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SPACE-ADAPTIVE REDUCED BASIS SIMULATION FOR TIME-DEPENDENT PROBLEMS

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Abstract. We address the task of model reduction of parametrized evolution equations. Detailed simulations of such partial differential equations are frequently expensive to compute due to the space resolution of the discretization and not suitable for multi-query-settings, i.e. multiple simulation requests with varying parameters. Reduced basis (RB) methods are increasingly popular methods to solve such parametrized problems. The currently existing RB-methods for time-dependent problems use identical dimensionality N of the reduced model for all timesteps. This may be suboptimal, as different solution structures may require different dimensionalities N at different times, or a prescribed error tolerance should be obtained.

In the current presentation, we extend a recently introduced RB-scheme, in order to adaptively choose N in time. This adjustment of the model dimension is based on a posteriori error estimators, which can be computed rapidly during the online simulation. We provide experimental insights based on two advection-diffusion problems. We demonstrate, that the trial-and-error process of the N-fixed approach for obtaining a desired model accuracy, can be circumvented by the N-adaptive approach. In examples, where the solution complexity is changing over time, the N-adaptive approach yields an overall gain in computation time.

1 Introduction

We address the task of model reduction for *parametrized* evolution equations. These are problems which are characterized by a parameter vector $\mu \in \mathscr{P}$ from some set of possible parameters $\mathscr{P} \subset \mathbb{R}^p$, and the evolution problem is to determine $u(t,\mu) \in L^2(\Omega)$ on an open bounded space domain $\Omega \subset \mathbb{R}^d$ and finite time interval $t \in [0,T], T > 0$ such that

$$\begin{aligned} \partial_t u(\mu) + \mathscr{L}(t,\mu)(u(t,\mu)) &= 0 \quad \text{in} \quad \Omega \times [0,T] && (1)\\ u(0,\mu) &= u_0(\mu) \quad \text{in} \quad \Omega && (2) \end{aligned}$$

and suitable boundary conditions are satisfied. Here $u_0(\mu) \in L^2(\Omega)$ are the parameter-dependent initial values, $\mathscr{L}(t,\mu)$ is the parameter dependent spatial differential operator. Discretization with finite element or finite volume schemes and first order time discretization, yields discrete solutions $u_H^k(\mu) \in \mathscr{W}_H, k = 0,\ldots,K$ in the H-dimensional discrete space $\mathscr{W}_H \subset L^2(\Omega)$ approximating $u(t^k,\mu)$ at the time instants $0 = t^0 < t^1 < \ldots < t^K = T$. These discretization schemes can compactly be expressed by the iteration

$$\begin{aligned} L_I^k(\mu)[u_H^{k+1}(\mu)] &= L_E^k(\mu)[u_H^k(\mu)] + b^k(\mu) && (3)\\ u_H^0(\mu) &= P[u_0(\mu)] && (4) \end{aligned}$$

for $k = 0,\ldots,K-1$, with initial data projection operator P, implicit discretization contributions in the operator $L_I^k(\mu)$ and explicit contributions in the operator $L_E^k(\mu)$. Such detailed simulations are frequently expensive to compute due to the space resolution and not suitable for use in multi-query settings, i.e. multiple simulation requests with varying parameters μ.

Reduced Basis Methods are increasingly popular methods to solve such parametrized problems, aiming at a problem-dependent simulation scheme, that approximates the detailed solutions $u_H^k(\mu)$ by efficiently computed reduced solutions $u_N^k \in \mathscr{W}_N$. Here $\mathscr{W}_N \subset L^2(\Omega)$ is an N-dimensional *reduced basis space* with suitable *reduced basis* $\Phi_N = \{\varphi_i\}_{i=1}^N$ which is generated in a problem specific way based on *snapshots* of detailed solutions for suitably chosen time instants k_i and parameters $\mu_i \in \mathscr{P}$, i.e. $\Phi_N \subset \operatorname{span}\{u_H^{k_i}(\mu_i)\}$. A reduced basis Φ_N is hierarchical in the sense, that for $1 \le N' \le N$ the bases $\Phi_{N'} := \{\varphi_i\}_{i=1}^{N'} \subset \Phi_N$ span N'-dimensional reduced spaces $\mathscr{W}_{N'} := \operatorname{span}(\Phi_{N'})$ which are nested by $\mathscr{W}_1 \subset \mathscr{W}_2 \subset \ldots \subset \mathscr{W}_{N-1} \subset \mathscr{W}_N$. An important focus of RB-methods is a posteriori error estimation of the model error $\left\|u_N^k(\mu) - u_H^k(\mu)\right\| \le \Delta^k(\mu)$ in suitable norms $\|\cdot\|$. The estimators $\Delta^k(\mu)$ can be rapidly computed during the reduced simulation and are rigorous and sharp upper bounds of the true error.

