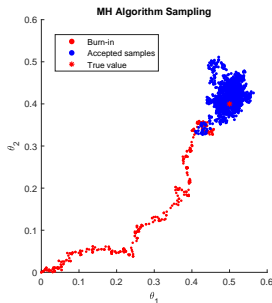
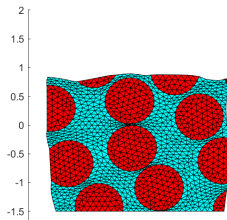
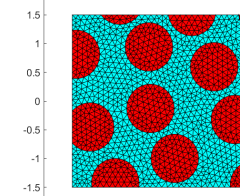
b) Identifying parameters,
inverse problems

linear elasticity

$$\xi = (\xi_1, \xi_2)$$

Bayes methods
Metropolis-Hastings method
surrogate models

(figures by L.Gaynutdinova)



Blaheta, Béréš, Domesová, Pan, A comparison of deterministic and Bayesian inverse with application in micromechanics, *Applications of Mathematics*, 2018

Solution methods for parametric problems

a) Monte Carlo methods

- + nonintrusive, multilevel Monte Carlo methods, universal
- time consuming (unless applied in parallel), generating samples, lack of guaranteed error bounds

b) Collocation methods (w.r.t. stochastic variables)

- + nonintrusive, sparse grids, nested grids (Clenshaw-Curtis quadrature)
- curse of dimensionality, discrete approximation measure, lack of guaranteed error bounds

c) Stochastic Galerkin methods / stochastic finite element methods

- + integral approximation measure, various post-processing of results, guaranteed error bounds
- intrusive (unless using double-orthogonal approximation polynomials), large linear systems, coupled problem, curse of dimensionality

Stochastic Galerkin method / stochastic FE method

As example

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

with $u(\mathbf{x}, \boldsymbol{\xi}) = 0$ on $\partial D \times \Gamma$.

Stochastic variational form. Find $u \in V = H_0^1(D) \times L_\rho^2(\Gamma) = L_\rho^2(\Gamma, H_0^1(D))$ (Bochner space) such that

$$\mathcal{A}(u, v) = \mathcal{F}(v), \quad v \in V.$$

Equality of moments.

Energy inner product and linear functional

$$\begin{aligned} \mathcal{A}(u, v) &= \int_{\Gamma} \int_D \nabla v(\mathbf{x}, \boldsymbol{\xi}) \cdot \mathbf{a}(\mathbf{x}, \boldsymbol{\xi}) \nabla u(\mathbf{x}, \boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\mathbf{x} d\boldsymbol{\xi} \\ \mathcal{F}(v) &= \int_{\Gamma} \int_D f(\mathbf{x}) v(\mathbf{x}, \boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\mathbf{x} d\boldsymbol{\xi}. \end{aligned}$$

Regularity and a priori convergence estimates

Babuska, Nobile, Tempone, Ghanem, Zouraris; Gittelsohn, 2009; Besspalov, Powell, Silvester, 2012

Discretization

$$\text{Solution } u(\mathbf{x}, \boldsymbol{\xi}) = \sum_{r,j=1}^{N_{\text{FE}}, N_{\text{pol}}} u_{(j-1)N_{\text{FE}}+r} \phi_r(\mathbf{x}) \psi_j(\boldsymbol{\xi})$$

Approximation basis functions $\phi_r(\mathbf{x}) \psi_j(\boldsymbol{\xi}) \in V^{\text{FE}} \times V^{\text{pol}} \subset V$

Finite element basis functions $\phi_r(\mathbf{x}) \in V^{\text{FE}} \subset H_0^1(D)$

Orthogonal w.r.t. weight ρ **polynomials** $\psi_j(\boldsymbol{\xi}) = \psi_{j_1}(\xi_1) \cdots \psi_{j_{N_\xi}}(\xi_{N_\xi}) \in V^{\text{pol}} \subset L_\rho^2(\Gamma)$

Polynomials

Hermite pol. $\rho(\xi) = \frac{1}{\sqrt{\pi}} e^{-\xi^2/2}$, **Legendre** pol. $\rho(\xi) = \frac{1}{2} \chi_{(-1,1)}$, etc.

