

# Introduction to the stochastic Galerkin approach for the solution of PDEs with parameters or uncertainties

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Michal Béréš

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Recapitulation of Random variable and Probability measure

Structure of the problem, discretization and suitable problems

System of equations and assembly

Approaches to the solution of the system

- 2D Darcy flow problem

$$\begin{cases} -\operatorname{div}(k(x; \mathbf{Z}) \cdot \nabla u(x; \mathbf{Z})) = f(x; \mathbf{Z}), & \forall x \in \mathcal{D} \\ u(x; \mathbf{Z}) = u_D(x; \mathbf{Z}), & \forall x \in \Gamma_D, \\ \frac{\partial u(x; \mathbf{Z})}{\partial n(x)} = u_N(x; \mathbf{Z}), & \forall x \in \Gamma_N \end{cases}$$

$\mathbf{Z}$  can be understood as  $\mathbf{Z} : \Omega \rightarrow \mathbb{R}^M$  and  $k(x; \mathbf{Z})$ ,  
 $u(x; \mathbf{Z}) : \mathcal{D} \times \mathbb{R}^M \rightarrow \mathbb{R}$

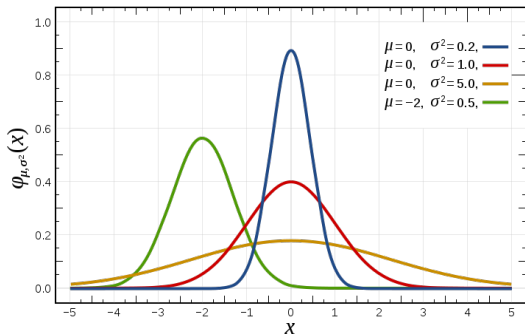
- **non-intrusive** approaches examines only point values of the solution (much easier to deploy)
  - PDE solution in fixed values of the parameter is handled as **black-box** by an existing software
  - Collocation or Monte Carlo methods
- stochastic Galerkin (SG) method is an **intrusive** approach
  - needs new framework for the solution of given problems
  - it provides error estimates

# Recapitulation of Random variable and Probability measure

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- continuous random variable  $Z$  is a map from sample space  $\Omega \rightarrow \mathbb{R}$
- can be described by probability density  $f : \mathbb{R} \rightarrow \mathbb{R}_0^+$ ,  $\int_{\mathbb{R}} f(x) dx = 1$
- distribution of a random variable defines a probability measure
  - in the case of a continuous random variable

$$\int_{\mathbb{R}} \dots dF_Z = \int_{\mathbb{R}} \dots f(x) dx = \mathbb{E}_Z(\dots)$$



- is a vector of  $M$  (let assume continuous) random variables  
 $\mathbf{Z} = (Z_1, \dots, Z_M)$
- can be described by joint probability density  $f_{\mathbf{Z}} : \mathbb{R}^M \rightarrow \mathbb{R}_0^+$ ,  
 $\int_{\mathbb{R}^M} f(x) dx = 1$
- random vector of independent random variables has joint probability density in form

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{i=1}^M f_{Z_i}(z_i)$$

- square integrable functions of a random vector  $\mathbf{Z}$  creates space

$$L^2_{dF\mathbf{Z}}(\mathbb{R}^M) := \left\{ f : \mathbb{R}^M \rightarrow \mathbb{R} : \int_{\mathbb{R}^M} f(\mathbf{z})^2 dF\mathbf{Z} < \infty \right\}$$

- with inner product

$$(u, v) := \int_{\mathbb{R}^M} u(\mathbf{z}) \cdot v(\mathbf{z}) dF\mathbf{Z} = \mathbb{E}_{\mathbf{Z}}(u(\mathbf{Z}) \cdot v(\mathbf{Z}))$$



- **orthogonal polynomial basis of  $L^2_{dFZ}$**
- polynomial chaos with respect to a random variable  $Z$
- set of polynomials of increasing degree  $\psi_i(Z)$  ( $i$  denotes degree of polynomial)
- orthogonal = satisfying  $\mathbb{E}_Z(\psi_i(Z)\psi_j(Z)) = \gamma_i\delta_{ij}$ , where  $\gamma_i = \mathbb{E}_Z(\psi_i(Z)^2)$
- generates basis of  $L^2_{dFZ}(\mathbb{R})$

- assume random vector  $\mathbf{Z}$  of **independent** random variables
- polynomial chaos for  $L^2_{dFZ}(\mathbb{R}^M)$  can be created by a product of 1d polynomials of  $Z_i$

$$\Psi_i(\mathbf{Z}) = \prod_{k=1}^M \psi_{i_k}(Z_k),$$

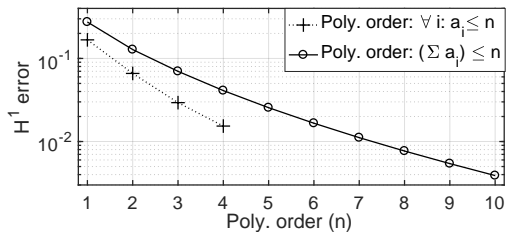
where  $i$  denotes the multi-index of size  $M$ .

