

Two Ways to Treat Time in Reduced Basis Methods

Silke Glas, Antonia Mayerhofer and Karsten Urban

Abstract In this chapter, we compare two ways to treat the time within reduced basis methods (RBMs) for parabolic problems: Time-stepping and space-time variational based methods. We briefly recall both concepts and review well-posedness, error control and model reduction in both cases as well as the numerical realization. In particular, we highlight the conceptual differences of the two approaches.

We provide numerical investigations focussing on the performance of the RBM in both variants regarding approximation quality, efficiency and reliability of the error estimator. Pro's and Con's of both approaches are discussed.

1 Introduction

Parametrized partial differential equations (PPDEs) often occur in industrial or financial applications. If simulations are required for many different values of the involved parameters (“multi-query”), fine discretizations that are needed for a good approximation may resolve in high dimensional systems and thus in (for many applications too) long computation times. The reduced basis method (RBM) is by now a well-known model reduction technique, which allows one to efficiently reduce the numerical effort for many PPDEs by precomputing a reduced basis in an offline phase (using a detailed model, sometimes called “truth”) and evaluating the reduced model (for new parameter values) highly efficient in the online phase.

Here, we focus on time-dependent problems of parabolic type in variational formulation and describe two different approaches. The maybe more standard one is

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

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

based upon a time-stepping scheme in the offline phase. The reduced basis is then usually formed by the POD-Greedy method, [3, 5], which results in a reduced time-stepping system for the offline phase. The second approach that we wish to discuss, is based upon the space-time variational formulation of the parabolic problem, in which the time is taken as an additional variable for the variational formulation. This results in a Petrov-Galerkin problem in $d + 1$ dimensions (if d denotes the spatial dimension). The reduced basis is then formed by a standard greedy approach resulting in a reduced space-time Petrov-Galerkin method, [13, 14].

The aim of this paper is to provide a comparison of these two methods in order to identify similarities and conceptual differences of the two approaches. It complements and completes a recent similar comparison in [2] for discrete instationary problems.

The remainder of this chapter is organized as follows. We start in Section 2 by reviewing both variational formulations of parabolic PDEs. A brief survey of the RBM is contained in Section 3. Section 4 is devoted to the description of the POD-Greedy/time-stepping method for the RBM, whereas Section 5 contains the space-time RBM. Our numerical experiments as well as the comparisons are presented in Section 6. We finish with some conclusions in Section 7.

2 Variational Formulations of Parabolic Problems

Let $V \hookrightarrow H$ be separable Hilbert spaces with continuous and dense embedding. The inner products and induced norms are denoted by $(\cdot, \cdot)_H$, $(\cdot, \cdot)_V$ and $\|\cdot\|_H$, $\|\cdot\|_V$, respectively. We identify H with its dual yielding a Gelfand triple $V \hookrightarrow H \hookrightarrow V'$.

Let $0 < T < \infty$ be the final time, $I := (0, T)$ the time interval and $\Omega \subset \mathbb{R}^d$ an open domain. We consider a linear, bounded operator $A \in \mathcal{L}(V, V')$ induced by a bilinear form $a(\cdot, \cdot) : V \times V \rightarrow \mathbb{R}$ as $\langle A\phi, \psi \rangle_{V' \times V} = a(\phi, \psi)$.^a We require the bilinear form to satisfy the following properties

$$|a(\phi, \psi)| \leq M_a \|\phi\|_V \|\psi\|_V, \quad \phi, \psi \in V \quad (\text{boundedness}) \quad (1a)$$

$$a(\phi, \phi) + \lambda \|\phi\|_H^2 \geq \alpha \|\phi\|_V^2, \quad \phi \in V \quad (\text{Gårding inequality}) \quad (1b)$$

with constants $M_a < \infty$, $\alpha > 0$, $\lambda \geq 0$. Then, we consider the parabolic initial value problem

$$\dot{u}(t) + Au(t) = g(t), \quad \text{in } V', \quad u(0) = u_0 \text{ in } H, \quad (2)$$

where $g \in L_2(I; V')$ and $u_0 \in H$ are given.

^a For simplicity, we restrict ourselves to Linear Time-Invariant (LTI) systems. However, much of what is said also holds for time-variant operators $A(t)$.

Semi-Variational Formulation

The maybe more standard approach consists of multiplying (2) with a test function $\phi \in V$ and form the inner product in H (i.e., in space only). This leads to an evolution problem in V' , i.e.,

$$\text{find } u(t) \in V : (\dot{u}(t), \phi)_H + a(u(t), \phi) = (g(t), \phi)_H, \quad \phi \in V, t \in I \text{ a.e.} \quad (3)$$

It is well-known that (3) is well-posed thanks to (1), see e.g. [15, Thm. 26.1]. Since the variational formulation is w.r.t. space only, we call it *semi-variational*.

Space-Time Variational Formulation

We now follow [12] for the description of a variational formulation of (2) w.r.t. space and time. This leads to a variational problem with different trial and test spaces \mathbb{X} and \mathbb{Y} , both being Bochner spaces, namely

$$\mathbb{X} := L_2(I; V) \cap H^1(I; V') = \{v \in L_2(I; V) : v, \dot{v} \in L_2(I; V')\}, \quad \mathbb{Y} := L_2(I; V) \times H,$$

with norms $\|v\|_{\mathbb{X}}^2 := \|v\|_{L_2(I; V)}^2 + \|\dot{v}\|_{L_2(I; V')}^2$ and $\|v\|_{\mathbb{Y}}^2 := \|v_1\|_{L_2(I; V)}^2 + \|v_2\|_H^2$, $v = (v_1, v_2) \in \mathbb{Y}$. Since $\mathbb{X} \hookrightarrow C(I; H)$, see, e.g. [15, Thm. 25.5], $u(0) \in H$ is well-defined for $u \in \mathbb{X}$.

The space-time variational formulation arises by multiplying (2) with test functions $v \in \mathbb{Y}$ and integrating w.r.t. time and space. This yields the linear operator $B \in \mathcal{L}(\mathbb{X}, \mathbb{Y}')$ defined as $\langle Bu, v \rangle_{\mathbb{Y}' \times \mathbb{Y}} = b(u, v)$ by (we omit the dependence on t in the integrands in the sequel)

$$b(u, v) := \int_I \langle \dot{u} + Au, v_1 \rangle_{V' \times V} dt + (u(0), v_2)_H, \quad u \in \mathbb{X}, v = (v_1, v_2) \in \mathbb{Y},$$

i.e., $b(\cdot, \cdot) : \mathbb{X} \times \mathbb{Y} \rightarrow \mathbb{R}$ and the right-hand side $f \in \mathbb{Y}'$ is defined by

$$\langle f, v \rangle_{\mathbb{Y}' \times \mathbb{Y}} := \int_I \langle g, v_1 \rangle_{V' \times V} dt + (u_0, v_2)_H, \quad v = (v_1, v_2) \in \mathbb{Y}.$$

Then, the space-time variational formulation of (2) reads

$$\text{find } u \in \mathbb{X} : \langle Bu, v \rangle_{\mathbb{Y}' \times \mathbb{Y}} = \langle f, v \rangle_{\mathbb{Y}' \times \mathbb{Y}}, \quad \forall v \in \mathbb{Y}. \quad (4)$$

Again, (1) yields well-posedness, e.g. [12, Thm. 5.1]. In fact, the operator B is boundedly invertible. The injectivity of the operator B is equivalent to

$$\beta_b := \inf_{w \in \mathbb{X}} \sup_{v \in \mathbb{Y}} \frac{|b(w, v)|}{\|w\|_{\mathbb{X}} \|v\|_{\mathbb{Y}}} > 0, \quad (\text{inf-sup condition}). \quad (5)$$

3 Parametrized Problems and the RBM

We introduce a general notation here, which will then be specified for both variational formulations. Let \mathcal{X}, \mathcal{Y} be Hilbert spaces, $\mu \in \mathcal{P} \subset \mathbb{R}^p$ a parameter and consider *parametric* forms $c : \mathcal{X} \times \mathcal{Y} \times \mathcal{P} \rightarrow \mathbb{R}$ as well as $h : \mathcal{Y} \times \mathcal{P} \rightarrow \mathbb{R}$. Then, the parameterized Petrov-Galerkin problem reads

$$\text{find } u(\mu) \in \mathcal{X} : c(u(\mu), v; \mu) = h(v; \mu) \quad \forall v \in \mathcal{Y}. \quad (6)$$

This framework obviously also includes the elliptic case $\mathcal{Y} = \mathcal{X}$. We briefly review the main ingredients of the RBM and refer to [6, 10] for recent surveys.

It is always assumed that a detailed discretization is available in the following sense: Let $\mathcal{X}^{\mathcal{N}} \subset \mathcal{X}$ and $\mathcal{Y}^{\mathcal{N}} \subset \mathcal{Y}$ be subspaces of finite, but large, dimension \mathcal{N} . The detailed problem (sometimes called “truth”) then reads

$$\text{find } u^{\mathcal{N}}(\mu) \in \mathcal{X}^{\mathcal{N}} : c(u^{\mathcal{N}}(\mu), v^{\mathcal{N}}; \mu) = h(v^{\mathcal{N}}; \mu) \quad \forall v^{\mathcal{N}} \in \mathcal{Y}^{\mathcal{N}}. \quad (7)$$

The “truth” solution $u^{\mathcal{N}}(\mu)$ is always assumed to be sufficiently close to $u(\mu)$. For well-posedness and stability of (7), a uniform inf-sup condition is required, e.g. [9].

The next step is the computation of a reduced basis formed by “snapshots” $\xi^i := u^{\mathcal{N}}(\mu^i)$, $1 \leq i \leq N \ll \mathcal{N}$, where the snapshot parameters $\mu^i \in \mathcal{P}$ are e.g. determined by a greedy procedure w.r.t. an efficiently computable error estimate $\Delta_N(\mu)$. The reduced trial space is then defined as $\mathcal{X}_N := \text{span}\{\xi^1, \dots, \xi^N\}$ and one needs some stable (possibly parameter-dependent) test space $\mathcal{Y}_N(\mu)$. The reduced problem reads

$$\text{find } u_N(\mu) \in \mathcal{X}_N : c(u_N(\mu), v_N; \mu) = h(v_N; \mu) \quad \forall v_N \in \mathcal{Y}_N(\mu). \quad (8)$$

In the above setting, it is easy to derive an error estimate which also results in the required error estimator $\Delta_N(\mu)$ defined by

$$\|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_{\mathcal{X}} \leq \frac{1}{\beta_c} \|r_N(\cdot; \mu)\|_{\mathcal{Y}} =: \Delta_N(\mu), \quad (9)$$

where $r_N(v; \mu) := h(v; \mu) - c(u_N(\mu), v; \mu) = c(u^{\mathcal{N}}(\mu) - u_N(\mu), v; \mu)$, $v \in \mathcal{Y}^{\mathcal{N}}$, is the *residual* and β_c is the inf-sup constant associated with the bilinear form c .

We call (8) *online efficient* if it can be solved with complexity independent of \mathcal{N} . In order to reach that goal, the following assumption is crucial: The forms are assumed to be separable in the parameter (sometimes called *affine decomposition*),

$$c(u, v; \mu) = \sum_{q=1}^{Q_c} \theta_q^c(\mu) c_q(u, v), \quad h(v; \mu) = \sum_{q=1}^{Q_h} \theta_q^h(\mu) h_q(v) \quad (10)$$

for some $Q_c, Q_h \in \mathbb{N}$, functions $\theta_q^c, \theta_q^h : \mathcal{P} \rightarrow \mathbb{R}$ and parameter-independent forms c_q, h_q that can be precomputed in the offline phase. The parameter-dependent functions θ_q^c, θ_q^h are assumed to be computable online efficient, i.e., with complexity independent of \mathcal{N} .

