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REDUCED BASIS SOLVER FOR STOCHASTIC GALERKIN FORMULATION OF DARCY FLOW WITH UNCERTAIN MATERIAL PARAMETERS

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Abstract: In this contribution, we present a solution to the stochastic Galerkin (SG) matrix equations coming from the Darcy flow problem with uncertain material coefficients in the separable form. The SG system of equations is kept in the compressed tensor form and its solution is a very challenging task. Here, we present the reduced basis (RB) method as a solver which looks for a low-rank representation of the solution. The construction of the RB consists of iterative expanding of the basis using Monte Carlo sampling. We discuss the setting of the sampling procedure and an efficient solution of multiple similar systems emerging during the sampling procedure using deflation. We conclude with a demonstration of the use of SG solution for forward uncertainty quantification.

Keywords: stochastic Galerkin method, reduced basis method, Monte Carlo method, deflated conjugate gradient method

MSC: 65C05, 65M60, 65M70

1. Introduction

This contribution briefly outlines the solution of stationary Darcy flow problem with uncertain hydraulic conductivity. The solution is obtained using the stochastic Galerkin (GM) method. A significant part of the contribution is the demonstration of the usage of SG solution for forward uncertainty quantification.

The work presented here is a continuation of author's results presented in [1].

2. Stochastic Galerkin method

We start with the problem setting. Let us assume a physical domain $\mathcal{D}$ and random vector $\boldsymbol{Z}$ (on sample space Ω) consisting of M independent standard normal

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random variables. We assume the hydraulic conductivity field as a function of both points in domain $\mathcal{D}$ and random vector $\boldsymbol{Z}$, more specifically in the form

$$k\left(x,\boldsymbol{Z}\right)=\sum_{m=1}^{M}\underbrace{\chi_{\mathcal{D}_m}\left(x\right)}_{k_m^D(x)}\underbrace{\exp\left(\sigma_m Z_m+\mu_m\right)}_{k_m^S(\boldsymbol{Z})}=\sum_{m=1}^{M}k_m^D\left(x\right)k_m^S\left(\boldsymbol{Z}\right).$$

I.e. piecewise constant function with the value of constant on each of M subdomains $\mathcal{D}_m$ governed by m-th element of random vector $\boldsymbol{Z}$. The model problem (steady Darcy flow) than takes the form

$$\begin{cases}-\mathrm{div}_x\left(k\left(x,\boldsymbol{Z}\right)\nabla_x u\left(x,\boldsymbol{Z}\right)\right)=f\left(x\right) & \forall x\in\mathcal{D},\boldsymbol{Z}\in\mathbb{R}^M,\\ u\left(x,\boldsymbol{Z}\right)=u_0\left(x\right) & \forall x\in\Gamma_D,\boldsymbol{Z}\in\mathbb{R}^M,\\ -k\left(x,\boldsymbol{Z}\right)\frac{\partial u(x,\boldsymbol{Z})}{\partial n(x)}=g\left(x\right) & \forall x\in\Gamma_N,\boldsymbol{Z}\in\mathbb{R}^M.\end{cases}$$

For testing purposes, we choose the decomposition into subdomains via thresholding of the Gaussian random field realisation, see Figure 1.