Reduced basis methods in particular have been applied successfully to various elliptic and parabolic problems, almost exclusively based on finite element discretizations. For linear elliptic problems we refer to [5], linear parabolic equations are treated in [2], extensions to nonlinear equations [8, 1] or systems [6] have been developed. Recently, we have proposed an RB-formulation for linear finite volume schemes [3] in case of so called *affine parameter dependence* of the data functions. We extended the finite volume RB-scheme to explicit discretizations with general parametric dependence and demonstrated its applicability [4].

The currently existing RB-methods for time-dependent problems use identical dimensionality $N^k := N$ for all timesteps k. This may be suboptimal, as different solution structures may require different dimensionalities N^k at different times. Given a certain desired error threshold $\varepsilon > 0$, a too large N will result in an unnecessarily good simulation result with unnecesarily large simulation time. On the contrary, a too small N may result in an intolerable error estimator value and require refined simulation. Hence it may be favourable in time-dependent simulations, to choose the model depth N^k during the reduced simulation.

The current presentation is structured as follows. In Section 2 we extend the RB-scheme of [3], in order to adaptively choose N^k. The previous and new approach will subsequently be denoted *N-fixed* and *N-adaptive*. In Section 3 we provide experimental insights based on the RB-scheme applied on two advection-diffusion problems. We conclude in Section 4.

2 N-Adaptive RB-Scheme

We assume to have given a reduced basis Φ_N. Without loss of generality, the basis functions φ_n are assumed to be orthonormal with respect to the $L^2(\Omega)$ inner product, i.e. $\langle \varphi_i, \varphi_j \rangle = \delta_{ij}$. The reduced solution $u_N^k(\mu)$ at time t^k is a linear combination of $N^k \leq N$ reduced basis functions $u_N^k(\mu) = \sum_{n=1}^{N^k} a_n^k \varphi_n$. The coefficient vectors $\mathbf{a}^k := (a_n^k)_{n=1}^{N^k}$ and dimensions N^k are defined by the reduced basis scheme. The scheme is identical to [3], except that at each timestep, the dimension N^{k+1} is adapted to a (possibly) new value depending on the current solution $u_N^k(\mu)$, error estimator $\Delta^k(\mu)$ and a desired threshold ε for the error estimator at end time.

Definition 2.1 (N-Adaptive RB-Scheme)**.** *We assume that an orthonormal reduced basis Φ_N and an evolution scheme of the form (3)–(4) are given. We further assume that a sequence $(N^k)_{k=0}^K$ is given or can be obtained during the simulation. The N-*adaptive RB-scheme *then proceeds in these steps:*

- *The initial coefficient vector is obtained as a projection of the detailed initial data*

$$\mathbf{a}^0 := (\langle P[u_0(\mu)], \varphi_n \rangle)_{n=1}^{N^0}.$$

- *For each $k = 0, \ldots, K-1$ and given N^{k+1} we determine the next coefficient vector $\mathbf{a}^{k+1}$ by solving*

$$\mathbf{L}_I^k(\mu)\mathbf{a}^{k+1} = \mathbf{L}_E^k(\mu)\mathbf{a}^k + \mathbf{b}^k(\mu)$$

with matrices and vectors

$$\mathbf{L}_I^k = \left(\left\langle \varphi_i, L_I^k(\mu)[\varphi_j] \right\rangle \right)_{i,j=1}^{N^{k+1}}, \quad \mathbf{L}_E^k = \left(\left\langle \varphi_i, L_E^k(\mu)[\varphi_j] \right\rangle \right)_{i,j=1}^{N^{k+1},N^k}, \quad \mathbf{b}^k = \left(\left\langle \varphi_i, b^k(\mu) \right\rangle \right)_{i=1}^{N^{k+1}}. \tag{5}$$

