

MoRePaS 2018

« *Model Reduction of Parametrized Systems IV* »

April 2018, 10-13, Centrale Nantes, Nantes, France

BOOK OF ABSTRACTS



PHOTO CREDITS

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Content

1	About <i>MoRePaS 2018</i>	2
1.1	Topics	2
1.2	Venue	2
1.3	Committees	2
1.4	Support	3
2	Program	5
3	Abstracts	9
3.1	Tuesday, April 10	9
3.2	Wednesday, April 11	19
3.3	Thursday, April 12	68
3.4	Friday, April 13	109
4	List of participants	119

1 About *MoRePaS 2018*

The conference *MoRePaS 2018*, hosted in Nantes, is the fourth edition of a series of conferences on Model Reduction of Parametrized Systems. Previous editions were held in Munster (2009), Gunzburg (2012) and Trieste (2015).

1.1 Topics

The conference aims at an international exchange of new concepts and ideas with respect to the following topics :

- Data-Assimilation and Data-Driven Methods
- Domain Decomposition Approaches
- Dynamic and Adaptive Approximations, Error Estimation
- High-Dimensional Parameter Spaces
- Interpolation Methods
- Krylov-Subspace, Rational Approximation and Interpolatory Methods
- Large-Scale Applications : Industry and Multiphysics Problems ; HPC
- Model Reduction for Optimization, Estimation, Control, and Uncertainty Quantification
- Multiscale Methods, Closure Approaches, Stabilization Methods
- Nonstationary Discontinuities and Internal Layers
- Proper Orthogonal Decomposition
- Proper Generalized Decomposition
- Reduced Basis Methods
- Statistical and Machine Learning Methods
- System-Theoretic and Structure-Preserving Methods
- Tensor Methods

1.2 Venue

The conference will be located at :

Ecole Centrale de Nantes ([Google Maps](#))

1 Rue de la Noë,
44300 Nantes, FRANCE

Contact : morepas2018@sciencesconf.org

1.3 Committees

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1.4 Support

The event is supported and organized in the framework of COST (European Cooperation in Science and Technology) initiative EU-MORNET : European Union Model Reduction Network (TD1307).

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2 Program

Tuesday, April 10

Time	Event
13 :00-13 :45	Welcome of participants
13 :45-14 :00	Opening
14 :00-14 :45	Plenary
	· Karen Veroy - <i>Certified Reduced Basis Methods for Variational Data Assimilation</i>
14 :45-16 :00	Session 1
	· Stephan Rave - <i>A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems</i>
	· Andreas Schmidt - <i>Parametric Model Order Reduction for Hamilton-Jacobi-Bellmann Equations and Applications to Feedback Control</i>
	· Babak Maboudi Afkham - <i>Model Reduction While Preserving A First Integral</i>
16 :00-16 :30	Coffee break
16 :30-17 :15	Plenary
	· Daniel Kressner - <i>Reduced basis methods : From low-rank matrices to low-rank tensors</i>
17 :15-18 :55	Session 2
	· Alexander Grimm - <i>Jointly optimal frequency/parameter sampling for modeling parameterized dynamical systems</i>
	· Francesca Bonizzoni - <i>Padé approximation for Helmholtz frequency response problems</i>
	· Maciej Balajewicz - <i>Discontinuity-aware model reduction using empirical flow map decomposition</i>
	· Andrea Manzoni - <i>Efficient reduction of large-scale unsteady Navier-Stokes flows on domains with variable shape</i>

Wednesday, April 11

Time	Event
08 :30-09 :15	Plenary
	· Benjamin Peherstorfer - <i>Data-Driven Multifidelity Methods for Monte Carlo Estimation</i>
09 :15-10 :30	Session 3
	· Traian Iliescu - <i>Data-Driven Filtered Reduced Order Modeling Of Nonlinear Systems</i>
	· Boris Kramer - <i>Estimation of Risk Measures with Reduced-Order Models</i>
	· Olivier Zahm - <i>Dimension reduction of the input parameter space of vector-valued functions</i>
10 :30-11 :00	Coffee break
11 :00-11 :45	Plenary
	· Olga Mula - <i>State estimation with reduced models and measurement data</i>
11 :45-12 :35	Session 4
	· Tommaso Taddei - <i>An adaptive Parameterized-Background Data-Weak Approach to state estimation</i>
	· Christian Soize - <i>Data-driven probabilistic learning on manifolds</i>
12 :35-14 :00	Lunch
14 :00-14 :45	Plenary
	· Kathrin Smetana - <i>Randomized Model Order Reduction</i>
14 :45-15 :35	Session 5
	· Oleg Balabanov - <i>Random Sketching for Model Order Reduction</i>
	· Patrick Heas - <i>Low-Rank Dynamic Mode Decomposition : Optimal Solution in Polynomial Time</i>
15 :35-16 :00	Poster Blitz I.A
	· Tommaso Taddei - <i>A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows</i>
	· Kenan Kergrene - <i>Goal-oriented proper generalized decomposition with application to the detection of delamination in composites</i>
	· James Nichols - <i>Greedy measurement selection for state estimation with reduced models</i>

	<ul style="list-style-type: none"> · Kevin Carlberg - Conservative model reduction for finite-volume models · Mickaël Abbas - Directional hyper-reduced model for evaluation of residual welding stresses · Francesco Ballarin - POD-Galerkin reduced order methods for inverse problems and multi-physics problems in fluid dynamics · Matteo Zancanaro - Advances in Hierarchical Model Reduction and combination with other reduction methods · Shfqat Ali and Saddam Hijazi - The effort of increasing Reynolds number in POD-Galerkin Reduced Order Methods : from laminar to turbulent flows · Mylena Mordhorst - Towards a stable and fast dynamic skeletal muscle model · Cécile Haberstich - Principal component analysis and optimal weighted least-squares method for training tree tensor networks · Federico Pichi - Reduced order methods for nonlinear parametric problems with branching solutions · Erwan Grelier - Statistical learning in tree-based tensor format · Carolina Introini - A reduced order Kalman filter for CFD applications · Alessandro Alla - Basis generation in optimal control problems · Zoi Tokoutsis - Reduced Basis Solutions of Parametrized Optimal Control Problems with Non-Affine Source Terms
16 :00-16 :30	Coffee break
16 :30-16 :55	Session 5
	<ul style="list-style-type: none"> · Bernard Haasdonk - Accelerating Implicit Integrators for Parametric ODE Systems by Greedy Kernel Approximation
16 :55-17 :30	Poster Blitz I.B
	<ul style="list-style-type: none"> · Nikhil Vaidya - Fast Estimation of Blood Vessel Cooling Effects in Hepatic Radio-Frequency Ablation using the Reduced Basis Method · Marco Tezzele - Parameter space and model reduction with shape parametrization, by means of active subspace and POD-Galerkin methods for industrial and biomedical applications · Kevin Tolle - Efficient Therapy Planning via Model Reduction for Laser-Induced Interstitial Thermotherapy · Andreas Buhr - Localized Reduced Basis Methods for Time Harmonic Maxwell's Equations · Simone Spada - Biogeochemical Oceanographic Data Assimilation : Dimensionality Reduced Kalman Filter for Mediterranean Sea Forecasting · Eva Vidlickova - Dynamical low rank approximation of random time dependent PDEs · Sofia Guzzetti - Reduced Models for Uncertainty Quantification in the Cardiovascular Network via Domain Decomposition · Amina Benaceur - A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems · Davide Pradovera - An efficient algorithm for Padé-type approximation of the frequency response for the Helmholtz problem · Niccolò Dal Santo - Multi space reduced basis preconditioners for large-scale parametrized PDEs · Stefan Banholzer - Certified POD-Based Multiobjective Optimal Control of Time-Variant Heat Phenomena · Stefan Hain, Alexander Nüsseler - Reduced basis method for parameter functions · Mazen Ali - Singular Value Decomposition on Intersection Spaces · Stefan Hain, Mladjan Radic - A hierarchical a-posteriori error estimator for the reduced basis method · Carmen Gräßle - Combining POD Model Order Reduction with Adaptivity · Christian Himpe - Parametric Model Order Reduction for Gas Flow Models · Daming Lou, Siep Weiland - Parametric model order reduction for large-scale and complex systems using Krylov subspace methods · Frank Naets - Parametric space-frequency reduction for second-order system models · Ward Rottiers - Parametric state-time reduction for the transient analysis of multi-physical systems
17 :30-18 :30	Poster session
18 :30-19 :30	Cocktail

Thursday, April 12

Time	Event
09 :15-10 :30	Session 6
	<ul style="list-style-type: none"> · Laura Iapichino - Greedy Controllability of Reduced-Order Linear Dynamical Systems