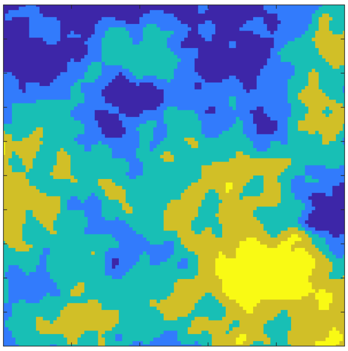

Figure 1: Illustration of decomposition into subdomains

2.1. Stochastic Galerkin matrix equations

The weak form of the problem takes the form

$$\begin{aligned}a\left(u_H,v\right)=&b\left(v\right),\ \forall v\in L^2\left(\Omega,H^1_{0,\Gamma_D}\left(\mathcal{D}\right)\right),\\ a\left(u_H,v\right)=&\int_{\mathbb{R}^M}\int_{\mathcal{D}}k\left(x,\boldsymbol{Z}\right)\nabla_x u_H\left(x,\boldsymbol{Z}\right)\cdot\nabla_x v\left(x,\boldsymbol{Z}\right)\,\mathrm{d}x\,\mathrm{d}F\boldsymbol{Z},\\ b\left(v\right)=&\int_{\mathbb{R}^M}\int_{\mathcal{D}}f\left(x\right)v\left(x,\boldsymbol{Z}\right)\,\mathrm{d}x\,\mathrm{d}F\boldsymbol{Z}-\int_{\mathbb{R}^M}\int_{\Gamma_N}g\left(x\right)v\left(x,\boldsymbol{Z}\right)\,\mathrm{d}x\,\mathrm{d}F\boldsymbol{Z}\\ &-\int_{\mathbb{R}^M}\int_{\mathcal{D}}k\left(x,\boldsymbol{Z}\right)\nabla_x u_0\left(x\right)\cdot\nabla_x v\left(x,\boldsymbol{Z}\right)\,\mathrm{d}x\,\mathrm{d}F\boldsymbol{Z}.\end{aligned}$$

The homogeneous part of the solution u_H lies in $L^2\left(\Omega, H^1_{0,\Gamma_D}(\mathcal{D})\right)$ which is isometrically isomorphic with $H^1_{0,\Gamma_D}(\mathcal{D}) \otimes L^2(\Omega)$. We choose the test space with the same tensor structure, i.e. $V_{h,K} := V_h \otimes V_K$, where the discretization of $H^1_{0,\Gamma_D}(\mathcal{D})$ are finite elements and the discretization of $L^2(\Omega)$ are polynomials

$$V_h = \{\varphi_1(x), \dots, \varphi_{N_D}(x)\} \subset H^1_{0,\Gamma_D}(\mathcal{D}), \quad V_K = \{\psi_1(\omega), \dots, \psi_{N_S}(\omega)\} \subset L^2(\Omega).$$

The dimension of $V_{h,K}$ is $N_D N_S$ with the basis

$$\xi_{i,j}(x,\omega) = \varphi_i(x)\psi_j(\omega) \quad \forall\, i = 1, \dots, N_D,\ j = 1, \dots, N_S.$$

Separable form of input data together with the tensor form of $V_{h,K}$ allow us to assemble the matrix in a compressed form. The resulting system of equations takes the form

$$\mathbb{A}\overline{u} = \overline{b}, \quad \mathbb{A} = \sum_{m=1}^{M} G_m \otimes K_m, \overline{b} = \sum_{m=1}^{M_b} \overline{g}_m \otimes \overline{k}_m,$$
$$(K_m)_{il} = \int_{\mathcal{D}} k^D_m(x)\nabla\varphi_i(x) \cdot \nabla\varphi_l(x)\,\mathrm{d}x,$$
$$(G_m)_{jn} = \int_{\mathbb{R}^M} k^S_m(\boldsymbol{Z})\psi_j(\boldsymbol{Z})\psi_n(\boldsymbol{Z})\,\mathrm{d}F\boldsymbol{Z}.$$

We simplify the right hand side as a sum over M_b ($M_b = M + 2$, M terms for Dirichlet boundary and one for forcing term and Neumann boundary) terms with vectors $\overline{g}_m$, $\overline{k}_m$, whose can be assembled in a similar way as G_m, K_m.

The system can be viewed as matrix equations, assuming reshaping $\overline{u}$ into $N_D \times N_S$ matrix $\boldsymbol{u}$

$$\sum_{m=1}^{M} K_m \boldsymbol{u} G^T_m = \sum_{m=1}^{M_b} \overline{k}_m \overline{g}^T_m. \tag{1}$$

3. Solving the stochastic Galerkin matrix equations

The solution of SG matrix equations (1) is quite a difficult task. We will solve it using conjugate gradients with Kronecker preconditioner (see [5]). With the full system, this could be prohibitively expensive ($N_D N_S$ dofs). Therefore, we reduce the test space via the reduced basis method.