For the above simulation scheme, efficient a posteriori error estimators can be computed. A simple $L^\infty([0,T],L^2(\Omega))$-error estimator has been given in [3], which is as well valid in the current N-adaptive case. We assume $\left\|L_E^k\right\| \leq C$ and $\left\|L_I^{-1}\right\| \leq 1$ (for the $L^2(\Omega)$-induced operator norms), which are satisfied for several typical PDE discretizations. Then, the following error estimate holds:

$$\|u_H(\mu) - u_N(\mu)\|_{L^\infty([0,t^k],L^2(\Omega))} \leq \Delta^k(\mu) \tag{6}$$

Here, $u_H(\mu), u_N(\mu) \in L^\infty([0,T],L^2(\Omega))$ denote functions, which are piecewise constant in time and coincide with u_H^k, resp. u_N^k on the time-slab $[t^k, t^{k+1})$. The error bound can be computed as

$$\Delta^k(\mu) := C \sum_{k'=0}^{k} \left\| R^k(\mu) \right\|. \tag{7}$$

As can be seen, the error bound consist of additive components $\left\|R^k(\mu)\right\|$ which are accumulated during the simulation in time. The computation is based on evaluations of suitably defined residuals $R^k(\mu) \in \mathscr{W}_H$.

The above simulation scheme, the residual norms and the error estimator can be computed in complexity independent of H, the dimensionality of $\mathscr{W}_H$. Instead they can be determined polynomial in N, in case of so called affine parameter dependence and a suitable offline-online decomposition. For details we refer to [3].

For the above N-adaptive approach, a heuristic rule for adjusting N^k must be defined. A simple strategy is to aim at a certain target for the a posteriori error estimator, e.g. linear development in time $T^k := k\frac{\varepsilon}{K}$ and define suitable

increases and decreases in model dimension depending on the deviation of the current estimator from the target curve. For the experiments, we apply

$$N^0 := N, \quad N^{k+1} := \max(\min(N^k + \delta N^k, N), 1). \tag{8}$$

with the increment (resp. decrement) δN^k

$$\delta N^k := \text{round}(S(\Delta^k(\mu) + K'(\Delta^k(\mu) - \Delta^{k-1}(\mu)) - T^{k+K'})). \tag{9}$$

Here, $K' \in \mathbb{N}$ is a parameter indicating the number of look-ahead timesteps and $S \in \mathbb{R}^+$ a factor in the slope of the N-increment. The above estimator simply assumes a linear growing of $\Delta^k(\mu)$ specified by a backward difference and the current value of $\Delta^k(\mu)$. The deviation of this linear extrapolation and the target value at time instant $k+K'$ are converted into a linear increment/decrement of N. This choice of the sequence of N^k is an ad-hoc procedure, which certainly leaves space for improvements.

Despite heuristics, an attractive conceptional aspect of the above scheme is equidistribution of error contributions. A widespread target in grid-adaptive numerical simulations is the use of local error estimators, which contribute additively to a global error estimator. The grid refinement/coarsening is performed such that the local error estimators are equally distributed over the domain Ω and a target threshold is reached [7]. In analogy, the above linear target for Δ^k corresponds to equally sized residual norms $\left\|R^k\right\|$ in time. Hence, the above adaptive scheme implicitly aims at an equal distribution of the residual norms over the time domain.

3 Experiments

The following experiments provide insights in the N-adaptive approach compared to the N-fixed approach. We consider rectangular domains $\Omega \subset \mathbb{R}^2$, with boundary decomposed into Dirichlet and Neumann segments $\partial\Omega = \Gamma_{\text{dir}} \cup \Gamma_{\text{neu}}$. We assume a linear advection-diffusion equation

$$\partial_t u(\mu) + \nabla \cdot (\mathbf{v}(\mu)u(\mu) - \delta(\mu)\nabla u(\mu)) = 0 \quad \text{in } \Omega \times [0,T] \tag{10}$$

with suitable initial data $u(\mu) = u_0(\mu)$ for $t = 0$, inhomogeneuos Dirichlet data $u(\mu) = u_{\text{dir}}(\mu)$ in $\Gamma_{\text{dir}} \times [0,T]$ and Neumann boundary data $\delta(\mu)\nabla u(\mu) \cdot \mathbf{n} = u_{\text{neu}}(\mu)$ in $\Gamma_{\text{neu}} \times [0,T]$. This can be discretized with cellwise constant functions and Finite Volume schemes, which results in a corresponding discretization space $\mathscr{W}_H$ and discretization operators L_I^k and L_E^k as presented in [3], using an Engquist-Osher flux for the convective contributions.