Complete polynomials (total degree $\leq d$) $N_{\text{pol}} = \binom{N_\xi + d}{N_\xi}$

Tensor product (degrees $\leq d_i$ at ξ_i) $N_{\text{pol}} = \prod_{i=1}^{N_\xi} (d_i + 1)$

Matrices

$$\begin{aligned}
 A_{(k-1)N_{FE}+s,(j-1)N_{FE}+r} &= \mathcal{A}(\psi_s \Phi_k, \psi_r \Phi_j) \\
 &= \int_{\Gamma} \int_D \nabla \psi_s \Phi_k \cdot \mathbf{a}(\mathbf{x}, \boldsymbol{\xi}) \nabla \psi_r \Phi_j \rho \, d\mathbf{x} d\boldsymbol{\xi} \\
 &= \int_{\Gamma} \Phi_k \Phi_j \rho \int_D \nabla \psi_s \cdot \mathbf{a}(\mathbf{x}, \boldsymbol{\xi}) \nabla \psi_r \, d\mathbf{x} d\boldsymbol{\xi}
 \end{aligned}$$

depend on data $\mathbf{a}(\mathbf{x}, \boldsymbol{\xi})$; e.g. (slide 5)

$$\begin{aligned}
 A_{(k-1)N_{FE}+s,(j-1)N_{FE}+r} &= \int_{\Gamma} \Phi_k \Phi_j \rho \int_D \sum_{l=0}^{N_a} a_l(\mathbf{x}) \rho_l(\boldsymbol{\xi}) \nabla \psi_s \cdot \nabla \psi_r \, d\mathbf{x} d\boldsymbol{\xi} \\
 &= \sum_{l=0}^{N_a} \int_{\Gamma} \rho_l(\boldsymbol{\xi}) \Phi_k \Phi_j \rho \, d\boldsymbol{\xi} \int_D a_l(\mathbf{x}) \nabla \psi_s \cdot \nabla \psi_r \, d\mathbf{x} \\
 &= \sum_{l=0}^{N_a} (\mathbf{G}_l)_{kj} \cdot (\mathbf{K}_l)_{sr}
 \end{aligned}$$

A is s.p.d. (unless, e.g., Gauss distribution and high degree approximation)

$$\mathbf{b}_{(k-1)N_{FE}+s} = \mathcal{F}(\psi_s \Phi_k) = \int_{\Gamma} \int_D f \psi_s \Phi_k \rho \, d\mathbf{x} d\boldsymbol{\xi}$$

Structures of matrices

Matrix A is not built. Sum of tensor products $A = \sum_{l=0}^{N_\xi} G_l \otimes K_l$

Examples:

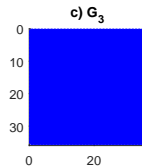
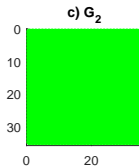
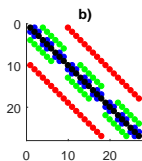
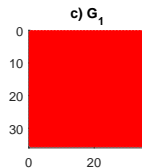
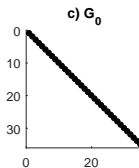
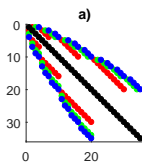
a) $a(\mathbf{x}, \boldsymbol{\xi}) = a_0(\mathbf{x}) + \sum_{i=1}^3 a_i(\mathbf{x}) \xi_i$, complete polynomials, $d = 4$

b) $a(\mathbf{x}, \boldsymbol{\xi}) = a_0(\mathbf{x}) + \sum_{i=1}^3 a_i(\mathbf{x}) \xi_i$, tensor product polynomials, $d_1 = d_2 = d_3 = 2$

c) $a(\mathbf{x}, \boldsymbol{\xi}) = \sum_{l=0}^3 a_l(\mathbf{x}) p_l(\boldsymbol{\xi})$, $N_a = 3$, complete polynomials, $d = 4$

G_0 , G_1 , G_2 , G_3

Every dot is a multiple
of an $N_{FE} \times N_{FE}$
"stiffness matrix" K_l



Structure of matrices

Linear $a(\mathbf{x}, \xi) = a_0(\mathbf{x}) + \xi_1 a_1(\mathbf{x}) + \xi_2 a_2(\mathbf{x})$:

$N_\xi = 2$, uniform distribution of ξ_j , Legendre polynomials, complete pol. $d = 2$

$$A = \begin{pmatrix} K_0 & \frac{1}{\sqrt{3}} K_1 & \frac{1}{\sqrt{3}} K_2 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} K_1 & K_0 & 0 & \frac{2}{\sqrt{15}} K_1 & \frac{1}{\sqrt{3}} K_2 & 0 \\ \frac{1}{\sqrt{3}} K_2 & 0 & K_0 & 0 & \frac{1}{\sqrt{3}} K_1 & \frac{2}{\sqrt{15}} K_2 \\ 0 & \frac{2}{\sqrt{15}} K_1 & 0 & K_0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} K_2 & \frac{1}{\sqrt{3}} K_1 & 0 & K_0 & 0 \\ 0 & 0 & \frac{2}{\sqrt{15}} K_2 & 0 & 0 & K_0 \end{pmatrix},$$

K_0 , K_1 , and K_2 are "stiffness matrices" corresponding to $a_0(\mathbf{x})$, $a_1(\mathbf{x})$, and $a_2(\mathbf{x})$, respectively

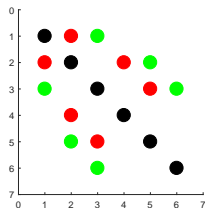
stiffness matrices

$$(K_i)_{rs} = \int_D a_i(\mathbf{x}) \nabla \psi_r(\mathbf{x}) \nabla \psi_s(\mathbf{x}) d\mathbf{x}$$

Jacobi matrices

$$(G_i)_{jk} = \int_\Gamma \xi_i \Phi_j(\xi) \Phi_k(\xi) \rho(\xi) d\xi$$

$$(G_0)_{jk} = \int_\Gamma \Phi_j(\xi) \Phi_k(\xi) \rho(\xi) d\xi = \delta_{jk}$$



Double orthogonal polynomials

p_0, p_1, p_2, \dots (infinite set) orthogonal on $\Gamma \subset \mathbb{R}$

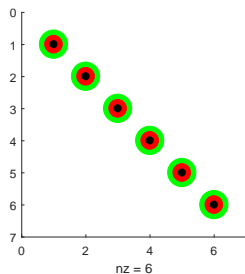
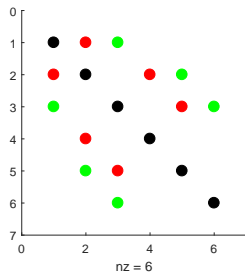
$$\int_{\Gamma} p_j(z) p_k(z) \rho(z) dz = \delta_{jk}$$

$\tilde{p}_1, \tilde{p}_2, \dots, \tilde{p}_m$ (finite set) double-orthogonal on $\Gamma \subset \mathbb{R}$,
Lagrange polynomials with the set of nodes - roots of p_m ,
all of the degree $m-1$

$$\int_{\Gamma} \tilde{p}_j(z) \tilde{p}_k(z) \rho(z) dz = \delta_{jk}$$

$$\int_{\Gamma} z \tilde{p}_j(z) \tilde{p}_k(z) \rho(z) dz = \delta_{jk}$$

A is block diagonal matrix with different blocks.



Solution methods

Conjugate gradient method with preconditioning

Preconditioning of $Au = b$ is getting M such that $M^{-1}Au = M^{-1}b$ is better solvable than $Au = b$, and $Mv = c$ is easy to solve. Also in an abstract form.

Preconditioning

1) Multigrid w.r.t. physical variable

[Brezina, et al., 2014](#), [Elman, Furnival, 2007](#)

2) Multilevel w.r.t. stochastic variable ... focused in this talk

3) Reduced basis, low rank approximations, rational Krylov subspace, etc.

vector $u \rightarrow$ tensorised matrix U , and

$$b = Au = \left(\sum_{i=0}^{N_a} G_i \otimes K_i \right) u \quad \text{is the same as} \quad B = \sum_{i=0}^{N_a} K_i U G_i^T$$

[Matthies et al., 2014](#); [Powell, Silvester, Simoncini, 2016](#); [Powell, Silvester, Simoncini, 2018](#); [Audouze, Nair, 2019](#)

