Adaptive Basis Enrichment for the Reduced Basis Method Applied to Finite Volume Schemes

Bernard Haasdonk — Mario Ohlberger

Institut für Numerische und Angewandte Mathematik, Universität Münster
Einsteinstrasse 62, 48149 Münster, Germany

{bernard.haasdonk, mario.ohlberger}@uni-muenster.de

ABSTRACT. *We derive an efficient reduced basis method for finite volume approximations of parameterized linear advection-diffusion equations. An important step in deriving a reduced finite volume model with the reduced basis technology is the generation of a reduced basis space, on which the detailed numerical simulations are projected. We present a new strategy for this reduced basis generation. We apply an effective exploration of the parameter space by adaptive grids based on an a posteriori error estimate. The resulting method gives a considerable improvement concerning equal distribution of the model error over the parameter space compared to uniform parameter selections. It is computationally very efficient in terms of small ratio of training-time over model-error.*

KEYWORDS: *reduced basis method, model reduction, parameterized equations, adaptive parameter grid, finite volume scheme, basis generation*

1. Introduction

Reduced basis methods [PAT 07] are increasingly popular methods for complexity reduction in problems, where parameterized PDEs are to be solved repeatedly for varying parameters. This means that high-dimensional finite element or finite volume approximations $u_H(\boldsymbol{\mu}) \in \mathcal{W}_H$ are to be calculated for varying parameter vectors $\boldsymbol{\mu} \in \mathcal{P}$ from a polygonal parameter domain. Examples for such applications are design, control, optimization, inverse modeling based on PDEs, etc. Instead of repeated computation of these expensive detailed simulations, a problem-specific finite dimensional subspace $\mathcal{W}_N \subset \mathcal{W}_H$ is chosen in a preprocessing step, which captures the solution variety under parameter changes. Based on this *reduced basis space $\mathcal{W}_N$*, a reduced model is devised, which inexpensively calculates $u_N(\boldsymbol{\mu}) \in \mathcal{W}_N$ as approximation of the unknown $u_H(\boldsymbol{\mu})$ for any new parameter vector. In this contribution we

focus on a reduced basis method for parameterized linear advection-diffusion equations, discretized by finite volumes.

The crucial ingredient for these methods is the choice of a *reduced basis* Φ_N which spans the reduced basis space. Methods for reduced basis construction are typically based on *snapshots*, i.e. $\{u_H(\boldsymbol{\mu}_i)\}_{i=1}^I$ for certain selected parameter vectors $\{\boldsymbol{\mu}_i\}_{i=1}^I$. Such *snapshots* are collected as basis vectors. Orthonormalization can be performed or proper orthogonal decomposition techniques may be used as a data compression step for large sets (time-sequences) of snapshots. Existing methods for basis construction by random parameter space sampling [GRE 05] or uniform parameter grids [HAA 06] reveal a breakdown of convergence of the global approximation error or high calculation times in case of very fine grids.

In this presentation we propose an accumulative basis construction scheme which is based on an adaptive grid in parameter space that is generated using an *a posteriori* error estimate for the reduced basis method derived in [HAA 06]. Our results indicate a considerable improvement over the fixed and uniformly refined grid approaches.

The article is organized as follows. In section 2 the reduced basis method based on a finite volume discretization is revisited and an *a posteriori* error estimate is cited. The new adaptive basis enrichment algorithm is formulated in section 3. Finally, in section 4 we give some numerical results that underline the good performance of the new basis enrichment approach in comparison with existing ones.

2. Reduced basis method for linear parameterized evolution equations

We consider the following parameterized convection diffusion equation with general initial data and boundary conditions.

Let $\Omega \subset \mathbb{R}^d$ denote a bounded polygonal space domain with boundary $\partial\Omega = \Gamma_{\mathrm{dir}} \cup \Gamma_{\mathrm{neu}}$ decomposed into Dirichlet and Neuman components and $[0, T_{\max}]$ be a time interval. For any parameter vector $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ the function $u(\mathbf{x}, t; \boldsymbol{\mu})$ denotes the solution of the parameterized advection-diffusion equation:

$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v}(\boldsymbol{\mu})u(\boldsymbol{\mu}) - d(\boldsymbol{\mu})\nabla u(\boldsymbol{\mu})) = 0 \ \text{ in } \Omega \times [0, T_{\max}], \tag{1}$$

$$u(\cdot, 0; \boldsymbol{\mu}) = u_0(\boldsymbol{\mu}) \ \text{ in } \Omega, \tag{2}$$

$$u(\boldsymbol{\mu}) = b_{\mathrm{dir}}(\boldsymbol{\mu}) \ \text{ in } \Gamma_{\mathrm{dir}} \times [0, T_{\max}], \tag{3}$$

$$(\mathbf{v}(\boldsymbol{\mu})u(\boldsymbol{\mu}) - d(\boldsymbol{\mu})\nabla u(\boldsymbol{\mu})) \cdot \mathbf{n} = b_{\mathrm{neu}}(u; \boldsymbol{\mu}) \ \text{ in } \Gamma_{\mathrm{neu}} \times [0, T_{\max}]. \tag{4}$$

In particular, the initial data u_0 is space-dependent, the velocity field $\mathbf{v}$, the diffusion coefficient d, the boundary value function b_{dir} and b_{neu} may be space and time dependent. The Neuman-boundary conditions are assumed to be affine in u, i.e. $b_{\mathrm{neu}}(u, \mathbf{x}, t; \boldsymbol{\mu}) = b_{\mathrm{neu},1}(\mathbf{x}, t; \boldsymbol{\mu})u(\mathbf{x}, t; \boldsymbol{\mu}) + b_{\mathrm{neu},0}(\mathbf{x}, t; \boldsymbol{\mu})$. This covers usual flow-conditions such as no-flow or outflow. The geometry and data is assumed to be sufficiently regular, such that the solution is well-defined.

For the finite volume approximations we introduce a discrete solution space as follows. Let $0 = t_0 < t_1 < \ldots < t_K = T_{\max}$ be a sequence of time instants with corresponding time-steps $\Delta t_k := t_{k+1} - t_k$ for $k = 1, \ldots, K - 1$. Furthermore, $\mathcal{T} = \{T_i\}_{i=1}^H$ denotes a convex polygonal tessellation of Ω. We denote by $\mathcal{W}_H := \operatorname{span}(\chi_{T_i}) \subset L^\infty(\Omega) \subset L^2(\Omega)$ the discrete space of cell-wise constant functions, where χ_{T_i} are the characteristic functions on the elements $T_i \in \mathcal{T}$. The space is equipped with the scalar product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$ inherited from $L^2(\Omega)$.

In the space $\mathcal{W}_H$, which is usually of high dimension $H = \dim(\mathcal{W}_H)$, a finite volume scheme can be formulated in the following form (cf. [HAA 06]). Let the discrete initial data $u_H^0 \in \mathcal{W}_H$ be given by a projection of the initial data to $\mathcal{W}_H$, i.e. $u_H^0 = P[u_0(\boldsymbol{\mu})]$. Then $u_H^k \in \mathcal{W}_H, k = 1, \ldots, K$ is defined using

$$L_I^{k-1}(\boldsymbol{\mu})[u_H^k] \;\; = \;\; L_E^{k-1}(\boldsymbol{\mu})[u_H^{k-1}] + b^{k-1}(\boldsymbol{\mu}). \tag{5}$$

Here $L_I^{k-1}(\boldsymbol{\mu})$ denotes an implicit discrete operator, $L_E^{k-1}(\boldsymbol{\mu})$ an explicit operator and $b^{k-1}(\boldsymbol{\mu})$ a source term coming from the discretization of the boundary conditions.

Let us for a moment suppose that we are given a low dimensional reduced basis space $\mathcal{W}_N \subset \mathcal{W}_H$. Then the reduced basis approximation $\{u_N^k(\boldsymbol{\mu}) \in \mathcal{W}_N\}_{k=0}^K$ is defined as a solution of the following problem

$$\int_\Omega (u_N^0 - P[u_0(\boldsymbol{\mu})])\varphi \;\; = \;\; 0 \quad \text{and} \tag{6}$$

$$\int_\Omega (L_I^{k-1}(\boldsymbol{\mu})[u_N^k] - L_E^{k-1}(\boldsymbol{\mu})[u_N^{k-1}] - b^{k-1}(\boldsymbol{\mu}))\varphi \;\; = \;\; 0 \tag{7}$$

for all $\varphi \in \mathcal{W}_N$ and all $k = 1, \ldots, K$.