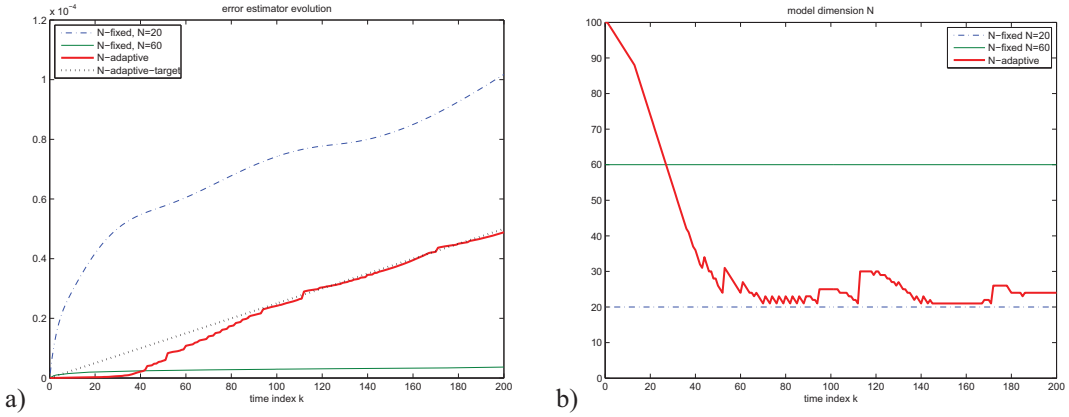
3.1 Setting 1

Our default problem is a model of a fuel cell gas diffusion layer. The computational domain is $\Omega = [0, 10^{-3}] \times [0, 2 \cdot 10^{-4}]$ discretized with a 200×40 Cartesian grid defining the finite volume cells. The time range with end time $T = 0.5$ is discretized with $K = 200$ time intervals such that the resulting time-step size satisfies the CFL condition and guarantees a stable simulation scheme.

The model is characterized by a 3-dimensional parameter space $\mu = (c_{\text{init}}, \beta, \delta) \in \mathscr{P} := [0,1] \times [0,1] \times [0, 5 \cdot 10^{-8}]$. Here, the first parameter c_{init} models the amplitude of a wave-shaped initial distribution $u_0(x,\mu)$. The second parameter models the Dirichlet value β at the inlet and $1-\beta$ at the outlet of the fuel cell component. The last parameter $\delta(x,\mu) := \delta$ models the global diffusivity of the gas diffusion layer. The velocity field $\mathbf{v}(x,\mu)$ is not parameter dependent, time-invariant, but spatially variant, precomputed as a pressure-gradient from an elliptic PDE. The boundary of the domain contains further no-flow and outflow boundaries with corresponding $u_{\text{neu}}(\mu)$, which does not involve parameters. The basis generation procedure is based on an equidistant 5^3 grid in parameter space and a greedy basis extension procedure resulting in a reduced basis Φ_N of $N = 100$ reduced basis vectors. For further details on the model and basis generation procedure, we refer to [3].

For the N-adaptive RB-scheme, we set the look-ahead timestep number $K' = 20$ and the slope-factor $S = 10$, a comment on this choice will follow below. Qualitative results of the corresponding N-adaptive RB simulation are depicted in Fig. 1 for the parameter choice $\mu = (1,0,0)^T$. The left plot a) illustrates the error estimator evolution for the N-fixed approach for the two choices $N = 20, 60$, the estimator development for the N-adaptive approach and the target line for the estimator. The right plot b) illustrates the adaptively adjusted model order N during time and the dimension of the two N-fixed models. As expected, the N-fixed approach may result in either an overly fine model ($N = 60$) or in a too coarse model ($N = 20$), which requires recomputation of a model with higher N. This trial and error process of choosing a correct value of N can obviously be prevented with N-adaptivity. The error estimator is steered in such a way, that it approximately reaches the desired prescribed tolerance level at end time. This in turn is a rigorous upper bound on the true simulation error.

Experimentally, there is a tradeoff between the approximation accuracy of the error estimator to the target line, and the variability of the model order in time. This can be adjusted by variation of S, the factor in the N-increment (9) and K', the look-ahead range. For example, the variability of the N-curve can be reduced by decreasing S with the consequence of a less tight matching of the error estimator target curve.



a) b)

Figure 1: N-fixed and N-adaptive RB simulation results over time for time-invariant example. a) Error estimator development, b) model order N.

