A Reduced Basis Method for Parameter Functions using Wavelet Approximations

Antonia Mayerhofer and Karsten Urban

Abstract We consider parameterized parabolic partial differential equations (PDEs) with variable initial conditions, which are interpreted as a parameter function within the Reduced Basis Method (RBM). This means that we are facing an infinite-dimensional parameter space. We propose to use the space-time variational formulation of the parabolic PDE and show that this allows us to derive a two-step greedy method to determine offline separately the reduced basis for the initial value and the evolution. For the approximation of the initial value, we suggest to use an adaptive wavelet approximation. Online, for a given new parameter function, the reduced basis approximation depends on its (quasi-)best N-term approximation in terms of the wavelet basis. A corresponding offline-online decomposable error estimator is provided. Numerical experiments show the flexibility and the efficiency of the method.

1 Introduction

The reduced basis method (RBM) is a well-known model reduction method for parameterized partial differential equations (PDE) within multi-query and/or realtime context situations. Of course, the structure and the dimension of the parameter set $\mathscr{D}$ has significant influence on the efficiency of any RBM. Typically, one has $\mathscr{D} \subset \mathbb{R}^P$ with P being "reasonably" small. In some applications, however, P may be large, even infinite. Such a case occurs if one faces a parameter *function* so that $\mathscr{D} \subset H$ with H being a function (Hilbert) space of infinite dimension.

Antonia Mayerhofer
Ulm University, Institute for Mathematical Finance, Helmholzstr. 18, 89081 Ulm, Germany
e-mail: antonia.mayerhofer@uni-ulm.de

Karsten Urban
Ulm University, Institute for Numerical Mathematics, Helmholtzstr. 20, 89081 Ulm, Germany
e-mail: karsten.urban@uni-ulm.de

We consider a particularly relevant class of problems involving parameter functions, namely parabolic problems with variable initial conditions, i.e., we consider the initial condition as a parameter. One possible application are pricing and hedging problems in finance, where the payoff is used as a parameter, see [4, 5]. Using a parameterized initial value in an evolution equation is a challenge by itself for standard RBM-techniques such as the POD-Greedy method [3], since usually the error is propagating over time.

This is the reason why we rely on the space-time variational formulation for parabolic problems introduced in [6] and being used within the RB-framework e.g. in [9, 10]. Within this framework, we show that we can separate the treatment of the initial value parameter function from additional parameters the PDE may have. We introduce a 2-stage Greedy method for computing a corresponding reduced basis in the offline phase.

The issue remains how to approximate a parameter *function*, an ∞-dimensional object (expansion in a separable Hilbert space). We propose an adaptive wavelet approximation for the parameter function online. We show that several ingredients for the RB approximation can be precomputed in the offline phase and how to realize an online-efficient approximation for a new parameter function. Numerical results show the flexibilty, efficiency and the approximation quality of the proposed method.

The remainder of this chapter is organized as follows. In Section 2, we recall those main facts of the RBM that we need here. Section 3 is devoted to a brief survey of the space-time variational formulation for parabolic problems as well as its parametric variant. Our suggested RBM for problems with parameter functions is detailed in Section 4 also including the description of the use of an adaptive wavelet approximation. We report our numerical results in Section 5 and finish with some conclusions in Section 6. We refer to [4] to more details on the presented material.

2 Reduced Basis Method

Let $\mathscr{D}$ be some parameter space. Consider the parametrized PDE

$$\text{find } u \equiv u(\mu) \in X: \quad b(u,v;\mu) = f(v;\mu) \quad \forall\, v \in Y; \quad \mu \in \mathscr{D}, \tag{1}$$

where $b : X \times Y \times \mathscr{D} \to \mathbb{R}$ is a parameter-dependent bilinear form and $f : Y \times \mathscr{D} \to \mathbb{R}$ a parameter dependent linear form. We assume well-posedness of (1). For discrete (but high-dimensional) trial $X^{\mathscr{N}} \subset X$ and test $Y^{\mathscr{N}} \subset Y$ spaces with $\dim(X^{\mathscr{N}}) = \dim(Y^{\mathscr{N}}) = \mathscr{N} \gg 0$ and every $\mu \in \mathscr{D}$, an associated $\mathscr{N}$-dimensional (detailed) linear system has to be solved that is given by

$$\text{find } u^{\mathscr{N}} \equiv u^{\mathscr{N}}(\mu) \in X^{\mathscr{N}}: \quad b(u^{\mathscr{N}},v;\mu) = f(v;\mu) \quad \forall v \, \in Y^{\mathscr{N}}. \tag{2}$$

Again we assume well-posedness for this detailed system.

In a multi-query or real-time context, the solution of this detailed system (sometimes called “truth”) is often too costly. In order to reduce the system, we consider the solution subset (“manifold”) $M(\mathscr{D}) = \{u(\mu^{\mathscr{N}}) \in X^{\mathscr{N}} : \ \mu \in \mathscr{D}\}$. The RBM aims to approximate $M(\mathscr{D})$ by a lower dimensional space $X_N \subset X^{\mathscr{N}}$ where, $\dim(X_N) = N \ll \mathscr{N}$. The reduced problem then reads

$$\text{find } u_N \equiv u_N(\mu) \in X_N : \quad b(u_N, v; \mu) = f(v; \mu) \quad \forall\, v \in Y_N \tag{3}$$

with an appropriate test space Y_N (which may also be parameter-dependent, i.e., $Y_N(\mu)$). Hence, a linear system of dimension N needs to be solved.