**tensor product polynomials** of maximal degree  $n$  are polynomials with

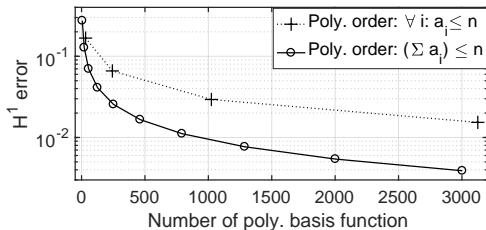
$$i_k \leq n, \forall k = 1, \dots, M$$

**complete polynomials** of maximal degree  $n$  are polynomials with

$$|i| = \sum_{k=1}^M i_k \leq n$$



**Figure 1:** Error dependence on the max. degree of the PC basis



**Figure 2:** Error dependence on the size of the PC basis

Let  $\{\psi_i\}$ ,  $\psi_{-1} = 0$ ,  $\psi_0 = 1$  be polynomials related to probability measure  $dFZ$  (single random variable), then

$$\psi_{i+1}(Z) = (Z - \alpha_i) \psi_i(Z) - \beta_i \psi_{i-1}(Z),$$

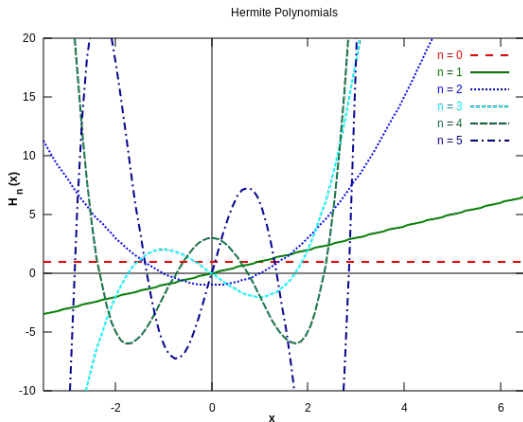
$$\alpha_i = \frac{\mathbb{E}_Z(Z \psi_i(Z) \psi_i(Z))}{\mathbb{E}_Z(\psi_i(Z) \psi_i(Z))}, \beta_i = \frac{\mathbb{E}_Z(\psi_i(Z) \psi_i(Z))}{\mathbb{E}_Z(\psi_{i-1}(Z) \psi_{i-1}(Z))}$$

- evaluation of orthogonal polynomials of higher degree can be numerically unstable
  - do not evaluate weights of the polynomials ( $a_0 + a_1x + \dots$ ), numerically unstable (infeasible for degree 20 and more in int32)
  - recurrence formula for computing the point values of the polynomial is favorable

- polynomial chaos basis for standard normal random variable consist of Hermite polynomials

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$$\psi_{i+1}(Z) = 2Z\psi_i(Z) - i\psi_{i-1}(Z)$$



# Structure of the problem, discretization and suitable problems

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- 2D Darcy flow problem

$$\begin{cases} -\operatorname{div}(k(x; \mathbf{Z}) \cdot \nabla u(x; \mathbf{Z})) = f(x; \mathbf{Z}), & \forall x \in \mathcal{D} \\ u(x; \mathbf{Z}) = u_D(x; \mathbf{Z}), & \forall x \in \Gamma_D, \\ \frac{\partial u(x; \mathbf{Z})}{\partial n(x)} = u_N(x; \mathbf{Z}), & \forall x \in \Gamma_N \end{cases}$$

$\mathbf{Z}$  can be understood as  $\mathbf{Z} : \Omega \rightarrow \mathbb{R}^M$  and  $k(x; \mathbf{Z})$ ,  
 $u(x; \mathbf{Z}) : \mathcal{D} \times \mathbb{R}^M \rightarrow \mathbb{R}$

- randomness in  $f$  and boundary conditions affects the right hand side
  - if  $k$  is deterministic, we obtain decoupled system = matrix of the resulting system of equations is block diagonal
- randomness in material  $k$  affects the matrix of the resulting system of equations
  - we obtain coupled system



- 2D Darcy flow problem

$$\begin{cases} -\operatorname{div}(k(x; \mathbf{Z}) \cdot \nabla u(x; \mathbf{Z})) = f(x), & \forall x \in \mathcal{D} \\ u(x; \mathbf{Z}) = u_D(x), & \forall x \in \Gamma_D, \\ \frac{\partial u(x; \mathbf{Z})}{\partial n(x)} = u_N(x), & \forall x \in \Gamma_N \end{cases}$$

$\mathbf{Z}$  can be understood as  $\mathbf{Z} : \Omega \rightarrow \mathbb{R}^M$  and  $k(x; \mathbf{Z})$ ,  
 $u(x; \mathbf{Z}) : \mathcal{D} \times \mathbb{R}^M \rightarrow \mathbb{R}$