There are some notable limitations, that we observed in investigation of this example. First, we lose some acceleration methods for the N-adaptive approach, that can be applied in the N-fixed approach in certain cases. As the reduced system components are not time-dependent (N fixed and all data functions time-invariant), the solution of the sequence of reduced linear equation systems over time can be accelerated by precomputing the inverse or an LU-decomposition of the implicit system matrix. These precomputations seem prohibitive for the N-adaptive approach. Hence in these cases, an accelerated N-fixed approach is very likely to be faster than a non-accelerated N-adaptive approach. Second, in case of pure explicit discretization ($L_I^k = Id$, $\mathbf{L}_I^k = \mathbf{I}_N$), the reduced N-fixed scheme is already very fast (one matrix-vector multiplication), such that the N^k-estimation step of the adaptive approach is dominant and the N-adaptive approach will not result in a clear acceleration benefit.

3.2 Setting 2

As explained in the previous section, the N-adaptive approach is expected to be computationally beneficial mainly in cases, where the solution complexity is changing over time and we have time-variant data functions and implicit discretization components. In order to demonstrate this, we fix the unit square $\Omega = [0,1]^2$ discretized with an unstructured triangular grid consisting of 5248 triangles. The time discretization is specified by the end time $T = 2$ and $K = 500$ timesteps. The parametrization of the problem is given by $\mu = (c_1, c_2, \delta) \in \mathscr{P} := [0,1]^3$. Here, the first two parameters are amplitude coefficients in the Dirichlet boundary values

$$u_{dir}(t,\mu) = c_1 \sin(-\pi t)\chi_{[0,1)}(t) + c_2 \sin(-16\pi t + \pi)\chi_{[1,2)}(t) \tag{11}$$

modeling a low-frequency wave on $t \in [0,1]$ and a high-frequency wave on $t \in [1,2]$. The Dirichlet boundary consists of the left and lower boundary of the unit square, while the upper and right boundary are outflow boundaries. The initial data is consistenty chosen depending on the parameter c_1 as

$$u_0(x,\mu) = c_1 \sin(\pi x_1)\chi_{\{x_1<x_2\}}(x) + c_1 \sin(\pi x_2)\chi_{\{x_1\geq x_2\}}(x). \tag{12}$$

The velocity field is constant and parameter-independent $\mathbf{v}(\mu) := (1,1)^T$, the diffusivity is constant but parameter dependent $\delta(\mu) := \delta$. Therefore, the Dirichlet-values are transported diagonally into the domain. Hence, the solution is considered to be more difficult on the time range $t \in [1,2]$. Again, the reduced basis is generated by a uniform grid in parameter domain and a greedy search as described in [3]. We obtain a basis with $N = 64$ basis vectors. We choose the parameters of the N-estimation as $K' = 40, S = 10$.

Figure 2 presents the error estimator development a) and N-development b) over time for the time-variant advection example analogous to the previous example using $\mu = (1,1,1)^T$. Again we see, that the control of the error estimator towards a desired output works. The N-fixed approaches reveal a clear increase in the error estimator curve on the second half of the time interval, which reflects the structural difficulty of the solution. In contrast to this, we again see, that the N-adaptive approach nicely attaches to the target curve. The structural complexity of the solution after $t = 1$ is reflected in the chosen dimension N, as indeed, the required dimensionality is much higher at this time. The N-adaptive approach, therefore, nicely detects and adapts to the solution complexity in time.

Figure 3 illustrates a plot of the runtime over the true error $\|u_H(\mu) - u_N(\mu)\|_{L^\infty([0,T],L^2(\Omega))}$ for both the N-adaptive and the N-fixed approach with $\mu = (1,1,1)$. The times are averaged over 10 runs determined on a Lenovo Laptop with Intel Centrino Duo processor, 2.0 GHz, 1 GB RAM. The chosen model dimension for the N-fixed approach ranges from 8 to 32. For the N-adaptive approach the average resulting model dimensions range from 10.2 to 33.5. We observe 3 phases. For model dimension above a certain threshold (32 for this μ, right border of the plot), the error does not decrease any further as we reached the resolution accuracy of the reduced basis. For too low model