Let us note that the solution of [6], [7] in the given form still involves scalar products in the high dimensional space $\mathcal{W}_H$. Thus, in order to really obtain an efficient reduced model, problem [6], [7] has to be decomposed into a probably expensive offline-step that contains all scalar products in $\mathcal{W}_H$, and a very inexpensive online-step, that only contains operations of order polynomial in N. We refer to [HAA 06] for more details on this offline-online decomposition.

In the rest of the paper we will discuss a new approach for the generation of suitable reduced basis spaces. The construction is based on *a posteriori* error estimates for the reduced basis approximation of the form

$$\|u_H(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\| \leq \Delta(\boldsymbol{\mu}, \Phi_N), \tag{8}$$

where $\|\cdot\|$ denotes a suitable norm and $\Delta(\boldsymbol{\mu}, \Phi_N)$ is a close upper bound of the error that only depends on the parameter $\boldsymbol{\mu}$ and the reduced basis $\Phi_N := \{\varphi_n\}_{n=1}^N$ of the reduced space $\mathcal{W}_N$. Examples of such error estimates were given in [HAA 06], e.g. for the case of finite volume discretizations with coercive space discretization operators

$$\Delta(\boldsymbol{\mu}, \Phi_N) := \sum_{k=1}^K \Delta t_{k-1} \left\| R^k(\boldsymbol{\mu}) \right\|,$$

a)

ESGREEDY $(\Phi_0, M_{train}, \varepsilon_{tol}, M_{val}, \rho_{tol})$

1 $\Phi := \Phi_0$
2 **repeat**
3      $\boldsymbol{\mu}^* := \arg\max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
4   **if** $\Delta(\boldsymbol{\mu}^*) > \varepsilon_{tol}$
5   **then**
6              $\varphi := \text{ONBASISEXT}(u_H(\boldsymbol{\mu}^*), \Phi)$
7              $\Phi := \Phi \cup \{\varphi\}$
8      $\varepsilon := \max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
9      $\rho := \max_{\boldsymbol{\mu} \in M_{val}} \Delta(\boldsymbol{\mu}, \Phi)/\varepsilon$
10 **until** $\varepsilon \leq \varepsilon_{tol}$ **or** $\rho \geq \rho_{tol}$
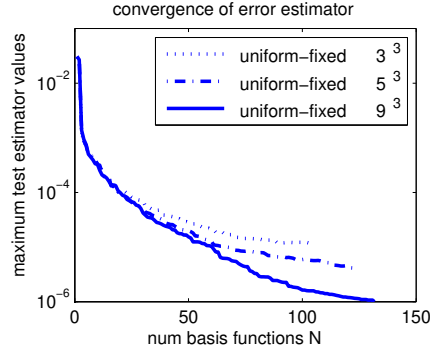11 **return** Φ, ε

b)

RBADAPTIVE $(\Phi_0, \mathcal{M}_0, \varepsilon_{tol}, M_{val}, \rho_{tol})$

1 $\Phi := \Phi_0, \mathcal{M} := \mathcal{M}_0$
2 **repeat**
3      $M_{train} := V(\mathcal{M})$
4      $[\Phi, \varepsilon] := \text{ESGREEDY}(\Phi, M_{train}, \varepsilon_{tol},$
5                          $M_{val}, \rho_{tol})$
6   **if** $\varepsilon > \varepsilon_{tol}$
7   **then**
8              $\boldsymbol{\eta} = \text{ELEMENTINDICATORS}(\mathcal{M}, \Phi, \varepsilon)$
9              $\mathcal{M} := \text{MARK}(\mathcal{M}, \boldsymbol{\eta})$
10             $\mathcal{M} := \text{REFINE}(\mathcal{M})$
11 **until** $\varepsilon \leq \varepsilon_{tol}$
12 **return** Φ

Figure 1. *a) The early stopping (ES) greedy search algorithm and b) the general adaptive RB-generation procedure.*

Figure 2. *Illustration of overfitting. The maximum error estimator on a random test-set is ploted over the dimension N of the reduced basis space for the* greedy *algorithm with a fixed training set corresponding to the vertices of a uniform Cartesian parameter grid with 3^3, 5^3, and 9^3 nodes.*

where the residual norms can be computed during the reduced simulation from

$$R^k(\boldsymbol{\mu}) := (\Delta t_{k-1})^{-1}(L_I^{k-1}[u_H^k] - L_E^{k-1}[u_H^{k-1}] - b^{k-1}(\boldsymbol{\mu})).$$

In the absence of such error estimates the following scheme can still be applied using $\Delta(\boldsymbol{\mu}, \Phi_N) := \|u_H(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|$ with the drawback of considerably higher computational demands.