Multilevel preconditioning with respect to stochastic variable

$$\left(A = \sum_{i=0}^{N_a} G_i \otimes K_i \right)$$

Mean based - diagonal blocks - [Powell, Elman, 2009; etc.](#)

$$M^{\text{mean}} = G_0 \otimes K_0$$

Kronecker product preconditioner - [Ullmann, 2010](#)

$$M^{\text{Kron}} = G_0 \otimes K_0 + \sum_{i=1}^{N_a} \beta_i G_i \otimes K_0, \quad \beta_i = \frac{\text{tr}(K_0^T K_i)}{\text{tr}(K_0^T K_0)}$$

Symmetric block Gauss-Seidel - [Bespalov, Loghin, Youngnoi, arXiv 2020](#)

$$M^{\text{SBGS}} = \left(G_0 \otimes K_0 + \sum_{i=1}^{N_a} L_i \otimes K_i \right) (G_0 \otimes K_0)^{-1} \left(G_0 \otimes K_0 + \sum_{i=1}^{N_a} L_i^T \otimes K_i \right), \quad L_i + L_i^T = G_i$$

Two-by-two blocks and Schur complement - [Sousedík, Ghanem, Phips, 2013](#)

Block diagonal preconditioner with large blocks - [P., Kubínová, 2020](#)

Overview - [Crowder, Adaptive and Multilevel Stochastic Galerkin Finite Element Methods, Ph.D. Thesis, 2020](#)

Numerical experiments

1D diffusion equation, $N_{FE} = 20$, complete polynomials, maximum degree d ,
 number of stoch. variables N_{ξ} , ξ_j uniformly distributed in $[-1, 1]$

Table: Mean based, Kronecker and SBGS preconditioning.

N_{ξ}	d	$\kappa(M^{-1}A)$				CG steps			
		no	mean	Kron	SBGS	no	mean	Kron	SBGS
1	1	252.8	2.1	1.6	1.1	39	10	8	5
1	3	317.5	3.1	2.0	1.2	71	13	9	5
1	7	345.4	3.7	2.3	1.2	103	14	10	5
2	1	256.2	2.1	1.6	1.1	56	10	8	5
2	3	335.5	3.9	2.5	1.3	99	14	11	6
2	7	387.9	6.1	3.6	1.5	125	17	13	6
3	1	262.6	2.1	1.6	1.2	60	10	7	5
3	3	372.6	4.2	2.8	1.4	112	14	11	6
3	7	462.6	7.8	5.0	1.8	142	20	15	7

Our contribution

Improving guaranteed spectral bounds for preconditioned matrix $M^{-1}A$ based on

- orthogonal polynomial properties
- data of problems associated to A and M - element-by-element
- for many kinds of distribution of data

[P., 2016](#); [Kubínová, P., 2020](#), [Plešinger, P., 2018](#)

Our approach - connected to and based on classical condition number estimates for algebraic multi-level (AML) preconditioning

[Eijkhout, Vassilevski, Axelsson, Neytcheva, Blaheta, Kraus](#)

Patterns of blocks of M :

$$M^C = \left(\begin{array}{c|c|c} X & & \\ \hline & X & \\ \hline & & X \\ \hline & & & X & \\ & & & & X & \\ & & & & & X \end{array} \right), \quad M^C = \left(\begin{array}{c|c|c} X & X & X \\ \hline X & X & \\ \hline X & & X \\ \hline & & & X & \\ & & & & X & \\ & & & & & X \end{array} \right)$$

Our contribution (cont.)

Patterns of blocks of M:

$$M^{TP} = \left(\begin{array}{ccc|ccc} X & & & & & \\ & X & & & & \\ & & X & & & \\ \hline & & & X & & \\ & & & & X & \\ & & & & & X \\ \hline & & & & & & X & \\ & & & & & & & X & \\ \hline & & & & & & & & X & \\ & & & & & & & & & X \end{array} \right), \quad M^C = \left(\begin{array}{c|cc|ccc} X & & & & & \\ \hline & X & & & & \\ \hline & & & X & & \\ \hline & & & & X & \\ & & & & & X & \\ & & & & & & X & \\ \hline & & & & & & & X & \\ & & & & & & & & X \end{array} \right),$$

