Non-Conforming Localized Model Reduction with Online Enrichment: Towards Optimal Complexity in PDE constrained Optimization

Mario Ohlberger and Felix Schindler

Abstract We propose a new non-conforming localized model reduction paradigm for efficient solution of large scale or multiscale PDE constrained optimization problems. The new conceptual approach goes beyond the classical offline/online splitting of traditional projection based model order reduction approaches for the underlying state equation, such as the reduced basis method. Instead of first constructing a surrogate model that has globally good approximation quality with respect to the whole parameter range, we propose an iterative enrichment procedure that refines and locally adapts the surrogate model specifically for the parameters that are depicted during the outer optimization loop.

Key words: Model reduction, reduced basis method, LRBMS, optimization, control, online enrichment, discontinuous Galerkin

MSC (2010)**: 35Q93, 65K10, 65N30**

1 Introduction

We are concerned with model reduction for parameter optimization of general elliptic multiscale problems, where the optimization functional is defined on a macro scale and the material design parameters are considered to have influence on the micro scale. Such optimization problems naturally arise, e.g., in optimal design of composed materials or in the design of technical devices that rely on multiscale processes, such as fuel cells or batteries. In previous works [13, 14] we considered such problems under the assumption of scale separation, or even local periodicity, which allowed us to suggest a model reduction approach based on the two scale limit equation of the homogenized problem. However, in many real applications such a structural assumption is too restrictive and hence more general approaches need to be de-

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veloped in general heterogeneous situations. In recent contributions, we introduced and analyzed the localized reduced basis multiscale method (LRBMS) [15, 16, 12] which is particularly designed to efficiently cope with general heterogeneous parameterized multiscale problems. In particular we developed an efficient localized a posteriori error estimator against the underlying true solution of the parameterized problem and demonstrated how this error estimator can be used to overcome the classical offline/online splitting of reduced basis (RB) methods, by means of the newly developed concept of online enrichment. The proposed method merely requires a very cheap preparation step and then iteratively enriches localized snapshot spaces using the localized a posteriori error information. In this contribution, we combine our development from the previous two approaches to suggest, for the first time, an efficient solution algorithm for parameter optimization of elliptic multiscale or large scale problems on the basis of our non-conforming localized model reduction approach with online enrichment.

In detail we look at the following multiscale or large scale optimization setting:

$$\left.\begin{aligned} \text{Find} \quad & \mu^* = \arg\min J\big(u^\varepsilon(\mu),\mu\big) \\ \text{subject to} \quad & C_j\big(u^\varepsilon(\mu),\mu\big) \leq 0 \quad \forall j = 1,\dots,m, \\ & \mu \in \mathscr{P} \end{aligned}\right\} \tag{1}$$

with a compact *parameter set* $\mathscr{P} \subset \mathbb{R}^P$ for $P \in \mathbb{N}$. In (1), the *state variable* $u^\varepsilon(\mu)$ is given as the solution of the following (parametrized) multiscale problem:

$$\left.\begin{aligned} -\nabla \cdot \big(A^\varepsilon(\mu)\nabla u^\varepsilon(\mu)\big) &= f(\mu) \quad (\text{in } \Omega) \\ u^\varepsilon(\mu) &= g_D \quad (\text{on } \partial\Omega) \end{aligned}\right\} \tag{2}$$

In (2), $\Omega \subset \mathbb{R}^d$ for $d = 1,2,3$ is a bounded domain and A^ε denotes a general multiscale diffusion tensor (the multiscale nature of which is denoted by $\varepsilon > 0$) without any further structural assumptions. We make use of the short notation $u(\mu) := u^\varepsilon(\mu) := u^\varepsilon(\cdot;\mu)$ and will use analogue expressions for all functions that depend on both spatial variables and parameters.

There is a large variety of numerical algorithms for general optimization problem such as (1), see for example [20]. Typically, these algorithms are based on necessary and/or sufficient optimality conditions for local optima which involve higher order derivatives of the participating functions. In order to obtain a reduced approximation of (1) it is thus not sufficient to provide fast approximations solely of the state $u(\mu)$, but also for derivatives with respect to the parameter μ.