4 Reduced Basis Methods with POD-Greedy

We start from the semi-variational formulation (3) and apply a semi-discretization in time, known as Rothe's method. To this end, set $\Delta t := \frac{T}{K}$ for some $K > 1$, $t^k := k\Delta t$ and we seek some approximation $u^k \approx u(t^k)$, where we omit the μ -dependency to shorten notation. This leads to a sequence of elliptic (time-independent) ordinary differential equations starting with $u^0 := u_0$. The standard θ -scheme then reads

$$\begin{aligned} \frac{1}{\Delta t} (u^{k+1} - u^k, v)_H + a(\theta u^{k+1} + (1-\theta)u^k, v; \mu) \\ = \theta g(v, t^{k+1}; \mu) + (1-\theta)g(v, t^k; \mu), \quad v \in V. \end{aligned}$$

“Truth”. The next step is a discretization in space by a standard Galerkin method using finite-dimensional spaces $V_h \subset V$ with large $\dim(V_h) = \mathcal{N}_h \in \mathbb{N}$. Then, the detailed or “truth” problem for a given parameter $\mu \in \mathcal{P}$ reads for an initial value $u_h^0 := \text{Proj}_{V_h} u^0$ to find $u_h^{k+1}(\mu) \in V_h$, such that for $v_h \in V_h$,

$$\begin{aligned} (u_h^{k+1}, v_h)_H + \Delta t \theta a(u_h^{k+1}, v_h; \mu) \\ = (u_h^k, v_h)_H + \Delta t (1-\theta) a(u_h^k, v_h; \mu) + \theta g(v_h, t^{k+1}; \mu) + (1-\theta)g(v_h, t^k; \mu), \end{aligned}$$

for $0 \leq k \leq K-1$. If $V_h = \text{span}\{\phi_i : i = 1, \dots, \mathcal{N}_h\}$, the latter equation can be written in matrix-vector form as follows. Let $M_h^{\text{space}} := [(\phi_i, \phi_j)_H]_{i,j=1, \dots, \mathcal{N}_h}$ denote the spatial mass matrix and $A_h^{\text{space}} := [a(\phi_i, \phi_j)]_{i,j=1, \dots, \mathcal{N}_h}$ the stiffness matrix, then we look for

$$u_h^{k+1} = \sum_{i=1}^{\mathcal{N}_h} \alpha_i^{k+1} \phi_i, \quad \alpha^{k+1} := (\alpha_i^{k+1})_{i=1, \dots, \mathcal{N}_h},$$

such that (with g^k and α_0 being the expansion coefficients of $g(t^k)$ and u_0)

$$\begin{aligned} (M_h^{\text{space}} + \theta \Delta t A_h^{\text{space}}(\mu)) \alpha^{k+1} = \\ = (M_h^{\text{space}} + (1-\theta) \Delta t A_h^{\text{space}}) \alpha^k + \Delta t (\theta g^{k+1} + (1-\theta)g^k), \end{aligned} \quad (11)$$

for $0 \leq k \leq K-1$ as well as $\alpha^0 := \alpha_0$. It is well-known that the θ -scheme is unconditionally stable for $\frac{1}{2} \leq \theta \leq 1$, whereas for $0 \leq \theta < \frac{1}{2}$ the space discretization has to satisfy additional properties, see e.g. [11, Thm. 11.3.1]. The choice $\theta = \frac{1}{2}$ results in the Crank-Nicolson scheme. Note, that (11) requires to solve a well-posed elliptic problem for each time step k , which easily follows from the assumption (1) on the bilinear form a and coercivity of $m(\phi, \psi) := (\phi, \psi)_H$. In fact, this implies that the matrix $M_h^{\text{space}} + \theta \Delta t A_h^{\text{space}}(\mu)$ is positive definite, e.g. [11, §11.3].

The system (11) is offline/online decomposable which is easily seen as long as the forms a and g are separable in the parameter. In fact, the mass inner product m is independent of the parameter.

Reduced Basis via POD-Greedy. The reduced basis is computed by the POD-Greedy method shown in Algorithm 1. This is a combination of the standard greedy

algorithm for the parameter search and a Proper Orthogonal Decomposition (POD) in time to select the time step containing the maximal information of the trajectory for the given parameter.

Algorithm 1 POD-Greedy algorithm, [5]

Require: Given $N_{\max} > 0$, $\mathcal{P}_{\text{train}} \subset \mathcal{P}$, $\varepsilon_{\text{tol}}, \ell = 1$

- 1: choose arbitrarily $\mu^\ell \in \mathcal{P}_{\text{train}}$; set $\Psi_\ell := \left\{ \frac{u^0(\mu^\ell)}{\|u^0(\mu^\ell)\|_V} \right\}$, $V_\ell := \text{span}(\Psi_\ell)$
- 2: **while** $\max_{\mu \in \mathcal{P}_{\text{train}}} \Delta_\ell(\mu) > \varepsilon_{\text{tol}}$ **do**
- 3: define $\mu^{\ell+1} := \arg\max_{\mu \in \mathcal{P}_{\text{train}}} \Delta_\ell(\mu)$
- 4: define $\tilde{\Psi}_{\ell+1} := \text{POD}\{u^k(\mu^{\ell+1}) - \text{Proj}_{V_\ell}(u^k(\mu^{\ell+1}))\}_{k=0, \dots, K}$
- 5: define $\Psi_{\ell+1} := \text{orthonormalize}(\Psi_\ell \cup \{\tilde{\Psi}_{\ell+1}\})$, $V_{\ell+1} := \text{span}(\Psi_{\ell+1})$, $\ell = \ell + 1$
- 6: **end while**
- 7: define $V_N := V_\ell$, $N_V := \dim(V_N)$
- 8: **return** V_N, N_V ;

Online Phase. The POD-Greedy method produces a reduced space $V_N \subset V$ of possibly small dimension $N := N_{\text{POD-G}} \ll \mathcal{N}_h$. Then, a reduced basis approximation for a new parameter $\mu \in \mathcal{P}$ is determined by a corresponding time-stepping scheme as follows. The reduced initial value $u_N^0 \in V_N$ is computed by $(u_N^0 - u_0, v_N)_V = 0$ for all $v_N \in V_N$. Then, for $0 \leq k \leq K - 1$, determine $u_N^{k+1}(\mu) \in V_N$ by

$$\frac{1}{\Delta t} (u_N^{k+1} - u_N^k, v_N)_H + a(\theta u_N^{k+1} + (1 - \theta)u_N^k, v_N; \mu) = f(v_N; \mu), \quad v_N \in V_N.$$

Obviously, this amounts solving a sequence of K reduced problems online.

Error Estimator/Indicator. As in the standard case in Section 3, an online efficient error estimator is needed both in Algorithm 1 and online for the desired certification of the RB approximation. Of course, such an estimator here also needs to incorporate the temporal evolution. In fact, there are several known choices for $\Delta_N(\mu)$ in Algorithm 1. A standard estimator for the error $e^k(\mu) := u_h^k(\mu) - u_N^k(\mu)$ at final time $T = t^K$ is given by, [4, Prop. 3.9]

$$\|e^K(\mu)\|_V \leq \|e^0(\mu)\|_V \left(\frac{\gamma_{\text{UB}}}{\alpha_{\text{LB}}} \right)^K + \sum_{k=0}^{K-1} \frac{\Delta t}{\alpha_{\text{LB}}} \left(\frac{\gamma_{\text{UB}}}{\alpha_{\text{LB}}} \right)^{K-k-1} \|r_N^k(\mu)\|_{V'} =: \Delta_N^K(\mu). \quad (12)$$

Here, α_{LB} is a lower bound for the coercivity constant of the implicit part of the operator, γ_{UB} an upper bound for the continuity constant of the explicit part and $r_N^k(\mu)$ is the residual at time step t^k . It can easily be seen that Δ_N^K is offline/online decomposable. There are some remarks in order.

Remark 1. (i) In our numerical experiments in Section 6 below, we use a finite element (FE) discretization. In that case, the estimator (12) can not be used. In fact, if $\alpha_{\text{LB}} < \gamma_{\text{UB}}$, then $\Delta_N^K(\mu)$ grows quickly with increasing K . This happens for FE discretizations in $V = H_0^1(\Omega)$, which we use here.

- (ii) For *symmetric* differential operators, the above estimate can be sharpened, [4, Prop. 3.11]. It allows to extend (12) to a μ -dependent norm on the whole trajectory. \diamond

According to this remark, we cannot use $\Delta_N^K(\mu)$ here. Thus, we follow the analysis in [4] and consider a weighted (sometimes called “space-time”) norm for $\omega := (\omega_k)_{k=0,\dots,K-1}$, $\omega_k > 0$ and $\sum_{k=0}^{K-1} \omega_k = T$ defined as

$$|e|_{\omega}^2 := \sum_{k=0}^{K-1} \omega_k \|e^k\|_V^2, \quad e = (e^k)_{k=0,\dots,K-1}. \quad (13)$$

A corresponding error *indicator* is defined as

$$\Delta_{N,\omega}^{\text{PST}} := \left(\sum_{k=0}^{K-1} \omega_k \|r_N^k(\mu)\|_{V'}^2 \right)^{1/2}. \quad (14)$$

The term “indicator” means that the error (in whatever norm) cannot be proven to be bounded in terms of $\Delta_{N,\omega}^{\text{PST}}$. However, even though the error of the POD-Greedy scheme cannot be guaranteed to decay monotonically, exponential convergence can be shown under additional assumptions, [3].

5 Space-Time Reduced Basis Methods

As we have seen in Section 2, the space-time variational formulation leads to a parameterized Petrov-Galerkin problem. Thus, the form is exactly as in the general RB-framework in (6). Note, that both $\mathbb{X} = H_{\{0\}}^1(I) \otimes V$ and $\mathbb{Y} = (L_2(I) \otimes V) \times H$ are tensor products, so that it is convenient to use the same structure for the detailed discretization, i.e., $\mathbb{X}^{\mathcal{N}} = S_{\Delta t} \otimes V_h$ and $\mathbb{Y}^{\mathcal{N}} = (Q_{\Delta t} \otimes V_h) \times V_h^b$, where $V_h \subset V$ is the space discretization as in Section 4 above and $S_{\Delta t} \subset H_{\{0\}}^1(I)$ as well as $Q_{\Delta t} \subset L_2(I)$ are temporal discretizations of step size Δt , [14].

Let us denote again by $V_h = \text{span}\{\phi_1, \phi_2, \dots, \phi_{\mathcal{N}_h}\}$ the detailed space discretization (e.g. by piecewise linear finite elements for $V = H_0^1(\Omega)$). Moreover, let $S_{\Delta t} = \text{span}\{\sigma^0, \sigma^1, \dots, \sigma^K\}$ and $Q_{\Delta t} = \text{span}\{\tau^1, \tau^2, \dots, \tau^K\}$ be the bases in time (e.g. piecewise linear σ^i and piecewise constant τ^i on the same temporal mesh, with the additional σ^0 for the initial value at $t = 0$).

The dimension of the arising test and trial spaces coincide, i.e., $\dim(\mathbb{X}^{\mathcal{N}}) = (K + 1)\mathcal{N}_h = \dim(\mathbb{Y}^{\mathcal{N}}) =: \mathcal{N}$. Exploiting the structure of the discretized spaces for the detailed solution $u^{\mathcal{N}} = \sum_{i=1}^{\mathcal{N}_h} \sum_{k=0}^K u_i^k \sigma^k \otimes \phi_i$ yields

^b It can be seen that $V_h \subset V \Leftrightarrow H$ is in fact sufficient, [8].

$$\begin{aligned} b(u^{\mathcal{N}}, (\tau^k \otimes \phi_j, 0); \mu) &= \sum_{i=1}^{\mathcal{N}_h} [(u_i^k - u_i^{k-1})(\phi_i, \phi_j)_H + \frac{\Delta t}{2} (u_i^k + u_i^{k-1})a(\phi_i, \phi_j; \mu)] \\ &= M_h^{\text{space}}(u^k - u^{k-1}) + \Delta t A_h^{\text{space}}(\mu) u^{k-1/2}, \end{aligned}$$

with mass and stiffness matrices $M_h^{\text{space}}, A_h^{\text{space}}(\mu)$ as above. On the right-hand side, we use a trapezoidal approximation as in [14] on a time grid $0 = t^0 < \dots < t^K = T$, $I^\ell := [t^{\ell-1}, t^\ell] = \text{supp}\{\tau^\ell\}$:

$$\begin{aligned} f((\tau^\ell \otimes \phi_j, 0); \mu) &= \int_I \langle g(t; \mu), \tau^\ell \otimes \phi_j(t, \cdot) \rangle_{V' \times V} dt = \int_{I^\ell} \langle g(t; \mu), \tau^\ell(t) \phi_j \rangle_{V' \times V} dt \\ &\approx \frac{\Delta t}{2} \langle g(t^{\ell-1}; \mu) + g(t^\ell; \mu), \phi_j \rangle_{V' \times V}. \end{aligned}$$

It turns out that this particular choice for the discretization results (again) in the Crank-Nicolson scheme involving an additional projection of the initial value, which requires a CFL condition to ensure stability. A detailed investigation of stable space-time discretizations can be found in [1].

Since the space-time variational approach yields a standard Petrov-Galerkin problem, the reduced basis trial and test spaces $\mathbb{X}_N = \text{span}\{\xi^1, \dots, \xi^N\}$, $\mathbb{Y}_N(\mu) := \text{span}\{\eta^1(\mu), \dots, \eta^N(\mu)\}$ can be constructed exactly following the road map in Section 3. Hence, we end up with a reduced problem of the form (8). In matrix-vector form, the resulting system matrix $B_N(\mu) := [b(\xi^i, \eta^j(\mu); \mu)]_{i,j=1,\dots,N}$ is of small dimension, but not symmetric. Moreover, $B_N(\mu)$ is uniformly invertible provided that the inf-sup condition in (5) holds for the RB spaces. It is not difficult to show that the arising non-symmetric linear system can also be written as minimization problem or in terms of normal equations (see [8] for details and further applications).

If normal equations are used, no (parameter dependent) reduced test space computation is required: Let $\mathbb{X}^{\mathcal{N}} = \text{span}\{\varphi_\ell : \ell = 1, \dots, \mathcal{N}\}$ and $\mathbb{Y}^{\mathcal{N}} = \text{span}\{\psi_m : m = 1, \dots, \mathcal{N}\}$ be the detailed bases, denote by $Y^{\mathcal{N}} := [(\psi_m, \psi_{m'})_{\mathbb{Y}}]_{m,m'=1,\dots,\mathcal{N}}$ the mass matrix of the test space $\mathbb{Y}^{\mathcal{N}}$ as well as the detailed system matrix by $B^{\mathcal{N}}(\mu) := [b(\varphi_\ell, \psi_m; \mu)]_{\ell,m=1,\dots,\mathcal{N}}$. Next, denote by $\xi^j = \sum_{\ell=1}^{\mathcal{N}} c_\ell^j \varphi_\ell$, $C := (c_\ell^j)_{\ell=1,\dots,\mathcal{N}, j=1,\dots,N} \in \mathbb{R}^{\mathcal{N} \times N}$ the expansion of the RB functions in terms of the detailed basis. Then,

$$B_N(\mu) := C^T B^{\mathcal{N}}(\mu) (Y^{\mathcal{N}})^{-1} (B^{\mathcal{N}}(\mu))^T C, \quad f_N(\mu) := C^T B^{\mathcal{N}}(\mu) (Y^{\mathcal{N}})^{-1} f^{\mathcal{N}}(\mu),$$

where $f^{\mathcal{N}}(\mu)$ contains the detailed basis coefficients of the right-hand side. The RB approximation $u_N(\mu) = \sum_{i=1}^N \alpha_i(\mu) \xi^i$, $\alpha(\mu) := (\alpha_i(\mu))_{i=1,\dots,N}$, is then determined by the solution of the linear system of size N , i.e.

$$B_N(\mu) \alpha(\mu) = f_N(\mu). \tag{15}$$

One can show that (15) admits an online/offline-separation, which is inherited from the separation of the forms a and g (in particular, we have $Q_b = Q_a$ and $Q_f = Q_g$). This means that (15) can be solved online efficient. Finally, the inf-sup stability of (15) is inherited from the detailed discretization.

6 Numerical Results

We provide some of our numerical investigations concerning the two approaches described above for a standard diffusion-convection-reaction problem with time dependent right-hand side. Since our focus is on the treatment of the time variable, we restrict ourselves to a 1d problem in space.

6.1 Data

Model problem. Let $d = 1$, $\Omega = (0, 1)$ and $V := H_0^1(\Omega) \hookrightarrow L_2(\Omega) =: H$. Consider the time interval $I = (0, 0.3)$ and the parameter set $\mathcal{P} := [0.5, 1.5] \times [0, 1] \times [0, 1] \subset \mathbb{R}^3$. For a parameter $\mu = (\mu_1, \mu_2, \mu_3)^T \in \mathcal{P}$ find $u \equiv u(\mu)$ that solves

$$\dot{u} - \mu_1 u'' + \mu_2 u' + \mu_3 u = g \quad \text{on } I \times \Omega, \quad (16a)$$

$$u(t, x) = 0 \quad \forall (t, x) \in I \times \partial\Omega, \quad (16b)$$

$$u(0, x) = u_0(x) := \sin(2\pi x) \quad \forall x \in \Omega. \quad (16c)$$

We set $g(t, x) := \sin(2\pi x)((4\pi^2 + 0.5) \cos(4\pi t) - 4\pi \sin(4\pi t)) + \pi \cos(2\pi x) \cos(4\pi t)$ for the right-hand side, which corresponds to the solution $u(t, x) := \sin(2\pi x) \cos(4\pi t)$ of (16) for $\mu^{\text{ref}} = (1, 0.5, 0.5) \in \mathcal{P}$. The parameter-separability is easily seen. We divide both Ω and I into 2^6 subintervals, i.e., $\mathcal{N}_h = 2^6 - 1$ and $K = 2^6$. The training set $\mathcal{P}_{\text{train}}$ is chosen as 17 equidistantly distributed points in \mathcal{P} in each direction.

“True” Norms. For the space-time RBM, the “true” error is measured in the natural discrete space-time norm, [13]

$$\|v\|_{\mathcal{N}}^2 := \|\bar{v}\|_{L_2(I;V)}^2 + \|\dot{v}\|_{L_2(I;V')}^2 + \|v(T)\|_H^2, \quad v \in \mathbb{X}^{\mathcal{N}} \subset \mathbb{X},$$

where $\bar{v} := \sum_{k=1}^K \tau^k \otimes \bar{v}^k \in L_2(I;V)$ and $\bar{v}^k := (\Delta t)^{-1} \int_{I^k} v(t) dt \in V$. Note, that $\|\bar{v}\|_{L_2(I;V)}$ is an $\mathcal{O}(\Delta t)$ -approximation of the $\mathbb{V} := L_2(I;V)$ -norm (due to the piecewise constant approximation \bar{v}^k).

For the POD-Greedy strategy, we consider the final time contribution $\|v(T)\|_V$ (corresponding to the left-hand side of (12)) as well as the “space-time norm” introduced in (13) for the specific weights $\omega_k := \Delta t$, $k = 0, \dots, K-1$, plus the final time contribution as “true” error, i.e.

$$|v|_{\Delta t}^2 := |(v(t^k))_{k=0, \dots, K-1}|_{\omega}^2 + \Delta t \|v(T)\|_V^2 = \sum_{k=0}^K \Delta t \|v(t^k)\|_{\bar{v}}^2.$$

This means that $|\cdot|_{\Delta t}$ is an $\mathcal{O}(\Delta t^2)$ -approximation of the $\mathbb{V} := L_2(I;V)$ -norm.

Remark 2. For later reference, we point out the fact that $|\cdot|_{\Delta t}$ is an $\mathcal{O}(\Delta t^2)$ -approximation of the norm $\|\cdot\|_{\mathbb{V}}$, whereas $\|\bar{v}\|_{L_2(I;V)}$ is only of the order $\mathcal{O}(\Delta t)$.

This means that it may happen that $|v|_{\Delta t} > \|v\|_{\mathcal{N}}$ even though $\|w\|_{\mathbb{X}} > \|w\|_{\mathbb{V}}$ for all $0 \neq w \in \mathbb{X}$. \diamond

Error Estimators/Greedy. For the error estimation in the space-time RBM, we use the residual-based error estimator $\Delta_N(\mu)$ in (9) with numerically estimated lower bound for the inf-sup constant, $\beta_{\text{LB}} = 0.2$. Of course, this is a relatively rough bound (independent of μ !) and performing e.g. a Successive Constraint Method (SCM, [7]) would improve the subsequent results. For the POD-Greedy scheme, we use the space-time error indicator $\Delta_N^{\text{PST}}(\mu)$ that arises from (14) by the choice $\omega_k \equiv \Delta t$ for the weights.

We emphasize that $\Delta_N(\mu)$ bounds the norm in $\mathbb{X} = H_{\{0\}}^1(I) \otimes V \subsetneq \mathbb{V} = L_2(I; V)$, whereas $\Delta_N^{\text{PST}}(\mu)$ is “only” an indicator, in particular it is not known to be an upper bound for any norm. In view of (12), we could expect that $\|e^K(\mu)\|_V$ might be a candidate, or –since $|\cdot|_{\Delta t}$ is a discrete $L_2(I; V)$ -norm– we could consider $\|e\|_{L_2(I; V)}$.

Comparison. We conclude that a direct and fair comparison is not easy because of the described methodological differences. Table 1 collects these differences and our choice for the experiments.

| | snapshot space | RB space | “true” error | error estimated by |
|------------|----------------------------------|----------------|---------------------------|---|
| space-time | $\mathbb{X}^{\mathcal{N}}$ | \mathbb{X}_N | $\ \cdot\ _{\mathcal{N}}$ | residual based, $\Delta_N(\mu)$ in (9) |
| POD-Greedy | $\{t^0, \dots, t^K\} \times V_h$ | V_N | $ \cdot _{\Delta t}$ | indicator $\Delta_N^{\text{PST}}(\mu)$ in (14) for $\omega_k \equiv \Delta t$ |

Table 1 Differences of space-time RBM and POD-Greedy sampling.

6.2 Results

Greedy Training. Within the framework of Table 1, the offline greedy error decay of both variants is shown in Figure 1. The red lines correspond to the space-time form, whereas the blue lines are for the POD-Greedy. Straight lines indicate the error, dotted ones the error estimator/indicator. The left figure shows the weak greedy using the error estimators/indicators. We observe exponential decay w.r.t. the RB dimension N in both cases – as predicted by the theory. At a first glance, it seems that the decay of POD-Greedy is much faster than the one for space-time. Note, however, that the online effort is related to N in a different way for both variants, see below. As mentioned above, the two variants are related to different norms. This is the reason why we performed a strong greedy using the $\|\cdot\|_{\mathcal{N}}$ -norm for both variants (right graph in Figure 1). We see a similar behavior – again referring to the different online work load. It is interesting, though, that at least in these experiments, POD-Greedy works very well even for the full norm – without theoretically foundation though. However, we can also see from the results that $\Delta_N^{\text{PST}}(\mu)$ is not an error bound since it is below the “exact” error for some N . Recall that $\Delta_N^{\text{PST}}(\mu)$ arises from the upper bound $\Delta_N^K(\mu)$ in (12) by setting involved coercivity and continuity constants to 1.

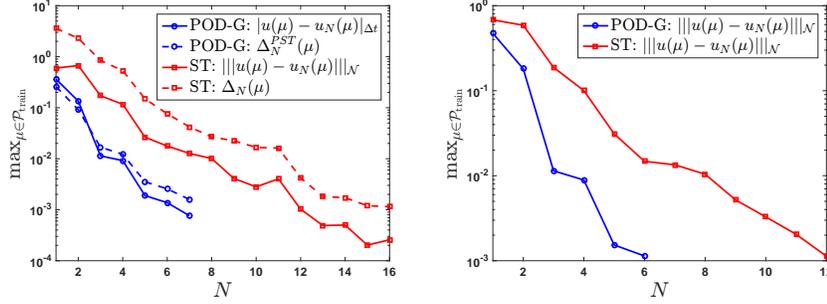


Fig. 1 RB-Greedy approximation error. Red: Space-Time (ST); blue: POD-Greedy (POD-G). Left: weak greedy, right: strong greedy w.r.t. $\|\cdot\|_{\mathcal{N}}$.

Moreover, note, that in the same spirit, we could easily lower the gap between the two red space-time lines by sharpen β_{LB} . The prescribed greedy-tolerance of 10^{-3} is reached for $N_{\text{POD-G}} = 6$ for POD-Greedy and for $N_{\text{ST}} = 12$ for space-time.

Online Phase. We test the RB approximations for two cases, namely for $\mathcal{P}_{\text{test}}^{\text{sym}} := \{(\mu_1, 0, 0) : \mu_1 \in [0.5, 1.5]\}$ (symmetric case) and $\mathcal{P}_{\text{test}}^{\text{non}} := \{(0.5, \mu_2, 0.75) : \mu_2 \in [0, 1]\}$ (non-symmetric case). The results are shown in Figure 2, the symmetric case in the top line, the non-symmetric in the bottom one.

First of all, both variants work as they should in the sense that the respective error measures are below the greedy tolerance of 10^{-3} .

The “true” error (solid red lines) is slightly smaller for the space-time variant in the symmetric case and very close to each other in the non-symmetric case.

We also compare the POD-Greedy error measure $|\cdot|_{\Delta_t}$. It is remarkable that this quantity is almost identical to $\|\cdot\|_{\mathcal{N}}$ for space-time. This means that the temporal derivative and the final time components of the solution are very-well approximated. Finally, regarding the result that for POD-Greedy the $|\cdot|_{\Delta_t}$ -lines turn out to be above the $\|\cdot\|_{\mathcal{N}}$ one, we recall Remark 2.

Finally, the error estimators/indicators are plotted as dash-dotted black lines. We observe, that the effectivities^c are of almost the same size. However, if we rely on the respective theory (i.e. $\|e\|_{\mathcal{N}}$ for space-time and $\|e(T)\|_V$ for POD-Greedy), the effectivity of space-time improves, see Figure 3.

Work Load/Effort. Finally, we compare the computational effort as well as the storage amount (offline and online) of both variants, see Table 2.

We recall that our chosen space-time method in the offline phase reduces to the Crank-Nicholson scheme. Hence, the offline complexities and storage requirements for the detailed solution of both variants indeed coincide (both linear in \mathcal{N}_h ; we count $187 \approx 3\mathcal{N}_h$ elements). The detailed solution requires K solves (corresponding to the number of time steps) of a sparse system of size \mathcal{N}_h . However, the space-time precomputations needed to form the online system, rely on the full dimension \mathcal{N} .

^c It is somehow misleading to use the term “effectivity” within the POD-Greedy framework, since usually effectivity is the ratio of *error bound* and error.

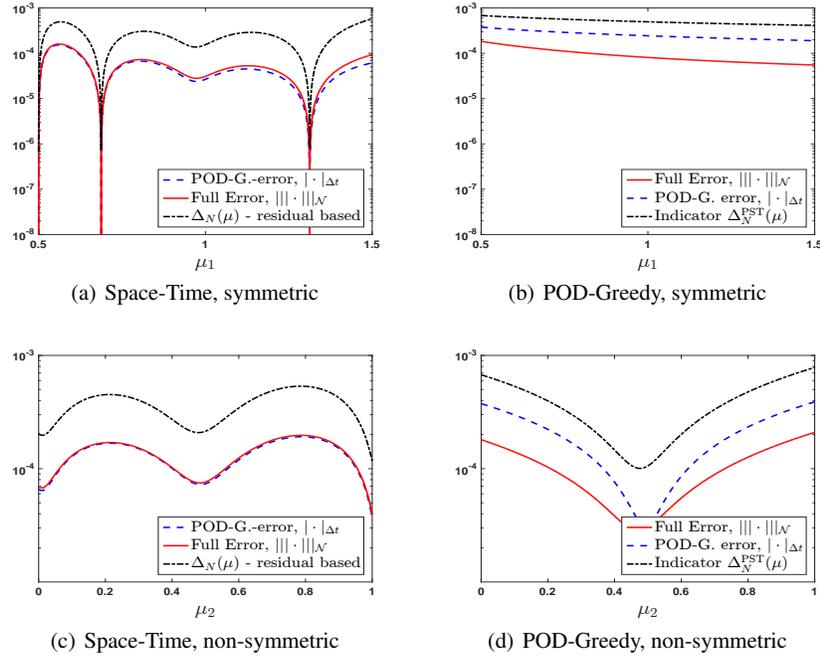


Fig. 2 RB approximation error on $\mathcal{P}_{\text{test}}$: Full error (red, solid), error estimator/indicator (black, dash-dotted) and the POD-Greedy error measure $|\cdot|_{\Delta t}$ (blue, dashed) for greedy tolerance $\tau_{\text{ol}} = 0.001$. Top line: symmetric case $(\mu_1, 0, 0)$; bottom: non-symmetric $(0.5, \mu_2, 0.75)$.

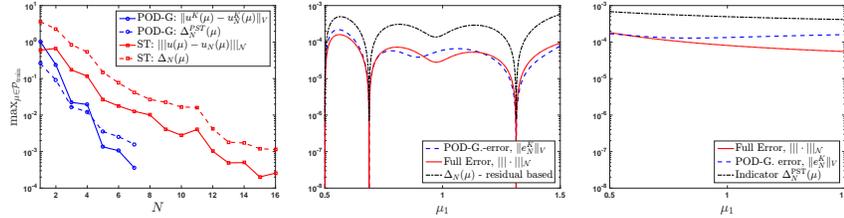


Fig. 3 Greedy error decay (left), space-time (middle) and POD-Greedy (right) using the final time for POD-Greedy training and error measure on the symmetric test set.

In the online-phase, POD-Greedy needs to store (for the LTI case) Q_a reduced matrices and KQ_g vectors of size $N_{\text{POD-G}}$ for the time-dependent right-hand side. The RB solution amounts to solve K densely populated reduced systems. In the LTI case, one may reduce this to the computation of one LU-decomposition and then K triangular systems, i.e., $\mathcal{O}(N_{\text{POD-G}}^3 + KN_{\text{POD-G}}^2)$ operations.

The space-time method usually requires more storage, either by storing a suitable test space or –as described above– by the setup of the normal equations using the affine decomposition (10). The normal equations need memory of size $\mathcal{O}(Q_b^2 N_{\text{ST}}^2 +$

| $\mathcal{O}() / \#$ | POD-Greedy | | Space-Time | |
|----------------------|------------------------------|---|------------------------------|--|
| | offline | online | offline | online |
| Solution | $K\mathcal{N}_h$ 4.032 | $N_{\text{POD-G}}^3 + KN_{\text{POD-G}}^2$ 2.520 | $K\mathcal{N}_h$ 4.032 | N_{ST}^3 1.728 |
| Storage | $\sim 3\mathcal{N}_h$ 187 | $Q_a N_{\text{POD-G}}^2 + KQ_g N_{\text{POD-G}}$ 528 | $\sim 3\mathcal{N}_h$ 187 | $Q_b^2 N_{\text{ST}}^2 + Q_b Q_f N_{\text{ST}}$ 2.352 |

Table 2 Offline and online effort of the RBMs. In our case, we have $N_{\text{POD-G}} = 6$, $N_{\text{ST}} = 12$, $\mathcal{N}_h = 63$, $Q_a = Q_b = 4$, $Q_f = Q_g = 1$, $K = 64$; the corresponding numbers are given in the respective 2nd row.

$Q_b Q_f N_{\text{ST}}$). The RB-solution requires the solution of one reduced linear system of dimension N_{ST} .

7 Conclusions

We have explained and compared both theoretically and numerically two different techniques to treat the time within the Reduced Basis Method (RBM). It is obvious that a fair and significant numerical comparison is a delicate task. In particular,

- different norms need to be considered;
- the choice of the error estimator/indicator within the POD-Greedy method has a significant impact;
- improving bounds for the involved constants will significantly improve the results;
- we only consider such space-time methods that are equivalent to a time marching scheme (here Crank-Nicholson). If this is not the case, the offline cost for the space-time scheme will significantly increase;
- $K = 64$ is a quite moderate number of time steps. The comparison may change for larger K and/or longer time horizons $[0, T]$;
- we only consider LTI-systems. Both the reduction rate and the storage depend on this assumption.

Despite all these facts, we do think that our study indeed shows some facts, namely:

1. The POD-Greedy method allows one to use *any* time-marching scheme offline. Even if the space-time discretization is chosen in such a way that it coincides with a time-stepping scheme, this variant has an increased offline complexity. If the full space-time dimension is needed, one may have to resort to tensor product schemes, [8].
2. In the online phase, the space-time method is more efficient concerning effort, whereas POD-Greedy uses less storage.
3. If a theoretical justification of an error bound in the full \mathbb{X} -norm is needed and Finite Elements shall be used, space-time seems to be the method of choice. If a Finite Volume discretization is chosen, POD-Greedy is more appropriate [5].

From these results, we tend to formulate the following recipe: If online computational time restrictions apply, the space-time approach is advisable even in those cases where it might cause an increased offline effort. — If online storage restrictions apply or the use of a specific time-marching scheme is necessary, the POD-Greedy approach is advisable.

References

1. Andreev, R.: Stability of space-time petrov-galerkin discretizations for parabolic evolution equations. Ph.D. thesis, ETH Zürich, Nr. 20842 (2012)
2. Baur, U., Benner, P., Haasdonk, B., Himpe, C., Maier, I., Ohlberger, M.: Comparison of methods for parametric model order reduction of instationary problems. Preprint MPIMD/15-01, Max Planck Institute Magdeburg (2015)
3. Haasdonk, B.: Convergence rates of the POD-greedy method. *ESAIM Math. Model. Numer. Anal.* **47**(3), 859–873 (2013)
4. Haasdonk, B.: *Reduced Basis Methods for Parametrized PDEs – A Tutorial Introduction for Stationary and Instationary Problems*. Reduced Order Modelling. Luminy Book series (2014)
5. Haasdonk, B., Ohlberger, M.: Reduced basis method for finite volume approximations of parametrized linear evolution equations. *M2AN Math. Model. Numer. Anal.* **42**(2), 277–302 (2008)
6. Hesthaven, J., Rozza, G., Stamm, B.: *Certified reduced basis methods for parametrized partial differential equations*. Springer Briefs in Mathematics. Springer, Cham (2016)
7. Huynh, D., Rozza, G., Sen, S., Patera, A.: A successive constraint linear optimization method for lower bounds of parametric coercivity and inf-sup stability constants. *C.R. Math. Acad. Sci. Paris* **345**(8), 473–478 (2007)
8. Mayerhofer, A.: *Reduced basis methods for parabolic pdes with parameter functions in high dimensions and applications in finance*. Ph.D. thesis, Ulm University (2016)
9. Nochetto, R., Siebert, K., Veiser, A.: Theory of adaptive finite element methods: An introduction. In: R. DeVore, A. Kunoth (eds.) *Multiscale, nonlinear and adaptive approximation*, pp. 409–542. Springer, Berlin (2009)
10. Quarteroni, A., Manzoni, A., Negri, F.: *Reduced basis methods for partial differential equations*, vol. 92. Springer, Cham (2016)
11. Quarteroni, A., Valli, A.: *Numerical approximation of partial differential equations*, vol. 23. Springer Science (2008)
12. Schwab, C., Stevenson, R.: Space-time adaptive wavelet methods for parabolic evolution problems. *Math. Comp.* **78**(267), 1293–1318 (2009)
13. Urban, K., Patera, A.: A new error bound for reduced basis approximation of parabolic partial differential equations. *C. R. Math. Acad. Sci. Paris* **350**(3-4), 203–207 (2012)
14. Urban, K., Patera, A.: An improved error bound for reduced basis approximation of linear parabolic problems. *Math. Comp.* **83**(288), 1599–1615 (2014)
15. Wloka, J.: *Partial differential equations*. Cambridge University Press (1987)