3.1. Reduced basis method

The reduced basis (RB) method aims at reducing the number of basis functions while keeping the same approximating properties. In the SG method, it makes sense to create the reduced basis W of V_h as it is the larger part of the basis and we have the tools to create a meaningful subspace of it. The resulting SG test space will take the form of $V_{h,K} \approx W \otimes V_K$, where W is the reduced basis of V_h.

The reduced basis should fulfill all the conditions needed for the discretized system to be well-posed (e.g. discrete inf-sup condition). In the case of our elliptic problem, we can pick any linearly independent reduced basis W and we obtain a valid system

$$\sum_{m=1}^{M} W^T K_m W \boldsymbol{y} G_m^T = \sum_{m=1}^{M_b} W^T \overline{k}_m \overline{g}_m^T, \quad \boldsymbol{u} \approx \tilde{\boldsymbol{u}} = W \boldsymbol{y}.$$

Approximation error of reduced basis W in the context of SG system can be expressed via residual with respect to the original system

$$R = \sum_{m=1}^{M} K_m W \boldsymbol{y} G_m^T - \sum_{m=1}^{M_b} \overline{k}_m \overline{g}_m^T. \tag{2}$$

The most difficult task is to build the reduced basis itself. We do this via Monte Carlo method.

3.2. Construction of the reduced basis via Monte Carlo sampling

The Monte Carlo (MC) approach to the reduced basis construction is based on iterative refinement of the reduced basis. We denote by W_l a reduced basis at iteration l with $W_0 = \emptyset$. The iterative construction can be summarized in the following steps:

1. draw N_{MC} samples $Z_1, \dots, Z_{N_{MC}}$ of random vector $\boldsymbol{Z}$
2. for every sample Z_j assemble and solve the reduced system of deterministic counterpart
$$W_l^T A_j W_l \widetilde{u}_j = W_l^T b_j$$
3. compute indicators for a sample selection based on the probability density function (pdf) of $\boldsymbol{Z}$ and the residual of reduced solutions $\widetilde{u}_j$
$$f_{\boldsymbol{Z}}(\boldsymbol{Z}_j) \left\| A_j W_l \widetilde{u}_j - b_j \right\|^2$$
4. select P (for simplicity, we use $P = 1$) highest values of identificators and compute solutions at corresponding samples Z_j
$$A_j u_j = b_j$$
5. use the collected solutions to expand the reduced basis W_l and check if the expanded reduced basis is good enough (e.g. with residual (2))

Computation of the reduced solutions and their residuals at samples $\boldsymbol{Z}_j$ is quite costly. We would like to avoid samples around those already contributing to the reduced basis, as they will not bring enough of “new information”. We propose avoiding already generated samples using sampling (changing Step 1) from a changed pdf (using Metropolis-Hastings algorithm)

$$\tilde{f}_l(\boldsymbol{Z}) \propto f(\boldsymbol{Z}) \min_{i=1,\dots,l} w_i(\boldsymbol{Z}), \;\; w_i(\boldsymbol{Z}) = 1 - \exp\left(- \|\boldsymbol{Z} - X_i\|^2_{\Sigma^{-1}} /2\right).$$

We choose the parameter Σ same as the covariance matrix of $\boldsymbol{Z}$. Illustration of altered pdf and comparison of generated samples can be seen in Figure 2. The benefits of this alternative sampling have diminishing returns when M increases, this can be seen in Figure 3.

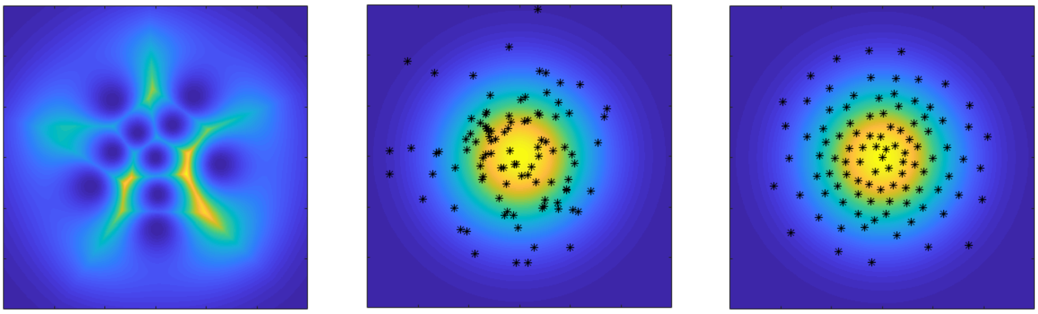

Figure 2: Illustration of altered pdf (left), crude MC samples (middle), samples using altered pdf (right)

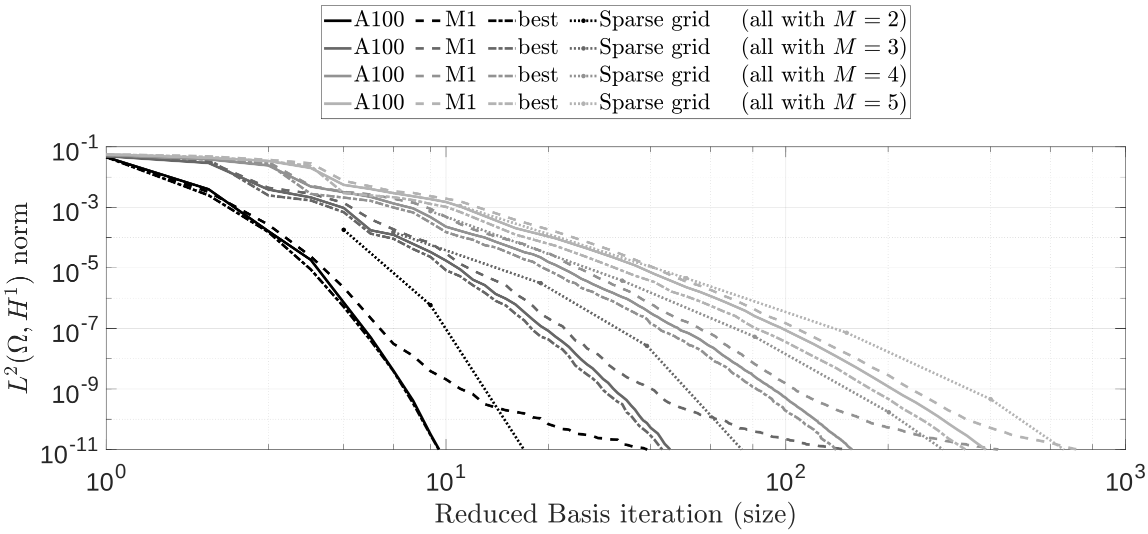

Figure 3: Efficiency of reduced basis construction using different N_{MC}, crude sampling and sampling using altered pdf, and comparison with optimal RB and sparse grid

In Figure 3, we demonstrate the efficiency of the MC approach to the construction of RB on a series of problems with an increasing number of subdomains/number of random variables and $\mu_m = 0, \sigma_m = 0.3$. We compare two variants: $M1$ - crude MC sampling with $N_{MC} = 1$ and $A100$ - sampling using altered pdf and $N_{MC} = 100$. We add a comparison with the optimal ("best") case of RB constructed from the singular value decomposition of the computed full solution and point selection using Smolyak nested sparse grids (see [3]). We measure the quality of RB in the terms of "true" $L^2(\Omega, H^1(\mathcal{D}))$ error of the resulting SG solution compared to pathwise deterministic solution on the same finite element grid. The "true" error is approximated using 1000 MC samples.

3.3. Deflated conjugate gradients

During the construction of RB, we encounter a solution of many similar systems. We propose the use of deflated conjugate gradients (DCG) [4] with the current iteration of reduced basis W_l as a deflation space to speed up the solution. The main part of the deflation is to project preconditioned residual using the projector $P = I - W_l \left(W_l^T A_j W_l\right)^{-1} W_l^T A_j$. This is fairly cheap as the reduced basis W_l has only a small number of columns.

We show the reduction of the number of iterations when using deflation on a problem with 5 subdomains and $\mu_m = 0, \sigma_m = 0.3$ using target precision of the reduced basis 10^{-6} and precision for the solution of deterministic problems 10^{-9}. We test three very different preconditioners (additive Schwarz, incomplete Cholesky factorization with no filling allowed, and diagonal) to demonstrate that the benefit of the use of DCG is independent of used preconditioner. The comparison of the number of iterations with and without the use of deflation can be seen in Figure 4. The total number of saved iterations is over 80% for all tested preconditioners, i.e. the solution of the series of problems is approximately 5x cheaper.

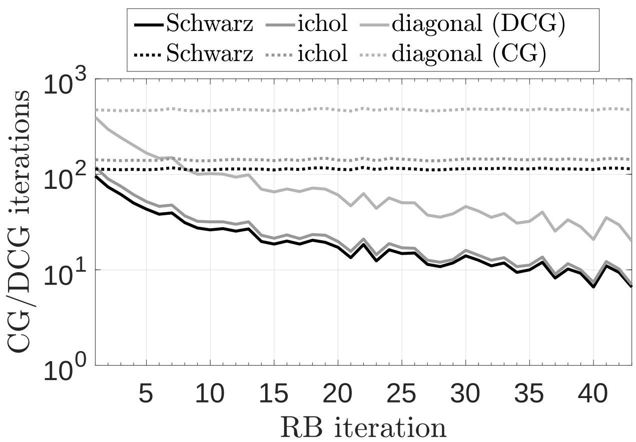

Figure 4: Comparison of number of iterations needed to solve the deterministic problems

4. Use of SG solution - TSX experiment

The main benefit of the SG solution is the result in form of a polynomial surrogate, i.e. an easy and cheap to evaluate approximation of the original problem. We can use this to perform extensive forward uncertainty quantification. We demonstrate this on a simplified tunnel sealing experiment (TSX) [2] modelled as stationary Darcy flow. We will be interested in the stochastic behaviour of pressure in different parts of the domain.

The problem domain is $\mathcal{D} = (0, 100) \times (0, 100) \setminus E$ (E is the ellipse with center $[50, 50]$ and height 2×1.75 and width 2×2.1875). The behaviour of pressure in the tunnel follows

$$\begin{cases} -\mathrm{div}_x \left(\left(\sum_{i=1}^{3} 1_{\mathcal{D}_i}(x) \, 10^{Z_i} \right) \nabla_x u(x, \boldsymbol{Z}) \right) = 0 & \forall\, x \in \mathcal{D}, \boldsymbol{Z} \in \mathbb{R}^3, \\ u(x, \boldsymbol{Z}) = 3 \cdot 10^6 & \forall\, x \in \Gamma_1, \boldsymbol{Z} \in \mathbb{R}^3, \\ u(x, \boldsymbol{Z}) = 0 & \forall\, x \in \Gamma_2, \boldsymbol{Z} \in \mathbb{R}^3, \end{cases}$$

where $Z_1 \sim \mathcal{N}\left(-16, \frac{1}{3}\right)$, $Z_2 \sim \mathcal{N}\left(-18, \frac{1}{3}\right)$, $Z_3 \sim \mathcal{N}\left(-21, \frac{1}{3}\right)$, Γ_1 is the outer boundary of the rectangle, Γ_2 is boundary of cut-out ellipse, and $\mathcal{D}_i$ (1-yellow, 2−teal, 3−blue) are marked in Figure 5.

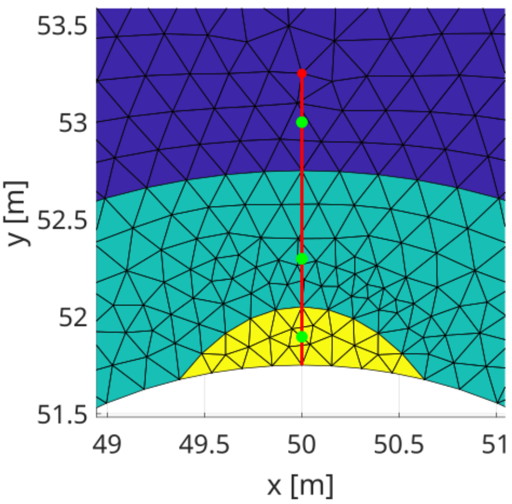

Figure 5: Problem geometry

4.1. Results of forward uncertainty quantification

In Figure 5, we can see a marked red line. We are mainly interested in the behaviour of pressure on this line. Figure 6 shows the comparison of the solution at mean values with the mean value of the stochastic results supplemented by 25%, 50% and 75% quantiles. Note the great difference between the solution at mean values and the mean value of the stochastic solution. The distribution of the pressure at each point on the selected line can be found in Figure 7. Finally, we include

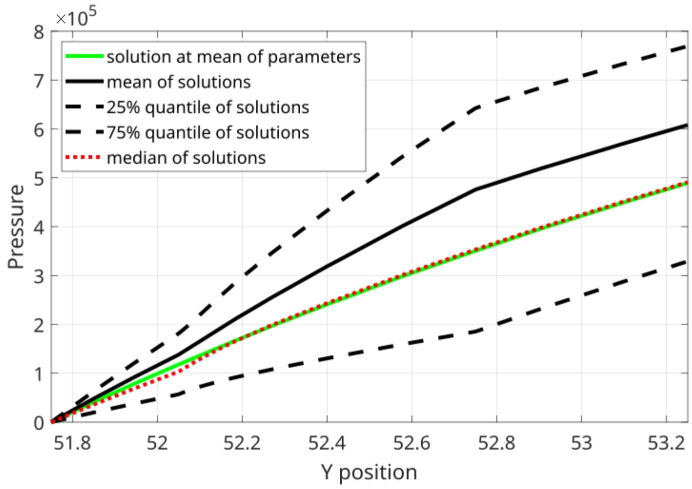

Figure 6: Behaviour on vertical line

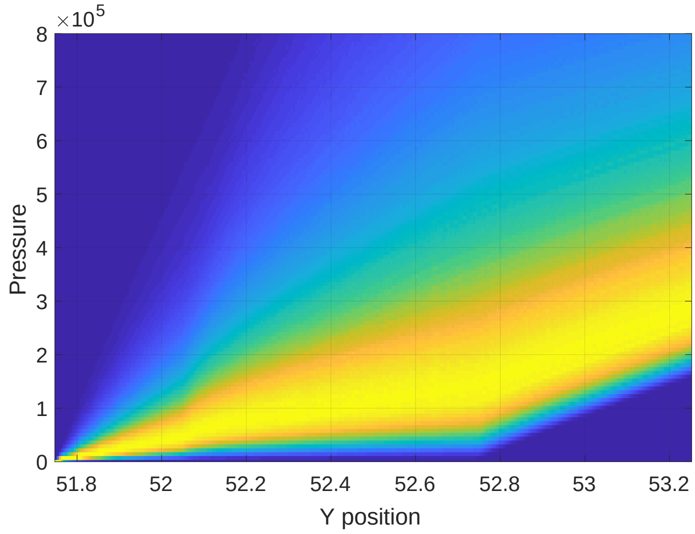

Figure 7: Behaviour on vertical line - distribution at each point

2-dimensional distributions of $\log_{10}$ of pressure for pairs of three selected points (black dots in Figure 8/green dots in Figure 5), see Figure 9. We choose to present $\log_{10}$ of pressures as the two dimensional distributions of pressures were very hard to read.

4.2. Overview of results

The presented results are mainly academic as we used a fairly simplified model. But we can draw some general conclusions. First, the behaviour of the mean value of the stochastic result can be wildly different from the result at the mean values of parameters. The medians are also different, but only slightly in our model. Second, it is very important to choose positions of "real-life" measurements carefully as we can easily pick measurements with overlapping information (as is clearly visible in Figure 8).

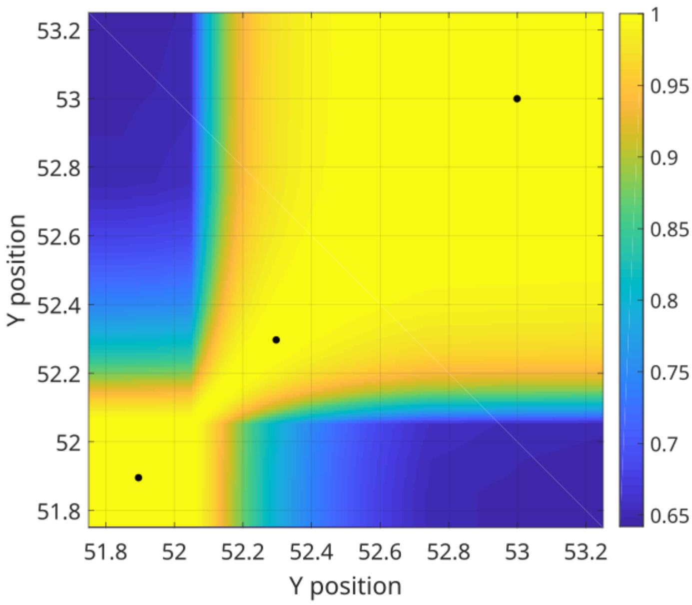

Figure 8: Behaviour on vertical line - correlation between points

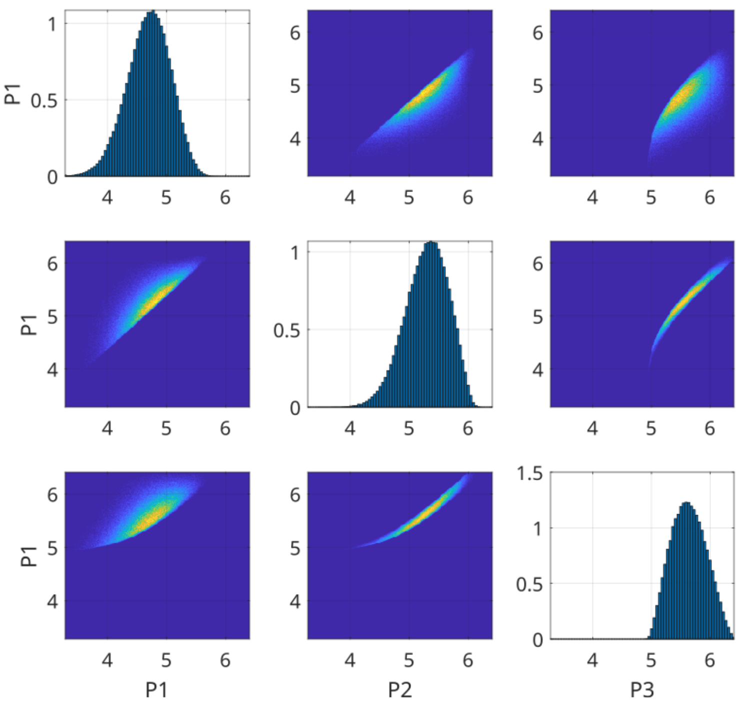

Figure 9: 2-dimensional distributions of $\log_{10}$ of pressure for pairs of selected points

5. Conclusions

The stochastic Galerkin method can be used to create a very precise polynomial surrogate model. Its main drawback is the need for the solution of a very large system of linear equations. In this contribution, we focus on reducing the SG system of equations using the reduced basis method. We present a sampling approach to the construction of the reduced basis, which is demonstrated to be very efficient. Moreover, we demonstrate that the series of similar deterministic systems, we need to solve during the reduced basis construction, can be solved almost five times cheaper using the deflated conjugate gradients. In Section 4, we showed a sample of the SG solution usage for forward uncertainty quantification. This type of analysis can be helpful in e.g. design of experiments.

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References

[1] Béreš, M.: A comparison of approaches for the construction of reduced basis for stochastic Galerkin matrix equations. Appl. Math. **65** (2020), 191–225.

[2] Chandler, N., A., Cournut, A., and Dixon, D.: The five year report of the Tunnel Sealing Experiment: an international project of AECL, JNC, ANDRA and WIPP. Tech. rep., 2002.

[3] Petras, K.: Smolyak cubature of given polynomial degree with few nodes for increasing dimension. Numer. Math. **93** (2003), 729–753.

[4] Saad, Y., Yeung, M., Erhel, J., and Guyomarc'h, F.: A deflated version of the conjugate gradient algorithm. SIAM J. Sci. Comput. **21** (2000), 1909–1926.

[5] Ullmann, E.: A Kronecker product preconditioner for stochastic Galerkin finite element discretizations. SIAM J. Sci. Comput. **32** (2010), 923–946.