- we can view  $k(x; \mathbf{Z})$ ,  $u(x; \mathbf{Z})$  from the perspective of Monte Carlo sampling
  - sample of  $\mathbf{Z}$  (e.g.  $\tilde{\mathbf{Z}}$ ) gives us a sample of  $k(x; \tilde{\mathbf{Z}}) \in L^\infty(\mathcal{D})$  and  $u(x; \tilde{\mathbf{Z}}) \in H^1(\mathcal{D})$
- then  $u(x; \mathbf{Z}) \in L^2_{dF\mathbf{Z}}(\mathbb{R}^M, H^1(\mathcal{D}))$

$$L^2_{dF\mathbf{Z}}(\mathbb{R}^M, H^1(\mathcal{D})) := \left\{ f : \mathbb{R}^M \rightarrow H^1(\mathcal{D}) : \int_{\mathbb{R}^M} \|f(\mathbf{Z})\|_{H^1(\mathcal{D})}^2 dF\mathbf{Z} < \infty \right\}$$

- $L^2_{dF\mathbf{Z}}(\mathbb{R}^M, H^1(\mathcal{D}))$  is isometrically isomorphic with tensor product space  $H^1(\mathcal{D}) \otimes L^2_{dF\mathbf{Z}}(\mathbb{R}^M)$

- we want to find the solution in the space  $V = V_D \otimes V_S$   
( $V_D = H^1(\mathcal{D})$ ,  $V_S = L^2_{dFZ}(\mathbb{R}^M)$ )
- we need to solve the following

$$\begin{cases} \text{Find } u = \sum_{i=1}^{\infty} u_{D,i} \cdot u_{S,i} \in V_D \otimes V_S, \forall v_D \in V_D, v_S \in V_S : \\ a(u, v) = b(v), v = v_D \cdot v_S \end{cases},$$

$$a(u, v) := a(u_D \cdot u_S, v_D \cdot v_S) = \sum_{r=1}^R a_{D,r}(u_D, v_D) \cdot a_{S,r}(u_S, v_S)$$

$$b(v) := b(v_D \cdot v_S) = \sum_{r=1}^S b_{D,r}(v_D) \cdot b_{S,r}(v_S)$$

$$a(u, v) := \int_{\mathbb{R}^M} \int_{\mathcal{D}} k(x; \mathbf{Z}) \cdot \nabla_x u(x; \mathbf{Z}) \cdot \nabla_x v(x; \mathbf{Z}) \, dx \, dF\mathbf{Z},$$

$$b(v) := \int_{\mathbb{R}^M} \int_{\mathcal{D}} f(x) \cdot v(x; \mathbf{Z}) \, dx \, dF\mathbf{Z},$$

- we use discretization as tensor product of basis functions on domain and basis functions on sample space

$$\langle \varphi_1(x), \dots, \varphi_{N_D}(x) \rangle \otimes \langle \psi_1(\mathbf{Z}), \dots, \psi_{N_P}(\mathbf{Z}) \rangle \subset V_H :$$

$$\langle \varphi_1(x), \dots, \varphi_{N_D}(x) \rangle \subset H_0^1(\mathcal{D}) \text{ and}$$

$$\langle \psi_1(\mathbf{Z}), \dots, \psi_{N_P}(\mathbf{Z}) \rangle \subset L_{dF\mathbf{Z}}^2(\mathbb{R}^M)$$

- As basis functions on physical domain we can take standard finite elements functions (piece-wise linear)
- For basis functions on sample (random parameter) space we choose polynomial chaos basis

- recall the

$$a(u, v) := \int_{\mathbb{R}^M} \int_{\mathcal{D}} k(x; \mathbf{Z}) \cdot \nabla_x u(x; \mathbf{Z}) \cdot \nabla_x v(x; \mathbf{Z}) \, dx \, dF\mathbf{Z}$$

- if we have separable form of the material field

$$k(x; \mathbf{Z}) = \sum_{m=1}^N k_m(x) \cdot g_m(\mathbf{Z})$$

- than resulting system of equation is also separable

$$(\mathbb{A})_{ij,kl} = \sum_{m=1}^N \left( \int_{\mathcal{D}} k_m(x) \nabla \varphi_j(x) \nabla \varphi_l(x) \, dx \right) \cdot \left( \int_{\mathbb{R}^M} g_m(\mathbf{Z}) \psi_i(\mathbf{Z}) \psi_k(\mathbf{Z}) \, dF\mathbf{Z} \right),$$

