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Mario Ohlberger, Kathrin Smetana

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A NEW HIERARCHICAL MODEL REDUCTION-REDUCED BASIS TECHNIQUE FOR ADVECTION-DIFFUSION-REACTION PROBLEMS

MARIO OHLBERGER* AND KATHRIN SMETANA*

*Institute for Computational and Applied Mathematics (ICAM)

University of Muenster

Einsteinstrasse 62, 48149 Muenster, Germany

e-mail: mario.ohlberger@uni-muenster.de, www.math.uni-muenster.de/u/ohlberger

e-mail: kathrin.smetana@uni-muenster.de, www.math.uni-muenster.de/u/smetana

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Abstract. We extend previous work on the Hierarchical Model Reduction-Reduced Basis (HMR-RB) approach to an advection-diffusion-reaction problem. In comparison to the Boussinesq approach we do not neglect the dependency on the vertical direction but enhance the solution for the horizontal direction with appropriately chosen basis functions living on the vertical one. This is done by a combination of the frameworks of hierarchical model reduction [4] and the reduced basis methods [3]. We derive a new a posteriori error estimate and demonstrate in numerical experiments that few basis functions suffice to get good approximations.

1 INTRODUCTION

Many phenomena in fluid dynamics, as for example groundwater, river, and blood flow, have dominant spatial directions along which the essential dynamics occur. Along the other, transverse direction the velocity of the fluid varies often only slightly. Hence in the Boussinesq approach the velocity of the fluid is assumed to be constant in this direction and the dimension of the model is reduced by at least one full dimension. However there are many situations, e.g. a bridge pier in the river or a strong rainfall event in the context of groundwater flow, where this assumption is not true. So, the idea is to reduce the model not by a full dimension but rather step by step. This can be done by the Hierarchical Model Reduction (HMR) approach, which was introduced by Vogelius and Babuška in [5] and generalized by Perotto, Ern, and Veneziani in [4]. Here the solution p of an elliptic problem is approximated by $p_m(x, y) = \sum_{k=1}^m \bar{p}_k(x) \phi_k(y)$, where the $\{\phi_k(y)\}_k$ are orthonormal basis functions, living on the transverse direction. Of course the central question is how to choose the functions $\{\phi_k(y)\}_k$. In [4] sine functions are a priori chosen. The idea of the HMR-RB approach, introduced in [2], is to choose the basis

functions a posteriori, adapted to the problem at hand. Therefore a parameter dependent 1D problem is derived from the original one, where the variable x and the behavior of the solution in x direction are considered as parameters. To find the optimal parameters, we adapt methods common in the framework of the reduced basis (RB) method [3], having been developed to tackle parameter dependent problems efficiently.

The contribution of this work is the extension of the HMR-RB approach to advection-diffusion-reaction problems and the presentation of a new a posteriori error estimator. In the next section we briefly recall the HMR approach. Afterwards we describe the HMR-RB approach consisting of the derivation of the parameter dependent 1D problem and the presentation of the algorithm adapt-HMR-POD for the construction of the basis functions. In section 4 we derive a new efficient and reliable a posteriori error estimator. Then we present numerical examples and finally close with concluding remarks. But first we would like to specify the problem we deal with.

We consider an advection-diffusion-reaction problem. Let $\Omega \subset \mathbb{R}^2$ be the computational domain with Lipschitz boundary $\partial\Omega$ and outer normal n . Let $\Sigma_R, \Sigma_D \subset \partial\Omega$ be two relatively open, pairwise disjoint one-dimensional Lipschitz manifolds, such that $\partial\Omega = \Sigma_R \cup \Sigma_D$. Here Σ_R is the Robin and Σ_D is the Dirichlet boundary. We assume for the sake of simplicity $|\Sigma_D| > 0$ and homogeneous Dirichlet boundary conditions. See [2] for the treatment of nonhomogeneous Dirichlet boundary conditions. So, we consider the following problem for p

$$\begin{aligned} -\nabla \cdot (k \nabla p - \mathbf{b} p) + dp &= f && \text{in } \Omega, \\ p &= 0 && \text{on } \Sigma_D, \\ -(k \nabla p - \mathbf{b} p) \cdot n &= g_R(p) && \text{on } \Sigma_R. \end{aligned} \quad (1)$$

To guarantee well-posedness of the problem we assume $k \in L^\infty(\Omega)$ with $0 < c_1 \leq k \leq c_2$ for constants $c_1, c_2 \in \mathbb{R}^+$, $\mathbf{b} \in [H^{1,\infty}(\Omega)]^2$, $d \in L^\infty(\Omega)$, $f \in L^2(\Omega)$ and $d + 1/2 \nabla \cdot \mathbf{b} \geq 0$ and $\mathbf{b} \cdot n \leq 0$ on Σ_R . The Robin boundary conditions are assumed to be affine in p by

$$g_R(p) = g_{R,1} p - g_{R,2}$$

where $g_{R,1} \in L^\infty(\Sigma_R)$ and $g_{R,2} \in L^2(\Sigma_R)$. Let furthermore be $V = \{v \in H^{1,2}(\Omega) \mid v = 0 \text{ on } \Sigma_D\}$. Then we define for $v, w \in V$ the bilinear form