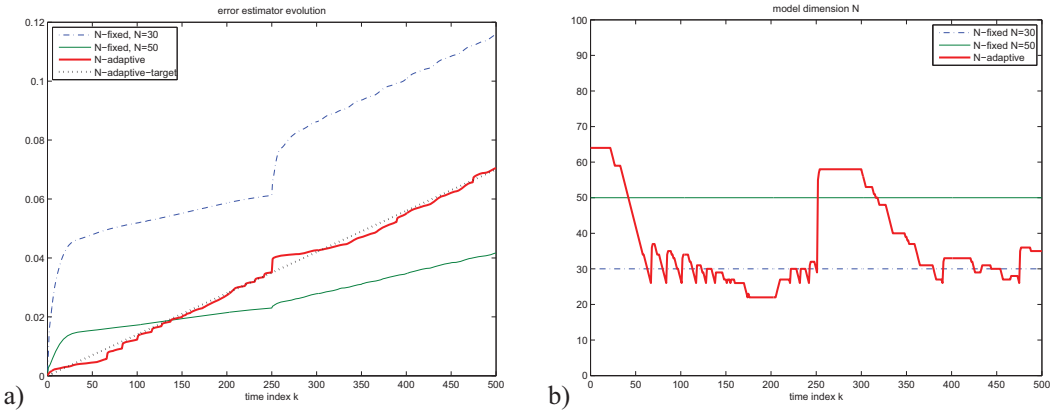


Figure 2: N-fixed and N-adaptive RB simulation results over time for time-variant advection example. a) Error estimator development, b) model order N.

dimension (less than 8 in this example, left border of the plot), the N-fixed approach is so fast, that the additional overhead of N-estimation in the N-adaptive approach results in a slower adaptive simulation scheme. In the range between these values, the curve of the N-adaptive approach is below the N-fixed approach. Hence, the adaptive approach results in lower true error for the same computational time. Obviously, the N-adaptive approach realizes a runtime gain over the N-fixed approach despite the additional estimation-overhead. Replacing the computational time with the average dimension N over time would result in an even more expressed but qualitatively identical plot. Hence the N-adaptive approach does distribute the dimension N over time, such that the resulting error is smaller than taking this average N as fixed dimension.

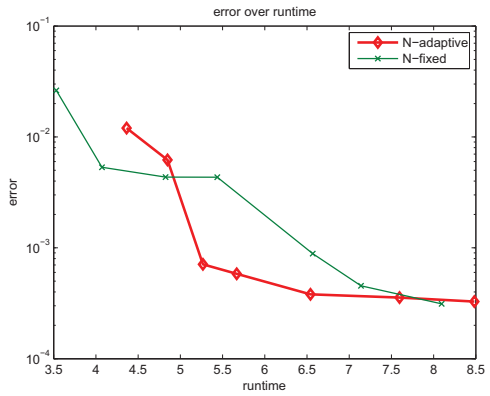


Figure 3: Error over runtime [s] for N-fixed and N-adaptive RB simulations.

4 Conclusions

We have presented an extension of an RB-scheme for time-dependent problems, which supports varying model dimension N^k over time. A heuristic way of choosing N^k based on a linear growing target for the error estimator has been presented as one particular instance. This scheme can be interpreted as an equidistribution strategy of the residual norms in time. The resulting N-adaptive approach allows to steer the error-estimators to desired target curves. By this, multiple simulation runs for trial-and-error with N-fixed simulations can be prevented. Due to the rigorosity of the error estimators, this final error estimator value is a strict upper bound on the true (but unknown) error. In the presented approach there are some parameters that can be chosen. They realize a tradeoff between the variability of the model dimension and the smoothness of the error-estimator curve. Hence, the error estimator can be forced to attach more closely to the target line, by accepting a larger varying/oscillating model dimension curve. The N-adaptive approach has a computational overhead by estimation of the model dimension. Still, the N-adaptive approach can also be demonstrated to be beneficial in terms of runtime for obtaining a certain error. We have demonstrated this speed advantage for a problem that is sufficiently complex, contains implicit discretization components and has time-varying data functions. Obviously, one perspective is development of more more sophisticated rules for the adjustment of the model dimension N and application to other a posteriori error estimators. Increasing and decreasing the model dimension is actually only one particular way of adjusting the reduced space during time. A more complex and attractive question therefore is optimal subspace selection over time.

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