	<ul style="list-style-type: none"> · Igor Pontes Duff - <i>Balanced truncation model reduction for polynomial control systems</i> · Felix Schindler - <i>True error control for localized model reduction with online enrichment in PDE constrained optimization</i>
10 :30-11 :00	Coffee break
11 :00-11 :45	Plenary
	<ul style="list-style-type: none"> · Markus Bachmayr - <i>Reduced Bases and Low-Rank Methods</i>
11 :45-12 :35	Session 7
	<ul style="list-style-type: none"> · Reinhold Schneider - <i>Variational Monte Carlo for the Hierarchical Tensor Representation</i> · Asma Toumi - <i>Tensor Empirical Interpolation Method for multivariate functions</i>
12 :35-14 :00	Lunch
14 :00-15 :40	Session 8
	<ul style="list-style-type: none"> · Kevin Carlberg - <i>Space-time least-squares Petrov-Galerkin projection for nonlinear model reduction</i> · Giovanni Stabile - <i>Stabilised finite volume POD-Galerkin ROMs of the incompressible Navier-Stokes equations</i> · Cédric Herzet - <i>Beyond Petrov-Galerkin projection by using “multi-space” priors</i> · Julia Brunken - <i>Model reduction based on optimally stable variational formulations of parametrized transport equations</i>
15 :40-16 :00	Poster Blitz II.A
	<ul style="list-style-type: none"> · Silke Glas - <i>Model Reduction for Hamilton-Jacobi-Bellman Equations resulting from Intraday Trading of Electricity</i> · Patrick Héas - <i>Optimal Kernel-Based Dynamic Mode Decomposition</i> · Sebastian Ullmann - <i>Stochastic Galerkin reduced basis methods for parametrized elliptic PDEs with random data</i> · Ion Gosea - <i>Data-driven model reduction of descriptor linear systems in the Loewner framework</i> · Olena Burkovska - <i>Model order reduction for parametrized nonlocal variational inequalities</i> · Dominik Garmatter - <i>Reduced basis methods for MREIT</i> · Denise Degen - <i>A Geoscientific Application of the Certified Reduced Basis Method</i> · Y. Yue - <i>On the Interpolation of Reduced Order Models</i> · Maria Cruz Varona - <i>Some Aspects of Systems Theory and Model Order Reduction for Nonlinear Systems</i> · Fabrizio Di Donfrancesco - <i>A CFD supported Reduced Order Model using a goal-oriented domain restriction</i> · Steffen W. R. Werner - <i>Computing the Hankel-Norm Approximation of Large-Scale Descriptor Systems</i> · Sébastien Riffaud - <i>Reduced-order model approximating the BGK model based on Proper Orthogonal Decomposition</i>
16 :00-16 :30	Coffee break
16 :30-17 :00	Poster Blitz II.B
	<ul style="list-style-type: none"> · Stefano Grivet-Talocia - <i>Data-driven parameterized modeling of LTI systems with guaranteed stability</i> · Christopher Bach - <i>Reduced-order model assisted optimization of automotive structures with nonlinearities</i> · Nicolas Montes - <i>PGD Variational vademecum for robot motion planning. A dynamic obstacle case</i> · Benjamin Fröhlich - <i>Shape Finding in Structural Optimization with Parametrically Reduced Finite-Element Models</i> · Fahad Alsayyari - <i>A Reduced Order Modeling Approach for Reactor Physics Problems Using Locally Adaptive Sparse Grids</i> · Sara Grundel - <i>Clustering Model Order Reduction for Water Networks</i> · Mikel Balmaseda - <i>Geometrically nonlinear autonomous reduced order model for rotating structures</i> · Harshit Bansal - <i>Model Order Reduction for convection dominated problems</i> · Zoran Tomljanovic - <i>Sampling-free parametric model reduction of systems with structured parameter variation</i> · Babak Maboudi Afkham - <i>Symplectic Model Reduction with respect to Energy Inner Product</i> · Sridhar Chellappa - <i>Adaptive POD-DEIM model reduction based on an improved error estimator</i> · Lyes Nechak - <i>On the reducibility of linear dynamic systems with hybrid uncertainties</i> · Romain Hild - <i>Towards real time computation of 3D magnetic field in parametrized Polyhelix magnets using a reduced basis Biot-Savart model</i> · Felipe Galarce - <i>Enhancing Hemodynamics Measurements with Mathematical Modeling</i> · Cleophas Kweyu - <i>Fast Solution of the Nonlinear Poisson-Boltzmann Equation using the Reduced Basis Method and Range-Separated Tensor Format</i> · Dennis Grunert - <i>Faster A-posteriori Error Estimation for Second Order Mechanical Systems</i>
17 :00-18 :00	Poster session
19 :00-23 :55	Gala Dinner

Friday, April 13

Time	Event
08 :30-09 :15	ACOM Plenary
	· Volker Mehrmann - <i>Reduced order energy based modeling in energy transport networks</i>
09 :15-10 :30	Session 9
	· Manuela Hund - <i>$H_2 \times L_2$ -optimal model order reduction of parametric linear time-invariant systems</i>
	· Petar Mlinaric - <i>H_2-optimal structure-preserving model order reduction for second-order systems</i>
	· Xingang Cao - <i>A Bilinear H_2 Model Order Reduction Approach to Linear Parameter-Varying Systems</i>
10 :30-11 :00	Coffee break
11 :00-12 :40	Session 10
	· Masayuki Yano - <i>Model reduction of parametrized aerodynamic flows : discontinuous Galerkin reduced basis empirical quadrature procedure</i>
	· Michael Schneier - <i>A Leray Regularized Ensemble-Proper Orthogonal Decomposition Method for Parameterized Convection-Dominated Flows</i>
	· Jean-Baptiste Wahl - <i>High Reynolds Aerothermal Simulations and Reduced Basis</i>
	· Gerrit Welper - <i>h and hp Adaptive Interpolation of Transformed Snapshots for Parametric Functions with Jumps</i>
12 :40-12 :50	Closing remarks
12 :50-14 :15	Lunch

3 Abstracts

3.1 Tuesday, April 10

Karen Veroy, RWTH Aachen University (14 :00-14 :45)	10
<i>Certified Reduced Basis Methods for Variational Data Assimilation</i>	
Stephan Rave, University of Münster (14 :45-15 :10)	11
<i>A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems</i>	
Andreas Schmidt, University of Stuttgart (15 :10-15 :35)	12
<i>Parametric Model Order Reduction for Hamilton-Jacobi-Bellmann Equations and Applications to Feedback Control</i>	
Babak Maboudi Afkham, Ecole Polytechnique Fédérale de Lausanne (15 :35-16 :00)	13
<i>Model Reduction While Preserving A First Integral</i>	
Daniel Kressner, EPFL (16 :30-17 :15)	14
<i>Reduced basis methods : From low-rank matrices to low-rank tensors</i>	
Alexander Grimm, Virginia Tech (17 :15-17 :40)	15
<i>Jointly optimal frequency/parameter sampling for modeling parameterized dynamical systems</i>	
Francesca Bonizzoni, University of Vienna (17 :40-18 :05)	16
<i>Padé approximation for Helmholtz frequency response problems</i>	
Maciej Balajewicz, University of Illinois at Urbana-Champaign (18 :05-18 :30)	17
<i>Discontinuity-aware model reduction using empirical flow map decomposition</i>	
Andrea Manzoni, Politecnico di Milano (18 :30-18 :55)	18
<i>Efficient reduction of large-scale unsteady Navier-Stokes flows on domains with variable shape</i>	

Certified Reduced Basis Methods for Variational Data Assimilation

S. Boyaval¹, M. Grepl², M. Kärcher³, N. Nellesen², and K. Veroy²

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³*NavVis GmbH, Munich, Germany*

We propose a certified reduced basis approach for strong- and weak-constraint variational data assimilation for parametrized PDE models. We consider here the case in which the behavior of the system is modelled by a parametrised PDE where certain model inputs (e.g., model parameters, or in the time-dependent case, the initial condition) are unknown and where the model itself may be imperfect. We consider (i) the standard strong-constraint approach, which uses the given observational data to estimate the unknown model inputs, and (ii) the weak-constraint formulation, which additionally provides an estimate for the model error, and thus can deal with imperfect models. Since the model error is a distributed function, the variational data assimilation formulation generally leads to a large-scale optimization problem that must be solved for every given parameter instance. To solve the problem efficiently, various reduced order approaches have therefore recently been proposed (see, e.g., [2]). Here, we build upon recent results on RB methods for optimal control problems to generate certified reduced order approximations for the state, adjoint, initial condition, and model error. In particular, we derive a posteriori error estimates for the error of the reduced basis approximation with respect to the underlying high-dimensional variational data assimilation problem [1]. We present numerical results for both three- and four-dimensional variational data assimilation (3D- and 4DVAR).

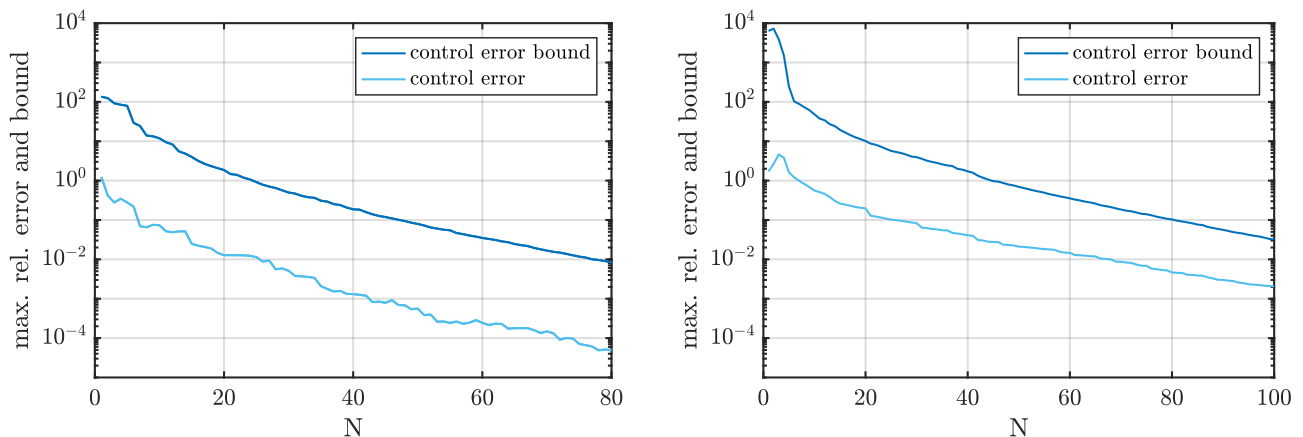


Figure 1: Maximum relative control error and error bound over number of greedy iterations N for strong-constraint (left) and weak-constraint (right) 4DVAR.

References

- [1] M. Kärcher, S. Boyaval, M. A. Grepl, and K. Veroy. Reduced basis approximation and a posteriori error bounds for 4D-VAR data assimilation. *arXiv preprint arXiv:1802.02328*, 2018.
- [2] R. Ștefănescu, A. Sandu, and I. M. Navon. POD/DEIM reduced-order strategies for efficient four dimensional variational data assimilation. *Journal of Computational Physics*, 295:569–595, 2015.

A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems

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²*Applied Mathematics, University of Münster, Germany*

Despite the many successes of Reduced Basis methods and similar projection-based model reduction techniques, the application of these methods to problems with moving features of low regularity remains a largely unresolved challenge [3]. Problems with free boundary $\Gamma(t) \subset \mathbb{R}^d$ also fall into this category when an Eulerian point of view is taken by embedding the solution $u(t)$ into a common function space on \mathbb{R}^d via extension with some constant function outside the moving domain $\Omega(t)$. As is easily seen, the approximation of these extended solution trajectories by low-dimensional linear spaces is bound to fail due to the moving discontinuity at $\Gamma(t)$ (e.g. [3]). Hence, model reduction methods need to be considered which are based on nonlinear approximation spaces.

In this contribution we introduce such a nonlinear Reduced Basis approximation scheme for parabolic free boundary problems of the form

$$\partial_t u(t) - \alpha \Delta u(t) = 0 \text{ in } \Omega(t), \quad V_\Gamma(t)u(t) + \alpha \partial_n u(t) = 0 \text{ on } \Gamma(t), \quad (1)$$

where the normal velocity V_Γ of $\Gamma(t)$ determined by the mean curvature $H(t)$ of $\Gamma(t)$ and the offset between $u(t)$ and some reference u_{ext} :

$$V_\Gamma(t) = -\beta H(t) + \gamma(u(t) - u_{\text{ext}}) \text{ on } \Gamma(t). \quad (2)$$

For instance, such problems arise from modelling of osmotic cell swelling [1].