3. Basis construction by adaptive parameter grids

The general goal of basis construction is a rapid calculation of a small basis Φ_N which implies a low error $\|u_H(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|$ over $\boldsymbol{\mu} \in \mathcal{P}$ with suitable problem-specific norm. Let us now suppose that an upper bound of the error is given as stated in [8], where the upper bound $\Delta(\boldsymbol{\mu}, \Phi_N)$ is cheap to calculate.

The standard *greedy* algorithm [PAT 07] is based on a finite training set of parameters $M_{train} \subset \mathcal{P}$, a given desired error tolerance $\varepsilon_{tol} > 0$ and optionally an initial choice of basis Φ_0, which is to be extended. It is an accumulative basis construction procedure. It consecutively determines the $\boldsymbol{\mu}^* \in M_{train}$ that is worst resolved with the current reduced basis (as measured by $\Delta(\boldsymbol{\mu}, \Phi_N)$), performs a detailed simulation $u_H(\boldsymbol{\mu}^*)$ and uses this for extension of the basis Φ_N, until the error over M_{train} is less than ε_{tol} (see Figure 1a)). As demonstrated in Figure 2, the resulting algorithm tends to overfitting for large N if the training set is kept fixed, i.e. the convergence rate breaks down if N increases. On the other hand, if larger and larger training sets are chosen, the breakdown of the convergence rate is shifted more and more towards larger values of N. Unfortunately, such a procedure usually comes with an immense increase in computational costs.

Stimulated by this observation, we propose an extension of the *greedy* algorithm, Figure 1a), which prevents overfitting on the training set by monitoring an additional validation-error and performing an early stopping if the validation-training-error ratio exceeds a certain limit ρ_{tol}. Such cases of detected overfitting indicate that M_{train} is too small for the desired model accuracy. Our adaptive approach, Figure 1b), is based on a grid $\mathcal{M}$ in parameter space, the vertices $V(\mathcal{M})$ of which are taken as training set of the greedy algorithm. In case of detected overfitting we conclude a necessary refinement of the parameter grid. In the spirit of FEM-adaptivity, element-indicators are calculated, which are related to the model-error on these parameter cells. A marking and refinement strategy results in uniform or adaptive grid refinement. A subsequent restart of the greedy search over the now extended set of grid-vertices is performed until the desired accuracy is obtained.

In particular, in the case of adaptive refinement, we first define preliminary element indicators $\tilde{\eta}(e)$ for elements $e \in \mathcal{M}$ of the parameter mesh by taking the maximum of the error estimator values in the vertices $\boldsymbol{\mu} \in V(e)$ and the barycenter $\boldsymbol{\mu} = c(e)$ of an element e, i.e.

$$\tilde{\eta}(e) := \left(\max_{\boldsymbol{\mu} \in V(e) \cup \{c(e)\}} \Delta(\boldsymbol{\mu}, \Phi_N) \right).$$

As is well known for adaptive methods, such an indicator may have problems detecting local maxima of the error in cases where the starting parameter mesh is too coarse to resolve the main structures. In order to circumvent such problems we finally define the element indicators $\eta(e)$ as