- it is natural for the Karhunen-Loève decomposition of the random field

$$k(x; \mathbf{Z}) = \sum_{m=1}^M k_i(x) \cdot Z_i$$

or material field with given interfaces

- in other cases it can be obtained by a projection into polynomial chaos

$$k(x; \mathbf{Z}) \approx \sum_{m=1}^N k_i(x) \cdot \Psi_i(\mathbf{Z})$$

# System of equations and assembly

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- After discretization we get following Galerkin system of equations:

$$\mathbb{A} \cdot \bar{u}_H = \bar{b},$$

$$(\mathbb{A})_{ij,kl} = \sum_{m=1}^N \int_{\mathcal{D}} k_m(x) \nabla \varphi_j(x) \nabla \varphi_l(x) dx \cdot \int_{\mathbb{R}^M} g_m(\mathbf{Z}) \psi_i(\mathbf{Z}) \psi_k(\mathbf{Z}) dF\mathbf{Z},$$

$$\mathbb{A} = \sum_{m=1}^N G_m \otimes K_m,$$

$$(K_m)_{ij} = \int_{\mathcal{D}} k_m(x) \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) dx,$$

$$(G_m)_{ij} = \int_{\mathbb{R}^M} g_m(\mathbf{Z}) \psi_i(\mathbf{Z}) \psi_j(\mathbf{Z}) dF\mathbf{Z}.$$



$$\bar{b} = \bar{g} \otimes \bar{f}$$

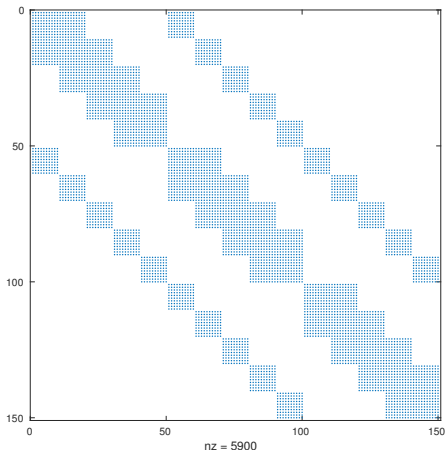
$$(\bar{g})_i = \int_{\mathbb{R}^M} \psi_i(\mathbf{Z}) dF\mathbf{Z}$$

in this case  $\bar{g}$  has only one nonzero value in the first position

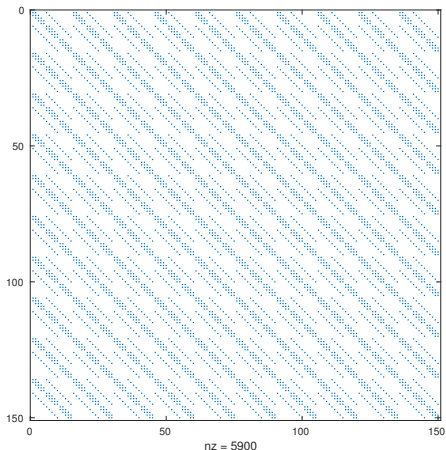
$$(\bar{f})_i = \int_D f(x) \cdot \varphi_i(x) dx$$

- Note: with non-homogeneous boundary conditions the r.h.s will have the general form

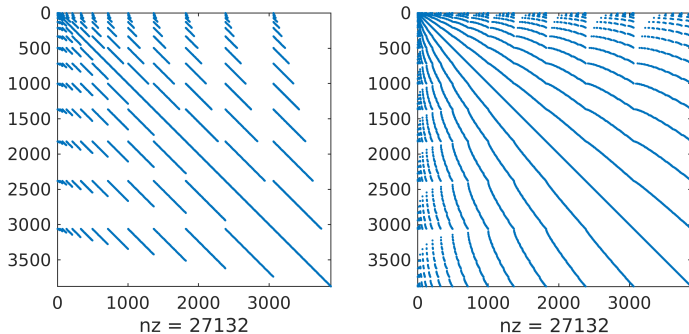
$$\bar{b} = \sum_{i=1}^{NN} \bar{g}_i \otimes \bar{f}_i$$



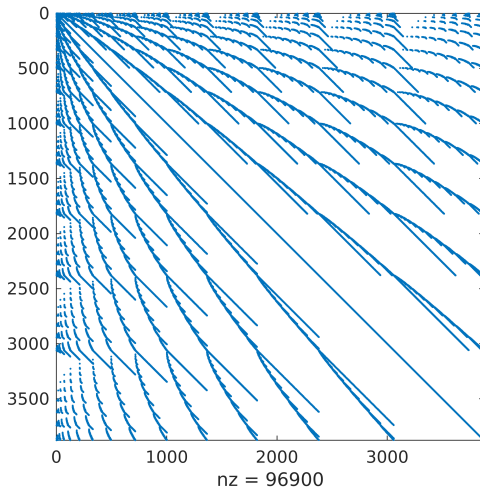
**Figure 3:** Permuted system matrix for physical domain discretization 4x4 and 10 polynomial chaos basis function



**Figure 4:** System matrix for physical domain discretization  $4 \times 4$  and 10 polynomial chaos basis function



**Figure 5:** Sparsity pattern of  $G_i, g_i = \exp(Z_i)$



**Figure 6:** Sparsity pattern of  $\sum_i G_i$

assume normalized Hermite polynomials  $\psi_i(\mathbf{Z}) = \prod_{j=1}^M \psi_{i,j}(Z_j)$

$$(G_m)_{k,l} = \int_{\mathbb{R}^M} \psi_k(\mathbf{Z}) \psi_l(\mathbf{Z}) \exp(a_m Z_m + b_m) dF\mathbf{Z} = \int_{\mathbb{R}} \psi_{k,m}(Z_m) \psi_{l,m}(Z_m) \exp(a_m Z_m + b_m) dFZ_m \prod_{i \neq m} \int_{\mathbb{R}} \psi_{k,i}(Z_i) \psi_{l,i}(Z_i) dFZ_i,$$

where  $\prod_{i \neq m} \int_{\mathbb{R}} \psi_{k,i}(Z_i) \psi_{l,i}(Z_i) dFZ_i$  is either 0 if some of the polynomials  $\psi_{k,i}$  do not equal  $\psi_{l,i}$  or 1 otherwise. The rest of the formula can be evaluated according to the following

$$\int_{\mathbb{R}} f(Z) \exp(aZ + b) dFZ = \int_{\mathbb{R}} f(Z) \exp(aZ + b) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{Z^2}{2}\right) dZ = \exp\left(\frac{a^2}{2} + b\right) \int_{\mathbb{R}} f(Z) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(Z-a)^2}{2}\right) dZ = \exp\left(\frac{a^2}{2} + b\right) \int_{\mathbb{R}} f(Z) dF\tilde{Z},$$

where  $\tilde{Z} \sim \mathcal{N}(a, 1)$ .

$\int_{\mathbb{R}} f(Z) dF\tilde{Z}$  can be precisely computed using the Gauss-Hermite quadrature rule or evaluated analytically (if  $f$  is polynomial), but the analytic formula can be numerically unstable.

$$\mathbb{A} = \sum_{m=1}^N G_m \otimes K_m,$$

Matrix multiplication

$$\mathbb{A}x = \text{vec} \left( \sum_{m=1}^N K_m \tilde{x} G_m^T \right),$$

where  $\tilde{x}$  is reshaped  $x$  into a matrix of corresponding dimensions.

# **Approaches to the solution of the system**

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- Krylov method with a suitable preconditioner with a low-rank compression in each iteration [7, 2, 4, 6]
  - preconditioners: block diagonal [15], Kronecker [18] hierarchical Schur [17]
- Generalized Spectral Decomposition, where the problem is treated as an extended eigenvalue problem and the solution is built using the power-type method [10, 9, 14, 11, 13, 12] (even nonlinear problems)
- low rank tensor approximation (also for multiple independent parameters): approximates the solution using the tensor train or hierarchical Tucker format [5, 1, 3].
- reduced basis (RB) approach - construction of the RB using the rational Krylov approximations [16]; using MC sampling [19], using sampling via sparse grids is presented in [8]

- assume a low rank approximation of the solution

$$\mathbf{x} \approx \mathbf{x}_k = W_k \mathbf{y}_k,$$

where  $W_k = [w_1, \dots, w_k] \in \mathbb{R}^{N_d \times k}$  is a **Reduced basis** of size  $k$  ( $k$  orthonormal vectors)

- here  $W_k$  approximates “deterministic” part of the solution  $\mathbf{x}$  (given by matrices  $K_m$ )
- matrix  $\mathbf{y}_k$  can be obtained using the Galerkin condition on the residual of  $\mathbf{x}_k$

$$R_k := \sum_{m=1}^M K_m (W_k \mathbf{y}_k) G_m^T - \sum_{m=1}^M f_m g_m^T$$

$$W_k^T R_k = 0 \Rightarrow \sum_{m=1}^M W_k^T K_m W_k \mathbf{y}_k G_m^T = \sum_{m=1}^M W_k^T f_m g_m^T$$

which is a system of equations of much lower dimension (can be easily solved by e.g. PCG)

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# Reduced basis solver

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- assume a low rank approximation of the solution

$$\mathbf{x} \approx \mathbf{x}_k = W_k \mathbf{y}_k,$$

where  $W_k = [w_1, \dots, w_k] \in \mathbb{R}^{N_d \times k}$  is a **Reduced basis** of size  $k$  ( $k$  orthonormal vectors)

- here  $W_k$  approximates “deterministic” part of the solution  $\mathbf{x}$  (given by matrices  $K_m$ )
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$$R_k := \sum_{m=1}^M K_m (W_k \mathbf{y}_k) G_m^T - \sum_{m=1}^M f_m g_m^T$$

$$W_k^T R_k = 0 \Rightarrow \sum_{m=1}^M W_k^T K_m W_k \mathbf{y}_k G_m^T = \sum_{m=1}^M W_k^T f_m g_m^T$$

