Adaptive Localized Model Reduction

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(joint work with Stephan Rave, Felix Schindler)

Many physical, chemical, biological or technical processes can be described by means of partial differential equations. Due to nonlinear dynamics, interacting processes on different scales, and possible parametric or stochastic dependencies, an analysis and prediction of the complex behavior is often only possible – if at all – with severe simplifications. This is in particular true if not only single forward problems are considered, but beyond that uncertainty quantification, parameter estimation or optimization in engineering applications are investigated.

It has been proven that modern algorithmic approaches such as higher order adaptive modeling and model order reduction combined with efficient software design for highly parallel environments outperforms the pure gain of increasing compute power. Hence, there is a need for algorithmic improvement, both concerning a reduction of the overall computational complexity and concerning new parallelization paradigms in order to exploit the computational resources of nowadays computer architectures in an optimal manner.

A mathematical key ingredient to achieve "optimal" numerical methods is error control via rigorous a posteriori error estimates. Such error estimates can not only be used to certify approximate solutions, but rather are the essential building block in the construction of problem adapted optimal solution spaces and related adaptive numerical methods. Examples of such optimal methods are e.g. particularly tuned mesh-adaptive finite element schemes for the approximation of PDEs or reduced basis methods (weak greedy algorithms) for the approximation of parameterized PDEs.

As a particular example we investigate model reduction for spatially resolved Li-ion batteries [14] based on POD basis construction for the state space reduction and empirical interpolation [2, 4] to deal with the non-linear electrochemical reaction kinetics. Numerical experiments demonstrate a speedup of the online computational complexity with respect to the underlying finite volume approximation by a factor of about 280. In that sense the reduced basis approach is very efficient. On the other hand, this online efficiency comes with the price of an enormous offline complexity, both with respect to CPU time and with respect to storage requirements. These observations motivate the development of new model reduction paradigms that overcome the classical offline/online splitting of projection based model reduction technique. An attempt towards this goal is the development of localized model reduction methods, such as e.g. the reduced basis element method [11], the reduced basis hybrid method [7], the port reduced static condensation reduced basis element method [17], or ArbiLoMod, a new approach for handling problems with arbitrary local modifications [3].

In this contribution we focus on the localized reduced basis methods (LRBM), which were first introduced in the context of elliptic heterogeneous multiscale problems in [9] and later applied in the context of two phase flow in porous media in

[8]. As demonstrated in [1], such an approach has the potential to reduce the offline cost at the price of a decreased online efficiency. It was also shown that depending on the choice of the macro mesh for the localization, the resulting localized reduced basis method can be seen as an interpolation of a classical reduced basis method and a Discontinuous Galerkin approximation on the underlying fine grid. First results for an application of LRBM to the fully non-linear Li-ion battery model were given in [13]. Although this approach allowed for balancing of offline and online complexity, it still maintained the paradigm of offline/online splitting.

In a more recent approach [16] we overcome this paradigm by allowing for local basis enrichment in the online-phase. Within this new conceptual approach we do not aim at first constructing a reduced basis that has good approximation properties with respect to the whole solution manifold of the parameterized system and then using it for fast online evaluations. We rather think of an iterative enrichment procedure, where the reduced space is updated during the online phase in an appropriate manner, while the user explores the solution manifold. To achieve this goal we allow for carefully selected adaptive local problem solves in the online phase, based on localized a posteriori error estimation. To this end, we derive robust and efficient a posteriori error estimates for the localized reduced basis approximation against the true solution of the underlying PDE. The a posteriori error estimate is based on conservative flux reconstruction for elliptic equations, following the approach in [5] and on the additional usage of elliptic reconstructions in the case of parabolic problems [6, 15]. Several numerical experiments for elliptic and parabolic applications demonstrate the applicability of the approach.

The numerical results were obtained with the newly developed model reduction algorithms implemented in the open-source Python software package pyMOR (see http://pymor.org and [12]).

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