As the solution of such optimization problems usually requires repeated evaluations of the underlying multiscale partial differential equation (PDE) for different sets of parameters, model reduction is applied to increase computational efficiency. In this contribution we are concerned with a localized generalization of the RB approach [8]. The application of the RB approach to parameter optimization of elliptic PDEs was first presented in [17], and generalized to multiscale problems in [13]. A posteriori error estimates for reduced approximation of linear - quadratic optimiza-

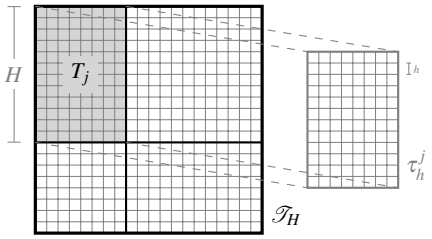

Fig. 1 Sketch of domain decomposition into macro elements $T_j \in \mathscr{T}_H$ for the definition of the LRBMS and the underlying fine grids $\tau_h^j \subset \mathscr{T}_H$ that are used for the construction of the local approximation spaces.

tion problems and parametrized optimal control problems with control constraints were studied, e.g., in [19, 21, 7, 4]. In the context of optimal control and mesh adaptivity of the underlying finite element discretizations we refer to [11, 2, 18, 9] and the references therein.

The rest of this paper is organized as follows: In Section 2 we introduce a weak formulation of the underlying parameterized multiscale problem in broken Sobolev spaces employing a non-conforming discontinuous Galerkin (DG) variational formulation. Based on this non-conforming setting, we then introduce in Section 3 localized reduced spaces and related localized RB surrogate models, both for the state equation and for the equations that characterize the derivatives of the state with respect to the parameters. Finally, in Section 4, a new iterative solution concept based on successively enhanced surrogate models is proposed and discussed.

2 Non-Conforming weak formulation of the parameterized multiscale problem

In order to derive a suitable non-conforming weak formulation for our model reduction approach, we first assume that a non-overlapping decomposition of the underlying domain Ω is given by a coarse triangulation $\mathscr{T}_H$ with cells $T_j \in \mathscr{T}_H$, $j = 1, \dots N_H$. Furthermore, each macro cell T_j is further decomposed by a local fine resolution triangulation τ_h^j, that resolves all fine scale features of the multiscale problem. We then define the global fine scale partition τ_h as the union of all its local contributions, i.e., $\tau_h = \bigcup_{j=1}^{N_H} \tau_h^j$. Hence, τ_h is a nested refinement of $\mathscr{T}_H$ as schematically depicted in Figure 1. Let $H^1(\tau_h) := \{v \in L^2(\Omega) \mid v|_t \in H^1(t) \ \forall t \in \tau_h\}$ denote the broken Sobolev space on τ_h, which naturally inherits the decomposition $H^1(\tau_h) = \bigoplus_{j=1}^{N_H} H^1(\tau_h^j)$.

Definition 1 (Weak solution of the multiscale problem in broken spaces).
We call $u(\mu) \in H^1(\tau_h)$ weak solution of (2), if

$$a_{\mathrm{DG}}\big(u(\mu), v; \mu\big) = L_{\mathrm{DG}}(v; \mu) \qquad \text{for all } v \in H^1(\tau_h). \tag{3}$$

Here, the DG bilinear form a_{DG} and the right hand side L_{DG} are given as

$$a_{\mathrm{DG}}(v,w;\mu) := \sum_{t\in\tau_h}\int_t A^\varepsilon(\mu)\nabla v\cdot\nabla w - \sum_{e\in\mathscr{F}_h^I}\int_e \{A^\varepsilon(\mu)\nabla v\cdot\mathbf{n_e}\}[w]$$
$$- \sum_{e\in\mathscr{F}_h^I}\int_e \{A^\varepsilon(\mu)\nabla w\cdot\mathbf{n_e}\}[v] + \sum_{e\in\mathscr{F}_h^I}\frac{\sigma_e(\mu)}{|e|^\beta}\int_e [v][w],$$
$$L_{\mathrm{DG}}(v;\mu) := \sum_{t\in\tau_h}\int_t fv + \sum_{e\in\mathscr{F}_h^D}\int_e \left(\frac{\sigma_e(\mu)}{|e|^\beta}v - A^\varepsilon(\mu)\nabla v\cdot\mathbf{n}\right) g_D,$$

where the parametric positive penalty function $\sigma_e(\mu):\mathscr{P}\to\mathbb{R}$ and the averages and jumps $\{\cdot\}$ and $[\cdot]$ across inner and boundary interfaces $e\in\mathscr{F}_h^I\cup\mathscr{F}_h^D$ are chosen similar to SWIPDG [6, 16].