The RBM is divided into an offline and an online phase. In the offline phase, bases spanning the reduced system X_N, Y_N are generated by computing detailed solutions $u(\mu^i) \in X^{\mathscr{N}}$ for a well-chosen sample set of parameters $\mu^1, \dots, \mu^N \subset \mathscr{D}$ along with a reduced stable test space Y_N. The reduced system is then solved online for new values of the parameters $\mu \in \mathscr{D}$. The goal is that the reduced system is *online-efficient*, which means it can be solved with an amount of work independent of the detailed dimension $\mathscr{N}$.

In order to reach the latter goal, a standard assumption is to require that the forms b and f are decomposable w.r.t. the parameter (sometimes called “affine decomposition”), i.e., there exist Q_b, $Q_f \in \mathbb{N}$ and functions $\theta_q^b, \theta_q^f : \mathscr{D} \to \mathbb{R}$ such that

$$b(u, v; \mu) = \sum_{q=1}^{Q_b} \theta_q^b(\mu) b_q(u, v), \quad f(v; \mu) = \sum_{q=1}^{Q_f} \theta_q^f(\mu) f_q(v) \tag{4}$$

with (bi-)linear forms b_q and f_q independent of μ. First, the reduced trial functions $u^i := u^{\mathscr{N}}(\mu^i) \in X^{\mathscr{N}}$ and corresponding inf-sup-stable test functions $v^i \in Y^{\mathscr{N}}$, $i = 1, \dots, N$, are computed. Then, the parameter-independent components are computed and stored, e.g.

$$b_q(u^i, v^j) = \sum_{k,l=1}^{\mathscr{N}} \alpha_{i;k}\, \tilde{\alpha}_{j;l}\, b_q(\varphi_k^{\mathscr{N}}, \tilde{\varphi}_l^{\mathscr{N}}),$$

where $\varphi_k^{\mathscr{N}}$, $\tilde{\varphi}_l^{\mathscr{N}}$ are the basis functions of the detailed spaces $X^{\mathscr{N}}$, $Y^{\mathscr{N}}$ and $\alpha_{i;k}$, $\tilde{\alpha}_{j;l}$ are the expansion coefficients of the reduced basis functions u^i, v^j in terms of the detailed basis functions. The linear forms $f_q(v^j)$ are precomputed in a similar fashion. In the online phase, only $\theta_q^b(\mu)$ and $\theta_q^f(\mu)$ need to be evaluated for a new parameter μ and the sums in (4) can be computed with complexity independent of $\mathscr{N}$, i.e., online-efficient.

3 Space-Time Variational Formulation for Parabolic Problems

We follow e.g. [6, 9, 10] for the introduction of space-time variational formulations for parabolic PDEs in terms of Bochner(-Lebesgue) spaces. Let $H \hookrightarrow V$ be densely embedded Hilbert spaces. By identifying H with its dual H', we obtain the Gelfand triple $V \hookrightarrow H \hookrightarrow V'$, i.e., the scalar product $(\cdot,\cdot)_H$ on H generates the duality pairing $\langle\cdot,\cdot\rangle_{V'\times V}$. We denote the induced norms on V and H by $|\cdot|_V$ and $|\cdot|_H$, respectively. We seek the solution in

$$\mathbb{X} := \{u \in L_2(I;V) : \dot{u} \in L_2(I;V')\}, \quad I := (0,T) \subset \mathbb{R},$$

equipped with the graph norm $\|u\|^2_{\mathbb{X}} := \|u\|^2_{L_2(I;V)} + \|\dot{u}\|^2_{L_2(I;V')}$.

The parameter spaces are assumed to be of the form $\mathscr{D} = \mathscr{D}_0 \times \mathscr{D}_1 \subset H \times \mathbb{R}^P$, where $\mu_0 \in \mathscr{D}_0$ accounts for the initial value (i.e., a function) and $\mu_1 \in \mathscr{D}_1$ for parameters in the PDE. To be more specific, consider a parameter-dependent bilinear form $a : V \times V \times \mathscr{D}_1 \to \mathbb{R}$ with induced linear operator $\mathscr{A}(\mu_1) \in \mathscr{L}(V,V')$ as $\langle \mathscr{A}(\mu_1)\phi,\psi\rangle_{V'\times V} = a(\phi,\psi;\mu_1)$ for $\phi,\psi \in V$. Then, given a non-parametric right-hand side $g \in L_2(I;V')$, we seek $u(t) \in V$, $t \in I$ such that for $\mu = (\mu_0,\mu_1) \in \mathscr{D}$

$$\dot{u}(t) + \mathscr{A}(\mu_1)u(t) = g(t) \quad \text{in } V', t \in I \text{ a.e.}, \qquad u(0) = \mu_0 \quad \text{in } H. \tag{5}$$

We assume that there exist constants $C_a(\mu_1) > 0$, $\alpha_a(\mu_1) > 0$ and $\lambda_a(\mu_1) \in \mathbb{R}$ such that for all $\phi,\psi \in V$

$$|a(\phi,\psi;\mu_1)| \leq C_a(\mu_1)|\phi|_V|\psi|_V \qquad \text{(continuity)}, \tag{6}$$

$$a(\phi,\phi;\mu_1) + \lambda_a(\mu_1)|\phi|^2_H \geq \alpha_a(\mu_1)|\phi|^2_V \qquad \text{(Gårding inequality)}. \tag{7}$$

Remark 1. (i) For $u \in \mathbb{X}$ the initial condition in (5) is meaningful since $\mathbb{X} \hookrightarrow \mathscr{C}(\bar{I};H)$, [7, III. Prop. 1.2].