$$a(w, v) := \int_{\Omega} k \nabla w \nabla v - \int_{\Omega} \mathbf{b} w \nabla v + \int_{\Omega} d w v + \int_{\Sigma_R} g_{R,1} w v \quad (2)$$

and the linear functional

$$f(v) := \int_{\Omega} f v + \int_{\Sigma_R} g_{R,2} v. \quad (3)$$

So, the corresponding weak formulation of (1) is: Find $p \in V$ so that there holds

$$a(p, v) = f(v) \quad \forall v \in V. \quad (4)$$

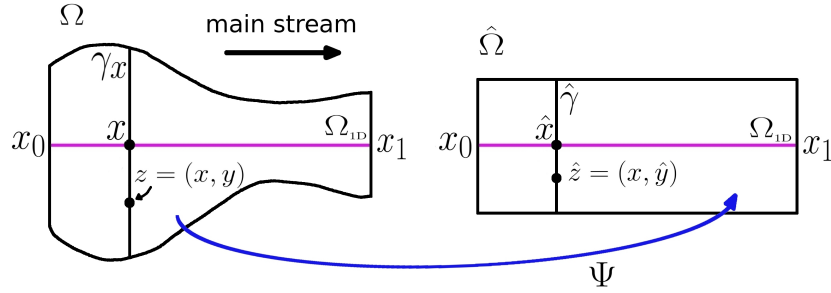


Figure 1: The mapping $\Psi : \Omega \rightarrow \hat{\Omega}$, [4]

2 THE HIERARCHICAL MODEL REDUCTION APPROACH

We use the hierarchical model reduction framework introduced by Perotto, Ern, and Veneziani [4], which is briefly described in this section — cf. [2, 4] for details. Let us assume that Ω can be described as a two-dimensional fiber bundle

$$\Omega = \bigcup_{x \in \Omega_{1D}} \{x\} \times \gamma_x,$$

with Ω_{1D} being the dominant direction and γ_x the transverse fiber associated with $x \in \Omega_{1D}$. For the sake of simplicity, we suppose $\Omega_{1D} =]x_0, x_1[$. For any $x \in \Omega_{1D}$ we define the mapping

$$\psi_x : \gamma_x \rightarrow \hat{\gamma}$$

between the fiber γ_x and a reference fiber $\hat{\gamma}$ with $\hat{\gamma} =]y_0, y_1[$. Then a point $z = (x, y) \in \Omega$ is mapped on $\hat{z} = (x, \hat{y}) \in \hat{\Omega}$ via the mapping $\Psi : \Omega \rightarrow \hat{\Omega}$ with $\hat{y} = \psi_x(y)$ for $y \in \gamma_x$ as shown in Fig. 1. We assume that ψ_x is a C^1 -diffeomorphism, that the mapping Ψ is differentiable relative to z and that $0 \in \gamma_x$ for all x . Finally we introduce the notations

$$\mathcal{D}_1(z) = \partial_x \psi_x, \quad \text{and} \quad \mathcal{D}_2(z) = \partial_y \psi_x.$$

Now we carry this splitting of the space over to a splitting of the functions. Therefore we initially define the two spaces

$$V_{1D} := \{v \in H^{1,2}(\Omega_{1D}) \mid v = 0 \text{ on } \Sigma_{D,side}\} \quad \text{and} \quad V_{\hat{\gamma}} := \{v \in H^{1,2}(\hat{\gamma}) \mid v = 0 \text{ on } \Sigma_{D,top}\}.$$

Then we introduce a set of basis functions $\{\phi_k\}_{k \in \mathbb{N}} \in V_{\hat{\gamma}}$, which are orthonormal with respect to the $L^2(\hat{\gamma})$ -inner product. Combining them with V_{1D} defines the reduced space

$$V_m = \left\{ v_m(x, y) = \sum_{k=1}^m \bar{v}_k(x) \phi_k(\psi_x(y)), \text{ with } \bar{v}_k(x) \in V_{1D}, x \in \Omega_{1D}, y \in \gamma_x \right\}, \quad (5)$$

where $m \in \mathbb{N}$ is the model order. Our reduced problem reads: Find $p_m \in V_m$ so that for all $v_m \in V_m$ there holds

$$\int_{\Omega} k \nabla p_m \nabla v_m - \int_{\Omega} \mathbf{b} p_m \nabla v_m + \int_{\Omega} d p_m v_m + \int_{\Sigma_R} g_{R,1} p_m v_m = \int_{\Omega} f v_m + \int_{\Sigma_R} g_{R,2} v_m.$$

We can rewrite p_m as $p_m(x, y) = \sum_{l=1}^m \bar{p}_l(x) \phi_l(\psi_x(y))$. The test functions $v_k(x, y)$ are chosen as $v_k(x, y) = v(x) \phi_k(\psi_x(y))$, $k = 1, \dots, m$, with $v(x)$ being an arbitrary function in V_{1D} . Transforming Ω to $\hat{\Omega}$ via Ψ we get the following problem (cf. [2, 4] for detailed computations): Find $\bar{p}_l(x) \in V_{1D}$ for $l = 1, \dots, m$ so that for all $v(x) \in V_{1D}$ and $\phi_k(\hat{y})$ with $k = 1, \dots, m$ there holds

$$\begin{aligned} \sum_{l=1}^m \int_{\Omega_{1D}} A_{lk}(x) \frac{d\bar{p}_l(x)}{dx} \frac{dv(x)}{dx} + B_{1,lk}(x) \frac{d\bar{p}_l(x)}{dx} v(x) + B_{2,lk}(x) \bar{p}_l(x) \frac{dv(x)}{dx} + D_{lk}(x) \bar{p}_l(x) v(x) dx \\ + G_{lk}(x_0) p_l(x_0) v(x_0) = \int_{\Omega_{1D}} F_k(x) v(x) + G_k(x_0), \end{aligned}$$

with

$$\begin{aligned} A_{lk}(x) &= \int_{\hat{\gamma}} k(x, \psi_x^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k(\hat{y}) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| d\hat{y}, \\ B_{1,lk}(x) &= \int_{\hat{\gamma}} k(x, \psi_x^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k'(\hat{y}) \mathcal{D}_1(x, \psi_x^{-1}(\hat{y})) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| d\hat{y}, \\ B_{2,lk}(x) &= \int_{\hat{\gamma}} \left[k(x, \psi_x^{-1}(\hat{y})) \phi_l'(\hat{y}) \phi_k(\hat{y}) \mathcal{D}_1(x, \psi_x^{-1}(\hat{y})) \right. \\ &\quad \left. - b_1(x, \psi_x^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k(\hat{y}) \right] |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| d\hat{y}, \\ D_{lk}(x) &= \int_{\hat{\gamma}} \left[k(x, \psi_x^{-1}(\hat{y})) \phi_l'(\hat{y}) \phi_k'(\hat{y}) \left\{ [\mathcal{D}_1(x, \psi_x^{-1}(\hat{y}))]^2 + [\mathcal{D}_2(x, \psi_x^{-1}(\hat{y}))]^2 \right\} \right. \\ &\quad \left. - \mathbf{b}(x, \psi_x^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k'(\hat{y}) \cdot \begin{pmatrix} \mathcal{D}_1(x, \psi_x^{-1}(\hat{y})) \\ \mathcal{D}_2(x, \psi_x^{-1}(\hat{y})) \end{pmatrix} \right. \\ &\quad \left. + d(x, \psi_x^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k(\hat{y}) \right] |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| d\hat{y} \\ &\quad + g_{R,1}(x, \psi_x^{-1}(y_0)) \phi_l(y_0) \phi_k(y_0) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(y_0))|, \\ G_{lk}(x_0) &= \int_{\hat{\gamma}} g_{R,1}(x_0, \psi_{x_0}^{-1}(\hat{y})) \phi_l(\hat{y}) \phi_k(\hat{y}) |\mathcal{D}_2^{-1}(x_0, \psi_{x_0}^{-1}(\hat{y}))| d\hat{y}, \\ F_k(x) &= \int_{\hat{\gamma}} \left[f(x, \psi_x^{-1}(\hat{y})) \phi_k(\hat{y}) \right] |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| d\hat{y} \\ &\quad + g_{R,2}(x, \psi_x^{-1}(y_0)) \phi_k(y_0) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(y_0))|, \\ G_k(x_0) &= \int_{\hat{\gamma}} g_{R,2}(x_0, \psi_{x_0}^{-1}(\hat{y})) \phi_k(\hat{y}) |\mathcal{D}_2^{-1}(x_0, \psi_{x_0}^{-1}(\hat{y}))| d\hat{y}. \end{aligned}$$

For the numerical computation of $p_m(x, y)$ we introduce a partition \mathcal{T}_H on Ω_{1D} with elements $\mathcal{T}_i = (x_{i-1}, x_i)$ of width $H_i = x_i - x_{i-1}$ and maximal step size $H := \max_{\mathcal{T}_i} H_i$ and a suitable conforming Finite Element space $V_{1D}^H \subset V_{1D}$, such that $\dim(V_{1D}^H) = N_H < \infty$. Then the discrete reduced space V_m^H can then be defined as

$$V_m^H = \left\{ v_m^H(x, y) = \sum_{k=1}^m \bar{v}_k^H(x) \phi_k(\psi_x(y)), \text{ with } \bar{v}_k^H(x) \in V_{1D}^H, x \in \Omega_{1D}, y \in \gamma_x \right\}.$$

Let $\varphi_{xi}(x)$, $1 \leq i \leq N_H$ be a basis of V_{1D}^H . Then the solution p_m^H of our discrete reduced problem can be written as $p_m^H(x, y) = \sum_{l=1}^m \left(\sum_{i=1}^{N_H} \bar{p}_l^i \varphi_{xi}(x) \right) \phi_l(\psi_x(y))$ and the discrete reduced problem reads: Find $p_m^H \in V_m^H$ so that for all v_m^H there holds

$$\int_{\Omega} k \nabla p_m^H \nabla v_m^H - \int_{\Omega} \mathbf{b} p_m^H \nabla v_m^H + \int_{\Omega} d p_m^H v_m^H + \int_{\Sigma_R} g_{R,1} p_m^H v_m^H = \int_{\Omega} f v_m^H + \int_{\Sigma_R} g_{R,2} v_m^H. \quad (6)$$

After all the question remains, how the basis functions $\{\phi_k\}_{k \in \mathbb{N}}$ can be chosen. An option are a priori chosen functions [4] as sine functions or Legendre polynomials or functions being adjusted to the original problem, as it is done in the next section.