3 Localized model reduction for PDE constrained optimization

Our non-conforming localized model reduction approach is based on the construction of appropriate low dimensional local approximation spaces $U_N^j\subset H^1(\tau_h^j)$ of local dimensions N_j that form the global reduced solution space via

$$U_H^N = \bigoplus_{j=1}^{N_H} U_N^j, \qquad N := \dim(U_H^N) = \sum_{j=1}^{N_H} N_j. \tag{4}$$

Once such a reduced approximation space is constructed, the LRBMS approximation is defined as follows.

Definition 2 (The localized reduced basis multiscale method). We call $u_N(\mu)\in U_H^N$ a localized reduced basis multiscale approximation of (3) if it satisfies

$$a_{\mathrm{DG}}(u_N(\mu),v_N;\mu) = L_{\mathrm{DG}}(\mu;v_N) \qquad \text{for all } v_N\in U_H^N. \tag{5}$$

Note that (5) is a globally coupled reduced problem, where all arising quantities can nevertheless be locally computed w.r.t the local reduced spaces U_N^j.

To simplify the presentation, we assume in the sequel that the bilinear form a_{DG} and the right hand side L_{DG} are affinely decomposable (see [5] and the references therein for the treatment of general nonlinear operators), which allows for an efficient offline/online splitting of the resulting reduced problem:

$$a_{\mathrm{DG}}(u,v;\mu) = \sum_{q=1}^{Q_A}\theta_q^A(\mu)a_{\mathrm{DG}}^q(u,v), \qquad L_{\mathrm{DG}}(\mu;v) = \sum_{q=1}^{Q_L}\theta_q^L(\mu)L_{\mathrm{DG}}^q(v). \tag{6}$$

In order to solve the overall optimization problem, we will also need to compute parameter derivatives of the state $u_N(\mu)$. Equations for these quantities are established by differentiating the defining equation (5) of $u_N(\mu)$ with respect to μ_i. Due to linearity and the chain rule, we obtain the following weak formulation for $\partial_{\mu_i}u_N(\mu)\in U_H^N$, for all $v_N\in U_H^N$:

$$a_{\mathrm{DG}}(\partial_{\mu_i}u_N(\mu),v_N;\mu) = -\partial_{\mu_i}a_h(u_N(\mu),v_N;\mu) + \partial_{\mu_i}L_{\mathrm{DG}}(\mu;v). \tag{7}$$

Since a_{DG} and L_{DG} are affinely decomposable, we have

$$\partial_{\mu_i} a_h(u,v;\mu) = \sum_{q=1}^{Q_A} \partial_{\mu_i}\theta_q^A(\mu) a_{\mathrm{DG}}^q(u,v), \quad \partial_{\mu_i} L_{\mathrm{DG}}(\mu;v) = \sum_{q=1}^{Q_L} \partial_{\mu_i}\theta_q^L(\mu) L_{\mathrm{DG}}^q(v).$$

Hence, we can reuse both the same reduced spaces and precomputed reduced system matrices as for the approximation of $u_N(\mu)$. Thus, the computational overhead to compute the parameter derivatives is of the same order as the cost to compute a reduced state equation. Higher order derivatives can be computed analogously by further differentiation of (7).

In recent contributions [10, 1, 16, 3] we discussed several possibilities to construct local reduced spaces U_N^j from global or localized snapshot computations. Thereby, in the concept presented above, it is possible to use finite volume, DG or conforming finite element approximations on the underlying fine partition τ_h or restrictions thereof to a local neighborhood of the macro elements $T_j \in \mathscr{T}_H$. In what follows, we consider the iterative construction of reduced approximation spaces and related surrogate models based on localized a posteriori error control and local enrichment as recently introduced in [16]. In these circumstances we obtain the following estimate on the error w.r.t. the unknown weak solution of (2).