$$\eta(e) := \gamma(e) s(e) + \tilde{\eta}(e)/\varepsilon,$$

where $\gamma(e) > 0$ denotes a weighting parameter depending on the local mesh size, $s(e)$ counts the number of precedent refinement steps that did not lead to a refinement of element e and ε is the maximum error estimator on $V(\mathcal{M})$. Thus, elements that are not detected by the point evaluation of the estimator are penalized from one refinement step to the next, which asymptotically leads to a refinement of all elements. In each refinement step a fixed fraction $\Theta \in (0, 1]$ of the elements is refined, where the elements with the highest estimator value $\eta(e)$ are chosen. The refinement of an ele-
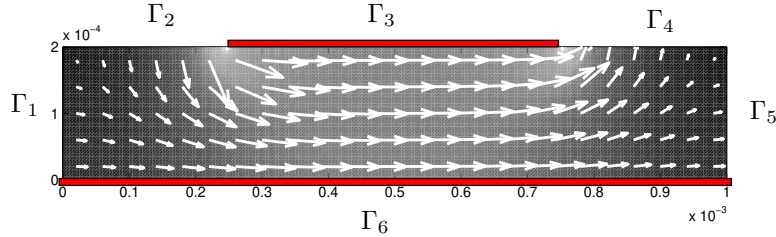
Figure 3. *Illustration of the geometry and velocity field of the advection-diffusion model problem. At Γ_3 and Γ_6 no-flow boundary conditions are prescribed, at Γ_5 outflow conditions. The remaining boundaries are assigned Dirichlet values.*

ment e in a Cartesian mesh in p dimensions is done by subdivision into 2^p congruent sub-elements.

4. Experimental results

We apply the basis construction method to the parameterized advection-diffusion problem [1]-[4], discretized by a finite volume reduced basis scheme [6], [7], and choose the L^2 *a posteriori* error estimator from [HAA 06] as error measure $\Delta(\boldsymbol{\mu}, \Phi_N)$. In particular, we choose the model problem described in [HAA 06, Sec. 7] for our numerical experiments concerning the basis enrichment. The model represents an instationary advection-diffusion problem in the gas-diffusion layer of a fuel-cell (see Figure 3). The velocity field is precomputed and the detailed discretization $u_H(\boldsymbol{\mu})$ is obtained by an implicit/explicit finite volume scheme of first order in space and time. The problem is characterized by a three-dimensional parameter space modeled by $(c_{init}, \delta, \beta) \in [0, 1] \times [0, 5 \cdot 10^{-8}] \times [0, 1]$. The first parameter c_{init} is the amplitude of a sinus-shaped initial-data distribution, δ is the global diffusion coefficient on the domain, and $\beta, 1 - \beta$ model the concentrations at the boundary of two gas-inlets. For details we refer to the above reference.

We generate bases with three approaches. First, the vertices of a uniform fixed Cartesian grid are chosen as the training set M_{train} without any refinement (uniform-fixed). Second, a uniform Cartesian grid is used with global refinement during the basis-construction (uniform-refined) and third, a Cartesian grid with adaptive refinement (adaptive-refined) is applied. For an initial experiment we use a restricted two-dimensional parameter space $\mathcal{P} = [0, 1] \times [0, 5 \cdot 10^{-8}]$ for the parameters $\boldsymbol{\mu} = (\beta, \delta)$ and fix $c_{init} = 1$. The resulting errors $\Delta(\boldsymbol{\mu}, \Phi_N)$ over the 2D parameter space are visualized logarithmically in Figure 4. The fixed grid approach in a) clearly demonstrates overfitting with respect to the grid-vertices and error values varying over several orders of magnitude. In particular, it has a low error in the upper (high diffusivity) and very high errors in the lower part (low diffusivity) of the parameter domain. The uniformly refined approach in b) is slightly advantageous concerning these aspects. The adaptively refined grid approach in c) demonstrates considerable improvements concerning equal distribution of the error and the prevention of overfitting. Quantita-
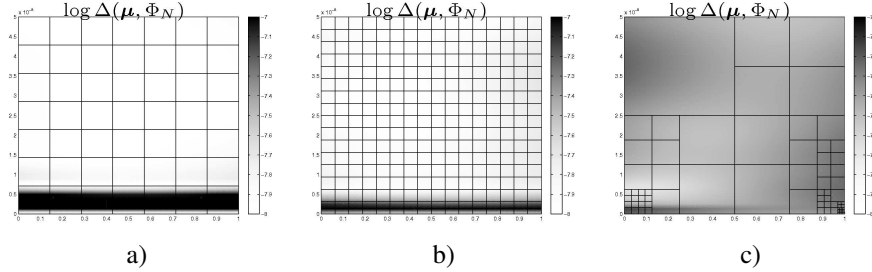
Figure 4. *Demonstration of the overfitting phenomenon for a basis of size $N = 130$ in two-dimensional parameter space $\boldsymbol{\mu} = (\beta, \delta) \in \mathcal{P} = [0,1] \times [0, 5 \cdot 10^{-8}]$ with a) the uniform-fixed, b) the uniform-refined and c) the adaptive-refined grid approach.*
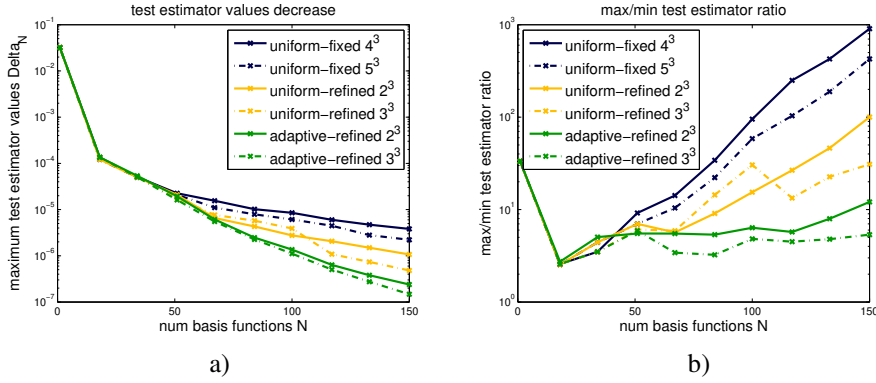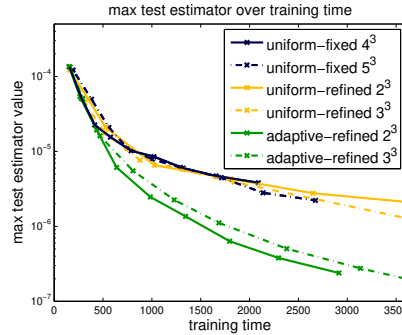

