

Matrix Equations, Sparse Solvers: M-M.E.S.S.-2.0.1 — Philosophy, Features and Application for (Parametric) Model Order Reduction

Peter Benner*

Martin Köhler*

Jens Saak*

March 5, 2020

Abstract

Matrix equations are omnipresent in (numerical) linear algebra and systems theory. Especially in model order reduction (MOR) they play a key role in many balancing based reduction methods for linear dynamical systems. When these systems arise from spatial discretizations of evolutionary partial differential equations, their coefficient matrices are typically becoming large and sparse. Moreover, the numbers of inputs and outputs of these systems are typically far smaller than the number of spatial degrees of freedom. Then, in many situations the solutions of the corresponding large-scale matrix equations are observed to have low (numerical) rank. This feature is exploited by M-M.E.S.S. to find successively larger low-rank factorizations approximating the solutions. This contribution describes the basic philosophy behind the implementation and the features of the package, as well as its application in the model order reduction of large-scale linear time-invariant (LTI) systems and parametric LTI systems.

1 Introduction

The M-M.E.S.S. toolbox [51] for MATLAB[®] (or package for GNU Octave) in version 2.0.1 focuses on the solution of large-scale symmetric algebraic and differential matrix equations and their application in model order reduction (MOR) and linear-quadratic regulator (LQR) problems. The basis for all considerations and problem formulations are linear dynamical systems of the form

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \quad (\Sigma)$$

where $E, A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$, $D \in \mathbb{R}^{p \times m}$, and $x(t) \in \mathbb{R}^n$, for all time instances $t \in [0, T]$. We assume that E is invertible, and often in addition that (Σ) is asymptotically stable.

Some of the supported matrix equations have applications in H_∞ -control, where the slightly more structured system

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + B_1u(t) + B_2w(t), \\ y(t) &= C_1x(t) + D_{11}u(t) + D_{12}w(t), \\ z(t) &= C_2x(t) + D_{21}u(t) + D_{22}w(t), \end{aligned} \quad (\Sigma_\infty)$$

is considered.

M-M.E.S.S. aims at systems, where $n \in \mathbb{N}$ is too large to store an $n \times n$ matrix in the computer's memory. This will usually be accounted for by the facts, that $p, m \ll n$ and E, A are sparse, or have a sparse realization that we can exploit in computations. We present more details about the exploitable structures in Section 2.

Similarly, for systems (Σ_∞) the matrices B_1, B_2, C_1, C_2 are considered thin and rectangular and the parts $D_{ij}, i, j \in \{1, 2\}$ correspondingly small.

*Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany, {benner, koehlerm, saak}@mpi-magdeburg.mpg.de

The contribution of this document is two-fold. On the one hand, we give the first concise introduction to M-M.E.S.S., its general philosophy and current features. On the other hand, we show how the software, that is in core intended for the solution of large-scale matrix equations, can be employed in the implementation of basic parametric model order reduction (PMOR) methods for systems of the form (Σ) .

Before moving on to the historical evolution of the package, we state the equations that can currently be solved by M-M.E.S.S.. The following is a list of all equations for which at least one solver function exists:

Algebraic Lyapunov equations

$$\begin{aligned} 0 &= APE^\top + EPA^\top + BB^\top \\ 0 &= A^\top QE + E^\top QA + C^\top C \end{aligned} \quad (\text{CALE})$$

Algebraic Riccati equations

$$\begin{aligned} 0 &= APE^\top + EPA^\top + BB^\top - EPC^\top CPE^\top \\ 0 &= A^\top QE + E^\top QA + C^\top C - E^\top QBB^\top QE \end{aligned} \quad (\text{CARE})$$

$$\begin{aligned} 0 &= \tilde{A}PE^\top + EP\tilde{A}^\top + \tilde{B}_1\tilde{B}_1^\top - EP\left(\tilde{C}_1^\top\tilde{C}_1 - \tilde{C}_2^\top\tilde{C}_2\right)PE^\top \\ 0 &= \tilde{A}^\top QE + E^\top Q\tilde{A} + \tilde{C}_1^\top\tilde{C}_1 - E^\top Q\left(\tilde{B}_1\tilde{B}_1^\top - \tilde{B}_2\tilde{B}_2^\top\right)QE \end{aligned} \quad (\mathcal{H}_\infty - \text{ARE})$$

In the last pair of equations, the matrix \tilde{A} is sparse plus low-rank (splr), i.e. $\tilde{A} = A + UV^\top$, where U, V are tall and skinny. Moreover the matrices $\tilde{B}_1, \tilde{B}_2, \tilde{C}_1, \tilde{C}_2$ are derived from the given system data by scaling and potentially rotation of the matrices B_1, B_2, C_1, C_2 .

For finite time horizon linear-quadratic control problems, one needs to solve differential Riccati equations. We restrict to providing only the controller equations here, while the dual ‘‘filter-type’’ equations are supported as well.

Autonomous differential Riccati equations

$$-E^\top \dot{Q}(t)E = A^\top Q(t)E + E^\top Q(t)A + C^\top C - E^\top Q(t)BB^\top Q(t)E \quad (\text{ADRE})$$

Non-autonomous differential Riccati equations

$$\begin{aligned} -E(t)^\top \dot{Q}(t)E(t) &= (A(t) + \dot{E}(t))^\top Q(t)E(t) + E(t)^\top Q(t)(A(t) + \dot{E}(t)) \\ &+ C(t)^\top C(t) - E(t)^\top Q(t)B(t)B(t)^\top Q(t)E(t) \end{aligned} \quad (\text{NDRE})$$

The last equations are formulated for the time-varying counterpart of (Σ) , i.e. the system where all matrices are allowed to depend on time as well. Both DREs contain the case of differential Lyapunov equations. Optimized solvers for those are still work in progress and must at the moment be implemented by setting either B , or C (in the dual equation) to zero and thus eliminating the quadratic term. Available solution methods in M-M.E.S.S. are described in Section 2.

Classic Lyapunov equation based balanced truncation is known to preserve asymptotic stability of the original system in the reduced-order model. Other balancing-based methods have been developed to preserve other properties like passivity or contractivity. For these special balancing-type MOR methods, other matrix equations need to be solved that do not have a tailored solver in M-M.E.S.S., yet. Still, they can be reformulated into one of the types above. In order to have a more complete picture, what equations can be solved with the current M-M.E.S.S., we list them here, but get back to them in Section 3 and describe their reformulations into the special cases above and why they can still be solved using M-M.E.S.S..

Positive real balancing

$$\begin{aligned} 0 &= APE^\top + EPA^\top + (EPC^\top - B)(D + D^\top)^{-1}(EPC^\top - B)^\top \\ 0 &= A^\top QE + E^\top QA + (E^\top QB - C^\top)(D + D^\top)^{-1}(E^\top QB - C^\top)^\top \end{aligned} \quad (\text{PRARE})$$

Bounded real balancing

$$\begin{aligned} 0 &= APE^\top + EPA^\top + BB^\top + (EPC^\top + BD^\top)(I - DD^\top)^{-1}(EPC^\top + BD^\top)^\top \\ 0 &= A^\top QE + E^\top QA + C^\top C + (E^\top QB + C^\top D)(I - D^\top D)^{-1}(E^\top QB + C^\top D)^\top \end{aligned} \quad (\text{BRARE})$$

Linear-quadratic Gaussian balancing

$$\begin{aligned} 0 &= APE^\top + EPA^\top + BB^\top - (EPC^\top + BD^\top)(I + DD^\top)^{-1}(EPC^\top + BD^\top)^\top \\ 0 &= A^\top QE + E^\top QA + C^\top C - (E^\top QB + C^\top D)(I + D^\top D)^{-1}(E^\top QB + C^\top D)^\top \end{aligned} \quad (\text{LQGARE})$$

1.1 A brief history of M-M.E.S.S.

Early days, the LyaPack years The package M-M.E.S.S. originates in the work of Penzl [14, 44, 45] around the year 2000. More precisely, we understand M-M.E.S.S. as a continuation and successor of Penzl's LyaPack-toolbox [46] for MATLAB. While most of the basic ideas from the original package have been preserved, some features have been abandoned and some have been altered to improve efficiency and reliability.

The treatment of generalized state-space systems, i.e. systems (Σ) with nontrivial, i.e. non-identity, E -matrices have been added first. These changes still happened under the LyaPack-label in versions 1.1–1.8 until about 2007.

Transition to M-M.E.S.S. and present The transition to the relabeled M-M.E.S.S.-1.0 package included a complete reorganization of the process data. Also, LyaPack used string manipulations and `eval`-calls to mimicked function pointers, which we replaced by proper function handles supported in modern MATLAB and GNU Octave. Moreover, the formulation of the low-rank alternating directions implicit (LR-ADI) iteration, which always was the heart and soul of LyaPack, was greatly updated to allow for cheaper evaluation of stopping criteria and an iteration inherent generation of real solution factors, which could only be achieved through post-processing in LyaPack.

The necessity for an a priori selection of shift parameters for convergence acceleration used to be a major point of criticism regarding the ADI based solvers. The selection of shift generation methods was extended in M-M.E.S.S. and especially a new method that automatically generates the shifts during the iteration [32] was added, which makes the solvers accessible also to non-experts.

Other than that version 1.0 saw general code modernization to support optimized features in MATLAB and to be 100% GNU Octave compatible.

The two major contributions of version 2.0 were the inclusion of the RADI iteration[7] for (CARE) and several solvers for differential Riccati equations in both the autonomous (ADRE) and non-autonomous (NDRE) cases.

Moreover, over time more system classes, including specially structured differential algebraic equation (DAE) based systems and second-order systems, have been added.

Future development plans The most immediate upcoming feature in the near future is the inclusion of Krylov subspace projection methods for algebraic Lyapunov [55, 57] and Riccati equations [58, 37, 56]. The infrastructure and solvers are under current development and the feature is going to be part of version 3.0. The plans for the more distant future include, inclusion of low-rank solvers for Sylvester equations [12] and non-symmetric AREs [13], as well as the discrete-time counterparts of the existing equations, i.e. Stein equations [30, 36, 12, 32, 48] and discrete time Riccati equations. Also, more complex sets of equations like Lur'e equations [47] and Lyapunov-plus-positive equations [18, 8, 54] are currently investigated and will be added if solvers can be implemented in a robust and efficient way using the M-M.E.S.S. infrastructure.

1.2 Structure of this chapter

The following section introduces M-M.E.S.S. and its basic implementation philosophy. It further elaborates on supported system structures beyond the basic form in (Σ) and describes current basic features of the package. Section 3 is dedicated to the description of MOR methods contained or demonstrated in M-M.E.S.S., while

usfs	default	so_1 / so_2	dae_1	dae_2	dae_1/2/3_so
System	standard / generalized state-space form	second-order 1st / 2nd companion form	semi-explicit index-1 DAE	semi-explicit index-2 Stokes-type DAEs	semi-explicit second-order index-1/2/3 DAEs using companion form
Demos	FDM [46], Rail [15]	TripleChain [62, 50]	DAE1 (BIPS Power-systems model [23])	DAE2 Stokes [53], Kármán vortex shedding [65]	constrained TripleChain

Table 1: Supported system structures via user-supplied function sets (usfs).

Section 4 shows how the existing tools in M-M.E.S.S. can be used to implement basic PMOR methods from the literature. The last section shows some results on a selection of the above equations for a set of benchmark examples. Furthermore, the usage of M-M.E.S.S. in parametric model order reduction is demonstrated.

2 M-M.E.S.S. — Philosophy and Features

The M-M.E.S.S. philosophy relies on three simple principles:

abstract state-space system All routines assume to work on a system of the form (Σ) , or (Σ_∞) . For a simple spatially discretized parabolic PDE, (Σ) is exactly given by the sparse matrices describing the semi-discretized system. For other systems, (Σ) may be a dense, inaccessible realization, like, e.g. a projection to a hidden manifold for a Stokes-type DAE system.

implicit reformulation When the system matrices are potentially dense or even inaccessible, or otherwise prohibitive to use, the matrices are never formed explicitly, but only their actions are expressed in terms of the original data. For the aforementioned DAEs this means, only the given semi-explicit system matrices are employed, but the algorithm runs as if it was formulated on the hidden manifold, i.e. for the implicit ordinary differential equation. This technique is often also called *implicit index-reduction*. For second-order systems, similarly, it is sometimes prohibitive to work with the double-sized phase-space realization in companion form. Again, all operations are executed only using the original second-order matrices, while solutions live in the double sized space.

operation abstraction The abstraction of operations is realized via the so-called user-supplied function sets (usfs), which we have inherited from LyaPack. In comparison to LyaPack we have slightly extended this set of functions. At the same time, we have removed the necessity to provide empty functions, which are now automatically replaced by a `do_nothing` function. While making things far more complicated in, e.g. the `default` case (see Table 1), where all matrices are expected to be available, this allows to hide the actual matrix realization from the algorithms. This way, in principle, the algorithms can run matrix-free with respect to A and E as demonstrated in [16].

The basic structure and design, of M-M.E.S.S., was decided when object-oriented features in MATLAB were in their early stages and essentially absent in GNU Octave. Still some of the design follows object-oriented paradigms. We mimic the object-orientation by passing three central data-structures through all relevant functions. These three items of type `struct` are

eqn This structure essentially holds all relevant information about the underlying system (Σ) , or (Σ_∞) and determines which equation in the dual pair we are aiming to solve, by `eqn.type='N'`, or `eqn.type='T'` representing the transposition on the left multiplication by A .

oper The operator structure, generated by the function `operatormanager`, holds all function handles for the relevant operations with the system matrices A and E . A list of these operations can be found in Table 2. Most functions in the list are accompanied by two functions, with appendices `_pre` and `_post`, called at the beginning and the end of a function working with them. They are intended for the generation and clean up of helper data, like the pre-factorization of matrices, when a sparse direct solver is used, or the generation of a preconditioner for an iterative solver.

function call	operation
<code>Y = oper.mul_A(eqn, opts, opA, B, opB)</code>	$Y = A^{\text{opA}} B^{\text{opB}}$
<code>Y = opr.mul_E(eqn, opts, opE, B, opB)</code>	$Y = E^{\text{opE}} B^{\text{opB}}$
<code>Y = oper.mul_ApE(eqn, opts, opA, p, opE, B, opB)</code>	$Y = (A^{\text{opA}} + pE^{\text{opE}}) B^{\text{opB}}$
<code>X = oper.sol_A(eqn, opts, opA, B, opB)</code>	$A^{\text{opA}} X = B^{\text{opB}}$
<code>X = oper.sol_E(eqn, opts, opE, B, opB)</code>	$E^{\text{opE}} X = B^{\text{opB}}$
<code>X = oper.sol_ApE(eqn, opts, opA, p, opE, B, opB)</code>	$(A^{\text{opA}} + pE^{\text{opE}}) X = B^{\text{opB}}$
<code>result = oper.init(eqn, opt, oper, f1, f2)</code>	general initialization and sanity checks
<code>[W, res0] = oper.init_res(eqn, opts, oper, V)</code>	Compute initial residual factor W from V , and $\text{res0} = \ W\ $
<code>[eqn, opts, oper] = eval_matrix_functions(eqn, opts, oper, t)</code>	In the time-varying case, fix all the above to time instance t .
<code>n = oper.size(eqn, opts, oper)</code>	Returns the dimension n in (Σ) .

Table 2: User supplied function names and their actual operation.

opts The actual options structure is a structure of structures, i.e. it has a substructure for each algorithm/function, but also holds central information on the top level. For example `opts.norm` defines the norm that should consistently be used in all operations and hierarchy levels of the potentially cascaded algorithms, while substructures like `opts.adi`, or `opts.shifts` provide the specific control parameters for the LR-ADI algorithm and the shift computation.

Note that for all matrix operations in the usfs, we allow for corresponding `_pre` and `_post` functions. Other functions like `init` or `size` do not support `_pre` and `_post`.

While the function handles in `oper` work on the original A from (Σ) , sometimes it is necessary to actually work with low-rank updated versions of A in the form $A + UV^T$. We have seen an example in $(\mathcal{H}_\infty - ARE)$, where \tilde{A} is in the very form. Another prominent appearance is the Newton-Kleinman iteration (see [31] for classic iteration and [14] for the low-rank version) for (CARE), where in iteration j , the step equation (for the second equation in the pair) takes the form

$$(A - BK_{j-1})^T X_j E + E^T X_j (A - BK_{j-1}) = [C \ K_{j-1}]^T [C \ K_{j-1}].$$

Therefore, most solvers in M-M.E.S.S. assume that this structure can be given. The flag `eqn.haveUV` set to a non-zero value indicates that this is the case. Then the fields `eqn.U` and `eqn.V` need to hold the corresponding dense rectangular matrices of compatible dimensions. Similarly, the field `eqn.haveE` indicates that a non-trivial, i.e. non-identity E matrix is present and needs to be used via the function handles in Table 2.

Note that it is prohibitive to form $A + UV^T$ explicitly, since even for very sparse A it can easily be a dense matrix. Especially, it is prohibitive to use direct solvers based on matrix decompositions on it, since then even if $A + UV^T$ manages to preserve some sparsity, the fill-in will make the triangular factors dense. Therefore, all linear systems with $A + UV^T$ are solved via the Sherman-Morrison-Woodbury matrix-inversion formula (see, e.g. [26, Section 2.1.4]) in M-M.E.S.S..

solver	description	reference
algebraic Lyapunov equations		
mess_lradi	The low-rank alternating directions implicit (LR-ADI) iteration in residual based formulation and with automatic shift selection for (CALE).	[32]
algebraic Riccati equations		
mess_lrn	An inexact Kleinman-Newton iteration with line search for (CARE).	[65]
mess_lrradi	The RADI iteration for (CARE)	[7]
mess_lrri	A low-rank version of the Riccati iteration [34] for ($\mathcal{H}_\infty - ARE$)	
differential Riccati equations		
mess_bdf_dre	Low-rank formulation of backward differentiation formulas for large-scale differential Riccati equations (ADRE), (NDRE)	[33]
mess_rosenbrock_dre	Low-rank formulation of Rosenbrock methods for large-scale differential Riccati equations (ADRE)	[33]
mess_splitting_dre	Splitting schemes for large-scale differential Riccati equations (ADRE), (NDRE)	[59, 60]

Table 3: Solver functions with algorithm and feature descriptions and latest and most feature complete literature references.

2.1 Available solver functions and underlying methods

We provide two solvers for the standard cases in (CALE) and (CARE) that are purely matrix-based, intended for large-scale sparse matrix coefficients and classic 2-term low-rank factorizations of the constant terms and cores in the quadratic terms. The functions are called `mess_lyap` and `mess_care` and mimic the calls of `lyap` and `care` from MATLAB’s control systems toolbox, or the GNU Octave control package, for dense matrices.

Other than that, we have the functions in Table 3 that allow for more flexible tuning, solve a large variety of equations and, especially, benefit from the full potential of the user supplied functions. In the table we give references to the most state of the art presentations of the algorithms in the literature, on which our implementations are based.

3 Model Order Reduction in M-M.E.S.S.

The basic model order reduction (MOR) facilities in M-M.E.S.S. are limited. Still, all building blocks for projection-based MOR using balancing methods, where matrix equations are most obviously applied, are available. For the sake of completeness and to fix our notation, we repeat the basics of projection based MOR. Given a state-space system of the form (Σ), we search for the two rectangular transformation matrices $V, W \in \mathbb{R}^{n \times r}$ that define the actual oblique projection $T = V(W^T V)^{-1} W^T$, but transform the system into the reduced coordinates directly. The reduced-order model then takes the form

$$\begin{aligned} \hat{E} \dot{\hat{x}}(t) &= \hat{A} \hat{x}(t) + \hat{B} u(t), \\ \hat{y}(t) &= \hat{C} \hat{x}(t) + D u(t), \end{aligned} \tag{ROM}$$

where $\hat{E} = W^T E V$, $\hat{A} = W^T A V \in \mathbb{R}^{r \times r}$, $\hat{B} = W^T B \in \mathbb{R}^{r \times m}$, and $\hat{C} = C V \in \mathbb{R}^{p \times r}$.

The number of actual MOR routines in M-M.E.S.S. is rather limited. In version 2.0.1, we have `mess_balanced_truncation` implementing classic Lyapunov balancing [39, 61, 35], for systems (Σ) realized with sparse E and A ([14, 28, 50]), and `mess_tangential_irka` implementing the tangential iterative Krylov algorithm (IRKA) [27] for first and second order systems. Our Gramian computation methods are integrated in a range of MOR software packages, though. While `sssMOR` [19] directly calls M-M.E.S.S.-1.0.1, for other packages like `MOREMBS` [22] and `MORPACK` [40] we have contributed tailored versions of our algorithms.

Also, we provide tools like a square root method (SRM) function to compute the transformation matrices V and W from given Gramian factors. This function currently only uses the classic Lyapunov balancing error bound in the adaptive mode. This is subject to change in future versions.

3.1 IRKA and classic balanced truncation

Consider that all matrices in (Σ) are available. As an example we use the Steel Profile benchmark [15, 42], included in M-M.E.S.S., using the version with $n = 1357$. Then computing the reduced order matrices E_r , A_r , B_r , C_r for maximum reduced order 25 using the tangential IRKA [27] is as easy as calling:

```
eqn = getrail(1);
opts.irka.r = 25;
[Er, Ar, Br, Cr] = mess_tangential_irka(eqn.E_, eqn.A_, eqn.B, eqn.C, opts)
```

This will use default values for maximum iteration numbers and stopping criteria, which can be refined via the `opts.irka` structure. For a list of available options see `help mess_tangential_irka`.

Analogously, to compute a (Lyapunov) balanced truncation approximation of maximum order 50 and with an absolute H_∞ -error tolerance of 10^{-2} for the same model the simplest call is:

```
eqn = getrail(1);
[Er, Ar, Br, Cr] = mess_balanced_truncation(eqn.E_, eqn.A_, eqn.B, eqn.C, 50, ...
    1e-2);
```

Note that Lyapunov balancing leaves the D matrix untouched in general, while it is absent in this example anyway. Note, further, that the interface may change slightly in future releases to make it more consistent with that of the IRKA function and to allow for the addition of the other balancing methods.

The balanced truncation approximation can be achieved in a step by step procedure first computing the two Gramian factors, then applying them in the square root method to determine V and W , and finally compressing the large-scale matrices to the reduced-order system matrices. This can all be executed using the procedural building blocks of `mess_balanced_truncation`. The example `bt_mor_rail_tol` in the `DEMOS/Rail` folder, residing in the main installation folder of M-M.E.S.S.-2.0.1, demonstrates this procedure. The step-wise approach can also be used for a number of structured systems like second-order systems, or semi-explicit DAE systems, while `mess_balanced_truncation` only supports generalized systems with invertible E , and all coefficients given explicitly as matrices, at the moment. See Table 4 for an overview of demonstration examples explaining these procedures.

3.2 Further variants of balanced truncation

We have shown the Riccati equations defining the Gramians employed in positive-real, bounded-real, and linear-quadratic Gaussian balanced truncation in equations (PRARE), (BRARE), (LQGARE) in the Introduction. Assuming, we have computed the Gramian factors, the reduced-order models can be derived, along the lines of the demonstration examples from Table 4. This can be done using the same M-M.E.S.S. function at least for a fixed desired reduced order. The error bound based order decision in the square root method needs adaptation to the specific error bound in some cases, though, see e.g. [2, Section 7.5] for a comparison of the bounds and procedures.

Here, we restrict ourselves to presenting how the specially structured Riccati equations can be solved with the existing functionality in M-M.E.S.S..

3.2.1 Positive-real balancing

For positive-real systems, by definition $D + D^T$ is positive-definite, when it is invertible. This is always the case when the Riccati equations exist and do not degenerate to a set of Lur'e equations. Then we can decompose

Example	Description	References
bt_mor_DAE1_to1	Balanced truncation for a semi-explicit power systems model of differential index 1	[23]
bt_mor_DAE2	Balanced truncation for Stokes and Oseen equations of index 2	[29, 17]
BT_TripleChain	First-order and structure-preserving balanced truncation for a model with three coupled mass-spring-damper chains	[62, 50, 49]
BT_sym_TripleChain	As above, but exploiting state-space symmetry of the tailored companion form first-order reformulation	
BT_DAE3_S0	First-order and structure-preserving balanced truncation for a variant of the above system that has a constraint turning it into an index-3 DAE	[52, 63, 64]

Table 4: Demonstration examples for balanced truncation of structured systems in M-M.E.S.S..

$D + D^T$ into Cholesky factors, i.e. $R^T R = D + D^T$. Using these Cholesky factors, we define

$$\tilde{E} = E, \quad \tilde{A} = A + UV^T, \quad \tilde{B} = BR^{-1}, \quad \tilde{C} = R^{-T}C,$$

with $U = \tilde{B}$ and $V^T = \tilde{C}$, and a straight forward calculation shows that (PRARE) can be rewritten in the form

$$\begin{aligned} 0 &= \tilde{A}P\tilde{E}^T + \tilde{E}P\tilde{A}^T + \tilde{B}\tilde{B}^T + \tilde{E}P\tilde{C}^T\tilde{C}P\tilde{E}^T \\ 0 &= \tilde{A}^T Q\tilde{E} + \tilde{E}^T Q\tilde{A} + \tilde{C}^T\tilde{C} + \tilde{E}^T Q\tilde{B}\tilde{B}^T Q\tilde{E}. \end{aligned}$$

This resembles the Riccati case in $(\mathcal{H}_\infty - ARE)$ with a low-rank updated matrix A and only the positive quadratic term present. This case is supported by the `mess_lrrri` routine. Note that $D + D^T$ is of small dimension, such that this reformulation is always feasible.

3.2.2 Bounded-real balancing

The bounded-real assumptions guarantee that $I - DD^T$ and $I - D^T D$ are symmetric positive definite. Therefore, we can decompose them into Cholesky factors, i.e. $R^T R = I - DD^T$ and $L^T L = I - D^T D$. Now, we define

$$\tilde{E} = E, \quad \tilde{A} = A + UV^T, \quad \tilde{B} = BL^{-1}, \quad \tilde{C} = R^{-1}C,$$

with $U = BD^T$ and $V^T = (I - DD^T)^{-1}C$ and another technical, but straight forward, calculation shows that (BRARE) can be rewritten in the form

$$\begin{aligned} 0 &= \tilde{A}P\tilde{E}^T + \tilde{E}P\tilde{A}^T + \tilde{B}\tilde{B}^T + \tilde{E}P\tilde{C}^T\tilde{C}P\tilde{E}^T \\ 0 &= \tilde{A}^T Q\tilde{E} + \tilde{E}^T Q\tilde{A} + \tilde{C}^T\tilde{C} + \tilde{E}^T Q\tilde{B}\tilde{B}^T Q\tilde{E}. \end{aligned}$$

This, again, falls into the class of equations in $(\mathcal{H}_\infty - ARE)$ with a low-rank updated matrix A and only the positive square term present. As mentioned above, this case is supported by the `mess_lrrri` routine. For the same reason as above, this reformulation can always be done.

3.2.3 Linear-quadratic Gaussian balancing

For linear-quadratic Gaussian balanced truncation, an important special case (see, e.g. [11, 41, 38, 3]) is $D = 0$. In that case (LQGARE) obviously reduces to the standard Riccati equation (CARE) that can be solved using `mess_lrrnm` or `mess_lrradi`. The corresponding M-M.E.S.S. workflow is demonstrated in the `lqgbt_mor_FDM` example for a simple heat equation model semi-discretized by the finite difference method.

On the other hand, when $D \neq 0$, it is, by standard assumptions in M-M.E.S.S., real and all eigenvalues of DD^\top and $D^\top D$ are non-negative. Therefore, $I + DD^\top$ and $I + D^\top D$ are symmetric and positive definite and analogous to the above, we can decompose into Cholesky factorizations $R^\top R = I + DD^\top$ and $L^\top L = I + D^\top D$. We now define

$$\tilde{E} = E, \quad \tilde{A} = A + UV^\top, \quad \tilde{B} = BL^{-1}, \quad \tilde{C} = R^{-1}C,$$

with $U = -BD^\top$ and $V^\top = (I + DD^\top)^{-1}C$. An analogous calculation to the bounded-real case shows that (LQGARE) can be rewritten in the form

$$\begin{aligned} 0 &= \tilde{A}P\tilde{E}^\top + \tilde{E}P\tilde{A}^\top + \tilde{B}\tilde{B}^\top - \tilde{E}P\tilde{C}^\top\tilde{C}P\tilde{E}^\top \\ 0 &= \tilde{A}^\top Q\tilde{E} + \tilde{E}^\top Q\tilde{A} + \tilde{C}^\top\tilde{C} - \tilde{E}^\top Q\tilde{B}\tilde{B}^\top Q\tilde{E}. \end{aligned}$$

Due to the differing signs, here, we end up with a standard Riccati equation (CARE), just like in the case $D = 0$. Again the transformation is always feasible in the sense of M-M.E.S.S. applicability.

4 Parametric Model Order Reduction using M-M.E.S.S.

Parametric MOR (PMOR) aims to preserve symbolic parameters in the original system description also in the reduced-order model. In the most general case that means the system

$$\begin{aligned} E(\mu)\dot{x}(\mu, t) &= A(\mu)x(\mu, t) + B(\mu)u(t), \\ y(\mu, t) &= C(\mu)x(\mu, t) + D(\mu)u(t), \end{aligned} \tag{\Sigma(\mu)}$$

is transformed into

$$\begin{aligned} \hat{E}(\mu)\hat{x}(\mu, t) &= \hat{A}(\mu)\hat{x}(\mu, t) + \hat{B}(\mu)u(t), \\ \hat{y}(t) &= \hat{C}(\mu)\hat{x}(\mu, t) + D(\mu)u(t). \end{aligned} \tag{ROM(\mu)}$$

By default, M-M.E.S.S.-2.0.1 does not support PMOR. It is, however, very easy to implement basic PMOR routines building up on the methods from the previous section. The key ingredient, that at the same time establishes the link to the previous section in many methods, is the necessity to evaluate standard MOR problems in certain training points for given parameter values $\mu^{(i)}$ ($i = 1, \dots, k$), e.g. on a sparse-grid in the parameter domain. While piecewise MOR approaches (e.g. [4]) aim to find constant global (with respect to the parameter) transformation matrices V and W to derive (ROM(μ)), other methods aim to establish it by interpolation of some kind. The literature basically provides three approaches interpolating different system features, see, e.g., [10] for further categorization of PMOR methods:

- matrix interpolation, i.e. function interpolation of the parameter-dependent coefficient matrices, or the transformation matrices, (e.g. [43, 25, 24, 1]),
- interpolation of the transfer functions in the parameter variable [5],
- interpolation of system poles (e.g. [9, 66]).

We demonstrate the basic steps for piecewise and interpolatory methods along the lines of [4, 5] in the remainder of this section and give numerical illustrations in Section 5.

4.1 Piecewise MOR

We have mentioned above that the aim, here, is to find V and W constant, such that $\hat{E}(\mu) = W^\top E(\mu)V$, $\hat{A}(\mu) = W^\top A(\mu)V$, $\hat{B}(\mu) = W^\top B(\mu)$, $\hat{C}(\mu) = C(\mu)V$. The strong point of this method is that it trivially allows the ROMs in the parameters $\mu^{(i)}$ to vary in their reduced-order. This is due to the fact that

$$V = \begin{bmatrix} V^{(1)} & \dots & V^{(k)} \end{bmatrix} \quad \text{and} \quad W = \begin{bmatrix} W^{(1)} & \dots & W^{(k)} \end{bmatrix},$$

with $V^{(i)}$ and $W^{(i)}$ the transformation matrices at parameter sample $\mu^{(i)}$. This concatenation should be followed by a rank truncation to eliminate linear dependencies.

It essentially does not matter how the single transformation matrices have been generated. We follow the presentation in [4], where IRKA is used. In the numerical experiments we also compare to versions using balanced truncation in the training samples.

4.2 Interpolation of transfer functions

The representation of $(\Sigma(\mu))$ in frequency domain after Laplace transformation in the time variable (t) , leads to the transfer function

$$H(\mu, s) = C(\mu)(sE(\mu) - A(\mu))^{-1}B(\mu).$$

The IRKA method seeks to interpolate this function in s -direction and the well known balanced truncation error bound limits the approximation error to this function for fixed μ . Therefore, it is an obvious task to try and preserve these features by interpolation in μ -direction. Baur and Benner meet this goal in [5] for local balanced truncation approximations of $(\Sigma(\mu))$, achieving both stability preservation and an error bound, i.e. the selling points of balanced truncation. Moreover their method shares the flexibility with respect to the ROM orders, since the interpolation is done via the transfer function, that has fixed dimension independent of the realization of the system. On the other hand, interpolation on matrix manifolds and with respect to system invariants need to fix the dimensions of those objects.

For simplicity we restrict ourselves to the case of scalar parameters. The approach in [5] defines $(\text{ROM}(\mu))$ via its transfer function, which is chosen as an interpolant of the form

$$\begin{aligned} \hat{H}(\mu, s) &= \sum_{i=1}^k \ell_i(\mu) \hat{H}^{(i)}(s) = \sum_{i=1}^k \ell_i(\mu) \hat{C}^{(i)} (s\hat{E}^{(i)} - \hat{A}^{(i)})^{-1} \hat{B}^{(i)} \\ &= \sum_{i=1}^k \hat{C}^{(i)}(\mu) (s\hat{E}^{(i)} - \hat{A}^{(i)})^{-1} \hat{B}^{(i)} \end{aligned}$$

with scalar coefficients functions $\ell_i(\mu)$, $\hat{H}^{(i)}(s)$ the transfer function of the ROM at parameter sample $\mu^{(i)}$ and $\hat{C}^{(i)}(\mu) = \ell_i(\mu) \hat{C}^{(i)}$. One can use the last identity to define the matrices for the ROM-realization

$$\hat{E} = \begin{bmatrix} \hat{E}^{(1)} & & \\ & \ddots & \\ & & \hat{E}^{(k)} \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} \hat{A}^{(1)} & & \\ & \ddots & \\ & & \hat{A}^{(k)} \end{bmatrix}, \quad \hat{B} = \begin{bmatrix} \hat{B}^{(1)} \\ \vdots \\ \hat{B}^{(k)} \end{bmatrix},$$

$$\hat{C}(\mu) = [\hat{C}^{(1)}(\mu) \quad \dots \quad \hat{C}^{(k)}(\mu)],$$

such that

$$\hat{H}(\mu, s) = \hat{C}(\mu) (s\hat{E} - \hat{A})^{-1} \hat{B}.$$

Note that the parameter could as well be put into \hat{B} . The specific choice of Lagrange polynomials is not necessary. We present experiments with both classic polynomial interpolation and spline interpolation in the next section. Since we are dealing with scalar coefficient functions here, it is advisable for a modern MATLAB-implementation to exploit the power of Chebfun [21, 20]. We do this for the polynomial interpolation and the generation of the grid of training parameters, while the splines use our own implementation.

5 Numerical Experiments

The experiments reported here have been executed in MATLAB R2019a on a Lenovo X380 Yoga equipped with an Intel[®] i7 8770 and 32GB of main memory running 64bit Linux based on Ubuntu 18.04. The experiments use M-M.E.S.S.-2.0.1 [51] and Chebfun version 5.7.0 [21, 20].

The source code of the implementations used to compute the presented results can be obtained from:

<https://doi.org/10.5281/zenodo.3678213>

and is authored by Jens Saak and Steffen W. R. Werner.

For easier comparison with the other reported software packages, all experiments use the thermal block benchmark introduced in a separate chapter of this volume. It describes a simple heat transfer model on the domain depicted in Figure 1a. Here, we investigate the one parameter version of the benchmark. That means, the heat transfer coefficients on the four circular sub-domains are given as 0.2μ , 0.4μ , 0.6μ , and 0.8μ for a single scalar parameter $\mu \in [10^{-6}, 10^2] = M \subset \mathbb{R}$. The full order model has dimension $n = 7488$ and one

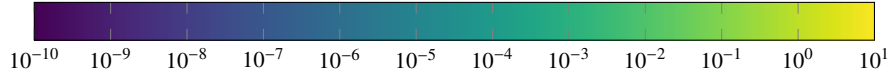
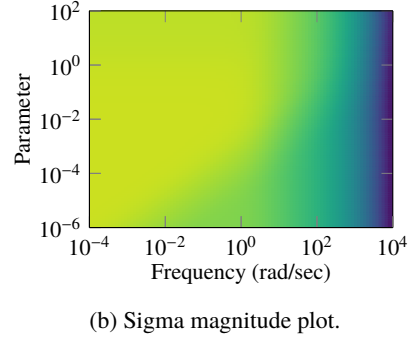
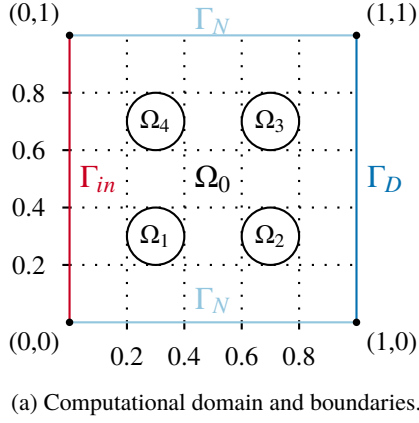


Figure 1: Computational domain and sigma magnitude plot for the thermal block model.

Method	ROMs	Full	One-sided
Piecewise			
BT(10^{-4})	9/12/15/13/12/9/8/9/8/7	102 (52)	200 (36)
BT(20)	20/20/20/20/20/20/20/20/20/20	199 (64)	200 (72)
IRKA	20/20/20/20/20/20/20/20/20/20	200 (132)	200 (132)
Lagrange			
BT(10^{-4})	9/9/12/15/12/9/8/8/7/7	96	–
IRKA	20/20/20/20/20/20/20/20/20/20	200	–
B-Spline			
BT(10^{-4})	9/9/12/15/12/9/8/8/7/7	96	–
IRKA	20/20/20/20/20/20/20/20/20/20	200	–

Table 5: Reduced orders of the training-sample ROMs and final ROM (numbers in () are after additional truncation with tolerance 10^{-6}).

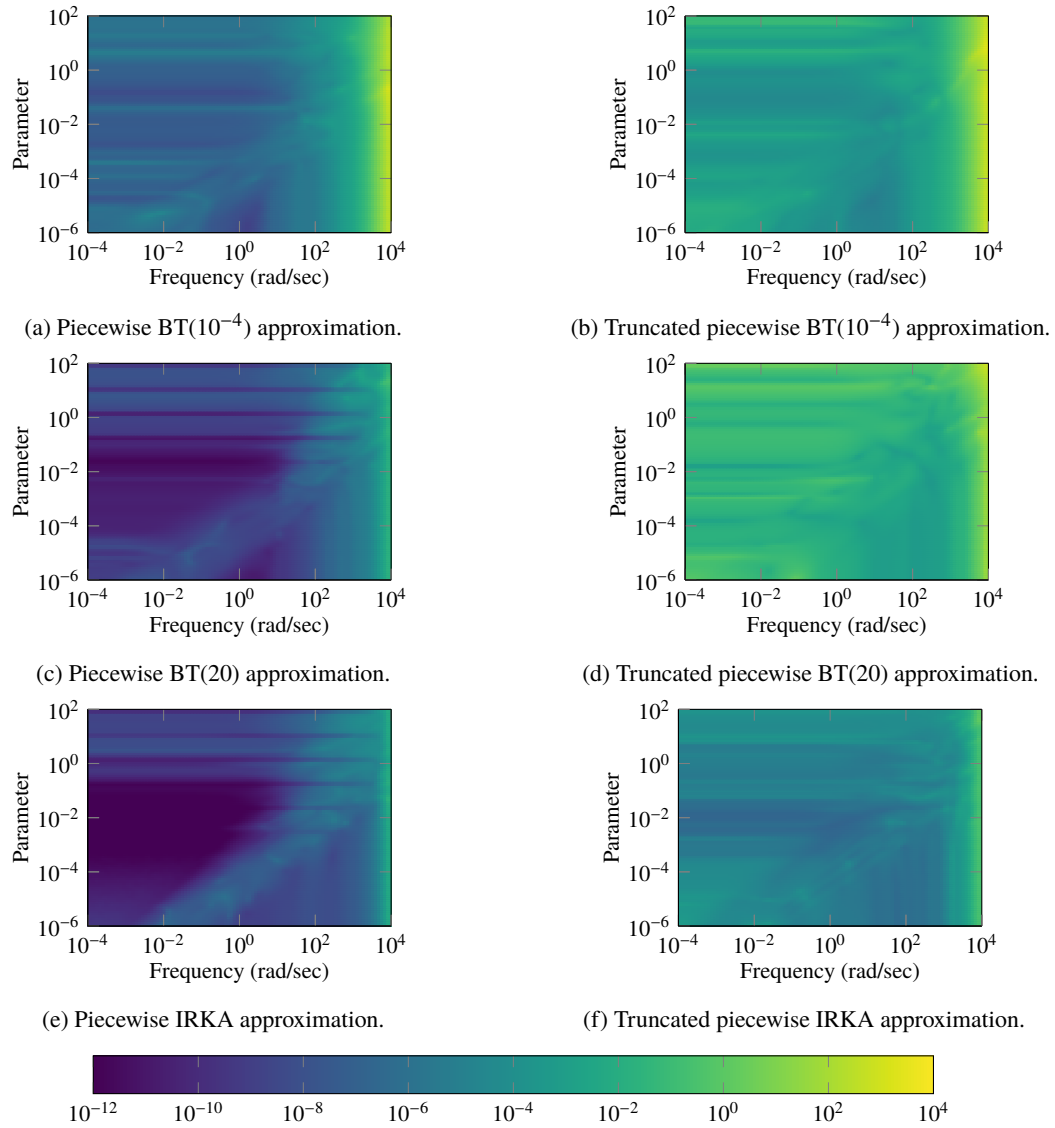


Figure 2: Relative sigma-magnitude errors of different piecewise parametric reduction approaches for the thermal block model.

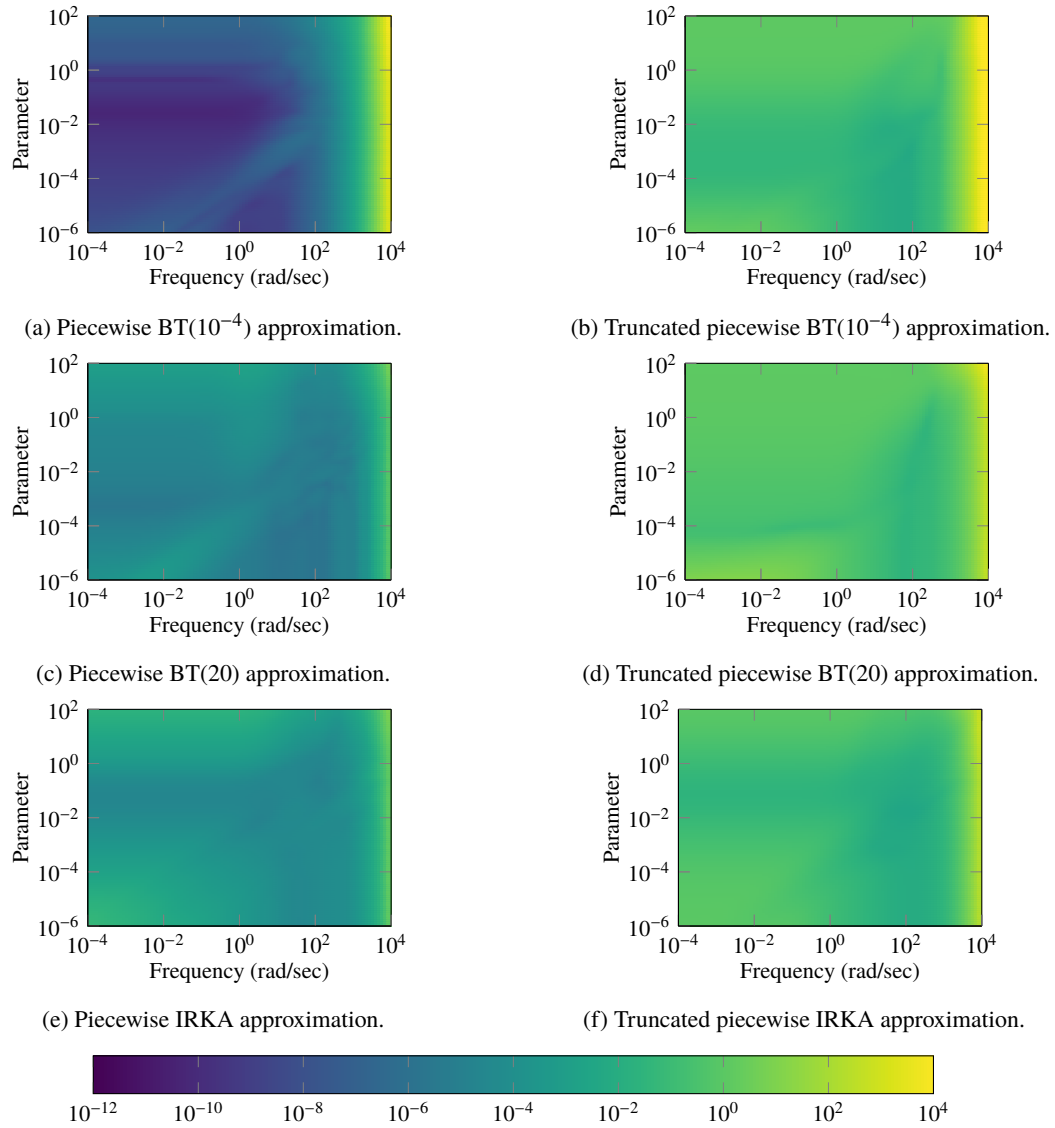


Figure 3: Relative sigma-magnitude errors of different piecewise parametric one-sided reduction approaches for the thermal block model.

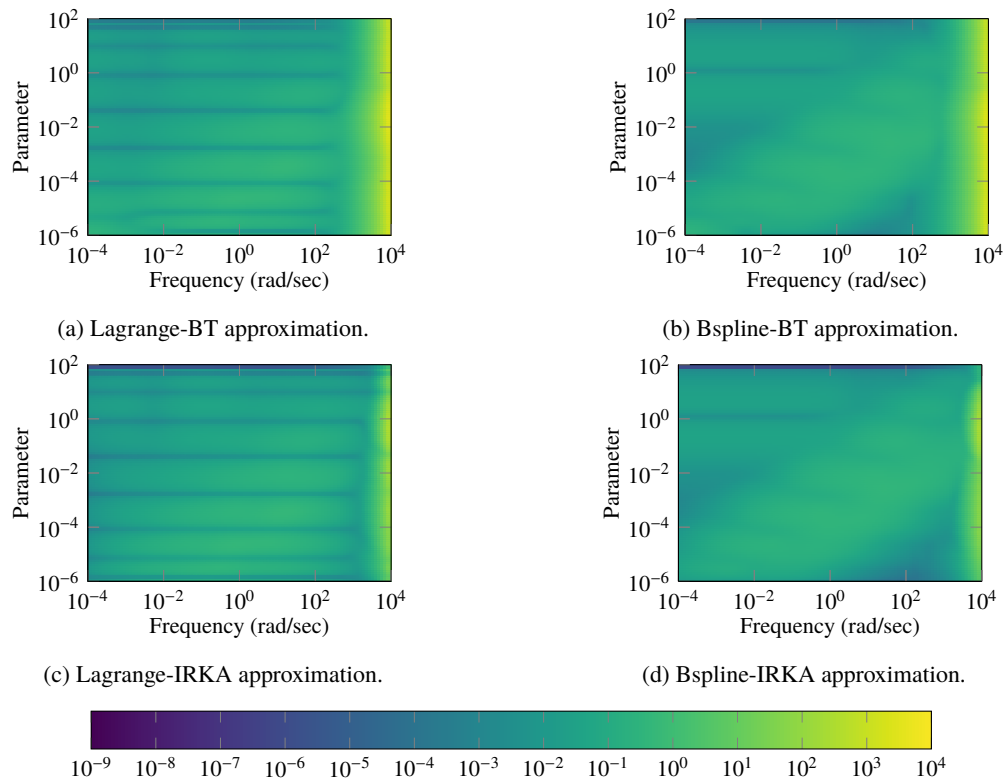


Figure 4: Relative sigma-magnitude errors of different transfer function interpolation methods for parametric reduction for the thermal block model.

input but 4 outputs. In Figure 1b we present the sigma-magnitude plot of the full order model (FOM), i.e. we plot $\|H(\mu, s)\|_2 = \sigma_{\max}(H(\mu, s))$ over the full parameter range and the frequency range $[10^{-4}, 10^4]$. The plot is based on 100 logarithmically equi-spaced sample points (logspace-generated) in each direction. We also use this sampling for all relative sigma-magnitude error plots in the other figures. The error plots analogously show $\|H(\mu, s) - \hat{H}(\mu, s)\|_2 / \|H(\mu, s)\|_2$.

Excluding the 10 000 evaluations for the pre-sampling of the original transfer function, all computations for generation of the ROMs and evaluation of the approximation errors can be executed in less than 8 minutes.

We compare both IRKA and classic (Lyapunov) balanced truncation (BT) in the piecewise as well as the transfer function interpolation context. For IRKA we use fixed order $r = 20$ in all training samples, while for BT we run in two modes. Since we have the BT error-bound that allows for adaptive processing, i.e. automatic choice of the reduced order, we do that with absolute error tolerance 10^{-4} . On the other hand, for a more fair comparison to IRKA we also run BT for fixed order $r = 20$. We refer to these two modes as BT(10^{-4}) and BT(20) in the following.

For the piecewise approaches we use 10 logarithmically equi-spaced (logspace-generated) parameter samples in M as the training positions. For the interpolatory approaches we choose 10 Chebyshev-roots generated by Chebfun. We have mentioned the final rank-truncation after basis concatenation in Section 4.1. We use a tolerance equal to `eps` in the standard case. Alternatively, to further compress the final parametric ROM, we truncate with tolerance 10^{-6} and refer to this approach by the name *truncated piecewise*.

For the training, BT can not reuse information from previous samples very easily. On the other hand, IRKA can be initialized with the ROM from the previous parameter sample, which in most cases made it converge after less than 5 steps (mostly being stopped by criterion monitoring the relative change of the model in the \mathcal{H}_2 -norm). For further implementation details we refer to the scripts in the code package.

Although, BT guarantees the local ROMs in the sample points to preserve the asymptotic stability of the original model, and also IRKA preserves stability upon convergence, this feature is in general lost after concatenating the bases to the global one. Still, for a one-sided projection the stability of the global ROM can be preserved. Due to stability and symmetry of the thermal block model, Bendixson's theorem [6] guarantees this. Therefore, we compare to a one-sided approach that simply combines V and W into one matrix. The comparison can be found in Figures 2 and 3. And the corresponding ROM orders are given in the first block of Table 5.

For the interpolatory approaches, we compare Lagrange polynomials and variation diminishing B-splines of order 2. Here, we always use BT(10^{-4}) in the BT case, since the results are already hard to distinguish from the IRKA-based ones in this case and we do not expect much improvement from the higher local orders.

It can be seen from Table 5 that the piecewise BT models are, in parts significantly, smaller than the piecewise IRKA models. This comes at the price that the accuracy is not as good in parts of the domain. Nonetheless, e.g. the truncated one-sided BT(10^{-4}) approximation yields a relative error of below 1% on a majority (around 70%) of the investigated frequency-parameter domain with a model size that is 3.7 to 5.6 times smaller. There is a significant increase in error for those frequencies, where the transfer function has very small values (see Figure 1b) that can be considered to be on the noise level.

The results are very satisfactory and so are the computation times. This indicates that the implementations can be used for larger and more challenging examples, that we can not report here due to space restrictions.

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