$$M^{TP} = \left(\begin{array}{ccc|ccc} X & X & & & & \\ X & X & X & & & \\ & X & X & & & \\ \hline & & & X & X & \\ & & & X & X & X \\ & & & X & X & \\ \hline & & & & & & X & X \\ & & & & & & X & X & X \\ & & & & & & X & X \end{array} \right).$$

$$M^{TP} = \left(\begin{array}{ccc|cc} X & X & & X & \\ X & X & X & & X \\ & X & X & & \\ \hline X & & & X & X & \\ & X & & X & X & X \\ & & X & X & X & \\ \hline & & & & & & X & X \\ & & & & & & X & X & X \\ & & & & & & X & X \end{array} \right), \quad M^C = \left(\begin{array}{c|cc|ccc} X & X & X & & & \\ \hline X & X & & & & \\ X & & X & & & \\ \hline & & & X & & \\ & & & & X & \\ & & & & & X \end{array} \right).$$

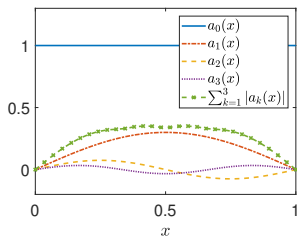
Our contribution (cont.)

Numerical experiment.

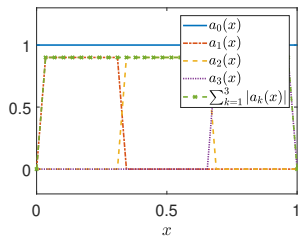
$$-(a(x, \xi)u(x, \xi))' = f(x),$$

$D = (0, 1)$, $N_\xi = 3$, $a(x, \xi) = a_0(x) + \xi_1 a_1(x) + \xi_2 a_2(x) + \xi_3 a_3(x)$,
 $\xi_i \in [-1, 1]$, $i = 1, 2, 3$.

Problem 1:



Problem 2:



Our contribution (cont.)

Table: Block-diagonal preconditioning of Problem 1 and Problem 2. New and classical bounds.

d	$\kappa(A)$	$\underline{c}_{\text{class}}$	\underline{c}	$\lambda_{\min}(M^{-1}A)$	$\lambda_{\max}(M^{-1}A)$	\bar{c}	\bar{c}_{class}	\bar{c}/\underline{c}
Problem 1								
1	458.42	0.76	0.80	0.83	1.17	1.20	1.24	1.51
2	498.47	0.68	0.73	0.76	1.24	1.27	1.32	1.75
...								
6	546.55	0.61	0.67	0.69	1.31	1.33	1.39	2.26
7	550.80	0.61	0.66	0.68	1.32	1.34	1.39	2.29
Problem 2								
1	947.79	-0.65	0.45	0.45	1.56	1.56	2.65	3.43
2	1596.34	-1.21	0.26	0.26	1.74	1.74	3.21	6.57
...								
6	4576.93	-1.71	0.10	0.10	1.90	1.90	3.71	19.34
7	5294.63	-1.74	0.09	0.09	1.91	1.91	3.74	21.80

P., 2015, 2016, 2017; Kubínová, P., 2020

Conclusion

- PDE with (stochastic) parameters - many methods, demanding
- Variational approach - stochastic Galerkin method
Preconditioning – a posteriori error estimates – adaptivity
 A posteriori error estimates
[Bespalov, Powell, Silvester, 2014; Eigel, Merdon, 2014; Khan, Bespalov, Powell, Silvester, 2020](#)
 Adaptivity
[Eigel, Gittelson, Schwab, Zander, 2014; P., 2015; Bespalov, Praetorius, Ruggeri, 2020](#)
- Relatively short history; many recent results; still developing
 Using as much information about A and M as possible
- Spectral estimates of $M^{-1}A$ (matrix pencil) - sharp new bounds based on element-by-element approach
[P., 2016; Kubínová, P., 2017; Plešinger, P., 2018](#)
- Estimates of all eigenvalues of preconditioned matrices
[Gergelits, Mardal, Nielsen and Strakoš, 2019; Gergelits, Nielsen, Strakoš, 2020;](#)
[Ladecký, P., Zeman, 2020; P., Ladecký, submitted](#)
 Our new method described in [Martin Ladecký's talk](#) at SNA 2021.

Thanks for your attention.

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