Theorem 1 (Localizable a posteriori error estimate). *With the assumptions and the notation of [16, Cor. 4.5], the following estimate on the full approximation error in the energy norm $|||v|||_{\overline{\mu}} := \sum_{t\in\tau_h}\int (A^\varepsilon(\overline{\mu})\nabla v)\cdot\nabla v$ holds for arbitrary $\overline{\mu},\hat{\mu}\in\mathscr{P}$,*

$$|||u(\mu)-u_N(\mu)|||_{\overline{\mu}} \leq \eta\left(u_N(\mu)\right) := C(\mu,\overline{\mu},\hat{\mu})\Bigg[\sum_{j=1}^{N_H}\left(\eta_j^{nc}(u_N(\mu))^2\right)^{1/2} + \sum_{j=1}^{N_H}\left(\eta_j^{r}(u_N(\mu))^2\right)^{1/2} + \sum_{j=1}^{N_H}\left(\eta_j^{df}(u_N(\mu))^2\right)^{1/2}\Bigg]$$

with a computable constant $C(\mu,\overline{\mu},\hat{\mu})>0$ and fully computable local indicators η_j^{nc}, η_j^{r} and η_j^{df} corresponding to the local non-conformity errors, residual errors, and diffusive flux reconstruction errors, respectively.

We refer to [16] for a more detail presentation and derivation of this result

4 A new iterative solution concept based on successively enhanced surrogate models

In classical model reduction approaches for PDE constrained optimization problems, a surrogate model to approximate the parameterized state equation is constructed in a so called offline phase and then successively used for fast evaluations of the state equation for parameters that are selected during the outer optimization loop (see, e.g., [17]). As the selected parameter values during the optimization loop are not known a priori, the surrogate models in such approaches need to be prepared

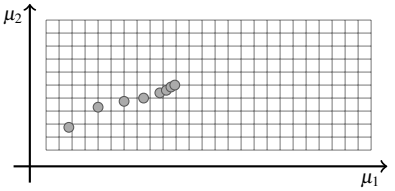

Fig. 2 Sketch of parameter selection during an optimization loop. For each selected parameter point $\mu = (\mu_1, \mu_2)$ an approximation of $u(\mu)$ and its derivatives with respect to μ need to be computed efficiently.

to uniformly approximate the state equation with respect to the whole parameter regime. This might lead to a quite expensive offline construction phase that involves a large number of usually global snapshot computations for suitably selected parameter values. In an optimization loop, however, typically only parameters along a path towards the optimal parameter are depicted, as sketched in Figure 2. Based on the concept of local enrichment from [16] we thus suggest a new iterative procedure to successively built up or enhance the surrogate model (5), (7) by using only localized snapshot computations for the parameters that are selected during the optimization loop. The resulting approach is thus tailored towards the specific optimization problem in an a posteriori manner.

In more detail, in a first step we initialize the local reduced spaces U_N^j with a classical polynomial coarse scale DG basis of prescribed order, thus ensuring that any reduced solution of the state equation is at least as good as a DG solution on the coarse triangulation $\mathscr{T}_H$. We then optionally employ a discrete weak Greedy algorithm with only very few (typically one) global snapshot computations and enrich U_N^j accordingly. Finally, $U_H^N = \bigoplus_{j=1}^{N_H} U_N^j$ and a related initial surrogate model is constructed as sketched in Section 3 above.

During the following optimization loop, given any $\mu \in \mathscr{P}$ from the optimization algorithm, we compute a reduced solution $u_N(\mu) \in U_H^N$ and efficiently assess its quality using the localized a posteriori error estimator $\eta(\mu) := (\sum_{j=1}^{N_H} \eta_j(\mu)^2)^{1/2}$ derived in [15, 16]. If the estimated error is above a prescribed tolerance, $\Delta > 0$, we start an intermediate local enrichment phase to enhance the surrogate model in the SEMR (solve $\rightarrow$ estimate $\rightarrow$ mark $\rightarrow$ refine) spirit of adaptive mesh refinement. We refer to Algorithm 4.1 and [16] for a detailed description and evaluation of this enrichment procedure that only involves local snapshot computations for the given parameter μ on some local neighborhoods $\omega(T_j), T_j \in \mathscr{T}_H$ with Dirichlet boundary values obtained from the insufficient previous reduced surrogate. The algorithm calls a routine `OPT` that performs one optimization step with a descent method based on the old parameter value, the corresponding state and its derivatives with respect to the parameters. It returns the new parameter value and `success=true`, if the optimization criteria has been met.