(ii) We assume that g is parameter-independent just for ease of presentation. All what is said here extends to parameter-dependent right-hand sides as well.

The test space is chosen as $\mathbb{Y} := L_2(I;V) \times H$ equipped with the graph norm $\|v\|^2_{\mathbb{Y}} = \|v_1\|^2_{L_2(I,V)} + |v_2|^2_H$, $v = (v_1,v_2) \in \mathbb{Y}$. For $w \in \mathbb{X}$, $v = (z,h) \in \mathbb{Y}$ and $\mu \in \mathscr{D}$, we define

$$b(w,v;\mu) := \int_I \langle \dot{w}(t), z(t)\rangle_{V'\times V}\, dt + \int_I a(w(t),z(t);\mu_1)dt + (w(0),h)_H, \tag{8}$$

$$f(v;\mu) := \int_I \langle g(t), z(t)\rangle_{V'\times V}\, dt + (\mu_0,h)_H. \tag{9}$$

The variational formulation of the parameterized parabolic PDE is then given by

$$\text{find } u \in \mathbb{X} : \quad b(u,v;\mu) = f(v;\mu) \quad \forall\, v \in \mathbb{Y}. \tag{10}$$

Note, that (10) and (5) are in fact equivalent. Well-posedeness was shown e.g. in [6, Thm. 5.1]. The linear operator $\mathscr{B}(\mu) : \mathbb{X} \to \mathbb{Y}'$ induced by $\langle \mathscr{B}(\mu)u,v\rangle := b(u,v;\mu)$, $v \in \mathbb{Y}$, is thus injective, which implies the inf-sup condition with a lower inf-sup-bound β_{LB}, i.e.,

$$\inf_{u\in\mathbb{X}} \sup_{v\in\mathbb{Y}} \frac{b(u,v;\mu)}{\|u\|_{\mathbb{X}}\|v\|_{\mathbb{Y}}} \geq \beta(\mu) \geq \beta_{\mathrm{LB}} > 0. \tag{11}$$

The lower inf-sup-bound plays a major role in the a-posteriori error estimation of the space-time RBM.

4 Reduced Basis Method for Parameter Functions

Recall, that the parameter $\mu_0 \in \mathscr{D}_0$ is the initial value, i.e., a parameter function in an infinite-dimensional parameter set (function space). We are now going to introduce an approach to deal with this challenge.

4.1 Using the Initial Value as Parameter in a Space-Time Setting

We start by separating the (bi-)linear forms in (8,9):

$$\begin{aligned} b(u,v;\mu) &= \int_I \langle \dot{u}(t), z(t) \rangle_{V' \times V}\, dt + \int_I a(u(t), z(t); \mu_1) dt + (u(0), h)_H \qquad (12) \\ &=: b_1(u,z;\mu_1) + (u(0),h)_H \\ f(v;\mu) &= \int_I \langle g(t), z(t) \rangle_{V' \times V}\, dt + (\mu_0, h)_H =: g_1(z) + (\mu_0, h)_H \qquad (13) \end{aligned}$$

for $\mu = (\mu_0, \mu_1) \in \mathscr{D}$, $u \in \mathbb{X}$ and $(z,h) \in \mathbb{Y}$. Note, that $b(\cdot,\cdot;\mu)$ only depends on μ_1, whereas $f(\cdot;\mu)$ only depends on μ_0, the latter one just for convenience.

The detailed discretization is induced by $\mathbb{X}^{\mathscr{N}} \subset \mathbb{X}$ and $\mathbb{Y}^{\mathscr{N}} \subset \mathbb{Y}$ with $\dim(\mathbb{X}^{\mathscr{N}}) = \dim(\mathbb{Y}^{\mathscr{N}}) = \mathscr{N}$. We assume well-posedness and uniform stability of the truth problem, [4]. Note, that $\mathbb{X} = H^1(I) \otimes V$ and $\mathbb{Y} = L_2(I) \otimes V \times H$ are tensor products, so that it is convenient to construct the detailed spaces accordingly,

$$\begin{aligned} \mathbb{X}^{\mathscr{N}} &= (E_0^1 \oplus E_1^{\mathscr{K}}) \otimes V^{\mathscr{J}} = (E_0^1 \otimes V^{\mathscr{J}}) \oplus (E_1^{\mathscr{K}} \otimes V^{\mathscr{J}}) =: Q^{\mathscr{J}} \oplus W^{\mathscr{L}}, \\ \mathbb{Y}^{\mathscr{N}} &= (F^{\mathscr{K}} \otimes V^{\mathscr{J}}) \times V^{\mathscr{J}} =: Z^{\mathscr{L}} \times V^{\mathscr{J}}, \quad \dim(W^{\mathscr{L}}) = \mathscr{L} := \mathscr{J}\mathscr{K}. \end{aligned}$$