## Reduced rational Krylov subspaces

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- series of symmetric positive definite (SPD) matrices  $\{K_m\}_{m=1,\dots,M}$  and a nonzero vector  $v$
- the first iteration generates addition to the basis:

$$\langle K_1^{-1}v, \dots, K_M^{-1}v \rangle$$

- the second iteration generate addition to the basis:

$$\langle K_1^{-1}K_1^{-1}v, K_1^{-1}K_2^{-1}v, \dots, K_M^{-1}K_{M-1}^{-1}v, K_M^{-1}K_M^{-1}v \rangle$$

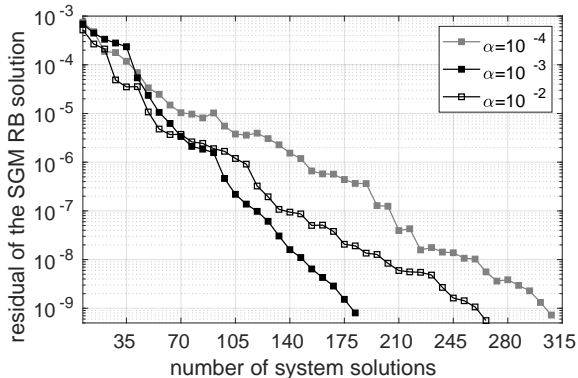
- starting vector from  $\hat{f}_m = K_0^{-1} f_m$
- using matrices  $\{K_0^{-1} (K_m + \alpha_m K_0)\}$
- full RRKS scheme is impractical because in each subsequent iteration we need to construct larger bases
- the remedy to this is to iteratively select a vector  $v$  from the current basis and expand the basis only by the first iteration of the RRKS
- during the orthogonalisation step, calculate weights corresponding to the norm of independent part of the vector
  - next direction according to the calculated weights



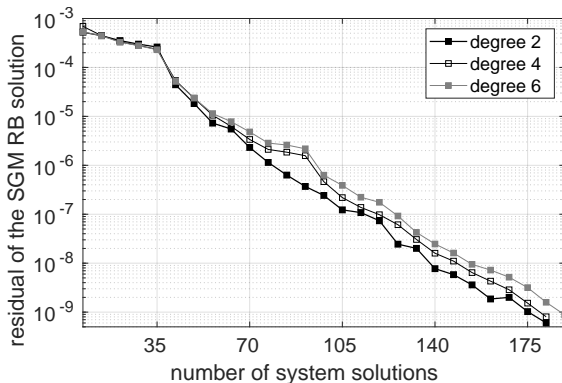
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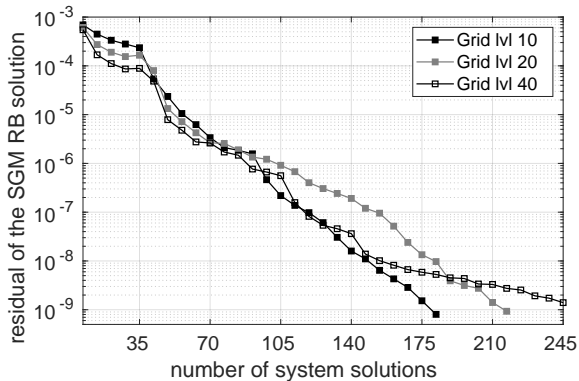


**Figure 1:** different values of  $\alpha$  (degree 4, grid level 10)



**Figure 2:** different maximal degree of polynomial chaos (grid lvl 10)





**Figure 3:** different grid levels (polynomial degree 4)

# Monte Carlo sampling

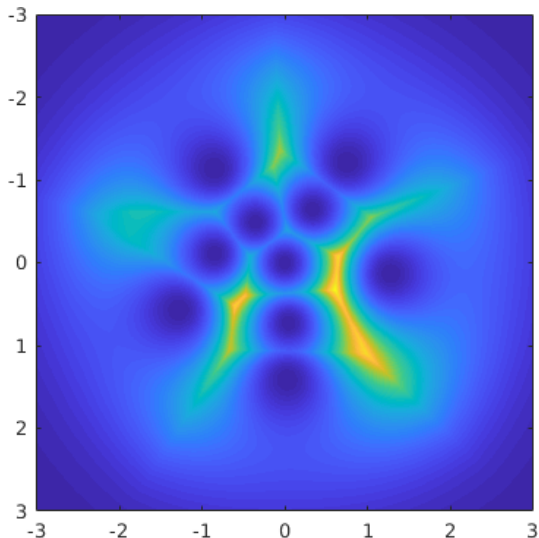
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We compare two random sampling procedures

- Crude MC
- Sampling using random process, which avoids already generated samples (MCMC)
  - assume sampling according to unscaled probability density  $f(x)$
  - each consecutive sample  $X_i$  is generated according to unscaled probability density

$$\bar{f}(x) = f(x) \cdot \min_{j=1 \dots i-1} \left\{ 1 - \exp \left( -\frac{1}{2} (x - X_j)^T \cdot \Sigma^{-1} \cdot (x - X_j) \right) \right\}$$

- these samples are generated using Metropolis Hastings method (we can take random sample of the chain, or the one with the highest value of  $\bar{f}(x)$ )