5 Conclusion and Outlook

In this contribution we proposed how to efficiently use the localized reduced basis multiscale method with local enrichment in the context of surrogate modeling for

Algorithm 4.1 Parameter optimization with adaptive enrichment.

Require: $\mu^{(0)} \in \mathscr{P}$, initial local bases ${\Phi_j}^{(0)}$, $\Delta_{\text{model}}, \Delta_{\text{opt}} > 0$, a marking strategy `MARK` and an orthonormalization procedure `ONB` (see [16, Sec. 5]), an optimization routine `OPT` (returning a new parameter and status of convergence).

$n \leftarrow 0$, $U_H^{N^{(0)}} \leftarrow \bigoplus_{j=1}^{N_H} \operatorname{span}\big({\Phi_j}^{(0)}\big)$

repeat

Solve (5), (7) *for* $u_N(\mu^{(n)}), \partial_{\mu_i} u_N(\mu^{(n)}) \in U_H^{N^{(n)}}, i = 1, \dots, P$.

$m \leftarrow n$

while $\eta(\mu^{(n)}) > \Delta_{\text{model}}$ **do**

for all $j = 1, \dots, N_H$ **do**

Compute local error indicators $\eta_j(\mu^{(n)})$ *according to [16, Cor. 4.5].*

end for

$\tilde{\mathscr{T}}_H \leftarrow \texttt{MARK}\big(\mathscr{T}_H, \{\eta_j(\mu^{(n)})\}_{j=1}^{N_H}\big)$

for all $T_j \in \tilde{\mathscr{T}}_H$ **do**

Solve locally on $\omega(T_j)$ *for enhanced local snapshot* $u_h^j(\mu^{(n)}) \in H^1(\tau_h^j)$.

${\Phi_j}^{(m+1)} \leftarrow \texttt{ONB}\big(\{{\Phi_j}^{(m)}, u_h^j(\mu^{(n)})\}\big)$

end for

$U_H^{N^{(m+1)}} \leftarrow \bigoplus_{T_j \in \tilde{\mathscr{T}}_H} \operatorname{span}\big({\Phi_j}^{(m+1)}\big) \oplus \bigoplus_{T_j \in \mathscr{T}_H \setminus \tilde{\mathscr{T}}_H} \operatorname{span}\big({\Phi_j}^{(m)}\big)$

Solve (5), (7) *for* $u^N(\mu^{(n)}), \partial_{\mu_i} u^N(\mu^{(n)}) \in U_H^{N^{(m+1)}}, i = 1, \dots, P$.

$m \leftarrow m+1$

end while

$(\mu^{(n+1)}, \texttt{success}) \leftarrow \texttt{OPT}\big(\mu^{(n)}, \Delta_{\text{opt}}, u^N(\mu_n), \{\partial_{\mu_i} u^N(\mu_n)\}_{i=1}^{P}\big)$

$n \leftarrow n+1$

until `success`

return optimal parameter $\mu^{(n)}$ and state $u^N(\mu^{(n)})$

the solution of large scale or multiscale PDE constrained optimization problems. The resulting approach iteratively constructs enhanced surrogate models specifically tailored to the solution of the optimization problem in an a posteriori manner and thereby overcomes offline/online splitting of traditional projection based model reduction approaches. A deeper numerical analysis of the presented approach as well as its thorough analysis in numerical experiments are subject to ongoing research.

References

1. Albrecht, F., Haasdonk, B., Kaulmann, S., Ohlberger, M.: The localized reduced basis multiscale method. In: Proceedings of Algoritmy 2012, Conference on Scientific Computing, Vysoke Tatry, Podbanske, September 9-14, 2012, pp. 393–403. Slovak University of Technology in Bratislava, Publishing House of STU (2012)
2. Benedix, O., Vexler, B.: A posteriori error estimation and adaptivity for elliptic optimal control problems with state constraints. Comput. Optim. Appl. **44**(1), 3–25 (2009)
3. Buhr, A., Engwer, C., Ohlberger, M., Rave, S.: ArbiLoMod, a simulation technique designed for arbitrary local modifications. arXiv e-prints (1512.07840) (2015). Http://arxiv.org/abs/1512.07840
4. Dedè, L.: Reduced basis method and error estimation for parametrized optimal control problems with control constraints. J. Sci. Comput. **50**(2), 287–305 (2012)