Here, E_0^1 contains the temporal basis function τ^0 (say) at $t = 0$ ($\dim(E_0^1) = 1$) and $E_1^{\mathscr{K}}$ collects the remaining basis functions in time.[1]All superscripts indicate the dimension of the spaces, so that $\mathscr{N} := \dim(\mathbb{X}^{\mathscr{N}}) = \mathscr{J} + \mathscr{L} = \dim(\mathbb{Y}^{\mathscr{N}})$. This discretization allows a 2-step computation for $\mu = (\mu_0, \mu_1) \in \mathscr{D}$ as follows:

$$\begin{aligned} &\text{(a) Find } q(\mu_0) \in V^{\mathscr{J}}: \quad (q(\mu_0), h)_H = (\mu_0, h)_H \qquad \forall h \in V^{\mathscr{J}}, \qquad (14) \\ &\text{(b) Find } w(\mu) \in W^{\mathscr{L}}: \quad b_1(w,z;\mu_1) = f_1(z; \mu_1, \tau^0 \otimes q(\mu_0)) \quad \forall z \in Z^{\mathscr{L}}, \qquad (15) \end{aligned}$$

with b_1 as in (12) and $f_1(z;\mu_1,w) := g_1(z) - b_1(w,z;\mu_1)$ with g_1 as in (13).

[1] If we use a function in space, say $q \in V^{\mathscr{J}}$, as initial value, we "embed" it into $Q^{\mathscr{J}}$, i.e., we set $\tau^0 \otimes q \in Q^{\mathscr{J}}$ with the temporal basis function τ^0 at $t = 0$.

The space-time variational approach allows us to use the standard RB-setting in Section 2 for the a posteriori error estimate in terms of the residual. It turns out that the separation in (14) is also crucial here. Let $u_N(\mu) \in \mathbb{X}_N \subset \mathbb{X}^{\mathcal{N}}$ (the RB-approximation to be detailed below), then we get for any $v = (z,h) \in \mathbb{Y}^{\mathcal{N}}$

$$\begin{aligned} r_N(v;\mu) &= f(v;\mu) - b(u_N(\mu),v;\mu) \\ &= g_1(z;\mu_1) - b_1(u_N(\mu),z;\mu_1) + (\mu_0 - u_N(0;\mu),h)_H \\ &=: r_{N,1}(z;\mu) + r_{N,0}(h;\mu). \end{aligned} \tag{16}$$

This separation of the residual allows us to control the error for the initial value ($t = 0$) and the evolution separately.

4.2 Wavelet Approximation for the Parameter Function

The initial value is a function in $\mathscr{D}_0 \subseteq H$. In principle, we could use any stable basis in H to represent the initial value. However, as indicated in Section 1, we do not want to fix any possible representation of μ_0 a priorily, [5], but adapt it during the online phase. Hence, we need a basis for H that allows for a rapid and local update of a given new μ_0. We have chosen wavelets. A detailed introduction to wavelets goes far beyond the scope of the present paper, we thus refer e.g. to [8] for details and sketch here just those ingredients that are particularly relevant in the RB-context.

Wavelets on the real line are usually formed via translation and dilation of a single (compactly supported) function $\psi : \mathbb{R} \to \mathbb{R}$, often called *mother wavelet*, i.e.,

$$\psi_\lambda(x) := 2^{j/2}\psi(2^j x - k), \quad x \in \mathbb{R}, \qquad j \in \mathbb{N}_0 \,(\text{the } \textit{level}), k \in \mathbb{Z}, \lambda = (j,k).$$

The simplest example is the *Haar wavelet*, where $\psi(x)^{\text{Haar}} := \begin{cases} 1, & 0 \le x < 0.5, \\ -1, & 0.5 \le x < 1. \end{cases}$ Then $\Psi^{\text{Haar}} := \{\psi_\lambda^{\text{Haar}} : \lambda \in \mathbb{Z} \times \mathbb{Z}\}$ is an orthonormal basis (ONB) for $L_2(\mathbb{R})$. If one only uses $\{(j,k) : j \in \mathbb{N}_0, 0 \le k < 2^j\}$ instead of $\mathbb{Z} \times \mathbb{Z}$, an ONB of $L_2(0,1)$ results. We denote such general index sets by Λ.

Definition 1. A countable set $\Psi := \{\psi_\lambda : \lambda \in \Lambda\} \subset H$ is called *wavelet basis*, if

(i) Ψ is a *Riesz basis* for H, i.e., there exist constants $0 < c_\Psi \le C_\Psi < \infty$ such that

$$c_\Psi \sum_{\lambda \in \Lambda} |d_\lambda|^2 \le \Big| \sum_{\lambda \in \Lambda} d_\lambda \psi_\lambda \Big|_H^2 \le C_\Psi \sum_{\lambda \in \Lambda} |d_\lambda|^2, \text{ (in short: } \|d\|_{\ell_2} \sim \|d^T \Psi\|_H); \tag{17}$$

(ii) Ψ has *local support*, i.e., $|\text{supp}(\psi_\lambda)| \sim 2^{-|\lambda|}$, $\lambda = (j,k)$, $|\lambda| := j$;

(iii) Ψ has $\tilde{d}$ *vanishing moments*, i.e., there exists some $r \in \mathbb{N}$ such that $((\cdot)^p, \psi_\lambda)_H = 0$ for $0 \le p < \tilde{d}$.

Remark 2. The Riesz representation theorem yields the existence of a *dual* wavelet basis $\tilde{\Psi}$ with the same properties but a possibly different d instead of $\tilde{d}$ in (iii). Typically, ψ_λ is a piecewise polynomial of degree d.

Nowadays, there is a whole variety of wavelet systems available, on general domains $\Omega \subset \mathbb{R}^d$, with arbitrary smoothness and additional properties. Definition 1 has several consequences. Just to mention a few (and without going into detail due to page restrictions):

(1) The wavelet coefficients d_λ decay fast with increasing level $|\lambda|$.
(2) The wavelet coefficients are small in regions where the function is smooth – they indicate regions of local non-smoothness (like isolated singularities).
(3) The *norm equivalence* (17) can be extended to scales of Sobolev spaces H^s around $s = 0$ and allow for an online-efficient computation of the residual, [1, 2].
(4) There are fast adaptive methods to approximate a given function in H (to be applied to approximate μ_0 online). Roughly speaking, one only needs higher level wavelets in regions where the function is locally non-smooth. The norm equivalence (17) ensures that this procedure converges very fast (see below).

Remark 3. It might be a first naive idea to choose a finite subset of wavelet-indices, say $\Lambda_M \subset \Lambda$, and use the corresponding expansion coefficients as a parameter set of dimension $|\Lambda_M|$. Of course, this severely limits the choice of initial conditions. If one is interested in a whole variety of such functions including localized effects, a sufficient approximation causes $|\Lambda_M|$ to be huge – thus making this idea computationally infeasible. Only if one has some knowledge on the shape of the initial value, one may a-priorily fix the approximation space, see e.g. [4, 5].

4.3 Online-Offline Reduced Basis Method

1st step Greedy: Adaptive approximation of the initial value. We start by collecting offline-information for the online initial value approximation given a new parameter function μ_0. We collect those information in a library $\mathbb{L}_{\text{init}}$ that is computed offline. The standard Jackson-estimate allows to truncate a wavelet expansion at a certain maximum level and to control the approximation error in terms of the Sobolev regularity. In fact, if we denote by S_j the subspace of H generated by all wavelets with level $|\lambda| \le j$, then

$$\inf_{v_j \in S_j} |v - v_j|_{L_2(\Omega)} \le C 2^{-js} |v|_{H^s(\Omega)}, \quad v \in H^s(\Omega),\ s \le d,$$

with d as in Remark 2, [8, (5.30)]. Hence, if we know (or fix) the regularity of all candidates for the initial values, we may fix a maximal level, say J. For all wavelets in the corresponding space S_J, we precompute the associated "snapshot" $q^\lambda \in Q^{\mathscr{I}}$ for the initial value by solving

$$(q^\lambda, \phi)_H = (\psi_\lambda, \phi)_H \quad \forall \phi \in S_J,\ |\lambda| \le J. \tag{18}$$

We thus obtain in the order of 2^J such initial value snapshots and store them in an *Initial Value Library* $\mathbb{L}_{\text{init}} = \{q^\lambda \ : \lambda \in \Lambda, |\lambda| \le J\}$.

2nd step Greedy: Evolution snapshots. Based upon the library $\mathbb{L}_{\text{init}}$, we precompute snapshots for the corresponding evolutions. This is done by an adapted standard Greedy scheme w.r.t. some training set $\mathscr{D}_1^{\text{train}} \subset \mathscr{D}_1$. The arising *Evolution Greedy* is detailed in Algorithm 1. Note, that the training phase is performed for each wavelet index λ with the respective training set $\{\psi_\lambda\} \times \mathscr{D}_1^{\text{train}}$. For each wavelet index λ, Algorithm 1 produces an RB space of the form $W^\lambda_{N(\lambda)} = \text{span}\{w^1_\lambda, \dots, w^{N(\lambda)}_\lambda\}$ of dimension $N(\lambda)$, where w^i_λ solves the space-time parabolic problem

$$b_1(w^i_\lambda, z; \mu^i_1) = g_1(z) - b_1(q^\lambda, z; \mu^i_1) \quad \forall\, z \in \mathbb{Y}^{\mathscr{N}} \tag{19}$$

for a parameter μ^i_1 chosen in the *i*-th step of Algorithm 1 with training set $\{\psi_\lambda\} \times \mathscr{D}_1^{\text{train}}$. We collect all such solutions of (19) in an *Evolution Library*

$$\mathbb{L}_{\text{evol}} := \{w^1_\lambda, \dots, w^{N(\lambda)}_\lambda \ : \lambda \in \Lambda, |\lambda| \le J\},$$

which consists of all RB bases of the evolutions with initial values in $\mathbb{L}_{\text{init}}$.

Algorithm 1 Evolution Greedy

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Require: training set $\mathscr{D}^{\text{train}} = \{\psi_\lambda\} \times \mathscr{D}_1^{\text{train}} \subset \mathscr{D}$, tolerance $\text{tol}_1 > 0$
Choose $\mu^1 \in \mathscr{D}^{\text{train}}$, $\mu^1 := (\psi_\lambda, \mu^1_1)$. Get precomputed $q^\lambda \in \mathbb{L}_{\text{init}}$
Compute $w(\mu^1) \in W^{\mathscr{L}}$ as in (19), $\Xi^\lambda_1 = \{w(\mu^1)\}$
for $\ell = 1, \dots, N^{\max}$ do
    $\mu^{\ell+1} = \arg \max_{\mu \in \mathscr{D}^{\text{train}}} \Delta^1_\ell(\mu)$
    if $\Delta^1_\ell(\mu^{\ell+1}) < \text{tol}_1$ then $N(\lambda) := \ell$ Stop end if
    Compute $w(\mu^{\ell+1}) \in W^{\mathscr{L}}$ as in (19)
    $S^{\ell+1}_1 := S^\ell_1 \cup \{\mu^{\ell+1}\}$, $\Xi^\lambda_{\ell+1} := \Xi^\lambda_\ell \cup \{w(\mu^{\ell+1})\}$
end for
return RB basis $\Xi^\lambda_{N(\lambda)}$
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We do not compute a reduced inf-sup stable test space $\mathbb{Y}_N$, since we use normal equations, see Remark 4 below. The space-time variational approach allows us to use a standard error estimator in Algorithm 1, i.e., the first part of (16),

$$\Delta^1_\ell(\mu) := \frac{\|r_{\ell,1}(\mu)\|_{Z'}}{\beta_{\text{LB}}}, \tag{20}$$

where β_{LB} is the lower bound of the inf-sup constant of the bilinear form b.

Orthonormalization. Note, that we are going to use combinations of RB bases stored in $\mathbb{L}_{\text{evol}}$ for the RB approximation online. This combinations of snapshots may not necessarily be linearly independent. We resolve this by performing an online orthonormalization that is prepared offline as follows. Denote the set of *all* functions that arise from the 2-step Greedy method by $W^{N_{\max}} := \{w^i : 1 \le$

$i \leq N_{\max}\}$, $N_{\max} = \sum_{\lambda\in\Lambda,|\lambda|\leq J} N(\lambda)$, and denote its Gramian matrix by $\mathbf{M} := [(w^i, w^j)_{\mathbb{X}}]_{i,j=1,\ldots,N_{\max}}$. We then compute an SVD, i.e., $\mathbf{M} = \mathbf{U}^T\mathbf{D}\mathbf{U}$. Setting $\mathbf{S} := \mathbf{U}^{-1}\mathbf{D}^{-1/2}$ obviously yields $\mathbf{S}^T\mathbf{M}\mathbf{S} = \mathbb{1}$. At a first glance, this might seem to be an overkill. However, in the online phase, we need to access to all rows and columns of $\mathbf{S}$ that correspond to the required RB snapshots in $\mathbb{L}_{\mathrm{evol}}$ that are significant for approximating the evolution for a new μ_0. Hence, we need to consider $W^{N_{\max}}$.

Online Phase: We need to adapt the online phase for the specific case of a parameter function μ_0. The main idea is to efficiently compute a (quasi-)best $N_0(\mu_0)$-term approximation to a given μ_0 by determining those $N_0(\mu_0)$ wavelets yielding the largest coefficients in absolute values. Let us denote by $\Lambda_N(\mu_0)$ the arising index set of dimension $N_0(\mu_0)$. Then, the computed approximation takes the form

$$u_{0,N}(\mu_0) = \sum_{\lambda\in\Lambda_N(\mu_0)} d_\lambda(\mu_0) q^\lambda, \qquad N_0(\mu_0) \equiv |\Lambda_N(\mu_0)|,$$

with $q^\lambda \in \mathbb{L}_{\mathrm{init}}$. The approximation error can be estimated as

$$\begin{aligned} \|\mu_0 - u_{0,N}(\mu_0)\|_H \leq \Delta_N^0(\mu_0) &:= \frac{\|r_{N,0}(\mu_0)\|_{H'}}{\beta_{\mathrm{LB}}} \\ &\leq \frac{1}{\beta_{\mathrm{LB}}} \Big\| \mu_0 - \sum_{\lambda\in\Lambda_N(\mu_0)} d_\lambda \psi_\lambda \Big\|_H = \frac{1}{\beta_{\mathrm{LB}}} \Big\| \sum_{\lambda\notin\Lambda_N(\mu_0)} d_\lambda \psi_\lambda \Big\|_H. \end{aligned} \tag{21}$$

For the evolutionary part, we use the reduced basis $\{w_\lambda^\ell : \lambda \in \Lambda_N(\mu), \ell = 1,\ldots,N(\lambda)\} \subset \mathbb{L}_{\mathrm{evol}}$ to span the reduced space, which is of dimension $N := N(\mu_0) = \sum_{\lambda\in\Lambda_N(\mu_0)} N_0(\lambda)$, i.e., we have to solve a linear system of dimension $N \times N$. Recall, that we have precomputed the SVD of the full Gramian matrix $\mathbf{M}$ along with the matrix $\mathbf{S}$ to orthogonalize the snapshots. Now, we pick the submatrix $\mathbf{S}_N$ of $\mathbf{S}$ consisting of the N rows and columns of $\mathbf{S}$ that correspond to the given initial value μ_0. We use this matrix $\mathbf{S}_N$ as a preconditioner for the system matrix $\mathbf{B}_N(\mu)$. The arising online phase is detailed in Algorithm 2.

Algorithm 2 Online Phase with Online Orthonormalization

```
Require: New parameter $\mu \in \mathscr{D}$, $N = N(\mu_0)$, $\mathbb{L}_{\mathrm{init}}$, $\mathbb{L}_{\mathrm{evol}}$, preconditioner $\mathbf{S}$.
1: Compute $\mathbf{B}_N(\mu)$, $\mathbf{F}_N(\mu)$ and pick $\mathbf{S}_N$ out of $\mathbf{S}$.
2: Orthogonalization: $\tilde{\mathbf{B}}_N(\mu) := \mathbf{S}_N^T\mathbf{B}_N(\mu)\mathbf{S}_N$, $\tilde{\mathbf{F}}_N(\mu) := \mathbf{S}_N^T\mathbf{F}_N(\mu)$.
3: if det($\tilde{\mathbf{B}}_N(\mu)) = 0$ then Delete zero rows/columns. end if
4: Solve $\tilde{\mathbf{u}}_N(\mu) = (\tilde{\mathbf{B}}_N(\mu))^{-1}\tilde{\mathbf{F}}_N(\mu) \to \mathbf{u}_N(\mu) = \mathbf{S}_N\tilde{\mathbf{u}}_N(\mu)$.
5: Compute $\Delta_N(\mu)$.
6: return RB solution $u_N(\mu)$, estimator $\Delta_N(\mu)$.
```

Remark 4. The online solution in line 4 of Algorithm 2 is performed by solving the corresponding normal equations. This is also the reason why we did not construct a reduced test space in the offline phase in (19). For details, we refer to [4].

Recall from (16) that the residual – and consequently also the error estimate Δ_N – can be split in two parts. The first part contains $\|\mu_0 - u_{0,N}(\mu_0)\|_H$ which is equivalent to the initial value error in (21). Since $\mu_0 - u_{0,N}(\mu_0)$ is a linear combination of wavelets, the Riesz basis property allows us to reduce this computation to a weighted sum of wavelet coefficients, which is clearly online-efficient.

The second part of the error estimator is easily seen to be offline-online decomposable and thus computable online-efficient. In addition, we obtain the following error bound

$$\|g_1 - b_1(u_N(\mu), \cdot; \mu_1)\|_{\mathbb{Y}'} \leq \Big|1 - \sum_{\lambda \in \Lambda_N(\mu_0)} d_\lambda(\mu_0)\Big| \|g_1(\cdot)\|_{\mathbb{Y}'} + \Big|\sum_{\lambda \in \Lambda_N(\mu_0)} d_\lambda(\mu_0)\Big| \mathrm{tol}_1, \quad (22)$$

for tol_1 defined as in Algorithm 1 and $d_\lambda(\mu_0)$ being the expansion coefficients of the approximate initial condition in terms of the basis function q^λ of $\mathbb{L}_{\mathrm{init}}$ in (18).

It is remarkable that the upper bound (22) can be evaluated *before* the RB approximation is actually computed, i.e., a-priori. This is important since the RB solution may not respect the chosen greedy tolerances. The reason is that the training set of the parameter function space contains single functions but linear combination of these functions need to be considered online. If the upper bound (22) indicates this, one may need to add some more basis functions by performing some few offline computations (in a multi-fidelity fashion).

5 Numerical Experiments

We aim at numerically investigating the influence of the right-hand side and of the error made in the approximation of the parameter function onto the RB error (estimator). In order to concentrate on these issues, we consider a univariate diffusion problem for $V := H_0^1(0,1)$ and $H := L_2(0,1)$, $I := (0, 0.3)$

$$\begin{aligned} \dot{u}(t,x) - \mu_1 u''(t,x) &= g(x) && \text{for } (t,x) \in (0,0.3) \times (0,1), \\ u(0,x) &= \mu_0(x) && \text{for } x \in (0,1). \end{aligned}$$

The parameter space is chosen as $\mathscr{D} = \mathscr{D}_0 \times \mathscr{D}_1 := L_2(0,1) \times [0.5, 1.5]$. For the right-hand side, we compare two settings. The first one is $g(t,x) = g_{\mathrm{zero}}(t,x) \equiv 0$, as the a-priori error bound (22) is minimal then. The second case is an instationary smooth right-hand side $g(t,x) = g_{\sin}(t,x) = \sin(2\pi x)\cos(4\pi t)$.

Truth. We use the space-time discretization that is equivalent to the Crank-Nicolson scheme, which is stable for $\Delta x = \Delta t = 2^{-6}$, [9]. Note, that this setting also allows us to compute the inf-sup constants analytically, so that our results are not influenced by any approximation errors in the constants. Finally, as in [9], we use the natural discrete norm for $w \in \mathbb{X}^{\mathscr{N}} \subset \mathbb{X}$ given as

$$|||w|||_{\mathscr{N}}^2 := \|\bar{w}\|_{L_2(I;V)}^2 + \|\dot{w}\|_{L_2(I;V')}^2 + \|w(T)\|_H^2,$$

for $\bar{w}^k := (\Delta t)^{-1} \int_{I^k} w(t)\, dt \in V$ and $\bar{w} := \sum_{k=1}^{\mathscr{K}} \tau_k \otimes \bar{w}^k \in L_2(I;V)$.

Parameter function. For the representation of the initial value, we use the Haar wavelets, see §4.2. The approximation error, i.e., the sum of those wavelet coefficients that are not used in the approximation, is computed up to a sufficiently high fixed level. For the online computations, we used $\mu_{0,\mathrm{smooth}} := x(1-x)$, which is smooth and allows for a sparse wavelet approximation. As a second example, we chose $\mu_{0,\mathrm{L2}} := |x-0.5|^{1/2} \in L_2(0,1) \setminus H_0^1(0,1)$. The space-time formulation allows us such a non-smooth initial condition, whose wavelet coefficients reflect the singularity of the derivative at $x = 0.5$.

Evolution Greedy. The tolerance was chosen as $\mathrm{tol}_1 = 0.001$ and the training set for $\mathscr{D}_1$ was set $\mathscr{D}_1^{\mathrm{train}} := \{0.5 + k\frac{1}{17} \ : \ k = 0, \ldots, 17\}$, $|\mathscr{D}_1^{\mathrm{train}}| = 18$. We fix the maximal level $J = 6$, which turned out to yield a sufficient resolution, i.e., $|\mathbb{L}_{\mathrm{init}}| = 2^6 = 64$. The Evolution Greedy is performed $|S_J| = 2^6$ times with $\mathscr{D}^{\mathrm{train}} = \{\psi_\lambda\} \times \mathscr{D}_1^{\mathrm{train}}$ for all $|\lambda| < 6$. For both right-hand sides we obtain 4 to 5 evolution reduced bases functions. The results concerning the following quantities are displayed in Figure 1.

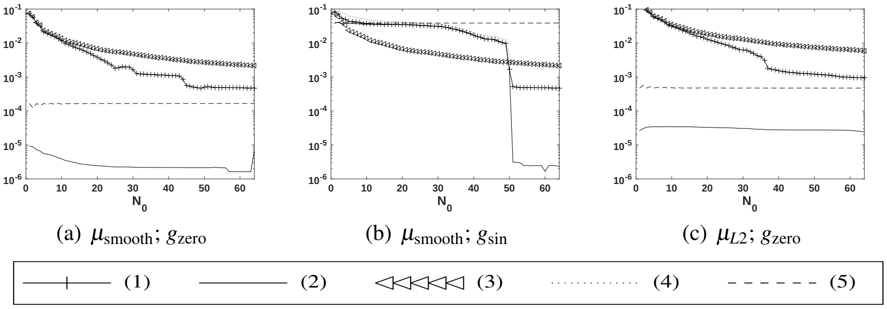
(1)	$\vert\vert\vert u(\mu) - u_{N_0+N}(\mu) \vert\vert\vert_{\mathscr{N}}$	Exact error of the RB-approximation
(2)	$\Delta_N^1(\mu)$	the RB error bound for the evolution in (20)
(3)	$\frac{1}{\beta}_{\mathrm{LB}}\big(\sum_{\lambda \notin \Lambda_N(\mu_0)} \vert d_\lambda\vert^2\big)^{1/2}$	sum of non-considered wavelet coefficients as upper bound for $\Delta_{N,0}(\mu_0)$ as in (21)
(4)	$\Delta_N^1(\mu) + \frac{1}{\beta}_{\mathrm{LB}}\big(\sum_{\lambda \notin \Lambda_N(\mu_0)} \vert d_\lambda\vert^2\big)^{1/2}$	full error bound Δ_N: sum of the latter two
(5)	Bound	a-priori bound, right-hand side of (22)

In Figure 1(a) (with smooth initial data and g_{zero}), we see almost no difference between (3) and (4), since the evolution error (estimator (2)) is very small, which should be expected for g_{zero}. Moreover, the difference between the full error estimator (4) and the true error (1) is quite small, the efficiency of the error estimator is quite good. The a-priori bound is reasonably good for $N_0 \geq 45$.

As we change the right-hand side to $g_{\sin}$ in Figure 1(b), the bound (5) immediately detects this. Until $N_0 = 50$, the error is dominated by the evolution and the error bound is quite sharp. However, as this part drops down, the initial value error (3) remains, which causes a slight decrease of efficiency.

The third case in Figure 1(c) uses a non-smooth initial data. As expected, the decay of the initial value error (3) is slow - we need many wavelets to represent μ_{L2} well. The evolution error (2) is almost negligible, which is also detected by the a-priori bound (5). However, even in this case, the full error estimator is sharp. Of course, the final RB-dimension depends on the initial value and its approximation. However, we have compared several configurations of initial value and right-hand side and found in all cases that N grows linearly with N_0 and the ratio is the same in all scenarios, [4].

In all cases, an expansion using $N_0 = 32$ wavelets already gives very good results. The detailed dimension was $\mathscr{N} = 4096$ and could be reduced to a maximum of $N = 160$, a factor of more than 25. Note, that we do not need a time-marching scheme online, but just the solution of one linear system.



(a) μ_{smooth}; g_{zero} (b) μ_{smooth}; $g_{\sin}$ (c) μ_{L2}; g_{zero}

Fig. 1 Error and estimators for different cases. Quantities (1)–(5) according to table above.

6 Conclusions

We presented a RBM for a parameter function as the initial value of a parabolic PDE. The space-time variational formulation allows us to separate the approximation of the initial condition from the error made in the evolution as time grows. We used an online adaptive wavelet approximation, which provides us with a great flexibility regarding both the size of the RB spaces as well as the approximation quality. We present an a-priori bound as well as an error estimator. Numerical results show the flexibility of the method and the efficiency of the a posteriori error bound.

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