3 THE HMR-RB APPROACH

The central idea of the HMR-RB approach is to use basis functions adapted to the problem at hand. A 1D problem is derived from the original problem by considering the variable x and the behavior of the solution in x direction as parameters. In order to find the optimal basis functions, techniques common in the framework of reduced basis methods are combined to derive the adapt-HMR-POD algorithm. In this section we firstly derive the 1D problem for the advection-diffusion-reaction problem and after this briefly outline the adapt-HMR-POD algorithm, being described in [2] in detail.

3.1 Formulation of a parameter dependent 1D problem

To realize the dimensional splitting we use test functions v of the form $v(\hat{x}, \hat{y}) = q(\hat{x}) \cdot \bar{v}(\hat{y})$, where the mapping Ψ is included in the test function. That is why we solve our original problem (4) in the space $\tilde{X}_1 = \{\tilde{v}_1(\hat{x}, \hat{y}) = \bar{v}(\hat{y}) \cdot e_1(\hat{x}), \bar{v}(\hat{y}) \in V_{\hat{\gamma}}, \hat{x} \in \Omega_{1D}, \hat{y} \in \hat{\gamma}\}$, leading to a reduced problem for $\tilde{p}_1(x, y)$. Rewriting $\tilde{p}_1(\Psi^{-1}(\hat{z})) = \bar{p}(\hat{y}) \cdot e_1(\hat{x})$ yields the reduced problem: Find $\bar{p}(\hat{y}) \in V_{\hat{\gamma}}$ so that for all $\bar{v}(\hat{y}) \in V_{\hat{\gamma}}$ there holds

$$\begin{aligned} & \int_{\hat{\gamma}} A(\hat{y}) \partial_{\hat{y}} \bar{p}(\hat{y}) \partial_{\hat{y}} \bar{v}(\hat{y}) + B_1(\hat{y}) \partial_{\hat{y}} \bar{p}(\hat{y}) \bar{v}(\hat{y}) + B_2(\hat{y}) \bar{p}(\hat{y}) \partial_{\hat{y}} \bar{v}(\hat{y}) + D(\hat{y}) \bar{p}(\hat{y}) \bar{v}(\hat{y}) d\hat{y} \\ & + G_1(y_0) \bar{p}(y_0) \bar{v}(y_0) = \int_{\hat{\gamma}} F(\hat{y}) \bar{v}(\hat{y}) d\hat{y} + G_2(y_0) \bar{v}(y_0), \end{aligned} \quad (7)$$

with

$$\begin{aligned}
A(\hat{y}) &= \int_{\Omega_{1D}} k(x, \psi_x^{-1}(\hat{y})) (e_1(x))^2 [\mathcal{D}_1^2(x, \psi_x^{-1}(\hat{y})) + \mathcal{D}_2^2(x, \psi_x^{-1}(\hat{y}))] |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| dx, \\
B_1(\hat{y}) &= \int_{\Omega_{1D}} k(x, \psi_x^{-1}(\hat{y})) \partial_x e_1(x) e_1(x) \mathcal{D}_1(x, \psi_x^{-1}(\hat{y})) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| dx, \\
B_2(\hat{y}) &= \int_{\Omega_{1D}} k(x, \psi_x^{-1}(\hat{y})) \partial_x e_1(x) e_1(x) \mathcal{D}_1(x, \psi_x^{-1}(\hat{y})) \\
&\quad - \mathbf{b}(x, \psi_x^{-1}(\hat{y})) (e_1(x))^2 \cdot \left(\frac{\mathcal{D}_1(x, \psi_x^{-1}(\hat{y}))}{\mathcal{D}_2(x, \psi_x^{-1}(\hat{y}))} \right) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| dx, \\
D(\hat{y}) &= \int_{\Omega_{1D}} \left[k(x, \psi_x^{-1}(\hat{y})) (\partial_x e_1(x))^2 - b_1(x, \psi_x^{-1}(\hat{y})) \partial_x e_1(x) e_1(x) + d(x, \psi_x^{-1}(\hat{y})) (e_1(x))^2 \right] \\
&\quad \cdot |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| dx + g_{R,1}(x_0, \psi_{x_0}^{-1}(\hat{y})) (e_1(x_0))^2 |\mathcal{D}_2^{-1}(x_0, \psi_{x_0}^{-1}(\hat{y}))|, \\
G_1(y_0) &= \int_{\Omega_{1D}} g_{R,1}(x, \psi_x^{-1}(y_0)) (e_1(x))^2 |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(y_0))| dx, \\
F(\hat{y}) &= \int_{\Omega_{1D}} f(x, \psi_x^{-1}(\hat{y})) e_1(x) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(\hat{y}))| dx \\
&\quad + g_{R,2}(x_0, \psi_{x_0}^{-1}(\hat{y})) e_1(x_0) |\mathcal{D}_2^{-1}(x_0, \psi_{x_0}^{-1}(\hat{y}))|, \\
G_2(y_0) &= \int_{\Omega_{1D}} g_{R,2}(x, \psi_x^{-1}(y_0)) e_1(x) |\mathcal{D}_2^{-1}(x, \psi_x^{-1}(y_0))| dx.
\end{aligned}$$

To get a 1D problem in \hat{y} we approximate the integrals over Ω_{1D} by a quadrature rule. The simplest one is a one point quadrature rule, where we evaluate the integrand in a quadrature point x^q and multiply it by the measure of Ω_{1D} . The crucial question is how to choose the quadrature point(s), or, in other words, for which points do we include global information from the data. To find the optimal quadrature points x_i^q , we perceive x_i^q as components of a parameter μ in the framework of reduced basis methods. We would like to recall that we assumed for the derivation of the 1D problem that $p(\Psi^{-1}(\hat{z})) \approx \bar{p}(\hat{y}) \cdot e_1(\hat{x})$, implying that $e_1(x)$ stands for the behavior of the solution in x direction. As this behavior is unknown, we regard the evaluations of $e_1(x)$ and $\partial_{\hat{x}} e_1(x)$ in x_i^q and optionally the values of e_1 on the left and right side of the boundary $e_1(x_0)$ and $e_1(x_1)$ as the other part of the parameter μ . So the parameter μ has the form $\mu = (x_1^q, e_1(x_1^q), \partial_x e_1(x_1^q), \dots, x_n^q, e_1(x_n^q), \partial_x e_1(x_n^q), e_1(x_0), e_1(x_1))$. The parameter space \mathcal{D} , containing all feasible parameter values of μ , is chosen as $\mathcal{D} = [\Omega_{1D} \times I_1 \times I_2]^n \times I_1 \times I_1$ for $I_1, I_2 \subset \mathbb{R}$. Then for each parameter vector $\mu \in \mathcal{D} \subset \mathbb{R}^P$ and all $\bar{v}(\hat{y}) \in V_{\hat{\gamma}} \bar{p}_{\mu}(\hat{y})$ is the

solution of the parameter dependent 1D advection-diffusion-reaction problem

$$\int_{\hat{\gamma}} A(\hat{y}; \mu) \partial_{\hat{y}} \bar{p}_{\mu}(\hat{y}) \partial_{\hat{y}} \bar{v}(\hat{y}) + B_1(\hat{y}; \mu) \partial_{\hat{y}} \bar{p}_{\mu}(\hat{y}) \bar{v}(\hat{y}) + B_2(\hat{y}; \mu) \bar{p}_{\mu}(\hat{y}) \partial_{\hat{y}} \bar{v}(\hat{y}) \quad (8)$$

$$+ D(\hat{y}; \mu) \bar{p}_{\mu}(\hat{y}) \bar{v}(\hat{y}) d\hat{y} + G_1(y_0; \mu) \bar{p}_{\mu}(y_0) \bar{v}(y_0) = \int_{\hat{\gamma}} F(\hat{y}; \mu) \bar{v}(\hat{y}) d\hat{y} + G_2(y_0; \mu) \bar{v}(y_0),$$

where the coefficient functions are defined as above. To compute $\bar{p}_{\mu}(\hat{y})$ numerically we introduce a partition τ_h of $\hat{\gamma}$ with elements $\tau_j = (\hat{y}_{j-1}, \hat{y}_j)$ of width $h_j = \hat{y}_j - \hat{y}_{j-1}$ and maximal step size $h := \max_{\tau_j} h_j$. Moreover let $V_{\hat{\gamma}}^h \subset V_{\hat{\gamma}}$ be a conforming Finite Element space with $\dim(V_{\hat{\gamma}}^h) = n_h < \infty$ and $\varphi_{y_j}(\hat{y})$, $1 \leq j \leq n_h$ a basis of $V_{\hat{\gamma}}^h$. Then $\bar{p}_{\mu}^h(\hat{y})$ denotes the solution of the discrete parameter dependent 1D problem. As we cannot compute $\bar{p}_{\mu}^h(\hat{y})$ for all parameter values $\mu \in \mathcal{D}$, we define a finite dimensional surrogate $\Xi_{train} \subset \mathcal{D}$ for whose parameters μ we compute the discrete solutions.

3.2 Construction of the basis functions — the adapt-HMR-POD algorithm

One goal of this subsection is to find a basis $\{\phi_k\}_k$, $1 \leq k \leq m$, with m as small as possible and $\|p - p_m^H\|_{H^{1,2}(\Omega)} \leq \varepsilon_{tol}$ for a given tolerance ε_{tol} . The other goal is to do this construction as cheap as possible. This results in the central question: How can we compute the optimal basis in the most efficient way. Most algorithms use either a Proper Orthogonal Decomposition (POD) and/or a Greedy approach for the generation of the basis. In short a POD determines the principal components of a given set of functions. The Greedy approach proceeds iteratively, enhancing in each loop the basis by the function which is worst approximated by the already chosen ones (cf. [3] for further details on the two approaches). In our proposed algorithm adapt-HMR-POD we use a combination of adjusted versions of those two approaches, exploiting the advantages of both. Obviously the computational costs accelerate with the increase of the sample size n_{train} , for which reason we want to be Ξ_{train} as small as possible. This can be done by adaptively refining the parameter space, which was introduced in [1]. As in [1] we use a hexaedral mesh, but in spite of choosing the vertices of the grid as the parameter values, we use randomly generated training sets in each element of the grid.

For the description of the algorithm we need some notations. M shall be a hexaedral, possibly non-conforming grid in the parameter space \mathcal{D} , e an element of M and N_M the number of elements in M . Moreover let Ξ_e be the randomly generated training set of an element e and n_{Ξ} the sample size of Ξ_e , which is identical for all elements. Ξ_M denotes the union of the training sets of all elements and n_{train} the sample size of Ξ_M . Inspired by [1] we use a

SOLVE \rightarrow ESTIMATE \rightarrow MARK \rightarrow REFINE

strategy. Let $\Delta_m^{\text{HMR}}(\mu)$ estimate the error between p and p_m^H in an appropriate norm, where $\Delta_m^{\text{HMR}}(\mu)$ is derived in the next section. Then the element indicator $\eta(e)$ is defined

Algorithm 1: $\text{adapt-para}(M, \Xi_M, s(M), m, \{\phi_k\}_1^{m-1}, \text{iter}, \varrho)$

foreach *element* $e \in M$ **do**
 Compute $\eta(e)$, $\xi(e)$ and $p_{y,e}$
end
for $i = 1:\text{iter}$ **do**
 $\mathcal{M} := \text{MARK}(\eta(M), \xi(M), \varrho)$
 $(\mathcal{M}, \Xi_M) := \text{REFINE}(\mathcal{M}, \Xi_M)$
 $s(M \setminus \mathcal{M}) = s(M \setminus \mathcal{M}) + 1$
 Compute $\eta(\mathcal{M})$, $\xi(\mathcal{M})$ and $p_{y,\mathcal{M}}$
end

as

$$\eta(e) := \min_{\mu \in \Xi_e} \Delta_m^{\text{HMR}}(\mu).$$

Now we fix $\theta \in (0, 1]$ and during each iteration the $\theta \cdot N_M$ elements with the smallest indicators $\eta(e)$ are refined. To guarantee that local structures in the data are resolved, we use an additional criterion in the marking strategy. We define

$$\xi(e) := \gamma(e) \cdot s(e),$$

where $\gamma(e)$ depends on $\text{diam}(e)$ and $s(e)$ counts the number of loops during which e has not been refined, since his last refinement. If $\xi(e) \geq \varrho$, where ϱ has been fixed, the element e is refined. During the refinement step all elements marked for refinement are bisected in every direction. In each new element as many new randomly generated parameter values are added as needed to attain the sample size n_Ξ . Before completing the description of Algorithm 1 adapt-para we still need some notations. iter denotes the number of refinement steps per basis function. $\eta(M)$, $\xi(M)$, and $s(M)$ contain the respective values for all elements of M . $p_{y,e}$ is the set of solutions of the parameter dependent 1D problem belonging to the parameter values of Ξ_e .

As $\Delta_m^{\text{HMR}}(\mu)$ estimates the error between p and p_m^H , it depends on m basis functions. That is why the algorithm adapt-para is run repeatedly in the Algorithm 2 adapt-HMR-POD . But for financial reasons adapt-para is only applied until a given maximal model order m_{\max} . The numerical experiments in [2] show that small values like $m_{\max} = 2$ are sufficient. In the end, we use a POD to determine the L^2 -orthonormal basis functions, demanding that $\varepsilon_{\text{tol}} \leq \varepsilon_{\text{POD}}^m$, where $\varepsilon_{\text{POD}}^m := \sqrt{\sum_{k=m+1}^{n_{\text{train}}} \lambda_{\text{POD}}^k}$ and λ_{POD}^k are the eigenvalues of the eigenvalue problem equivalent to the POD. This completes the outline of the adapt-HMR-POD algorithm.

Algorithm 2: adapt-HMR-POD($M_0, \Xi_{0,M}, iter, m_{\max}, \varepsilon_{\text{tol}}, \varrho$)

for $m=1:m_{\max}$ **do**

$p_{y,M} = \text{adapt-para}(M, \Xi_M, s(M), m, \{\phi_k\}_1^{m-1}, iter, \varrho)$
 $\{\phi_k\}_1^m := \text{POD}(p_{y,M}, m)$

end

$\{\phi_k\}_1^{m_{\text{POD}}} := \text{POD}(p_{y,M}, \varepsilon_{\text{tol}})$, so that $\varepsilon_{\text{POD}}^{m_{\text{POD}}} \leq \varepsilon_{\text{tol}}$.

4 A POSTERIORI ERROR ESTIMATION

The goal of this section is to derive an error estimator estimating the error between the discrete reduced solution p_m^H and a solution $p_{H \times h}$ computed using 2D FEM in an appropriate norm. First we need a FE space which is suitable for this comparison. We introduce a partition $P := \mathcal{T}_H \times \tau_h$ of $\hat{\Omega}$ induced by the partitions \mathcal{T}_H on Ω_{1D} and τ_h on $\hat{\gamma}$ with elements $T_{ij} := \mathcal{T}_i \times \tau_j$, $1 \leq i \leq N_H$, $1 \leq j \leq n_h$. Next we define a set of basis functions

$$\varphi_{ij}(x, \hat{y}) := \varphi_{xi}(x) \cdot \varphi_{yj}(\hat{y}), \quad 1 \leq i \leq N_H, 1 \leq j \leq n_h. \quad (9)$$

For the sake of simplicity we restrict ourself to the case where both $\varphi_{xi}(x)$ and $\varphi_{yj}(\hat{y})$ are piecewise linear. This implies that their product $\varphi_{ij}(x, \hat{y})$ is a standard bilinear quadrilateral element on T_{ij} . For this reason we introduce the space $\mathbb{Q}^k := \{u(x, \hat{y}) := \sum_{0 \leq l, n \leq k} c_{l,n} x^l \hat{y}^n\}$. Now we can introduce a FE space

$$V_{H \times h} := \{v \in C^0(\hat{\Omega}) : v|_{T_{ij}} \in \mathbb{Q}^1 \text{ and } v|_{\partial T_{ij}} \in \mathbb{P}^1\},$$

which coincides with the standard bilinear Finite Element space. Next we need a suitable norm. Let $a_s(w, v) := \frac{1}{2}(a(w, v) + a(v, w))$ denote the symmetric part of the bilinear form $a(w, v)$, specified in (2) for all $w, v \in V_{H \times h}$. Based on that we define a $V_{H \times h}$ -inner product and the induced $V_{H \times h}$ -norm

$$(\cdot, \cdot)_{V_{H \times h}} := a_s(\cdot, \cdot), \quad \|\cdot\|_{V_{H \times h}} := \sqrt{(\cdot, \cdot)}.$$

Then the error $e := p_{H \times h} - p_m^H$ satisfies the equation

$$a(e, v_{H \times h}) = r_{H \times h}^m(v_{H \times h}) \quad \forall v_{H \times h} \in V_{H \times h},$$

where

$$r_{H \times h}^m(v_{H \times h}) := f(v_{H \times h}) - a(p_m^H, v_{H \times h}) \quad \text{for } v_{H \times h} \in V_{H \times h},$$

with $f(v)$ specified in (3). Now we introduce the Riesz representation of $r_{H \times h}(v_{H \times h})$, denoted as $\mathcal{R}_m \in V_{H \times h}$, fulfilling the identity

$$(\mathcal{R}_m, v_{H \times h})_{V_{H \times h}} = r_{H \times h}^m(v_{H \times h}) \quad \forall v_{H \times h} \in V_{H \times h}.$$

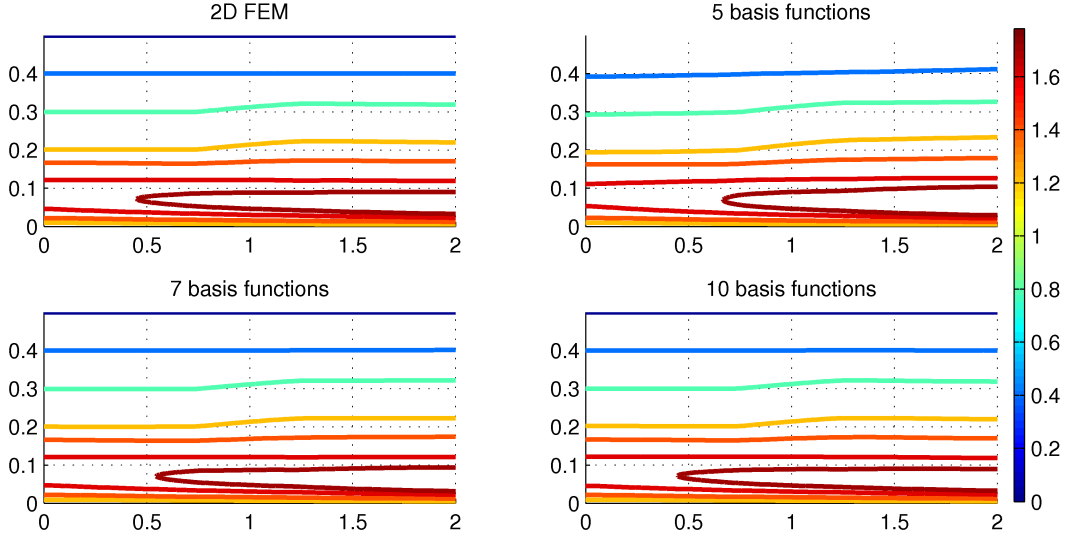


Figure 2: In comparison from left to right and top to bottom: the 2D FEM solution and the approximating solution for 5, 7 and 10 basis functions

And finally we define our error estimator

$$\Delta_m^{HMR} := \|\mathcal{R}_m\|_{V_{H \times h}}.$$

Efficiency and reliability of this estimator can be proved.

5 NUMERICAL EXPERIMENTS

As we are aiming at the application of the HMR-RB approach to unsaturated groundwater flow, we consider a test case quite similar to this situation. The diffusion coefficient exhibits an interface imitating the macroscopic interface between dry and wet soil in groundwater flow and the x -dependent advection coefficient points downwards like the gravitation term in the Richards equation. So we solve problem (4) on $\Omega = (0, 2) \times (0, 0.5)$ with a diffusion coefficient

$$k_1(x) = \begin{cases} 1 & 0 \leq x < 0.75 \\ -2x + 2.5 & 0.75 \leq x < 1.25 \\ 0 & \text{else} \end{cases}, \quad k_1(y) = \begin{cases} 1 & 0 \leq y \leq 0.1 \\ -9y + 1.9 & 0.1 < y < 0.2 \\ 0.1 & \text{else} \end{cases},$$

$$k_2(x) = \begin{cases} 2x - 1.5 & 0.75 < x \leq 1.25 \\ 1 & 1.25 < x \leq 2 \\ 0 & \text{else} \end{cases}, \quad k_2(y) = \begin{cases} 1 & 0 \leq y \leq 0.3 \\ -9y + 3.7 & 0.3 < y < 0.4 \\ 0.1 & \text{else} \end{cases},$$

$$k(x, y) = k_1(x)k_1(y) + k_2(x)k_2(y),$$

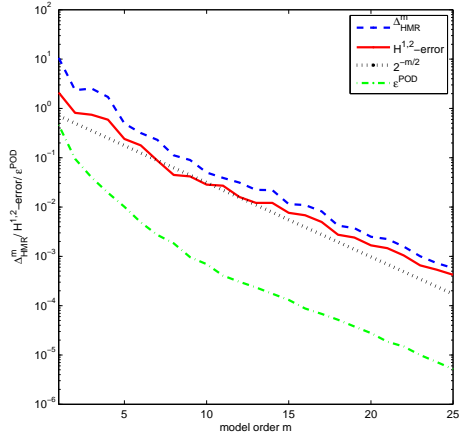


Figure 3: Comparison of Δ_{HMR}^m (dash), the computed $H^{1,2}$ -error (solid), and ε_{POD}^m (dash-dot) for increasing model order

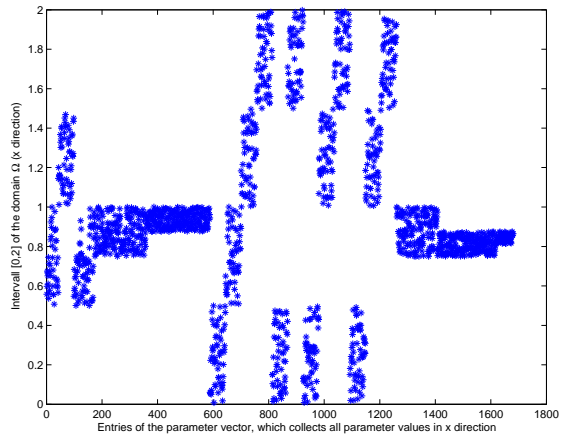


Figure 4: Adaptive refinement of the parameter space; distribution of the parameter values in $[0,2]$ — the x direction

an advection coefficient $\mathbf{b} = (0, 10x + 25)^t$ and a zero source term. We prescribe Dirichlet boundary conditions $g_D(x, y_1) = 0$ on the top and $g_D(x, y_0) = 1$ on the bottom and homogeneous Neumann boundary conditions on the left and right side of the domain. Typically the solution manifold, containing the solutions of the parameter dependent 1D problem (7) for all parameters $\mu \in \mathcal{D}$, is of very low dimension. However, due to the presence of the advection term and the interface in the diffusion coefficient we cannot expect that. To validate the proposed HMR-RB approach for this setting we first compare the isolines of the 2D FE solution using bilinear finite elements and the approximating solutions for five, seven, and ten basis functions in Fig. 2. Here we have used equidistant grids in x - and y -direction of mesh size $H = 0.005$ and $h = 0.0025$ both for the 2D FEM and the HMR-RB approach. We observe a perfect matching between the 2D FE solution and the approximating solution using ten basis functions. Also the solution produced by seven basis functions approximates the 2D FE solution quite well. This is a first hint that the approach seems also applicable to problems with advection. Moreover, we see in Fig. 3 that both the error estimator Δ_{HMR}^m (dash), the computed $H^{1,2}$ -error (solid), and the POD error ε_{POD}^m (dash-dot) show an exponential convergence rate of order $2^{-m/2}$ (dot) for an increasing model order m . This convergence rate is not as good as in smooth examples without interfaces (see [2]), but of course we could not have expected that. Furthermore, comparing the behavior of the error estimator Δ_{HMR}^m and the computed $H^{1,2}$ -error in Fig. 3 demonstrates that the error estimator is both reliable and efficient. At last we discuss the refinement of the parameter space. We have chosen $\mathcal{D} = [0, 2] \times [0, 4] \times [-10, 10]$, $n_{\Xi} = 7$, $m_{\max} = 2$, $iter = 3$ (2) for the iteration for the first (second) basis function, and $\theta = 0.25$. A sample size of $n_{\text{train}} = 1680$ is obtained. In Fig. 4 we can see where additional parameter values are put successively in the interval $[0, 2]$, meaning in the x -direction. What we see is that especially the interval $[0.75, 1]$ is refined, which is reasonable owing to the kink that the coefficient function exhibits here. So, we can say that the algorithm

adapt-HMR-POD refines the right regions in x -direction.

6 Conclusions

We have extended the HMR-RB approach to advection-diffusion-reaction problems. The numerical results show that the method is applicable to problems with advection. The next steps would be to study problems with a more dominant advection and also problems on more complex domains Ω , as the geometry strengthens the advective contribution. Furthermore we presented a new error estimator. As its computation is very expensive, its application is especially interesting in the case of parameter dependent problems where the construction of the basis functions can be done in a possibly costly offline phase. Here both the reliability and the efficiency of the error estimator will probably lead to a reduction of the model order m , which in turn reduces the online costs considerably.

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