5. Drohmann, M., Haasdonk, B., Ohlberger, M.: Reduced basis approximation for nonlinear parametrized evolution equations based on empirical operator interpolation. SIAM J. Sci. Comput. **34**, A937–A969 (2012). DOI 10.1137/10081157X
6. Ern, A., Stephansen, A.F., Zunino, P.: A discontinuous galerkin method with weighted averages for advection–diffusion equations with locally small and anisotropic diffusivity. IMA J. Numer. Anal. **29**(2), 235–256 (2009)
7. Grepl, M.A., Kärcher, M.: Reduced basis a posteriori error bounds for parametrized linear-quadratic elliptic optimal control problems. C. R. Math. Acad. Sci. Paris **349**(15-16), 873–877 (2011)
8. Haasdonk, B.: Reduced basis methods for parametrized PDEs – A tutorial introduction for stationary and instationary problems. In: Model Reduction and Approximation: Theory and Algorithms (to appear). SIAM, Philadelphia, PA. (2017)
9. Hintermüller, M., Hinze, M., Hoppe, R.H.W.: Weak-duality based adaptive finite element methods for PDE-constrained optimization with pointwise gradient state-constraints. J. Comput. Math. **30**(2), 101–123 (2012)
10. Kaulmann, S., Ohlberger, M., Haasdonk, B.: A new local reduced basis discontinuous Galerkin approach for heterogeneous multiscale problems. C. R. Math. Acad. Sci. Paris **349**(23-24), 1233–1238 (2011)
11. Liu, W., Yan, N.: A posteriori error estimates for distributed convex optimal control problems. Adv. Comput. Math. **15**(1-4), 285–309 (2001)
12. Ohlberger, M., Rave, S., Schindler, F.: Model reduction for multiscale lithium-ion battery simulation. In: B.K. et al. (ed.) Numerical Mathematics and Advanced Applications ENUMATH 2015, *Lecture Notes in Computational Science and Engineering*, vol. 112, pp. 317–331. Springer (2016)
13. Ohlberger, M., Schaefer, M.: A reduced basis method for parameter optimization of multiscale problems. In: Proceedings of Algoritmy 2012, Conference on Scientific Computing, Vysoke Tatry, Podbanske, September 9-14, 2012, pp. 272–281 (2012)
14. Ohlberger, M., Schaefer, M.: Error control based model reduction for parameter optimization of elliptic homogenization problems. In: Y. Le Gorrec (ed.) 1st IFAC Workshop on Control of Systems Governed by Partial Differential Equations, CPDE 2013; Paris; France; 25 September 2013 through 27 September 2013; Code 103235, vol. 1, pp. 251–256. International Federation of Automatic Control (IFAC) (2013)
15. Ohlberger, M., Schindler, F.: A-posteriori error estimates for the localized reduced basis multi-scale method. In: J. Fuhrmann, M. Ohlberger, C. Rohde (eds.) Finite Volumes for Complex Applications VII-Methods and Theoretical Aspects, *Springer Proceedings in Mathematics & Statistics*, vol. 77, pp. 421–429. Springer International Publishing (2014)
16. Ohlberger, M., Schindler, F.: Error control for the localized reduced basis multi-scale method with adaptive on-line enrichment. SIAM J. Sci. Comput. **37**(6), A2865–A2895 (2015)
17. Oliveira, I.B., Patera, A.T.: Reduced-basis techniques for rapid reliable optimization of systems described by affinely parametrized coercive elliptic partial differential equations. Optim. Eng. **8**(1), 43–65 (2007)
18. Rösch, A., Wachsmuth, D.: A-posteriori error estimates for optimal control problems with state and control constraints. Numer. Math. **120**(4), 733–762 (2012)
19. Tröltzsch, F., Volkwein, S.: POD a-posteriori error estimates for linear-quadratic optimal control problems. Comput. Optim. Appl. **44**(1), 83–115 (2009)
20. Vanderbei, R.J., Shanno, D.F.: An interior-point algorithm for nonconvex nonlinear programming. Comput. Optim. Appl. **13**(1-3), 231–252 (1999). Computational optimization—a tribute to Olvi Mangasarian, Part II
21. Vossen, G., Volkwein, S.: Model reduction techniques with a-posteriori error analysis for linear-quadratic optimal control problems. Numer. Algebra Control Optim. **2**(3), 465–485 (2012)