Similar to the ideas in [2], our method is based on a linear approximation space for $u(t)$ on a fixed reference domain $\hat{\Omega}$, nonlinearly transformed by deformation fields $\Psi(t) : \hat{\Omega} \rightarrow \Omega(t)$. By determining $\Psi(t)$ from the evolution of $V_\Gamma(t)$, the resulting model can be seen as an ALE reformulation of the original problem (1),(2). Our method is fully offline/online decomposed, and we show that it exactly preserves the total mass $\int_{\Omega(t)} u(t, x) dx$ over the entire simulation time interval. We will also discuss the issue of remeshing in the context of reduced order modelling, which becomes necessary in the presence of large deformations of $\Omega(t)$.

References

- [1] F. Lippoth and G. Prokert. Classical solutions for a one-phase osmosis model. *Journal of Evolution Equations*, 12(2):413–434, 2012.
- [2] M. Ohlberger and S. Rave. Nonlinear Reduced Basis Approximation of Parameterized Evolution Equations via the Method of Freezing. *C. R. Acad. Sci. Paris, Ser. I*, 351:901–906, 2013.
- [3] M. Ohlberger and S. Rave. Reduced Basis Methods: Success, Limitations and Future Challenges. In *Proceedings of ALGORITHM 2016, 20th Conference on Scientific Computing, Vysoké Tatry, Podbanske, Slovakia, March 13-18, 2016*, pages 1–12, 2016.

Parametric Model Order Reduction for Hamilton-Jacobi-Bellmann Equations and Applications to Feedback Control

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We investigate infinite horizon optimal control problems for parametrized partial differential equations. Due to the good robustness to unknown disturbances, we are interested in applying feedback control techniques. A very general framework for feedback control is given by the famous dynamic programming principle (DPP) of R. Bellman. The application of the DPP to such problems yields a nonlinear system of PDEs for the calculation of the value function, known as the Hamilton-Jacobi-Bellmann (HJB) equation. It is well-known that classical discretization techniques such as semi-Lagrangian schemes for this equation suffer severely from the curse of dimensionality, which renders these methods infeasible for applications that stem from semidiscretized PDEs.

We are thus interested in first reducing the dimension of the control problem by applying parametric model order reduction techniques, as it was introduced in [3] for nonparametric problems. By combining recent basis generation techniques (see [4, 2]) with adaptive methods in the parameter domain, we are able to reach very low dimensional subspaces that contain relevant information and are feasible for the DPP approach, see [1]. The numerical discretization requires us to find a suitable subset in the reduced domain, as well as a grid that captures the important parts. For this, we present a technique to construct nonuniform grids in the reduced domain based on statistical information. Furthermore, we propose an offline-online splitting of the scheme: In an expensive offline step we precalculate the basis and perform initial calculations that allow for a large speed-up in a subsequent online phase where feedback controls for new parameters can then be obtained rapidly. We do this by precalculating initial guesses for the value functions and function evaluations offline, which then substantially speed up the online calculation that uses a policy iteration scheme. Finally, we discuss numerical examples to illustrate the effectiveness of the proposed methods for feedback control of nonlinear PDEs in two space dimensions.

References

- [1] A. Alla, M. Gunzburger, B. Haasdonk, and A. Schmidta. Feedback control of parametrized PDEs via model order reduction and dynamic programming principle. Technical report, University of Stuttgart, 2017. In preparation.
- [2] A. Alla, A. Schmidt, and B. Haasdonk. *Model Order Reduction Approaches for Infinite Horizon Optimal Control Problems via the HJB Equation*, pages 333–347. Springer International Publishing, Cham, 2017.
- [3] K. Kunisch, S. Volkwein, and L. Xie. HJB-POD based feedback design for the optimal control of evolution problems. *SIAM Journal on Applied Dynamical Systems*, 3:701–722, 2004.
- [4] A. Schmidt and B. Haasdonk. Reduced basis approximation of large scale parametric algebraic Riccati equations. *ESAIM: Control, Optimisation and Calculus of Variations*, Feb 2017.

Model Reduction While Preserving A First Integral

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Reduced order models have offered a promise for accelerated evaluation of large-scale and parametric systems of partial differential equations (PDEs). However, many challenges still remain regarding the efficiency and stability of the solution, especially for time dependent and hyperbolic PDEs. Invariants, conservation laws and symmetries are a central part of many of such problems which conventional model reduction methods do not generally preserve. This results in a qualitatively wrong, and often unstable solution.

Many recent studies are dedicated to conservation of intrinsic structures over the course of model reduction. Preservation of such structure together with an appropriate time-integration of the reduced system can help with the stability and robustness of the reduced system over long time-integration. In the context of the Lagrangian and Hamiltonian systems works in [2, 1, 3] suggest construction of a reduced order configuration space and an approximated conservation law. This result in a physically meaning reduced system, where preserving the conservation law would be possible with an appropriate time-integration scheme. However, These methods are only limited to Lagrangian and Hamiltonian systems, and subsequently only conserve the Lagrangian and the Hamiltonian. A model reduction method that can preserve a general invariant is still remain as a domain of research.

Using skew-symmetric tensors [4], we have developed a model reduction method that preserves a first integral of a system of partial differential equations. This is obtained by restricting the reduced system to the manifold that satisfies the first integral. An appropriate time-integration scheme, can then ensure that the solution remains on this manifold. This leads to a compact reduced system that maintains robustness over long time-integration. The error in the evaluation of the first integral is constant in time and only depends on the accuracy of the reduced basis.

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Reduced basis methods: From low-rank matrices to low-rank tensors

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The purpose of this talk is to highlight the benefits of combining low-rank tensor techniques with reduced basis methods for solving parametrized problems.

In the first part of the talk, we describe a combination of the reduced basis method with low-rank tensor formats, such as the tensor train and hierarchical Tucker formats, for the efficient solution of parameter-dependent linear systems in the case of several parameters. This combination consists of three ingredients. First, the underlying parameter-dependent operator is approximated by an explicit affine representation in a low-rank tensor format. Second, a standard greedy strategy is used to construct a problem-dependent reduced basis. Third, the associated reduced parametric system is solved for all parameter values on a tensor grid simultaneously via a low-rank approach. This allows us to explicitly represent and store an approximate solution for all parameter values at a time. Once this approximation is available, the computation of output functionals and the evaluation of statistics of the solution becomes a cheap online task, without requiring the solution of a linear system.

In the second part of the talk, we described an adaptive multilevel strategy for low-rank tensor techniques, in the context of random diffusion problems. This adaptive scheme allows to equilibrate the error on all levels by exploiting analytic and algebraic properties of the solution at the same time.

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Jointly optimal frequency/parameter sampling for modeling parameterized dynamical systems

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We consider the model reduction problem for parametrized linear dynamical systems whose input-output mapping is described in the frequency domain as

$$\hat{y}(i\omega, p) = \mathcal{H}(i\omega, p)\hat{u}(i\omega).$$

$\hat{u}(i\omega)$ and $\hat{y}(i\omega, p)$ denote, respectively, Fourier transforms of the input forcing and the output quantity of interest (the latter also reflecting the system parameter dependence); p is a scalar parameter; and $\mathcal{H}(s, p)$ is the transfer function. The model reduction process we develop is data-driven and does not need intrusive access to internal dynamics; we only assume the ability to evaluate the transfer function $\mathcal{H}(s, p)$. For a *non-parameterized* dynamical system having a transfer function $\mathcal{H}(s)$ depending only on the frequency parameter s , interpolatory model reduction generates a reduced model whose transfer function interpolates $\mathcal{H}(s)$ at selected points that may be chosen optimally so as to minimize a global H_2 error measure [2]. Even though interpolatory methods have been extended to parametric systems, there exists no jointly optimal strategy for the combined selection of frequency and parameter samples minimizing a joint (global) error measure (except for some special cases [1]).

We attempt to close this gap in this work by introducing a framework for systematic selection of frequency and parameter interpolation points that jointly minimizes a global $\mathcal{H}_2 \otimes L_2$ norm corresponding to an H_2 error measure in the frequency and an L_2 error measure in the parameter domain:

$$\|\mathcal{H}\|_{\mathcal{H}_2 \otimes L_2} := \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_0^{2\pi} \left| \mathcal{H}(i\omega, e^{i\theta}) \right|^2 d\theta d\omega.$$

We show that if a reduced parametric model of the form $\hat{\mathcal{H}}(s, p) := \sum_{i=1}^{r_s} \sum_{j=1}^{r_p} \frac{\phi_{i,j}}{(s - \lambda_i)(p - \pi_j)}$ (with separable poles in s and p) is the best approximation to $\mathcal{H}(s, p)$ in the $H_2 \otimes L_2$ sense, then it satisfies

$$\begin{aligned} \hat{\mathcal{H}}(-\lambda_i, \pi_j^{-1}) &= \mathcal{H}(-\lambda_i, \pi_j^{-1}), \quad \text{for } i = 1, \dots, r_s \text{ and } j = 1, \dots, r_p, \\ \sum_{j=1}^{r_p} \phi_{i,j} \nabla_s \hat{\mathcal{H}}(-\lambda_i, \pi_j^{-1}) &= \sum_{j=1}^{r_p} \phi_{i,j} \nabla_s \mathcal{H}(-\lambda_i, \pi_j^{-1}), \quad \text{for } i = 1, \dots, r_s, \text{ and} \\ \sum_{i=1}^{r_s} \frac{\phi_{i,j}}{\pi_j} \nabla_p \hat{\mathcal{H}}(-\lambda_i, \pi_j^{-1}) &= \sum_{i=1}^{r_s} \frac{\phi_{i,j}}{\pi_j} \nabla_p \mathcal{H}(-\lambda_i, \pi_j^{-1}), \quad \text{for } j = 1, \dots, r_p. \end{aligned} \tag{1}$$

We note that these optimality conditions extend the Hermite interpolation conditions that appear in (non-parametric) \mathcal{H}_2 -optimal model reduction to the parametric case; Hermite interpolation at the mirror image of system poles still plays a fundamental role. We propose a numerical algorithm that produces a reduced model $\hat{\mathcal{H}}(s, p)$ satisfying the optimality conditions in (1).

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Padé approximation for Helmholtz frequency response problems

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This talk deals with the *Helmholtz frequency response function* \mathcal{S} defined on $K := [k_{min}^2, k_{max}^2] \subset \mathbb{R}^+$, (the interval of frequencies we are interested in), i.e. the map which associates to each $k^2 \in K$, $u(k^2, \cdot)$, the solution of the Helmholtz problem

$$-\Delta u - k^2 u = f \quad \text{in } D \subset \mathbb{R}^d \quad (d = 1, 2, 3) \quad (1)$$

endowed with either Dirichlet or Neumann homogeneous boundary conditions on ∂D . The solution $u(k^2, \cdot)$ belongs to the Hilbert space V , V being $H_0^1(D)$ or $H^1(D)$ depending on the imposed boundary conditions.

Due to the oscillatory behavior of the solutions, the finite element approximation of Helmholtz frequency response problems in mid- and high-frequency regimes is challenging: accurate approximations are possible only on very fine meshes or with high polynomial approximation degrees. For this reason, the direct numerical evaluation of the frequency response function for a whole range of frequencies is often out of reach.

The Helmholtz frequency response function \mathcal{S} is proved to be meromorphic in \mathbb{C} , with a pole of order one in every (single or multiple) eigenvalue of the Laplace operator with the considered boundary conditions (see [1]). To reduce the computational cost we propose a rational approximation technique, which approximates the Helmholtz frequency response function from evaluations only at few frequencies.

Following [1], we define the *Least Square (LS) Padé approximant* of \mathcal{S} , denoted as $\mathcal{S}_{[M/N]}$, as the ratio $\mathcal{S}_{[M/N]}(z) = \frac{\mathcal{P}_{[M/N]}(z)}{\mathcal{Q}_{[M/N]}(z)}$, where $\mathcal{Q}_{[M/N]} \in \mathbb{P}_N(\mathbb{C})$ is a polynomial of degree at most N , and $\mathcal{P}_{[M/N]} \in \mathbb{P}_M(\mathbb{C}; V)$, with $\mathbb{P}_M(\mathbb{C}; V) = \left\{ P(z) = \sum_{m=0}^M p_m(z) z^m, p_m \in V \right\}$, such that its Taylor series agrees (in the least square sense) with the power series of \mathcal{S} for as many terms as possible.

Let $R \in \mathbb{R}^+$, and define ν as the number of the isolated (simple) poles of \mathcal{S} contained in $\mathcal{B}(0, R)$. Letting the degree of the denominator N be fixed and exactly equal to ν , we prove exponential convergence of the Padé approximation error $\|\mathcal{S}(z) - \mathcal{S}_{[M/N]}(z)\|_V$, as M goes to infinity, on the compact subsets of $\mathcal{B}(0, R) \setminus G$, G being the set of all the (simple) poles of \mathcal{S} contained in $\mathcal{B}(0, R)$. (See [1])

Two algorithms to compute the Padé approximant are discussed. 2D numerical tests are provided that confirm the theoretical upper bound on the convergence error.

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Discontinuity-aware model reduction using empirical flow map decomposition

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It is well known that traditional linear dimensionality reduction techniques such as PCA/POD/DMD/etc. often fail to efficiently compress solutions characterized by moving sharp gradients, shocks or discontinuities. Such solutions arise in a wide range of important engineering applications including, for example, high-speed fluid flows, multi-phase flows with evolving material interfaces, computational finance and structural contact problems with evolving contact regions. Over the years, a large variety of discontinuity-aware reduction techniques have been developed. In the first class of such methods, the symmetry and transport reversal properties of certain hyperbolic PDEs are exploited. Other methods involve decomposition into global and advection modes governed by optimal mass transfer, or more direct modeling of discontinuities using basis splitting. Finally, other methods avoid the problem of modeling discontinuities entirely by domain decomposition where the full-order model is used to reconstruct regions containing the discontinuities. In this work, we summarize a new model reduction approach for solutions characterized by evolving (in both time and parameter space) sharp gradients, shocks or discontinuities [1, 2]. Key to our proposed approach is the observation that certain solutions can be approximated efficiently using a low-rank empirical flow map. This approach can be interpreted as a data-driven generalization of previous approaches based on symmetry reduction and optimal mass transport. The reproductive as well as predictive capabilities of the method are evaluated on several simple yet representative problems including 2D compressible flows governed by the Euler equations, American options pricing and image reconstruction (Fig. 1).

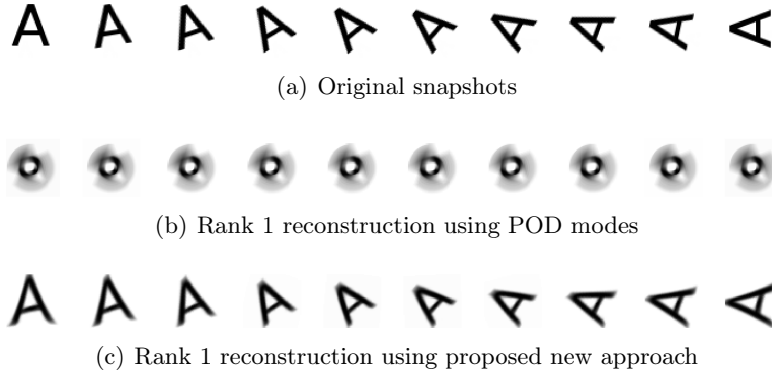


Figure 1: 90 degree CCW rotation of character “A”

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Efficient reduction of large-scale unsteady Navier-Stokes flows on domains with variable shape

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The efficient solution of large-scale fluid dynamics problems depending on both physical and geometrical parameters is a relevant task in several applications from engineering. In the last decade, reduced basis (RB) methods [5] have been applied to both steady and unsteady parametrized Navier-Stokes in several works, see e.g. [3, 1]. However, ensuring both accuracy and efficiency could be an involved task when facing problems defined on domains of varying shape. Moreover, what really makes the RB approximation of parametrized (Navier)-Stokes equations hard is ensuring the stability of the resulting problem. Here we propose a new, general and computationally cheap way to tackle both these issues. Regarding the way we handle shape variations, we generate domain (and mesh) deformations by means of a solid extension, obtained by solving a linear elasticity problem [4]. In this way, the knowledge of an analytical map between a reference domain and the physical, parameter-dependent domain, is not required. RB spaces are then generated by using either POD or greedy algorithms, relying on finite element snapshots evaluated over a set of reduced deformed configurations. To deal with unavoidable nonaffine parametric dependencies, we apply a matrix version of the empirical interpolation method, allowing to treat geometrical deformations in a non-intrusive, efficient and purely algebraic way. Regarding stability, we adopt a new algebraic least squares reduced basis (aLS-RB) method [2], which does not require to enrich the velocity space, as often done when dealing with a velocity-pressure formulation by using a Galerkin method. This method is shown to be stable (in the sense of a suitable inf-sup condition) and results in a cheaper, more convenient option both during the offline and the online stage of computation, compared to the existing G-RB methods.

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3.2 Wednesday, April 11

Benjamin Peherstorfer, University of Wisconsin Madison (08 :30-09 :15)	22
<i>Data-Driven Multifidelity Methods for Monte Carlo Estimation</i>	
Traian Iliescu, Virginia Tech (09 :15-09 :40)	23
<i>Data-Driven Filtered Reduced Order Modeling Of Nonlinear Systems</i>	
Boris Kramer, Massachusetts Institute of Technology (09 :40-10 :05)	24
<i>Estimation of Risk Measures with Reduced-Order Models</i>	
Olivier Zahm, Massachusetts Institute of Technology (10 :05-10 :30)	25
<i>Dimension reduction of the input parameter space of vector-valued functions</i>	
Olga Mula, Paris Dauphine University (11 :00-11 :45)	26
<i>State estimation with reduced models and measurement data</i>	
Tommaso Taddei, Université Pierre et Marie Curie (11 :45-12 :10)	27
<i>An adaptive Parameterized-Background Data-Weak Approach to state estimation</i>	
Christian Soize, Université Paris-Est (12 :10-12 :35)	28
<i>Data-driven probabilistic learning on manifolds</i>	
Kathrin Smetana, Twente (14 :00-14 :45)	29
<i>Randomized Model Order Reduction</i>	
Oleg Balabanov, Centrale Nantes and Universitat Politècnica de Catalunya (14 :45-15 :10)	30
<i>Random Sketching for Model Order Reduction</i>	
Patrick Heas, INRIA (Institut National de Recherche en Informatique et en Automatique) (15 :10-15 :35)	31
<i>Low-Rank Dynamic Mode Decomposition : Optimal Solution in Polynomial Time</i>	
Tommaso Taddei, Université Pierre et Marie Curie (15 :35-15 :40)	32
<i>A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows</i>	
Kenan Kergrene, École Polytechnique de Montréal (15 :35-15 :40)	33
<i>Goal-oriented proper generalized decomposition with application to the detection of delamination in composites</i>	
James Nichols, Université Pierre et Marie Curie (15 :35-15 :40)	34
<i>Greedy measurement selection for state estimation with reduced models</i>	
Kevin Carlberg, Sandia National Laboratories [Livermore] (15 :40-15 :45)	35
<i>Conservative model reduction for finite-volume models</i>	
Mickaël Abbas, EDF R&D, Institut des Sciences de la Mécanique et Applications Industrielles (15 :40-15 :45)	36
<i>Directional hyper-reduced model for evaluation of residual welding stresses</i>	
Francesco Ballarin, International School for Advanced Studies (15 :40-15 :45)	37
<i>POD-Galerkin reduced order methods for inverse problems and multi-physics problems in fluid dynamics</i>	
Matteo Zancanaro, International School for Advanced Studies (15 :45-15 :50)	38
<i>Advances in Hierarchical Model Reduction and combination with other reduction methods</i>	
Shfqat Ali and Saddam Hijazi, International School for Advanced Studies (15 :45-15 :50)	39

The effort of increasing Reynolds number in POD-Galerkin Reduced Order Methods : from laminar to turbulent flows

Mylena Mordhorst, University of Stuttgart (15 :45-15 :50)	40
<i>Towards a stable and fast dynamic skeletal muscle model</i>	
Cécile Haberstich, Centrale Nantes, LMJL UMR 6629, Nantes, France (15 :50-15 :55)	42
<i>Principal component analysis and optimal weighted least-squares method for training tree tensor networks</i>	
Federico Pichi, International School for Advanced Studies (15 :50-15 :55)	43
<i>Reduced order methods for nonlinear parametric problems with branching solutions</i>	
Erwan Grelier, Institut de Recherche en Génie Civil et Mécanique (15 :50-15 :55)	44
<i>Statistical learning in tree-based tensor format</i>	
Carolina Introi, Politecnico di Milano (15 :55-16 :00)	45
<i>A reduced order Kalman filter for CFD applications</i>	
Alessandro Alla, Pontificia Universidade Católica do Rio de Janeiro (15 :55-16 :00)	46
<i>Basis generation in optimal control problems</i>	
Zoi Tokoutsis, Aachen Institute for Advanced Study in Computational Engineering Science, Philips Research Eindhoven (15 :55-16 :00)	47
<i>Reduced Basis Solutions of Parametrized Optimal Control Problems with Non-Affine Source Terms</i>	
Bernard Haasdonk, University of Stuttgart (16 :30-16 :55)	48
<i>Accelerating Implicit Integrators for Parametric ODE Systems by Greedy Kernel Approximation</i>	
Nikhil Vaidya, Rheinisch-Westfälische Technische Hochschule Aachen, Philips Research [Netherlands] (16 :55-17 :00)	49
<i>Fast Estimation of Blood Vessel Cooling Effects in Hepatic Radio-Frequency Ablation using the Reduced Basis Method</i>	
Marco Tezzele, International School for Advanced Studies (16 :55-17 :00)	50
<i>Parameter space and model reduction with shape parametrization, by means of active subspace and POD-Galerkin methods for industrial and biomedical applications</i>	
Kevin Tolle, Friedrich-Alexander Universität [Erlangen-Nürnberg], Universität Trier (17 :00-17 :05)	51
<i>Efficient Therapy Planning via Model Reduction for Laser-Induced Interstitial Thermotherapy</i>	
Andreas Buhr, University of Münster (17 :00-17 :05)	52
<i>Localized Reduced Basis Methods for Time Harmonic Maxwell's Equations</i>	
Simone Spada, University of Trieste (17 :05-17 :10)	53
<i>Biogeochemical Oceanographic Data Assimilation : Dimensionality Reduced Kalman Filter for Mediterranean Sea Forecasting</i>	
Eva Vidlickova, Ecole Polytechnique Fédérale de Lausanne (17 :05-17 :10)	54
<i>Dynamical low rank approximation of random time dependent PDEs</i>	
Sofia Guzzetti, Department of Mathematics and Computer Science [Emory University] (17 :05-17 :10) .	55
<i>Reduced Models for Uncertainty Quantification in the Cardiovascular Network via Domain Decomposition</i>	
Amina Benaceur, ENPC - CERMICS, EDF R&D (17 :10-17 :15)	56
<i>A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems</i>	
Davide Pradovera, Ecole Polytechnique Fédérale de Lausanne (17 :10-17 :15)	57
<i>An efficient algorithm for Padé-type approximation of the frequency response for the Helmholtz problem</i>	

Niccolò Dal Santo, CMCS-EPFL (17 :10-17 :15)	58
<i>Multi space reduced basis preconditioners for large-scale parametrized PDEs</i>	
Stefan Banholzer, Department of Mathematics and Statistics, University of Konstanz (17 :15-17 :20) ...	59
<i>Certified POD-Based Multiobjective Optimal Control of Time-Variant Heat Phenomena</i>	
Stefan Hain, Institute of Numerical Mathematics, Ulm University - Alexander Nüsseler, Institute of Numerical Mathematics, Ulm University (17 :15-17 :20)	60
<i>Reduced basis method for parameter functions</i>	
Mazen Ali, Ulm University (17 :15-17 :20)	61
<i>Singular Value Decomposition on Intersection Spaces</i>	
Stefan Hain, Institute for Numerical Mathematics, Ulm University - Mladjan Radic, Institute for Numerical Mathematics, Ulm University (17 :20-17 :25)	62
<i>A hierarchical a-posteriori error estimator for the reduced basis method</i>	
Carmen Gräßle, University Hamburg (17 :20-17 :25)	63
<i>Combining POD Model Order Reduction with Adaptivity</i>	
Christian Himpe, Max Planck Institute for Dynamics of Complex Technical Systems (17 :20-17 :25)	64
<i>Parametric Model Order Reduction for Gas Flow Models</i>	
Daming Lou, Department of Electrical Engineering, Eindhoven University of Technology - Siep Weiland, Department of Electrical Engineering, Eindhoven University of Technology (17 :25-17 :30)	65
<i>Parametric model order reduction for large-scale and complex systems using Krylov subspace methods</i>	
Frank Naets, KU Leuven [Leuven], Member of Flanders Make (17 :25-17 :30)	66
<i>Parametric space-frequency reduction for second-order system models</i>	
Ward Rottiers, Department of Mechanical Engineering, KU Leuven, Member of Flanders Make (17 :25-17 :30)	67
<i>Parametric state-time reduction for the transient analysis of multi-physical systems</i>	

Data-Driven Multifidelity Methods for Monte Carlo Estimation

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Outer-loop applications, such as optimization, control, uncertainty quantification, and inference, form a loop around a computational model and evaluate the model in each iteration of the loop at different inputs, parameter configurations, and coefficients. Using a high-fidelity model in each iteration of the loop guarantees high accuracies but often quickly exceeds available computational resources because evaluations of high-fidelity models typically are computationally expensive. Replacing the high-fidelity model with a low-cost, low-fidelity model can lead to significant speedups but introduces an approximation error that is often hard to quantify and control. We introduce multifidelity methods that combine, instead of replace, the high-fidelity model with low-fidelity models. The overall premise of our multifidelity methods is that low-fidelity models are leveraged for speedup while occasional recourse is made to the high-fidelity model to establish accuracy guarantees. The focus of this talk is the multifidelity Monte Carlo method that samples low- and high-fidelity models to accelerate the Monte Carlo estimation of statistics of the high-fidelity model outputs. Our analysis shows that the multifidelity Monte Carlo method is optimal in the sense that the mean-squared error of the multifidelity estimator is minimized for the available computational resources. We provide a convergence analysis, prove that adapting the low-fidelity models to the Monte Carlo sampling reduces the mean-squared error, and give an outlook to multifidelity rare event simulation. Our numerical examples demonstrate that multifidelity Monte Carlo estimation provides unbiased estimators (“accuracy guarantees”) and achieves speedups of orders of magnitude compared to crude Monte Carlo estimation that uses a single model alone.

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Data-Driven Filtered Reduced Order Modeling Of Nonlinear Systems

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We propose a data-driven filtered reduced order model (DDF-ROM) framework for the numerical simulation of nonlinear systems [1]. The novel DDF-ROM framework consists of two steps: In the first step, we use explicit ROM spatial filtering [2] of the nonlinear PDE to construct a filtered ROM. This filtered ROM is low-dimensional, but is not closed (because of the nonlinearity in the given PDE). In the second step, we use data-driven modeling to close the filtered ROM, i.e., to model the interaction between the resolved and unresolved modes. To this end, we use a quadratic ansatz to model this interaction and close the filtered ROM. To find the new coefficients in the closed filtered ROM, we solve a least squares problem that minimizes the difference between the full order model data and our ansatz. We emphasize that the new DDF-ROM is built on general ideas of spatial filtering and optimization and is independent of restrictive phenomenological arguments, e.g., eddy viscosity.

We investigate the DDF-ROM in the numerical simulation of a channel flow past a circular cylinder. The DDF-ROM is significantly more accurate than the standard projection ROM (see Fig. 1). Furthermore, the computational costs of the DDF-ROM and the standard projection ROM are similar, both costs being orders of magnitude lower than the computational cost of the full order model. We also compare the new DDF-ROM with modern ROM closure models. The DDF-ROM is more accurate and significantly more efficient than these ROM closure models.

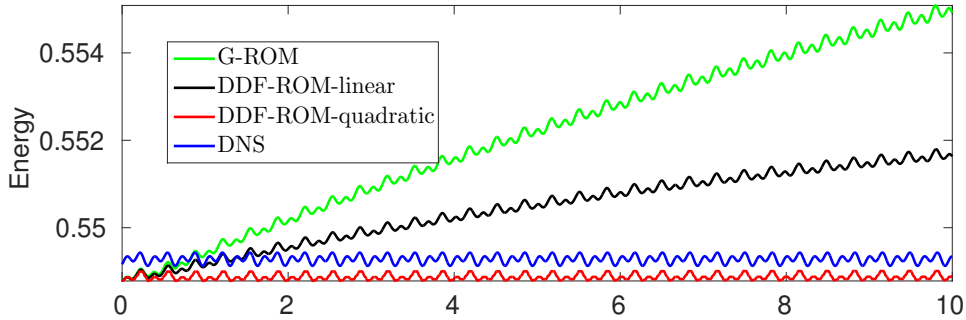


Figure 1: Plots of energy coefficients vs. time for the DDF-ROM. The DDF-ROM with a quadratic ansatz is dramatically more accurate than the standard Galerkin ROM (G-ROM).

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Estimation of Risk Measures with Reduced-Order Models

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We present recent results [1] on two reduced-order model (ROM) based approaches for the efficient and accurate evaluation of the Conditional-Value-at-Risk (CVaR) of quantities of interest (QoI) in engineering systems with uncertain parameters. CVaR is used to model objective or constraint functions in risk-averse engineering design and optimization applications under uncertainty. Evaluating the CVaR of the QoI requires sampling in the tail of the QoI distribution and typically requires many solutions of an expensive full-order model (FOM) of the engineering system. Our ROM approaches substantially reduce this computational expense.

Both ROM-based approaches use Monte Carlo (MC) sampling. The first approach replaces the computationally expensive FOM by inexpensive ROMs. The resulting CVaR estimation error is proportional to the ROM error in the so-called risk region, a small region in the space of uncertain system inputs. The second approach uses importance sampling (IS) and is effective even if the ROM has larger errors. ROM samples are used to estimate the risk region and to construct a biasing distribution. Few FOM samples are then drawn from this biasing distribution. Asymptotically as the ROM error goes to zero, the importance sampling estimator reduces the variance by a factor $1 - \beta \ll 1$, where $\beta \in (0, 1)$ is a parameter in the CVaR specification. Numerical experiments on a system of semilinear convection-diffusion-reaction equations illustrate the performance of the approaches.

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Dimension reduction of the input parameter space of vector-valued functions

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Approximation of multivariate functions is a difficult task when the number of input parameters is large. Identifying the directions where the function does not significantly vary is a key preprocessing step to reduce the complexity of the approximation algorithms.

Among other dimensionality reduction tools, the *active subspace* is defined by means of the gradient of a scalar-valued function, see [1]. It can be interpreted as the subspace in the parameter space where the gradient varies the most. In this talk, we propose a natural extension of the active subspace for vector-valued functions, e.g. functions with multiple scalar-valued outputs or functions taking values in function spaces. Our methodology consists in minimizing an upper-bound of the approximation error obtained using Poincaré-type inequalities, see [2].

We also compare the proposed gradient-based approach with the popular and widely used *truncated Karhunen-Loève decomposition* (KL). We show that, from a theoretical perspective, the truncated KL can be interpreted as a method which minimizes a looser upper bound of the error compared to the one we derived. Also, numerical comparisons show that better dimension reduction can be obtained provided gradients of the function are available.

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State estimation with reduced models and measurement data

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There is nowadays a growing amount of scientific and industrial applications where decisions need to be taken very fast or even in real time. In many cases, these decisions rely on predictions about the state of physical systems (blood flux in an artery, neutron population in a nuclear reactor, concentration of pollutants in a city...). Two reconstruction approaches can be considered:

- The first consists in using data from measuring devices and then reconstruct by interpolation or extrapolation.
- The second approach is based on the knowledge of a physical model, usually a parametrized Partial Differential Equation, whose solution gives an approximation of the state at every point of the domain.

Both approaches lead to incomplete and imperfect reconstructions because the system is usually too complex in order to perfectly sample or model it. This observation motivates to combine measurements and models in order to benefit from the advantages of both.

Investigations on this coupling are of growing interest in view of the emergence of very promising methods to treat large amounts of data (big data) that challenge the prominent role of modelling in many applications. In this talk, we will give an overview and present recent developments on state estimation methods based on reduced modelling. Our starting point will be the so-called Parametrized Background Data Weak (PBDW) method, recently introduced in [5]. After recalling its fundamental properties (optimality of the approximation [3], error bounds, stability), we will present a recent work on how to use the method in order to optimally select sensor locations and guarantee the stability of the reconstruction [4]. We will then discuss how to adapt the reduced model depending on the available measurement information. Finally, we will present applications to nuclear engineering [1, 2] and hemodynamics problems where understanding how to adapt the methodology for noisy measurements is a central question.

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An adaptive Parameterized-Background Data-Weak Approach to state estimation

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We present an Adaptive Parametrized-Background Data-Weak (PBDW) approach to the steady-state variational data assimilation (state estimation) problem, for systems modeled by partial differential equations. Given M noisy measurements of the state, the PBDW approach seeks an approximation of the form $u^* = z^* + \eta^*$, where the *background* z^* belongs to a N -dimensional *background space* informed by a parameterized mathematical model, and the *update* η^* belongs to a M -dimensional *update space* informed by the experimental observations.

We propose a Tikhonov regularization of the constrained statement originally presented in [Y Maday, AT Patera, JD Penn, M Yano, Int J Numer Meth Eng, 102(5), 933-965], and an adaptive procedure based on holdout validation, to effectively deal with noisy measurements. We further propose an user-defined update space, to improve convergence with respect to the number of measurements. Finally, we discuss an *a priori* error analysis for general linear functionals in the presence of noise, to identify the different sources of state estimation error and ultimately motivate the adaptive procedure.

We present results for a synthetic model problem in Acoustics, to illustrate the elements of the methodology and to prove its effectiveness.

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Data-driven probabilistic learning on manifolds

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A novel methodology [6] allows for generating realizations of a \mathbb{R}^n -valued random variable \mathbf{X} whose probability distribution $P_{\mathbf{X}}$ is unknown. The solely available information is a given dataset of $N \gg n$ independent realizations of \mathbf{X} , represented by a matrix $[x_d] \in \mathbb{M}_{n,N}(\mathbb{R})$, which is thus one sample of the $\mathbb{M}_{n,N}(\mathbb{R})$ -valued random variable $[\mathbf{X}]$ with probability distribution $P_{[\mathbf{X}]}$ for which the columns are N independent copies of \mathbf{X} . The probabilistic learning methodology proposed is based (1) on the construction of a diffusion-maps basis [1] represented by a matrix $[g] \in \mathbb{M}_{N,m}(\mathbb{R})$ with $m \ll N$, which allows for characterizing the local geometry structure of dataset $[x_d]$; (2) on the construction of a Reduced Itô Stochastic Differential Equation (R-ISDE) [6] on $\mathbb{M}_{n,m}(\mathbb{R})$ whose invariant measure $P_{[\mathbf{Z}]}$ is constructed as the projection $[X] = [Z][g]^T$ of the ISDE on $\mathbb{M}_{n,N}(\mathbb{R})$ associated with a dissipative Hamiltonian dynamical system [5, 6] for which the invariant measure is $P_{[\mathbf{X}]}$. The MCMC generator of realizations is given by solving the R-ISDE with a Stormer-Verlet algorithm and we then show [7] how a polynomial chaos representation of databases can be constructed. The method is robust and remains efficient for high dimension and large datasets. Based on such a methodology and introducing an additional formulation (based on nonparametric statistics) for the computation of conditional mathematical expectations, we present a novel methodology [2] for constructing the solution of probabilistic nonconvex constrained optimization problems under uncertainties, using only a fixed small number of function evaluations and probabilistic learning. Such a methodology brings together novel ideas to tackle an outstanding challenge in nonconvex optimization under uncertainties. Several examples are presented to highlight different aspects of the proposed probabilistic learning methodology, in particular for analyzing geophysics [3], complex flows in CFD [4, 8], and climate data.

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Randomized Model Order Reduction

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In this talk we show how randomization as used say in randomized linear algebra or compressed sensing can be exploited both for constructing reduced order models and deriving bounds for the approximation error.

We propose local approximation spaces for localized model order reduction procedures such as domain decomposition and multiscale methods, where those spaces are constructed from local solutions of the partial differential equation (PDE) with random boundary conditions [1]. Extending methods from randomized linear algebra [2] allows us to construct local spaces both for interfaces and subdomains that yield an approximation that converges provably at a nearly optimal rate and can be generated at close to optimal computational complexity. To realize the latter, we build the reduced spaces adaptively, relying on a probabilistic a posteriori error estimator.

Moreover, we propose a constant-free, probabilistic a posteriori error estimator for reduced order approximations such as the reduced basis approximation for parametrized PDEs. This error estimator does not require to estimate any stability constants and is both reliable and efficient at (given) high probability. Here, we rely on results similar to the restricted isometry property employed in compressed sensing [3]. In order to obtain an a posteriori error estimator that is computationally feasible in the online stage we employ the solution of a reduced dual problem with random right-hand side, exploiting the typically fast convergence of reduced order models.

Work in collaboration with A. Buhr (University of Münster), A. T. Patera (Massachusetts Institute of Technology), and O. Zahm (Massachusetts Institute of Technology)

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Random Sketching for Model Order Reduction

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For large-scale parameter-dependent problems, the cost of post-processing the snapshots can dominate the total computational cost of classical model order reduction methods. We propose a methodology for drastic reduction of the computational complexity. We show how the reduced order model can be constructed from a small set, called a sketch, of efficiently computable random projections of high-dimensional vectors. In this way, the heavy operations on large matrices and vectors can be avoided. Our algorithms are well suited for basically any computational environment. All operations, except solving linear systems of equations, are embarrassingly parallel. We provide a new version of Proper Orthogonal Decomposition that can be computed on multiple workstations with a communication cost independent of the dimension of the full problem. The reduced order model can even be constructed in a so-called streaming environment, i.e., under extreme memory constraints. In addition, we provide an efficient way for estimating the residual error. It does not require any assumption on the approximate solution and can be employed separately from the other part of the methodology. For example, it can be used for efficient estimation of the error associated with classical Galerkin projection. The new approach for error estimation is not only more efficient than the classical one but is also less sensitive to round-off errors.

Low-Rank Dynamic Mode Decomposition: Optimal Solution in Polynomial Time

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This work is concerned with linear approximations of high-dimensional dynamical systems of the form:

$$\begin{cases} x_t(\theta) = f_t(x_{t-1}(\theta)), & t = 1, \dots, T, \\ x_1(\theta) = \theta, \end{cases} \quad (1)$$

where $x_t(\theta) \in \mathbb{R}^n$ is the state variable, $f_t : \mathbb{R}^n \rightarrow \mathbb{R}^n$, and $\theta \in \mathbb{R}^n$ denotes an initial condition. We consider a data-driven approach relying on representative trajectories $\{x_t(\theta_i)\}_{t=1}^T$, $i = 1, \dots, N$, obtained by running (1) for N different initial conditions $\{\theta_i\}_{i=1}^N$ in a given set Θ . A linear approximation

$$\tilde{x}_t(\theta) = B_t \theta, \quad (2)$$

of $x_t(\theta)$ with $\text{rank}(B_t) \leq k \leq n$ is said *optimal* if $B_t = \left(\prod_{i=1}^{t-1} A_k^*\right) \in \mathbb{R}^{n \times n}$ with

$$A_k^* \in \arg \min_{A: \text{rank}(A) \leq k} \sum_{t=2, i=1}^{T, N} \|x_t(\theta_i) - Ax_{t-1}(\theta_i)\|_2^2. \quad (3)$$

Reduced models are then deduced by setting matrices $R, L \in \mathbb{C}^{n \times k}$ and $S \in \mathbb{C}^{k \times k}$ such that we have a decomposition $B_t = R(\prod_{i=1}^{t-1} S)L^\top$, lowering as much as possible the cost for computing (2). In particular, low-rank dynamic mode decomposition (DMD) of (1) is obtained in the case columns of matrices L and R gather the first k left and right eigen-vectors of A_k^* . If the latter is diagonalisable, a reduced model based on low-rank DMD presents an advantageous complexity scaling as $\mathcal{O}(kn)$.

This work deals with the off-line construction of reduced models of the form of (2) relying on (3). State-of-the-art polynomial-time algorithms are all sub-optimal. We show that we can compute in polynomial time a solution of (3) and the low-rank DMD of (1). We evaluated the proposed algorithms by numerical simulations using synthetic and physical data benchmarks. Details of this work can be found in [1].

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A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows

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For turbulent flows, estimation of the entire solution trajectory through a low-dimensional Reduced Order Model might be unfeasible due to the slow convergence of the Kolmogorov N -width, and due to the sensitivity of the dynamical system to perturbations. Nevertheless, it might still be possible to estimate the time-averaged solution and associated quantities of interest.

In this poster, we propose a Reduced-Basis technique for the estimation of long-time-averaged solutions of parametrized turbulent flows. The key elements of our approach are (i) a Greedy technique for the construction of a low-dimensional reduced space, and (ii) a constrained POD-Galerkin formulation of the reduced solution. The Greedy technique relies on a novel residual indicator for the error in the long-time-averaged solution.

We present a number of numerical examples to illustrate our approach, and to demonstrate the effectiveness of the error indicator.

Goal-Oriented Proper Generalized Decomposition with application to the detection of delamination in composites

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The poster will deal with the development of a mathematical formulation aiming at constructing adaptive reduced-order models tailored for the approximation of quantities of interest. The main idea is to formulate a constrained minimization problem that includes refined information in the goal functionals so that the resulting model be capable of delivering enhanced predictions of the quantities of interest [3]. The formulation will be applied to the so-called Proper Generalized Decomposition method [2, 1]. Such a paradigm represents a departure from classical goal-oriented approaches where the reduced model is first derived by minimization of the energy, or of the residual functional, and subsequently adapted via a greedy approach by controlling a posteriori error estimates measured in terms of quantities of interest using dual-based error estimates. In order to illustrate the efficiency of the proposed approach, we will consider the case of a delaminated composite material with the electrical conductivities of the different plies taken as parameter extra-coordinates in the PGD separation.

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Greedy measurement selection for state estimation

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Parametric PDEs of the general form

$$\mathcal{P}(u, a) = 0$$

are commonly used to describe many physical processes, where \mathcal{P} is a differential operator, a is a high-dimensional vector of parameters and u is the unknown solution belonging to some Hilbert space V .

Typically one observes m linear measurements of $u(a)$ of the form $\ell_i(u) = \langle w_i, u \rangle$, $i = 1, \dots, m$, where $\ell_i \in V'$ and w_i are the Riesz representers, and we write $W_m = \text{span}\{w_1, \dots, w_m\}$. The goal is to recover an approximation u^* of u from the measurements.

The solutions $u(a)$ lie in a manifold within V which we can approximate by a linear space V_n , where n is of moderate dimension. The structure of the PDE ensure that for any a the solution is never too far away from V_n , that is, $\text{dist}(u(a), V_n) \leq \varepsilon$. In this setting, the observed measurements and V_n can be combined to produce an approximation u^* of u up to accuracy

$$\|u - u^*\| \leq \beta^{-1}(V_n, W_m) \varepsilon$$

where

$$\beta(V_n, W_m) := \inf_{v \in V_n} \frac{\|P_{W_m} v\|}{\|v\|}$$

plays the role of a stability constant. For a given V_n , one relevant objective is to guarantee that $\beta(V_n, W_m) \geq \gamma > 0$ with a number of measurements $m \geq n$ as small as possible. We present results in this direction when the measurement functionals ℓ_i belong to a complete dictionary.

Conservative model reduction for finite-volume models

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We present a method for model reduction of finite-volume models that guarantees the resulting reduced-order model is conservative, thereby preserving the structure intrinsic to finite-volume discretizations [1]. The proposed reduced-order models associate with *optimization problems* characterized by (1) a minimum-residual objective function and (2) nonlinear equality constraints that explicitly enforce conservation over subdomains. *Conservative Galerkin* projection arises from formulating this optimization problem at the time-continuous level, while *conservative least-squares Petrov–Galerkin* (LSPG) projection associates with a time-discrete formulation. Figure 1 depicts possible decomposed meshes over which conservation can be enforced for a vertex-centered finite-volume model. We note that other recent works have also considered ROMs that associate with constrained optimization problems [3, 2], although none are conservative.

We equip these approaches with hyper-reduction techniques in the case of nonlinear flux and source terms, and also provide approaches for handling infeasibility. In addition, we perform analyses that include deriving conditions under which conservative Galerkin and conservative LSPG are equivalent, as well as deriving *a posteriori* error bounds.

On a parameterized quasi-1D Euler equation problem, the proposed method not only conserves mass, momentum, and energy globally, but also has significantly lower state-space errors than nonconservative reduced-order models such as standard Galerkin and LSPG projection.

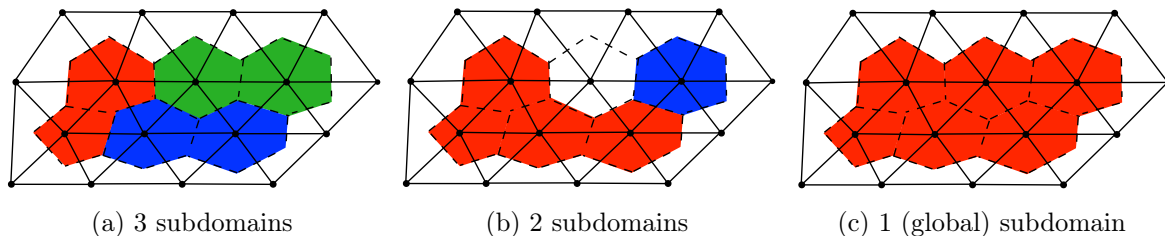


Figure 1: Examples of decomposed meshes. The propose method enforces conservation over each subdomain (denoted by colors). Note that 1 global subdomain enforces global conservation.

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Directional hyper-reduced model for evaluation of residual welding stresses

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The welding process produces strains and residual stresses that must be taken into account to evaluate the final quality of the assembly. For that, the simulation of the process by a thermomechanical computation is very widely used [1]. Numerical simulation uses many parameters (materials, heat source, boundary conditions) whose effects must be studied. But as the computation becoming very expensive, massive parametric studies quickly become unusable [4].

To reduce the computation time, we propose an approach based on the spatial and temporal similarity of thermal results, by a method of hyper-reduction on a *slice* of the domain.

We suppose the heat source is moves along the Ox axis, considering the domain $\Omega = [0, L_X] \times S$ it is possible to separate the variables (x, t) and variables (y, z) for the approximation of temperatures:

$$\mathbf{u}_{ROM}(x, y, z, t; \boldsymbol{\mu}) = \mathbf{u}^D + \sum_{i=1}^{N_S} \hat{\Psi}_k(y, z) \hat{\gamma}_k(x, t; \boldsymbol{\mu}) \quad (1)$$

We use SVD method to construct the basis $\hat{\Psi}_k(y, z)$. Each plane (y, z) of the mesh has a *directional* shape function $(\xi_j(x))$ for $j = 1, N_X$, the reduced coordinates $\hat{\gamma}_k$ are:

$$\hat{\gamma}_k(x, t; \boldsymbol{\mu}) = \sum_{j=1}^{N_X} \xi_j(x) \gamma_p(t; \boldsymbol{\mu}) \quad (2)$$

with $p = (j - 1)N_S + k$ and $k = 1, \dots, N_S$.

For the mechanical part, we use a more classical method using also hyper-reduction[2] . The domain of variations of the parameters being very wide, it is often necessary to carry out a correction finite elements on the reduced model. In addition, careful attention was given to the evaluation of quantities in post-treatment (reconstruction of the stresses field by gappy-POD). [4]

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POD–Galerkin reduced order methods for inverse problems and multi-physics problems in fluid dynamics

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In this talk we will focus on recent advances in reduced order modelling for parametrized problems in computational fluid dynamics, with a special attention to the case of inverse problems, such as optimal flow control problems and data assimilation, and multi-physics applications.

Among the former, we will discuss applications arising in environmental marine sciences and engineering [5], namely a pollutant control in the Gulf of Trieste, Italy and a solution tracking governed by quasi-geostrophic equations describing North Atlantic Ocean dynamic. Similar methodologies will also be employed in problems related to the modeling of the cardiovascular system [4].

Among the latter, we will present further recent developments on reduction of fluid-structure interaction problems, based on our earlier work in [1, 3]. Reduced order approaches for parametric optimal flow control will also be applied in combination with domain decomposition in view of further applications in multi-physics [2].

This work is in collaboration with Y. Maday (UPMC Université Paris 06, France), L. Jiménez-Juan (Sunnybrook Health Sciences Centre, Toronto, Canada), P. Triverio (University of Toronto, Canada), R. Mosetti (National Institute of Oceanography and Applied Geophysics, Trieste, Italy).

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Advances in Hierarchical Model Reduction and combination with other computational reduction methods

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In this work we present address the combination of the Hierarchical Model (Hi-Mod) reduction approach [2, 6, 5] with projection-based reduced order methods, exploiting either on Greedy Reduced Basis (RB) or Proper Orthogonal Decomposition (POD) [3], in a parametrized setting. The Hi-Mod approach, introduced in [2], is suited to reduce problems in pipe-like domains featuring a dominant axial dynamics, such as those arising for instance in haemodynamics. The Hi-Mod approach aims at reducing the computational cost by properly combining a finite element discretization of the dominant dynamics with a modal expansion in the transverse direction. In a parametrized context, the Hi-Mod approach has been employed as the high-fidelity method during the offline stage of model order reduction techniques based on RB or POD. The resulting combined reduction methods, which have been named Hi-RB and Hi-POD, respectively, will be presented with applications in diffusion-advection problems, fluid dynamics [1, 7] and optimal control problems [4], focusing on the approximation stability of the proposed methods and their computational performance.

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The effort of increasing Reynolds number in POD-Galerkin Reduced Order Methods: from laminar to turbulent flows

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We present different strategies to be able to increase Reynolds number in Reduced Order Methods (ROMs), from laminar to turbulent flows, in the context of the incompressible parametrised Navier-Stokes equations. The proposed methodologies are based on different full order discretisation techniques: the finite element method and the finite volume method. For what concerns finite element full order discretisations - which in this work aim to be used from low to moderate Reynolds numbers - the ROMs are based on classical stabilisation approaches like the Brezzi-Pitkaranta (BP), the streamline upwind Petrov-Galerkin (SUPG), the Galerkin least square (GALS) and then the Variational Multi-scale Method (VMS) [5, 2, 1]. For what concerns the finite volume full order simulations, which are performed using RANS-LES turbulence models, and aim to be used for higher Reynolds numbers flows, a reduced version of the eddy viscosity is included into the reduced order model [3, 4]. The proposed methodologies are tested on classic benchmark test cases.