Figure 5. *Quantitative comparison of the basis-generation approaches with respect to a) maximum test error and b) ratio of maximum to minimum test-error in dependence of the dimension N of the reduced basis space.*

tive results are illustrated in Figures 5 and 6 for the full 3D parameter space $\mathcal{P}$ and different initial grid sizes (vertex numbers ranging from 2^3 to 5^3). In Figure 5a) we demonstrate the improved model-error (measured as maximum error-estimator over a randomly generated test-set) for the refined approaches over the fixed grid setting. Figure 5b) quantifies the improvement of the error-distribution by monitoring the ratio of maximum to minimum test-error. Finally, in Figure 6 the maximum test-error decrease of Figure 5a) is related to the corresponding training time, i.e. the CPU time for the overall basis construction. For instance with respect to this last criterion, the adaptive refinement approach is consistently superior to the uniform grid approaches.

5. Conclusion

We addressed the task of reduced basis construction based on snapshots. If the training set for the greedy search is too small, overfitting of the reduced model can oc-

Figure 6. *Comparison of the basis-generation approaches with respect to maximum test-error over training time [s].*

cur. On the other hand, too large training sets lead to unnecessarily large computation times. The "right guess" of the training set size and the location of its points can be addressed by applying overfitting control and training set extension.

We demonstrated that adaptive grid-management with FEM-inspired refinement strategies can be used as one instant of training set extension. In particular, in comparison to fixed training set approaches, adaptive grid-refinement produces reduced bases with better model accuracy, more uniform distribution of the model-error over the parameter space and faster computation time for equal accuracy.

6. Acknowledgment

7. References

[GRE 05] GREPL M., PATERA A., "*A posteriori* error bounds for reduced-basis approximations of parametrized parabolic partial differential equations", *M2AN Math. Model. Numer. Anal.*, vol. 39, num. 1, 2005, p. 157-181.

[HAA 06] HAASDONK B., OHLBERGER M., "Reduced Basis Method for Finite Volume Approximations of Parametrized Evolution Equations", report num. 12/2006, 2006, University of Freiburg, Institute of Mathematics, Accepted for publication in M2AN Math. Model. Numer. Anal.

[PAT 07] PATERA A., ROZZA G., *Reduced Basis Approximation and a Posteriori Error Estimation for Parametrized Partial Differential Equations*, MIT, 2007, Version 1.0, Copyright MIT 2006-2007, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering.