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# Book of Abstracts

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Institute of Numerical Mathematics

# Monday, 20.03.23

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# Dictionary-based Online-adaptive Structure-preserving Model Order Reduction for Parametric Hamiltonian Systems

**R. Herkert**[1], **B. Haasdonk**[1], **and P. Buchfink**[1]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*

Reduced Basis (RB) methods applied to a non-linear time-dependent system often lead to a reduced basis, that is too large, such that no sufficient speed up can be realized compared to the high-order simulation. In general, the development of online-efficient RB methods for problems with slowly decaying Kolmogorov-n-widths is still a strongly investigated topic. To address this problem, we present symplectic dictionary-based online-adaptive methods for Hamiltonian systems. The idea is, that the reduced basis is adapted during the time-stepping of the reduced simulation. Basis vectors, that are no longer required to represent the current solution vector (because, they would have a zero coefficient) are removed from the basis and new basis vectors are added, that are necessary to get a good approximation for the next time steps.
We focus on the symplectic model order reduction of parametric Hamiltonian systems

$$\dot{x}(t) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \nabla_x H(x(t), \mu) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} L(\mu) x(t) + \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} f_{\mathrm{nl}}(x(t), \mu). \tag{1}$$

To compute a basis, a dictionary of snapshots $D_{\mathrm{X}} = \{x_1, ..., x_{N_{\mathrm{X}}}\}$ is constructed and during the online phase snapshots are selected from the dictionary. Then, the basis is computed from the selected snapshots. With an offline-online splitting this basis computation can be performed highly efficiently, such that the online-run-time is just depending on the number of selected snapshots (see [2]). Like this, we derive online-efficient versions of both classical basis generation techniques like POD as well as symplectic basis generation techniques, like the complex SVD-algorithm (see [1]).
In order to efficiently treat non-linearities in the right-hand side of (1) in combination with the SDEIM-algorithm (see [4]), a dictionary of non-linearity snapshots $D_{\mathrm{F}} = \{f_{\mathrm{nl}}(x_1), ..., f_{\mathrm{nl}}(x_{N_{\mathrm{F}}})\}$ and a dictionary of DEIM-indices $D_{\mathrm{P}} = \{i_1, ..., i_{N_{\mathrm{P}}}\}$ is computed. With an offline-online splitting an online-efficient version of the classical SDEIM-algorithm is obtained.
The snapshots are selected according to their distances in the parameter-time-space $\mathcal{P} \times [t_0\ t_e]$ to the parameter-time-coordinates of the time steps computed next (see [3]). The presented methods are tested on a linear and a non-linear wave-equation model. The influence of the basis changes on the conservation of the Hamiltonian is studied.

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# Structure-Preserving Model Reduction with Quadratic Manifolds

**P. Oehme**[1]

[1] *University of Münster*

The standard approaches to structure-preserving model order reduction nowadays make use of either linear subspaces [1, 3] or more complex spaces learned by the use of machine learning means such as autoencoders [5, 6]. The benefits of linear approximation are that these are simple to compute, explainable, and may possess other qualities like offline-online decomposability. Complex learned spaces require much more effort during computation, and usually lack the explainability attributed to their linear counterparts; what they make up in however, is their approximative quality by being able to model complex non-linear problems.
Lately, another method has been introduced: model order reduction with quadratic (and potentially arbitrary polynomial) solution manifolds as a generalization of modal derivatives [2, 4]. The hope for this procedure is to gain approximation quality in comparison to the linear subspace models while at the same time keeping the computation time lower and the final manifolds more explainable than the machine-learned results. As of right now these approaches lack a lot of the versatility of the previous ideas such as error estimators, computational time comparisons, and the availability of additional properties such as structure preservation during runtime. A first goal would hence be to achieve a quadratic manifold method conserving the structure of the underlying problem as an extension of the available methods.
This talk intends to give an introduction to data-driven quadratic manifold construction and the possibility of preserving the structure of a port-Hamiltonian system along its trajectory, as well as a few examples.

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# Parametric reduced order modelling for a 2D wildland fire model via the shifted POD based deep learning method

**Shubhaditya Burela**[1] **and Philipp Krah**[1,2]

[1] *Institute of mathematics, Technical University of Berlin*
[2] *I2M - Institut de Mathèmatiques de Marseille*

Forecasting the spread of forest fires has become an important aspect of civil protection [2]. To predict forest fires the wildland fire model [4] can be simulated over a range of different scenarios. To speed up the numerical simulations model order reduction (MOR) is unavoidable. Unfortunately, classical MOR techniques like proper orthogonal decomposition (POD) fail for the wildland fire model since it features moving flame fronts that cannot be captured with a linear subspace. To circumvent this, [1] proposes to use shifted proper orthogonal decomposition (sPOD). The sPOD [6, 5] decomposes transport fields by shifting the data field in so-called co-moving frames, in which the traveling wave is stationary and can be described with a few spatial basis functions, that are computed with help of the POD. In this work, we use the sPOD together with neural networks and show that we are able to learn the spread of forest fires. The low dimensional description of the wildland fire model is created once using the snapshot data, that has been simulated for a representative set of input parameters. Thereafter we train the neural networks to predict the wildland fire spread for any new parameter set. The approach proposed here closely follows [3] where a deep learning framework is employed to efficiently learn the nonlinear trial manifold from the snapshot data and subsequently predict the solutions at new parameter values. The proposed method is tested on 1D and 2D wildland fire models with varying burning rates and varying flame front shapes.

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# A certified wavelet-based physics-informed neural network for the solution of parameterized partial differential equations

**Lewin Ernst*** **and Karsten Urban†**

* Institute for Numerical Mathematics
Ulm University
Helmholtzstr. 20, 89081 Ulm, Germany
e-mail: lewin.ernst@uni-ulm.de

† Institute for Numerical Mathematics
Ulm University
Helmholtzstr. 20, 89081 Ulm, Germany

## ABSTRACT

Parameterized partial differential equations (PPDEs) arise to describe physical phenomena. These equations often have to be solved either in a multi-query or in a real-time context for different parameters resulting in the need for model order reduction. For transport- or wave-type problems it has been proven that the Kolmogorov $N$-width decay is poor ([4], [3]), such that linear model reduction techniques are bound to fail and nonlinear methods are needed. The recent success in solving various PDEs with neural networks (NNs), particularly with physics-informed NNs (PINNs) (see e.g. [5] [1]) suggests that they are a natural candidate for nonlinear model order reduction (MOR) techniques, although an a-posteriori error control is at least not trivial.

The goal of our approach is to construct PINNs along with a computable upper bound of the error, which is particularly relevant for model reduction of PPDEs. To this end, we suggest to use a weighted sum of expansion coefficients of the residual in terms of an adaptive wavelet expansion both for the loss function and an error bound, [2].

This approach is shown for the linear transport equation using an optimally stable ultra-weak formulation. Numerical examples show a very good quantitative effectivity of the wavelet-based error bound.

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# $N$-widths of the linear transport equation linked with the smoothness of boundary values

**Florian Arbes**[1] **and Constantin Greif**[2]

[2] *Ulm University, Institute of Numerical Mathematics, Helmholtzstr. 20, 89081 Ulm (Germany)*
[1] *IFE, Institute for Energy Technology, Instituttveien 18, 2007 Kjeller (Norway)*

It is well-known that the decay of the Kolmogorov $N$-width, given by $O(N^{-1/2})$, is slow for transport and wave phenomena with discontinuous initial values [3, 4]. However, when considering smooth boundary values this behaviour changes.
We analysed the $N$-width of the solution manifold of the linear transport equation

$$\partial_t \Phi + v\, \partial_x \Phi = 0, \quad \Phi(0, \cdot) = f,$$

where $v$ is the velocity and $\Phi$ the transported quantity. We considered the boundary value $f$ to be $p$-times weak differentiable, i.e. $f \in H^p$.
The $N$-width for the class $H^p$ of $p$-times weak differentiable functions was already investigated by Kolmogoroff and Pinkus [1, 2] and is approximately $O(N^{-p})$. Since the solution manifold is a subset of $H^p$, the result by Pinkus can be used as an upper bound. But how sharp is this upper bound?
We proved that the $N$-width for the transport problem can be bounded by $O(N^{-p-1/2})$.
We were also able to prove that $O(N^{-p-1/2})$ is the exact Kolmogorov $N$-width for some specific boundary functions $f \in H^p$. This tells us that approximating the solution manifold $\mathcal{M} \subset H^p$ for the transport problem is nearly as hard as approximating all of $H^p$.
For $f \in H^\infty$, we get an exponential decay.
Finally, we made some numerical experiments where we defined some $p$-times differentiable ramps that approximate the Heaviside function and observed the same decay. This is particular interesting, since in practice the error decay can be accelerated by first smoothing the initial values.

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# Tuesday, 21.03.23

1. O. Tugluk .....
2. C. Gahr .....
3. I. Prusak .....
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8. J. Schleuß .....

# Effects of Compression on Reduced Bases for Turbulent Flows

**O. Tugluk**[1]

[1]*METU/Ankara*

Recent advances in machine learning (ML), specifically deep neural nets (DNN), have resulted in unprecedented leaps in certain areas of research, such as natural language processing, image processing, and robotics to name a few. ML is, without a doubt, the fastest growing and the most prevalent artificial intelligence (AI) technique in use today.
Increased use of machine learning tools, while ever expanding, found comparatively little use in computational fluid dynamics (CFD), especially in turbulent flows. Underlying reasons for this are twofold, traditionally data for computationally complex turbulent flows is scarce, and size of the input to the machine learning model (the so- called feature vector) is very large when compared to more classical problems tackled with machine learning. In addition, when neural network (NN) based ML is used in a straightforward manner, i.e. continuously mapping the input flow field to a final flow state, the complexity of the underlying neural network (number of artificial neurons) can easily become untenable. Further complicating the situation is the so-called curse of dimensionality, which means the data required to train a ML model increases with increasing feature vector size. This increase in data requirement also adversely affects the training time for the ML model. How, then, can we overcome these obstacles and benefit from the ever-expanding machine learning research?
In this talk I will outline my approach to tackle the curse of dimensionality while building reduced order models for pipe flow. My approach leverages versatility and power of reduced basis methods; while aiming to further reduce model order by employing analysis preserving data compression techniques [1].

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# Data-driven non-intrusive reduced-order modeling for plasma turbulence via Operator Inference

**Constantin Gahr**[1], **Ionuţ-Gabriel Farcaş**[2], **and Frank Jenko**[1]

[1] *Max-Planck-Institute for Plasma Physics, 85748 Garching, Germany*
[2] *Oden Institute for Computational Engineering & Sciences, Austin, TX 78712, United States*

Turbulence simulations play a crucial role in the plasma physics community as they give insight into the underlying nonlinear dynamics. However, these simulations are computationally expensive. Reduced-order models provide a computationally cheaper alternative to the high-fidelity model exploiting the fact that in most physics and engineering problems, the dominant dynamics live on low-dimensional manifolds.
We focus on the Hasegawa-Wakatani equations, a plasma model describing two-dimensional drift-wave turbulence, and approximate it with a reduced order model learned via Operator Inference. Operator Inference is a data-driven non-intrusive model reduction method that learns low-dimensional reduced models with polynomial nonlinearities from trajectories of high-dimensional high-fidelity simulations. In addition, it can handle arbitrary nonlinearities by employing lifting transformations that map the given states into states with polynomial nonlinearities. In the present work, we perform one of the first systematic reduced-order modeling studies in plasma physics to ascertain whether Operator Inference can provide accurate and predictive reduced models for the Hasagawa-Wakatani system.

# A reduced order model for segregated fluid-structure interaction solvers based on a ALE approach

**Valentin Nkana[1], Giovanni Stabile[2], Andrea Mola[3], and Gianluigi Rozza[4]**

[1, 4] *Mathematics Area, mathLab, SISSA*
[2] *University of Urbino*
[3] *IMT Lucca*

Interactions between fluid and moving (deforming) structures are essential in many fields, such as aerospace, civil, and mechanical engineering, and numerical simulation has been one of the few available methods for studying this problem [1]. In civil engineering, wind-induced vibrations can cause the collapse of the construction, being the most studied example the Tacoma Narrows Bridge, which collapsed under 64 [km/h] wind conditions on November 7, 1940. To illustrate and understand this type of bluff body dynamics problem, the flow past a moving cylinder has received continued attention in the past few decades as a benchmark problem in fluid dynamics that serves to models such engineering applications [3]. The resolution to the above modeling problem is given by numerically solving the Navier-Stokes equations, which is computationally expensive (for data storage, data handling, and processor costs), even when implemented on modern advanced computing platforms. Therefore, it can be a significant challenge to deal with several situations such as fluid-structure interaction problems. Given this difficulty, we pay significant attention to reducing both storage and processing costs of non-linear state solutions by using reduced-order models.
This talk discusses the potentiality of reduced-order models in flow-induced vibration. The originality of this work is the study of the flow past an oscillating cylinder in finite volume methods (FVM) using a segregated approach based on a PIMPLE algorithm with dynamic mesh capability. We generate modes using the proper orthogonal decomposition (POD) technique. The full-order model (FOM) is the flow around a cylinder that can move in the vertical direction. We verify our results by comparing the velocities, pressure, and grid motion given by the FOM and the reduced-order model (ROM). Additionally, a deep analysis is done by comparing both the phase portraits and forces given by the high-fidelity problem with those given by the reduced-order model's using the open source libraries OpenFOAM [2] and ITHACA-FV [4]

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# An optimisation-based domain-decomposition reduced order model for the incompressible Navier-Stokes equations

**I. Prusak**[1], **M. Nonino**[2], **D. Torlo**[1], **F. Ballarin**[3], **and G. Rozza**[1]

[1]*Mathematics Area, mathLab, SISSA, Trieste, Italy*
[2]*Fakultät für Mathematik, Universität Wien, Vienna, Austria*
[3]*Department of Mathematics and Physics, Universitá Cattolica del Sacro Cuore, Brescia, Italy*

The aim of this work is to present a model reduction technique in the framework of optimal control problems for partial differential equations [2]. We combine two approaches used for reducing the computational cost of the mathematical numerical models: domain-decomposition (DD) methods and reduced-order modelling (ROM). In particular, we consider an optimisation-based domain-decomposition algorithm for the parameter-dependent stationary incompressible Navier-Stokes equations [5].
Firstly, the problem is described on the subdomains coupled at the interface and solved through an optimal control problem, which leads to the complete separation of the subdomain problems in the DD method. On top of that, a reduced model for the obtained optimal-control problem is built; the procedure is based on the Proper Orthogonal Decomposition technique and a further Galerkin projection [3].
The presented methodology is tested on two fluid dynamics benchmarks: the stationary backward-facing step and lid-driven cavity flow. The numerical tests show a significant reduction of the computational costs in terms of both the problem dimensions and the number of optimisation iterations in the domain-decomposition algorithm.
The aforementioned techniques could be promising in the context of more complex time–dependent problems and, more importantly, multi–physics problems, where either pre-existing solvers can be used on each subcomponent or we do not have direct access to the codes. In particular, in future, we are planning to extend the methodology presented in this paper to the nonstationary fluid–dynamics problems and, eventually, to Fluid–Structure interaction problems [4]. Moreover, this approach can be applied also to more complicated problems, where different types of numerical models are used in different subdomains [1].

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# Dictionary-based model reduction for state estimation

**A. Pasco**[1] **and A. Nouy**[1,§]

[1] *Centrale Nantes, Nantes Universite, Laboratoire de Mathematiques Jean Leray*
[§] *PhD supervisor*

We consider the problem of state estimation from $m$ linear measurements, where the state $u$ to recover is an element of the manifold $\mathcal{M}$ of solutions of a parameter-dependent equation. The state is estimated using a prior knowledge on $\mathcal{M}$ coming from model order reduction. Variational approaches based on linear approximation of $\mathcal{M}$, such as PBDW [3], yields a recovery error limited by the Kolmogorov $m$-width of $\mathcal{M}$. To overcome this issue, piecewise-affine approximations [2] of $\mathcal{M}$ have also be considered, that consist in using a library of linear spaces among which one is selected by minimizing some distance to $\mathcal{M}$. In this paper, we propose a state estimation method relying on dictionary-based model reduction, where a space is selected from a library generated by a dictionary of snapshots, using a distance to the manifold. The selection is performed among a set of candidate spaces obtained from the path of a $\ell_1$-regularized least-squares problem. Then, in the framework of parameter-dependent operator equations (or PDEs) with affine parameterizations, we provide an efficient offline-online decomposition based on randomized linear algebra [1], that ensures efficient and stable computations while preserving theoretical guarantees.

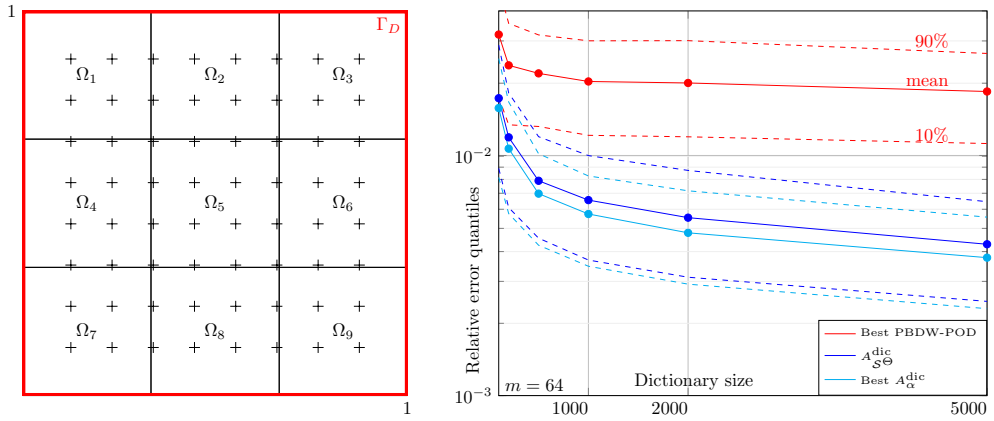


Figure 1: Dictionary-based state estimation applied to the thermal block problem parameterized by the thermal conductivity of the different subdomains (left). Sensors are located on a grid of $m = 64$ points. On the right, we compare our approach to the classical PBDW (red) using the best truncated POD modes as background space, on a test set of 500 snapshots. We distinguish the (randomized) residual-based (blue) and best (cyan) model selection of the regularization parameter.

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# Reduced Basis based Hierarchical Multiobjective Parameter Optimization

**M. Kartmann**[1]

[1] *Universität Konstanz*

In many applications there is not only one optimization goal of interest, but instead there are given $k \in \mathbb{N}$ contradicting objective functions $J_i$ ($i \in \mathbb{N}_{\leq k}$), which should be met optimally at the same time. For example, one can be interested in finding a good compromise between reaching several heat distributions $y_d^i$ ($i \in \mathbb{N}_{\leq k-1}$), while heating with the minimal cost necessary. This can be modeled by an *Multiobjective Parameter Optimization Problem* (MPOP) of the following form

$$\min_{(y,\mu)\in V\times P_{ad}} J(\mu) = \begin{bmatrix} \frac{1}{2}\left\|y(\mu) - y_d^1\right\|_H^2 \\ \vdots \\ \frac{1}{2}\left\|y(\mu) - y_d^{k-1}\right\|_H^2 \\ \nu_1\left\|\mu\right\|_1 + \frac{\nu_2}{2}\left\|\mu\right\|_2^2 \end{bmatrix}, \tag{MPOP}$$

where the state $y(\mu) = y \in V$ solves the parametrized PDE

$$A(\mu)y = f(\mu) \text{ in } V'. \tag{PDE($\mu$)}$$

In the setting above, $V, H$ are Hilbert spaces in the usual setting and $P_{ad} \subset \mathbb{R}^n$ is a compact set of admissible parameters. In contrast to single objective optimization the objective function is vector-valued $J : P_{ad} \to \mathbb{R}^k$,which results in the Pareto optimality concept [1]. The goal is to numerically approximate the set of all optimal compromises, the so-called Pareto set. For such problems the computational effort can be challenging due to (1) the presence of many objectives and the uncountableness of the Pareto set and due to (2) the presence of PDE constraints, which make the objective function evaluation expensive. To overcome these two challenges, we use two reduction techniques, which are (i) Hierarchical Multiobjective Optimization, which aims at a efficient description of the Pareto set, and (ii) Reduced Order Modelling (ROM) techniques, to speed up the PDE solves. To be precise, we are using the Reduced Basis (RB) method as a tool for reduced order modelling in combination with hierarchical variants of Continuation methods (CM) and Weighted sum methods (WSM) for the multiobjective optimization to obtain an approximation $J^r$ of the objective. Those variants aim at computing the boundary of the Pareto (critical) set by considering subsets of the objective functions and are based on a theoretical description of the hierarchical structure of the Pareto (critical) set ([2]). This has the advantage that objective components can be neglected for the computation of certain Pareto critical points and that the Pareto (critical) set is described completely by a smaller amount of points needed. Further, we consider how the inexactness due to the RB approximation in the objective translates into an error in the Pareto (critical) set.

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# Coupled Parameter and Data Dimension Reduction for Bayesian Inference

Qiao CHEN [1], Olivier ZAHM[1], Elise ARNAUD[1], and Ricardo BAPTISTA[2]

[1] *Inria, Université Grenoble-Alpes*
[2] *California Institute of Technology*

In this talk, we introduce a new method to jointly reduce the dimension of the parameter and the data space of high-dimensional Bayesian inverse problems. Recent dimension reduction methods commonly focus on the parameter space, yet many geophysical applications equally necessitate dimension reduction in the data space, which is done in practice through an independent upstream procedure. A recent work [1] considers dimension reduction for both data and parameters albeit treating the two spaces separately. However, choosing a low-dimensional informed parameter subspace influences which data subspace is informative and vice versa. We thus propose a coupled dimension reduction method based on the gradient of the generalised forward operator that maps between the parameter and data spaces. Our method computes in an offline phase a projector for a ridge approximation of the likelihood function to accelerate online multi-query posterior evaluations. We also show how our method can aid experimental design by localising effective sensor placements. Numerical experiments on a 2D shallow water model illustrate the benefits of our proposed method.

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Abstract:

In this talk, we study large-scale linear fractional stochastic systems representing, e.g., spatially discretized stochastic partial differential equations (SPDEs) driven by fractional Brownian motion (fBm) with Hurst parameter $ H>1/2 $. Such equations are more realistic in modeling real-world phenomena in comparison to frameworks not capturing memory effects. To the best of our knowledge, dimension reduction schemes for such settings have not been studied so far.

In this presentation, we investigate empirical reduced order methods that are either based on snapshots (e.g. proper orthogonal decomposition) or on approximated Gramians. In each case, dominant subspaces are learned from data. Such model reduction techniques are introduced and analyzed for stochastic systems with fractional noise and later applied to spatially discretized SPDEs driven by fBm in order to reduce the computational cost arising from both the high dimension of the considered stochastic system and a large number of required Monte Carlo runs.

# Generating reduced order models in parallel in time via random sampling

**J. Schleuß[1], K. Smetana[2], and L. ter Maat[3]**

[1] *Faculty of Mathematics and Computer Science, University of Münster, Einsteinstraße 62, 48149 Münster, Germany (julia.schleuss@uni-muenster.de)*
[2] *Department of Mathematical Sciences, Stevens Institute of Technology, 1 Castle Point Terrace, Hoboken, NJ 07030, United States of America (ksmetana@stevens.edu)*
[3] *Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands*

In this talk, we generate reduced basis functions defined in space that can be combined with time stepping schemes within model order reduction methods. We propose for the first time an embarrassingly parallel reduced basis construction in time [5]. Moreover, we especially target time-dependent partial differential equations (PDEs) with coefficients that are rough in both space and time.
In detail, we perform several simulations of the PDE for few time steps in parallel, starting at different, randomly drawn start points, prescribing random initial conditions. Applying a singular value decomposition to a subset of the so obtained snapshots yields the reduced basis. This facilitates constructing the reduced basis functions parallel in time. To select start time points for the temporally local PDE simulations, we suggest using a data-dependent probability distribution. To this end, we represent the time-dependent data functions of the PDE as matrices, where each column of a matrix corresponds to one time point in the grid of the time discretization. Subsequently, we employ column subset selection techniques from randomized numerical linear algebra [3] such as leverage score sampling.
Each local in time simulation of the PDE with random initial conditions approximates a local approximation space in one time point that is optimal in the sense of Kolmogorov (cf., e.g., [1, 4]). These optimal local approximation spaces are spanned by the left singular vectors of a compact transfer operator that maps arbitrary initial conditions to the solution of the PDE in a later point of time. By solving the PDE locally in time with random initial conditions, we construct local ansatz spaces in time that converge provably at a quasi-optimal rate and allow for local error control (cf. [2]).
Numerical experiments demonstrate that the proposed method can outperform existing methods like the proper orthogonal decomposition even in a sequential setting and is well capable of approximating advection-dominated problems.

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# Wednesday, 22.03.23

1. F. Arbes .....
2. H. Kleikamp .....
3. L. Renelt .....
4. I. Niakh .....
5. S. Schopper .....

# Reduced order modelling of solidification problems

**F. Arbes[1, 2], J. S. Dokken[3], C. Greif[4], Ø. Jensen[1], and K. A. Mardal[2, 3]**

[1] *Institute for Energy Technology (IFE)*
[2] *Department of Mathematics, University of Oslo (UiO)*
[3] *Center for Biomedical Computing, Simula Research Laboratory*

Reduced order models (ROMs) are a powerful tool to predict the state of a system within split seconds and hence are a popular choice to build digital twins that rely on numerical simulations [2]. However, advection driven problems are known to be difficult to model using a ROM, because they don't have a low rank representation in general [1].
My work investigates how this challenge transfers to the context of solidification problems and tries to answer when and to what extend ROMs work well. In solidification problems, a solidification front progresses through the domain with the advected enthalpy. Since the solid allows for only little movement, the convection only happens in the liquid part of the domain and thus the velocity field travels through the domain. Early investigations have uncovered large differences between alloy solidifications and pure metal solidifications in terms of the decay of the Kolmogorov $N-width$. Alloys consist of several metals that might have different melting points which causes the alloy to solidify over a large temperature range. The part of the domain with partially solidified material ('mushy zone') features growing crystals within a liquid that allows for some movement. It is suspected, that this diffuse interface improves the $N-width$.
To further investigate this, reduced spaces for 1D step functions that move in time have been studied. The results show that not only the PDE itself, but the smoothness of the solution is crucial for the decay of the Kolmogorov $N-width$ and thus the quality of a reduced space representation.

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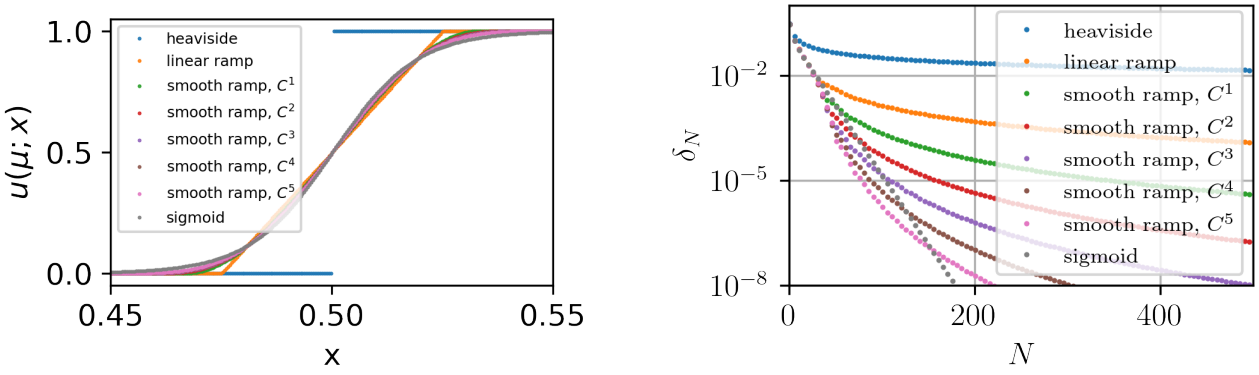


(a) Initial conditions of varying smoothness classes $C^k$

(b) Error decay, $\delta_N$-width

Figure 1: Magnitude of the velocity.

# Nonlinear model order reduction for parametrized transport-dominated PDEs using registration-based methods

**H. Kleikamp, M. Ohlberger, and S. Rave**

*Institute for Analysis and Numerics, University of Münster*

In this contribution, we describe a new approach for model order reduction of parametrized transport-dominated or hyperbolic partial differential equations (PDEs) [3]. These kinds of equations typically exhibit slowly decaying Kolmogorov $N$-widths of the corresponding solution manifolds due to sharp moving fronts or interacting discontinuous shocks, see for instance [5, 2]. Therefore, purely linear methods are not well-suited to obtain accurate reduced order models in these scenarios.
To tackle such problems, we propose an algorithm based on ideas from *computational anatomy* and *image registration*, see [1, 4]. In the *geodesic shooting* method, diffeomorphisms $\phi^v \colon \Omega \to \Omega$ over some set $\Omega \subset \mathbb{R}^d$ are encoded via corresponding vector fields $v \colon \Omega \to \mathbb{R}^d$ by the exponential map, i.e. $\exp(v) = \phi^v$. On the other hand, the diffeomorphism group $G$ acts on functions $u \colon \Omega \to \mathbb{R}$ by composition, i.e. $\phi \cdot u := u \circ \phi$. Using such diffeomorphic transformations, we register space-time solution snapshots $u_\mu$ for a set of parameters $\mu \in \mathcal{P}$ of the parametrized PDE onto a common (space-time) reference snapshot $u_{\text{ref}}$. To obtain a reduced order model, we apply linear model order reduction methods, such as the *proper orthogonal decomposition*, in the Hilbert space $V$ of vector fields, see [6]. Hereby, we extract a reduced space $V_N \subset V$ of vector fields, which, in turn, defines a subset $G_{V_N} \subset G$ of the diffeomorphism group via the exponential map, i.e. $G_{V_N} = \exp(V_N)$. During the online phase, elements $\phi_N \in G_{V_N}$ can act on the reference snapshot $u_{\text{ref}}$ to approximate snapshots for previously unseen parameter values. In other words, for a parameter $\mu \in \mathcal{P}$, we determine a reduced vector field $\tilde{v}_\mu \in V_N$, such that $u_\mu \approx u_{\text{ref}} \circ \exp(\tilde{v}_\mu)$. Different numerical experiments show the potential of the proposed method.

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# Localized Model Order Reduction for convection-dominated problems using an optimally stable discretization

**Lukas Renelt**[1], **Mario Ohlberger**[1], **and Christian Engwer**[1]

[1] *Institute for Analysis and Numerics, University of Münster, Germany*

In the numerical treatment of convection-dominated problems one needs to pay particular attention to the stability of the discretization. One stable approach is the enrichment of the test space by so-called *supremizers* leading to a nonsymmetric Petrov-Galerkin scheme. These supremizers are, however, expensive to compute since the (approximate) solving of PDEs is required. In the context of model order reduction this also poses an additional challenge since both a reduced trial and test space need to be constructed simultaneously while preserving the stability in the reduced problem (c.f. [2]).
We adapt the construction introduced by Brunken et al in [1] and also recently employed in [3]. There it is proposed to choose a test space first and then subsequently determine a corresponding trial space. This idea is computationally less complex and leads to optimally stable schemes. For parametrized problems we employ standard projection based techniques on the test space and again determine a corresponding (reduced) trial space afterwards which leads to an optimally stable reduced scheme. We show that the approach also allows the construction of local reduced spaces which is particulary desirable in the case of spatially strongly varying data functions. First numerical experiments with parametrized convection-diffusion-reaction problems as well as pure transport problems show the advantages and challenges of the proposed approach. A thorough analysis of the discrete system reveals the saddle point structure of the problem and gives a guideline for efficient solving.

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# A reduced basis method for contact problems formulated with Nitsche's method

**Idrissa Niakh[1,2,3], Guillaume Drouet[3], Virginie Ehrlacher[1,2], and Alexandre Ern[1,2]**

[1] *CERMICS, École des Ponts*
[2] *INRIA Paris*
[3] *EDF Lab Paris-Saclay*

We develop an efficient reduced basis method for the contact problem with friction formulated with Nitsche's method under the small deformation assumption. The key idea ensuring the computational efficiency of the method is to treat the nonlinearity resulting from the contact conditions by means of the Empirical Interpolation Method. The proposed method is applied to the Hertz contact problem between two half-disks with parameter-dependent radius. We also highlight the benefits of the present approach with respect to the mixed (primal-dual) formulation.

***Keywords*** — model reduction, variational inequalities, reduced basis method, contact problems, Nitsche's method, Tresca friction, Coulomb friction.

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# Comparison of Inconsistency Measures, Model Order Reduction Methods and Interpolation/Regression Methods for Parametric Model Order Reduction by Matrix Interpolation

**S. Schopper[1], Q. Aumann[2], and G. Müller[1]**

[1] *Technical University of Munich, School of Engineering and Design, Chair of Structural Mechanics, Arcisstr. 21, 80333 Munich, Germany*
[2] *Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg*

Simulations of complex dynamical systems using the Finite Element Method (FEM) can become computationally very expensive since large systems of equations have to be solved for multiple instances in time or frequency. To reduce the required effort, projection-based Model Order Reduction (MOR) methods can be used. These project the full solution into a lower-dimensional subspace and by this aim to reduce the computational effort required to solve the system while providing an accurate approximation of the full solution. [1]
A limitation of these methods occurs when parametric models are considered. In applications such as optimization or uncertainty quantification, one is interested in having a reduced model that can be evaluated with little computational effort and provides accurate results for a large range of parameters. Parametric Model Order Reduction (pMOR) methods are able to retain these parametric dependencies in the reduced model. Many of those methods require an affine representation of the parametric dependency though, which is difficult to realize for e.g. geometric parameters. [1]
One pMOR approach that is not limited to affine parametric dependencies is pMOR by matrix interpolation [2]. In this method, a generalized coordinate system is constructed from reduced bases collected over a set of samples, into which all reduced systems are transformed. In this coordinate system, the reduced operators can be interpolated to obtain the solution for queried parameter points with little computational effort. However, there are still some unanswered questions in this workflow:

- Depending on the reduced bases collected in the samples, a transformation to the generalized coordinate system may not be possible for some samples or basis vectors. For this purpose, a measure of incosistency is needed to assess whether this problem occurs.
- Once the reduced operators have been transformed into the generalized coordinate system, any interpolation or regression method can be used to predict the reduced operators for queried parameter points. Which methods are best suited for this task has not yet been studied in detail.
- Finally, any MOR method can be used to generate the required database of reduced operators. The properties of the MOR method used will also affect the workflow and accuracy of pMOR by matrix interpolation. Investigating these effects is another open task to be explored.

In this contribution, inconsistency measures, MOR methods and interpolation/regression methods for pMOR by Matrix Interpolation are compared to investigate the above questions.

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# Thursday, 23.03.23

1. L. Gkimisis .....
2. T. Ehring .....
3. H. Mu .....
4. F.A.B. Silva .....
5. E. Beurer .....
6. N. Reich .....
7. J. Henning .....

# Adjacency-based, non-intrusive reduced-order modeling for incompressible Navier Stokes and Fluid-Structure Interactions

**L. Gkimisis**[1], **T. Richter**[2], **and P. Benner**[1]

[1] *Computational Methods in Systems and Control Theory (CSC), Max Planck Institute for Dynamics of Complex Techincal Systems, Sandtorstrasse 1, 39106 Magdeburg, Germany*
[2]*Institute for Analysis and Numerics, Faculty of Mathematics, Otto-von-Guericke University Magdeburg - University Square 2, 39106 Magdeburg, Germany*

Non-intrusive model reduction has been developed to become a promising solution to system dynamics forecasting, especially in cases where data are collected from experimental campaigns or proprietary software simulations.
In this work, we present a method for non-intrusive model reduction, applied to fluid dynamics and fluid-structure interaction systems. The approach is based on the a priori known sparsity of the full-order system operators (e.g. of the discretized Navier-Stokes equations), which is dictated by grid adjacency information. In order to enforce this type of sparsity, we solve a "local", regularized least-squares problem for each degree of freedom on a grid, considering only the training data from adjacent nodes, thus making computation and storage of the inferred full-order operators feasible. After constructing the non-intrusive, sparse full-order model, the Proper Orthogonal Decomposition is used for its projection to a reduced dimension subspace. This approach differs from methods where data are first projected to a low-dimensional manifold [1, 2], since here the inference problem is solved for the original, full-order system.
We consider two applications in the context of incompressible fluid dynamics and fluid-structure interactions. The first corresponds to the construction of a quadratic, reduced order model for the flowfield prediction over a cylinder at a range of low Reynolds numbers. Increasing complexity, we examine a two-way coupled fluid-structure interaction benchmark; a purely data-driven, coupled fluid/structure model is constructed for the Hron-Turek fluid-structure interaction application [3]. Results considering the accuracy and predictive capabilities of the inferred reduced models (e.g. Figure 1) are analytically discussed.


(a) ROM with 50 and 5 DOFs for flow and structure response

(b) CFD-FSI solution

Figure 1: Contour plots for the Hron-Turek benchmark velocity along $x$ at the end of testing time.

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# Hermite kernel surrogates for the value function of high-dimensional nonlinear optimal control problems

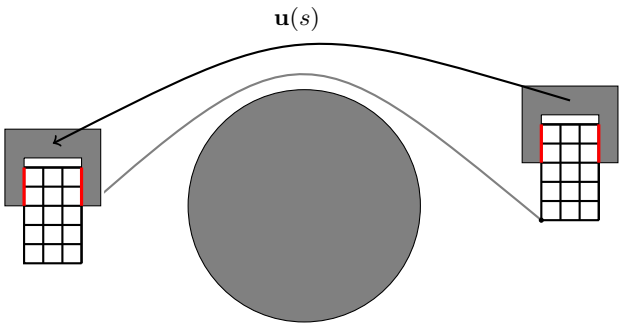
**Tobias Ehring** [1] **and Bernard Haasdonk**[1]

[1] *Institute of Applied Analysis and Numerical Simulation (IANS), University of Stuttgart*

Numerical methods for the optimal feedback control of high-dimensional dynamical systems typically suffer from the curse of dimensionality. In the current presentation, we devise a mesh-free data-based approximation method for the value-function based on [3] for optimal control problems of the form

$$\min_{\mathbf{u}\in\mathcal{U}_\infty} J(\mathbf{u}) = \min_{\mathbf{u}\in\mathcal{U}_\infty} \int_0^\infty r(\mathbf{x}(s)) + \mathbf{u}(s)^\top R\mathbf{u}(s)\,\mathrm{d}s$$
$$\text{subject to } \dot{\mathbf{x}}(s) = f(\mathbf{x}(s)) + g(\mathbf{x}(s))\mathbf{u}(s) \text{ and } \mathbf{x}(0) = x_0 \in \mathbb{R}^N,$$

which partially mitigates the dimensionality problem. The data comes from open-loop control systems, which are solved via the first-order necessary conditions of the problem, called the Pontryagin's maximum principle. In this, the most informative initial states for the open-loop process are chosen using a greedy selection strategy [2]. Furthermore, the approximation method is based on a greedy Hermite-interpolation scheme, and incorporates context-knowledge by its structure. Especially the value function surrogate is elegantly enforced to be 0 in the target state, non-negative and constructed as a correction of a linearized model. The algorithm is proposed in a matrix-free way, which circumvents the large-matrix-problem for multivariate Hermite interpolation. For finite time horizons, convergence of the corresponding scheme is proven for both the value-function and the surrogate as well as for the optimal vs. the surrogate controlled dynamical system. Experiments support the effectiveness of the scheme, using among others a new academic toy model with an explicit given value function. Another model problem (details in [1]) describes a gripper that has gripped a soft tissue, for example a fruit or piece of meat, and brings it optimally to a prescribed target position while avoiding an obstacle.

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# Model Reduction on Polynomially Embedded Manifolds

**P. Buchfink[2], S. Glas[1], and H. Mu[1]**

[1] *University of Twente, Department of Applied Mathematics*
[2] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*

For advection-dominated or wave-like problems, the decay of the Kolmogorov n-widths is expected to be slow, see e.g., [4, 5]. Thus, linear-subspace reduced order models (ROMs) of low dimension might yield inaccurate results. Recent advances in projection-based model reduction utilize autoencoders to build a nonlinear embedding from reduced-order space to full-order space. Those methods can achieve good accuracy for ROMs of low dimension, but the online evaluation (without employing hyper-reduction) scales with the size of the full-order models (FOMs). In this talk we consider ROMs constructed via polynomially embeddings. This bridges the aforementioned approaches in terms that we can achieve higher accuracy than the linear-subspace ROMs and the online evaluation of the ROM is independent of the size of the FOM.
Recent works in the direction of polynomially, especially quadratically, embedded manifolds consider intrusive model reduction with the projection matrix being the POD basis matrix [1], as well as non-intrusive model reduction with the projection matrix being either the POD basis matrix [3] or the state-dependent Jacobian matrix of the embedding [2]. Here, we compare intrusive reduced order models in terms of accuracy and computational cost with respect to the choice of the projection matrix. Additionally, we propose an algorithm to select the most significant basis from the polynomial library, so the reduced polynomial model obtained by the truncated library has a less computational cost and similar accuracy than those obtained from the entire library.
In the numerical example, we consider a linear transport equation (known to have slowly decaying Kolmogorov n-widths) and compare the polynomially embedded approach to linear-subspace model reduction with respect to accuracy and computational cost. Furthermore, we provide a thorough numerical comparison for the different choices of the projection matrix.

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# A Multi-Fidelity Ensemble Kalman Filter with Adaptive Reduced-Order Models

**F. A. B. Silva**[1], **C. Pagliantini**[1], **and K. P. Veroy-Grepl**[1]

[1] *CASA, Eindhoven University of Technology, 5600 MB, Eindhoven, The Netherlands*

The use of model order reduction techniques in combination with ensemble-based methods for estimating the state of systems described by nonlinear partial differential equations has been of great interest in recent years in the data assimilation community. Methods such as the multi-fidelity ensemble Kalman filter (MFEnKF) [2] and the multi-level ensemble Kalman filter (MLEnKF) [1] have been developed and implemented in several papers and are recognized as state-of-the-art techniques. However, the construction of low-fidelity models in the offline stage, prior to solving the data assimilation problem, leads these methods into a trade-off between the accuracy and computational cost of the approximate models. In our work, we investigate the use of adaptive reduced-basis techniques in which the approximation space is modified (but not retrained) online based on the information extracted from the full-order solutions. This has the potential to simultaneously ensure good accuracy and low cost for the employed models and thus improve the performance of the multi-fidelity/multi-level methods.

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# Randomized Residual-Based Error Estimators for Parametrized Equations

**Emil Beurer**[1]

[1] *University of Münster*

Note that my talk isn't about my own research, it is entirely based on [2].

In [2], an a posteriori error estimator for the approximation error between the full order model (FOM) and the reduced order model (ROM) is proposed. It is based on the residual, but in contrast to the classical approach it isn't reliant on stability constants (coercivity or inf-sup) and instead makes use of a randomized approach.

The error in the desired norm is approximated using Gaussian random vectors, where the covariance is chosen according to the norm. This approximation can then be rewritten in terms of the residual and solutions to dual problems which have these random vectors as their right-hand side. The method is inspired by a similar approach for ordinary differential equations from [1].

To solve these dual problems in an online efficient manner, a reduced dual space is constructed using a specialized greedy algorithm. The dimension of this reduced dual space is independent of the dimension of the ROM, but it grows with the desired effectivity of the estimator and with the prescribed probability of actually achieving that effectivity.

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# Development of a Software Library for Space-Time Variational Formulations

**M. Feuerle[1], J. Henning[1], T. Ingel[1], N. Reich[1,2], M. A. Reinhold[1], K. Urban[1], and J. Vorloeper[2]**

[1] *Ulm University, Institute for Numerical Mathematics, Ulm*
[2] *Ruhr West University of Applied Sciences, Institut Naturwissenschaften, Mülheim an der Ruhr*

The research group around Karsten Urban has been working on space-time variational formulations (mainly for partial differential equations) and accompanying model order reduction over the last decade. This resulted in several publications, including [1, 2, 3, 4, 5], among others. Up to this point the results of these works have been mostly based on separate implementations, partially in different programming languages.
Since early 2022 there has been a collaborative software development project between Ulm University (under the direction of Karsten Urban) and Ruhr West University of Applied Sciences (under the direction of Jürgen Vorloeper). The goal of this project is to unite already existing (and future) space-time and variational formulation related research work with its implementations in a joint software library in the programming language Python.
We want to present the concept of this project, what we have achieved so far and what we have planned in the future.

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# Model Order Reduction as an Enabler for Digital Twins of Manufacturing Equipment

**J. Henning**[1]

[1] *Ulm University, ATR Software GmbH*

The term *Digital Twin* is one of the most hyped buzzwords in the last few years in several application contexts, e.g., the industry 4.0. Until now, there is no universally accepted definition but all definitions of Digital Twins encapsulate the idea of a physical entity being replicated in a digital model and the presence of some form of interaction between the physical an the digital twin (see e.g., [1]). Typically, data from the real entity is captured and used to improve the quality of the digital model. The Digital Twin, on the other hand, is used to make predictions about the future which influence the control of the physical twin. Typically, Digital Twins contain various sub-models which describe various aspects of the real counterpart.

Parametrized partial differential equations (PPDEs) are one class of models that can be used to model a physical entity or process. These partial differential equations need to be constantly solved throughout the life cycle of a Digital Twin. Therefore, we are in a *multi-query* setting. Furthermore, the solving of the partial differential equations should, ideally, be possible in *real time*.

Model Order Reduction (MOR) is one tool that can be used to tackle the challenges described in the last paragraph. The idea of using MOR for Digital Twins is not new and can for example be found in [2]. In their publication, the authors describe a methodology for creating a Digital Twin of a single airplane. In this talk, we want to extend this methodology to a manufacturing setting with multiple machines and products that interact which each other. Furthermore, we want to elaborate which kind of PPDEs might be useful in this context, how they can be reduced, and in which areas the MOR approach still lacks practicality.

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# Friday, 24.03.23

1. T. Peters .....
2. M.N. Senn .....
3. A. Borghi .....
4. H. Fischer .....
5. A. Reinhold .....

# Symplectic Exponential Runge-Kutta-Methods for Solving Large Nonlinear Hamiltonian Systems

**Till Peters**[1]

[1] *Institute for Numerical Analysis, TU Braunschweig, Universitätsplatz 2, 38106 Braunschweig (Germany)*

We study stiff Hamiltonian systems of the form

$$y'(t) = My(t) + f(y(t)), \qquad y(t_0) = y_0, \qquad t \in [t_0, T] \tag{1}$$

with a Hamiltonian matrix $M \in \mathbb{R}^{2d\times 2d}$ and a suitable function $f : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. Here $M$ is called Hamiltonian if $M$ fulfills $(JM)^T = JM$ with the matrix $J = \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix}$. Moreover, $M$ forms the main part of the stiffness in system (1) by having only eigenvalues on the imaginary axis with large magnitude.

Exponential integrators are known to be useful for integrating stiff systems (1). These integrate the linear part of the differential equation exactly which can help to weaken the stiffness of the differential equation. Symplectic methods are suitable for integrating Hamiltonian systems because they preserve the symplectic flow of the system and provide good long-term results (see also [1]). Combining these two aspects, Mei und Wu show in [2] starting from symplectic Runge-Kutta-Methods how to generate symplectic exponential Runge-Kutta-Methods. For large dimensions $d$, the evaluation of the action of a matrix exponential on a vector is costly. A standard approach to reduce these costs is the use of Krylov subspace methods to approximate the matrix-vector-products of the form $e^M b$ with $M \in \mathbb{R}^{2d\times 2d}$ and $b \in \mathbb{R}^{2d}$. We investigate different Krylov subspace methods such as the standard Arnoldi method or different symplectic methods like the symplectic Lanczos method. Furthermore, we compare resulting approximative integrators in terms of accuracy in the matrix exponential approximation, accuracy in solving the system and preservation of the Hamiltonian structure.

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# On exponential integrators for large-scale Hamiltonian systems

**Peter Benner[1], Heike Faßbender[2], and Michel-Niklas Senn[2]**

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg (Germany)*

[2] *Institute for Numerical Analysis, TU Braunschweig, Universitätsplatz 2, 38106 Braunschweig (Germany)*

Hamiltonian systems are differential equations that exhibit a particular structure. This structure leads to geometric attributes e.g. energy conservation or symplectic flow maps. Such systems come along in physical problems like Maxwell's equations, molecular dynamics or wave equations. Simulating and analyzing these systems lead to differential equations of a high dimension that are computationally expensive to solve. We consider large and sparse Hamiltonian systems

$$\dot{y}(t) = J\nabla\mathcal{H}(y(t)), \quad y(0) = y_0, \quad J = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}, \tag{1}$$

where $\mathcal{H} : \mathbb{R}^{2n} \to \mathbb{R}$ is a $C^2$-function and $0_n$, $I_n$ are the zero and identity matrix of order $n$. A natural approach is to consider Krylov subspace based methods to approximate the solution of the orginal system by one of smaller dimension. In this work, only structure preserving approximation methods and a structure preserving integrator are considered in order to let the smaller systems and their solution of the differential equation inherit the relevant geometric properties of the original system. We recapitulate existing methods of this type and compare these with respect to the error in the energy conservation and the global error. We suggest to use such a method in the combination with model order reduction techniques for the studies of Hamiltonian systems to reduce the computational effort.

# $\mathcal{H}_2$ Optimal Model Order Reduction on Arbitrary Domains

**A. Borghi**[1] **and T. Breiten**[1]

[1]*Institut für Mathematik, Technische Universität Berlin, 10623 Berlin*

The optimal $\mathcal{H}_2$ approximation has been widely used for the development of efficient model order reduction algorithms. Well known examples are IRKA [2] and MIRIAm [1] respectively adopted in continuous and discrete time state-space systems. The idea is that given a SISO full order model with transfer function $G$, we want to find a reduced order model $\hat{G}_r$ such that

$$\|G - \hat{G}_r\|_{\mathcal{H}_2} = \min_{\dim(G_r)=r} \|G - G_r\|_{\mathcal{H}_2}. \tag{1}$$

This minimization process leads to the $\mathcal{H}_2$ optimal interpolation conditions

$$\begin{aligned} G\left(-\hat{\lambda}_j^*\right) = \hat{G}_r\left(-\hat{\lambda}_j^*\right),\ G'\left(-\hat{\lambda}_j^*\right) = \hat{G}_r'\left(-\hat{\lambda}_j^*\right) \quad &\text{(Continuous time)},\\ G\left(\frac{1}{\hat{\lambda}_j^*}\right) = \hat{G}_r\left(\frac{1}{\hat{\lambda}_j^*}\right),\ G'\left(\frac{1}{\hat{\lambda}_j^*}\right) = \hat{G}_r'\left(\frac{1}{\hat{\lambda}_j^*}\right) \quad &\text{(Discrete time)}. \end{aligned} \tag{2}$$

These results rely on the definition of a norm on a Hardy space. Referring to the cases in (2), these are spaces of functions analytic in the right half complex plane $\mathbb{C}_+$ and the outside of the closed unit disk $\mathbb{D}_+$, respectively.
In our work, we consider the Galerkin projection of a parametrized linear PDE in the weak form into a large finite dimensional subspace (see also [3]). In more detail, we look at equations of the form

$$\begin{aligned} (\mathbf{A}_1 + \mathbf{p}\mathbf{A}_2)x(\mathbf{p}) &= \mathbf{B},\\ y(\mathbf{p}) &= \mathbf{C}x(\mathbf{p}), \end{aligned} \tag{3}$$

where $\mathbf{A}_1, \mathbf{A}_2 \in \mathbb{C}^{n\times n}$, $\mathbf{B}, \mathbf{C}^\top \in \mathbb{C}^{n\times 1}$ and $(\mathbf{A}_1 + \mathbf{p}\mathbf{A}_2)$ is invertible for every $\mathbf{p} \in \mathbb{C}$. The rational function $y(\mathbf{p}) = \mathbf{C}(\mathbf{A}_1 + \mathbf{p}\mathbf{A}_2)^{-1}\mathbf{B}$ resembles the structure of a transfer function. However, $y$ can be analytic in sets that differ from $\mathbb{C}_+$ and $\mathbb{D}_+$. Hence, we propose a framework to derive first order interpolation conditions for $\mathcal{H}_2$ optimality in an arbitrary set $\mathbb{A}$. The theoretical background relies on conformal maps and generalizes Hardy spaces to functions that are analytic in $\mathbb{A}$. The objective is to eventually develop algorithms that can be used to find a reduced order rational function $\hat{y}$ that satisfies the $\mathcal{H}_2$ optimality conditions in $\mathbb{A}$.

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# Space-time goal-oriented error control for incremental proper orthogonal decomposition based reduced order modeling with dual-weighted residuals

**H. Fischer[1,2], J. Roth[1,2], A. Fau[2], and T. Wick[1,2]**

[1] *Leibniz Universität Hannover, Institute of Applied Mathematics, Welfengarten 1, 30167 Hannover, Germany*

[2] *Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay LMPS - Laboratoire de Mecanique Paris-Saclay, 91190 Gif-sur-Yvette, France*

In this presentation, we apply the dual-weighted residual (DWR) method [1, 2] to obtain a certified incremental proper orthogonal decomposition based reduced order model [4]. For the full order model, we utilize a tensor-product space-time discretization [6]. The first novelty of our work is the application of this space-time discretization to the reduced order model. Further, we introduce a novel approach that marries the space-time reduced order model and an incremental proper orthogonal decomposition (POD) [3, 5] based basis generation with a goal-oriented error control based on DWR estimates. We aim to solve the reduced system without any prior knowledge or exploration of the solution manifold such that no offline phase is required. Instead, we solve from the beginning on the reduced order model and –if necessary– update the reduced basis on-the-fly during the simulation with high fidelity finite element solutions by means of the incremental POD. For this purpose, we estimate the error in the cost functional and update the reduced basis if the estimate exceeds a given threshold. This allows an adaptive enrichment of the reduced basis in case of unforeseen changes in the solution behavior which is of high interest in engineering applications. Therefore, we are able to reduce the full-order solves to a minimum, which is demonstrated on numerical tests for the heat and wave equation. Additionally, since we rely on the DWR method, our approach is versatile and it is possible to apply this method to nonlinear or multiphysics problems where no error bounds are known. We conclude the talk with recent developments and preliminary extensions of our presented framework.

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# Space-time Variational Methods for Control Constrained Parabolic Optimal Control Problems

**Martin Alexander Reinhold**[1], **Nina Beranek**[1], **and Karsten Urban**[1]

[1] *Institute of Numerical Mathematics, Ulm University*

Optimal Control Problems with PDE constraints are not only highly relevant for a wide range of applications but also an interesting ongoing subject in research of numerical methods. In this talk we want to discuss problems of the form:

$$\min_{y\times u\in\mathcal{Y}\times\mathcal{U}} J(y,u) = \frac{1}{2}\|y-y_d\|_{L_2(I\times\Omega)} + \frac{\lambda}{2}\|u\|_{L_2(I\times\Omega)}$$

s.t:

$$By = Fu + c \quad \in \mathcal{Y}' \tag{1}$$

$$u_a \leq u \leq u_b \qquad a.e.\text{in } I\times\Omega, \tag{2}$$

where the constraint (1) is a parabolic time dependent PDE. We will also consider additional constraints of the control (2). Usually these type of problems are solved using time stepping schemes to solve the constraining PDE and the arising adjoint equation. But lately approaches using simultaneous space-time discretizations are investigated for these problems.

For parabolic PDEs it is known that these approaches can have significant advantages w.r.t. Model Order Reduction (MOR), which motivates the application of these methods to optimal control problems. In this talk we will discuss the application of a space-time variational formulation for the optimal control problem. We will discuss the approach in the infinite dimensional setting using Bochner-Lebesgue spaces and derive the optimality system in this setting. We show the application of a second order semi-smooth Newton method to solve the optimization problem and propose a discretization with a tensor type approach in space and time.

The talk concludes with a presentation of the implementation of the ideas mentioned above and some numerical examples. In an outlook we will discuss the possibility of MOR for this approach but also which challenges might occur when we want to apply these techniques in the context of optimal control problems.