**Figure 4:** Unscaled probability density after 10 samples ( $\Sigma = 10 \cdot I$ )

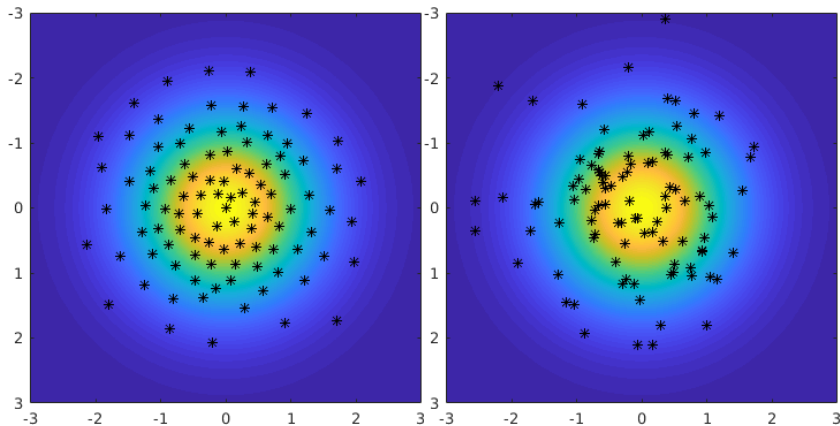
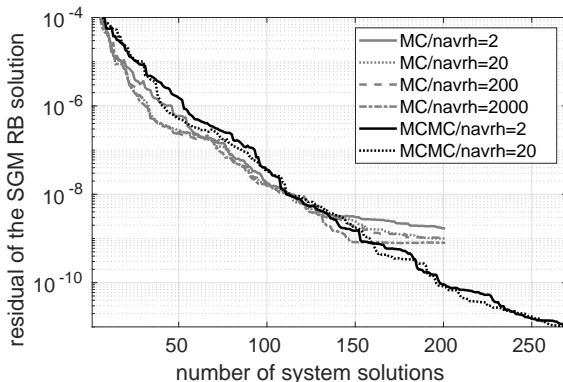


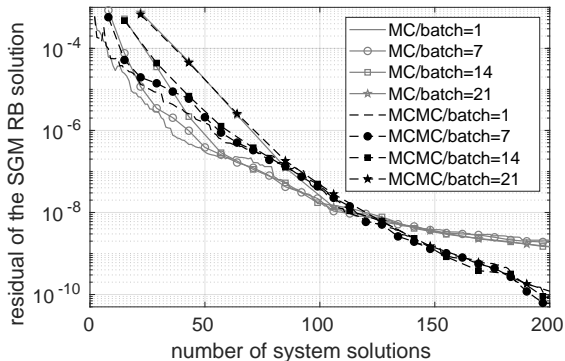
Figure 5: left MCMC, right MC

Loop until satisfactory reduced basis is obtained:

1. Propose  $n$  samples (MC or MCMC)
2. Calculate residual of reduced solution in this samples
3. Solve systems, using best  $N$  samples (largest residual error)
4. Add these  $N$  samples into the reduced basis (truncate if needed)

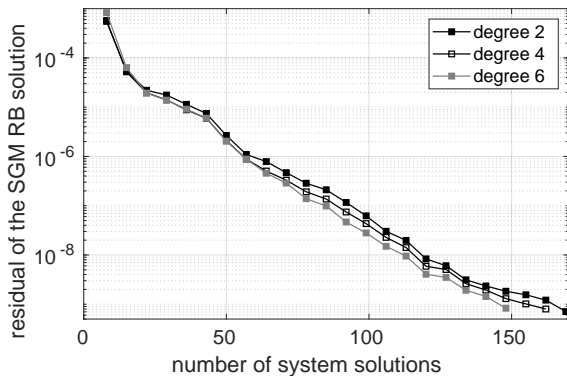


**Figure 6:** different number of proposal samples  $n$

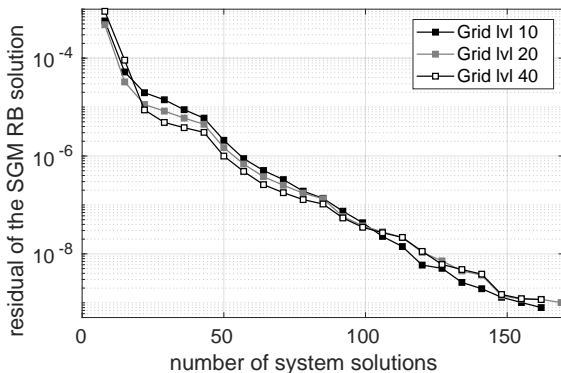


**Figure 7:** different number of parallel solutions  $N$

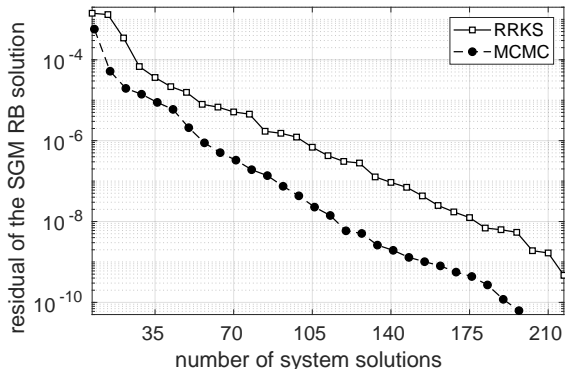




**Figure 8:** different maximal degree of polynomial chaos (grid lvl 10)



**Figure 9:** different grid levels (polynomial degree 4)



**Figure 10:** grid lvl 10, polynomial chaos degree 4

MCMC:

- better convergence (same rate, but shifted)
- easier to implement (it is possible to call black box solvers)
- random (different runs can differ)

RRKS:

- it solves the same systems (much cheaper assembly of systems and preconditioners)
- depends on the choice of  $\alpha$  (can be difficult)

## Deflated conjugate gradients

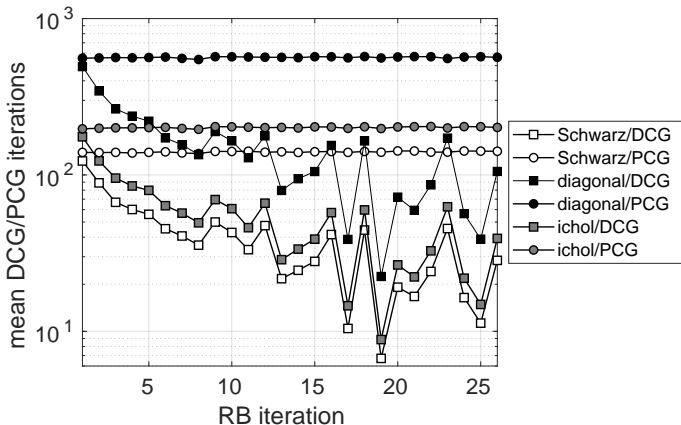
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- DCG method is an extension of the standard conjugate gradient (CG or PCG if using a preconditioner) method
- DCG method takes an additional parameter in the form of the deflation basis  $W$  (linearly independent, we will use orthonormal).
- the deflation basis  $W$  should be able to describe the sought solution reasonably well
- the DCG method looks for the solution outside of the deflation basis  $W$

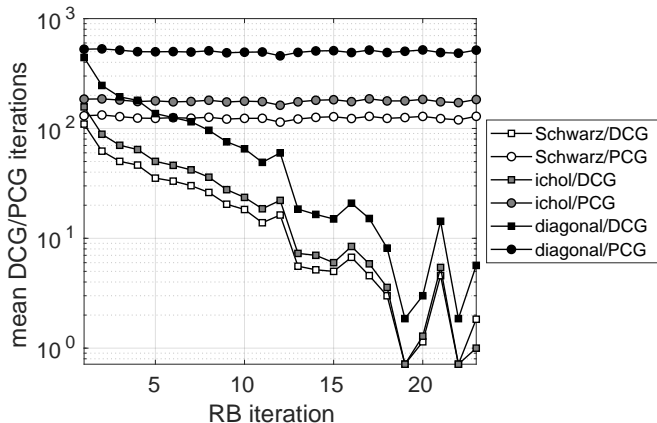
- DCG difference in comparison to the conjugate gradient implementation:
  - the residual of the initial guess should be orthogonal on  $W$  (e.g. by using  $x_0 = W (W^T A W)^{-1} W^T b$ )
  - in each iteration the DCG projects the preconditioned residual  $\tilde{z}_i = P z_i$  using the projector  $P = I - W (W^T A W)^{-1} W^T A$
- in our case the reduced basis  $W_i$  in  $i$ -th iteration of RB solver can be directly used as the deflation basis
- only significant additional cost compared to the standard CG method is the solution of systems with  $Q_i = W_i^T A W_i$  (in  $i$ -th iteration of the RB solver)
  - In our application, the size of the matrix  $Q_i$  (corresponding to a size of the RB) is reasonably small and we can use e.g. an explicit inversion.

- we test the solution of systems  $(K_m + \alpha K_0)$  using: Schwarz, diagonal and ichol preconditioner
  - the Schwarz preconditioner was set using 30 subdomains = equal column slices of our square domain of the size  $1/20$
  - the incomplete Cholesky preconditioner was build with no filling allowed





**Figure 11:** Num. of the DCG iterations compared to the PCG (mean DCG/PCG iterations per RB iter.)



**Figure 12:** Num. of the DCG iterations compared to the PCG (mean DCG/PCG iterations per RB iter.)

	Ad. Schwarz	diagonal	ichol (nofill)
RRKS savings in %	72.32%	73.47%	73.33%
MCMC savings in %	82.58%	83.48%	83.06%

**Table 1:** Computational savings using DCG with the RB as a deflation basis