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Towards a stable and fast dynamic skeletal muscle model

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Forward simulations of three-dimensional, continuum-mechanical skeletal muscle models are computationally demanding and expensive. To adequately represent the muscles' mechanical behaviour, a fully dynamic modelling framework based on the theory of finite hyperelasticity, which accounts for the highly nonlinear, anisotropic, viscoelastic and incompressible material behaviour, needs to be established. Discretisation of the governing equations by means of the finite element method yields a nonlinear second-order DAE system

$$\mathbf{M}\mathbf{u}''(t) = -\mathbf{D}\mathbf{u}'(t) - \mathbf{K}(\mathbf{u}(t)) + \mathbf{A}(\mathbf{u}(t))\mathbf{w}(t), \quad (1)$$

$$\mathbf{0} = \mathbf{G}(\mathbf{u}(t)). \quad (2)$$

This system represents a challenge for solution strategies as well as for the application of model order reduction techniques. In this contribution, we will compare different solution strategies (DAE index reduction, different solvers) as well as the performance of reduced order models obtained by means of Galerkin and Petrov-Galerkin projection using different projection and test spaces.

Principal component analysis and optimal weighted least-squares method for training tree tensor networks

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One of the most challenging tasks in computational science is the approximation of high-dimensional functions. Most of the time, only a few information on the functions is available, and approximating high-dimensional functions requires exploiting low-dimensional structures of these functions.

In this work, the approximation of a function u is built using point evaluations of the function, where these evaluations are selected adaptively. Such problems are encountered when the function represents the output of a black-box computer code, a system or a physical experiment for a given value of a set of input variables.

A multivariate function $u(x_1, \dots, x_d)$ defined on a product set $\mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_d$ can be identified with a tensor of order d . Here, we present an algorithm for the construction of an approximation of a function u in tree-based tensor format (tree tensor networks whose graphs are dimension partition trees). This approximation is parametrized by a set of low-order tensors, seen as multilinear vector-valued maps v_α , α being a node of a dimension partition tree T .

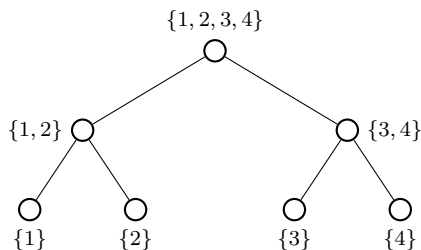


Figure 1: Example of a dimension partition tree T over $D = \{1, 2, 3, 4\}$

For example, an approximation v associated with the tree of the Figure 1 takes the form:

$$v = v_{1,2,3,4}(v_{1,2}(v_1(\phi_1(x_1)), v_2(\phi_2(x_2))), v_{3,4}(v_3(\phi_3(x_3)), v_4(\phi_4(x_4))))$$

where the $\phi_\nu : \mathcal{X}_\nu \rightarrow \mathbb{R}^{n_\nu}$, $\nu \in \{1, 2, 3, 4\}$ are the feature maps.

This algorithm relies on an extension of principal components analysis (PCA) to multivariate functions in order to estimate the tensors v_α . In practice, the PCA is realized on sample-based projections of the function u , using interpolation or least-squares regression.

Least-squares regression can provide a stable projection but it usually requires a high number of evaluations of u , which is not affordable when one evaluation is very costly. In [1], the authors proposed an optimal weighted least-squares method, with a choice of weights and samples that guarantee an approximation error of the order of the best approximation error using a minimal number of samples. We here present an extension of this methodology for the approximation in tree-based format, where optimal weighted least-squares method is used for the projection onto tensor product spaces. This approach will be compared with a strategy using standard least-squares method or interpolation (as proposed in [2]).

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Reduced order methods for nonlinear parametric problems with branching solutions

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The aim of this work is to show the applicability of the reduced basis model reduction in nonlinear systems undergoing bifurcations. Bifurcation analysis, i.e., following the different bifurcating branches, as well as determining the bifurcation point itself, is a complex computational task [4, 3]. Reduced Order Models (ROM) can potentially reduce the computational burden by several orders of magnitude, in particular in conjunction with sampling techniques.

In the first task we focus on nonlinear structural mechanics [2], and we deal with an application of ROM to Von Kármán plate equations, where the buckling effect arises, adopting reduced basis method. Moreover, in the search of the bifurcation points, it is crucial to supplement the full problem with a reduced generalized parametric eigenvalue problem, properly paired with state equations and also a reduced order error analysis. These studies are carried out in view of vibroacoustic applications (in collaboration with A.T. Patera at MIT). As second task we consider the incompressible Navier-Stokes equations [1], discretized with the spectral element method, in a channel and a cavity. Both system undergo bifurcations with increasing Reynolds - and Grashof - number, respectively. Applications of this model are contraction-expansion channels, found in many biological systems, such as the human heart, for instance, or crystal growth in cavities, used in semiconductor production processes. This last task is in collaboration with A. Alla and M. Gunzburger (Florida State University).

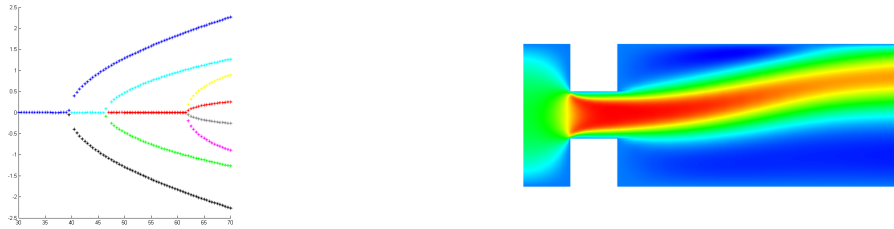


Figure 1: Bifurcation plot for the buckling of a rectangular plate (left) and the Coanda effect on the velocity field solution in an expansion channel problem held by Navier-Stokes equations (right).

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Statistical learning in tree-based tensor format

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Tensor methods are widely used tools for the approximation of high dimensional functions. Such problems are encountered in uncertainty quantification and statistical learning, where the high dimensionality imposes to use specific techniques, such as rank-structured approximations [1].

In this work, we introduce a statistical learning algorithm for the approximation in tree-based tensor format, which are tensor networks whose graphs are dimension partition trees (figure 1). This tensor format includes the Tucker format, the Tensor-Train format, as well as the more general Hierarchical tensor formats [4]. It can be interpreted as a deep neural network with a particular architecture [2].

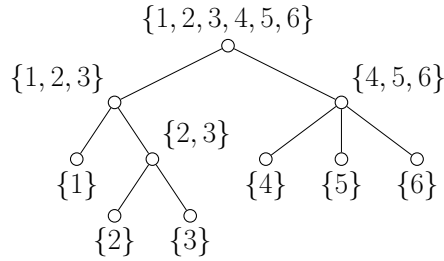


Figure 1: Example of a dimension partition tree T over $D = \{1, \dots, 6\}$.

The proposed algorithm uses random evaluations of a function to provide a tree-based tensor approximation, with adaptation of the tree-based rank by using a heuristic criterion based on the higher-order singular values to select the ranks to increase, and of the approximation spaces of the leaves of the tree.

We then present a learning algorithm for the approximation under the form

$$u(x) \approx v(z_1, \dots, z_m) \quad (1)$$

where v is a tensor in tree-based format and the $z_i = g_i(x)$, $1 \leq i \leq m$ are new variables. A strategy based on the projection pursuit regression [3] is proposed to compute the mappings g_i and increase the effective dimension m .

The methods are illustrated on different examples to show their efficiency and adaptability as well as the power of representation of the tree-based tensor format, possibly combined with changes of variables.

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A reduced-order Kalman filter for CFD applications

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In the last decade, the importance of numerical simulations for the analysis of complex engineering systems, such as thermo-fluid dynamics in nuclear reactors, has grown exponentially. In spite of the large experimental databases available for validation of mathematical models, in order to identify the most suitable one for the system under investigation, the inverse integration of such data into the CFD model is nowadays an ongoing challenge. In addition, such integration could tackle the problem of propagation of epistemic uncertainties, both in the numerical model and in the experimental data. In this framework, the data-assimilation method allows for the dynamic incorporation of observations within the computational model. Perhaps the most famous among these methods, due to its simple implementation and yet robust nature, is the Kalman filter. Although this approach has found success in fields such as weather forecast and geoscience, its application in Computational Fluid-Dynamics (CFD) is still in its first stages. In this setting, a new algorithm based on the integration between the segregated approach, which is the most common method adopted by CFD applications for the solution of the incompressible Navier-Stokes equations, and a Kalman filter modified for fluid-dynamics problems, while preserving mass conservation of the solution, has already been developed and tested in a previous work.

Whereas such method is able to robustly integrate experimental data within the numerical model, its computational cost increases with model complexity. In particular, in high-fidelity realistic scenarios the error covariance matrix for the model, which represents the uncertainties associated with it, becomes dense, thus affecting the efficiency and computational cost of the method. For this reason, due to the promised reduction of computational requirements recently investigated [1, 2], which combines model reduction and data-assimilation, in this work a combination of reduced order model and mass-conservative Kalman filter within a segregated approach for CFD analysis is proposed. The novelty lies in the peculiar formulation of the Kalman filter and how to construct a low-dimensional manifold to approximate, with sufficient accuracy, the high fidelity model. With respect to literature, in which the full-order Kalman filter is applied to a reduced model, the reduction is performed directly on the integrated model in order to obtain a reduced-order Kalman filter already optimised for fluid-dynamics applications. In order to verify the capabilities of this approach, this reduced-order algorithm has been tested against the lid-driven cavity test case.

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Basis generation in optimal control problems

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We consider numerical approximation for the control of linear PDEs for both open and closed loop. Since control problems are computationally very expensive, we use model order reduction techniques to reduce its complexity. The general idea is to find *basis functions*, which allow to project our dynamical system into a low-dimensional system. It is crucial that the basis functions have information about the underlying control problem. In this talk, we will focus on recent advances in the computation of the basis functions.

In the open-loop case, we consider Proper Orthogonal Decomposition (POD) which is a Galerkin approach where the basis functions are obtained upon information contained in time snapshots of the PDE related to given input data. This constitutes the bottleneck of the method. We also show that for POD in optimal control problems it is important to have knowledge about the controlled system at the right time instances. Therefore, we propose to determine the time instances (*snapshot locations*) by reformulating the optimality conditions and using a-posteriori error control (see [1]).

In the closed-loop case, we explore order reduction techniques for solving the algebraic Riccati equation (ARE), and investigating the numerical solution of the linear-quadratic regulator problem (LQR). A classical approach is to build a surrogate low dimensional model of the dynamical system, for instance by means of e.g. POD, and then solve the corresponding ARE. Alternatively, iterative methods can be used to directly solve the ARE and use its approximate solution to estimate quantities associated with the LQR. We propose a class of Petrov-Galerkin (see [2]) strategies that simultaneously reduce the dynamical system while approximately solving the ARE by projection. This basis functions will directly benefit information upon the value function which is fundamental to compute feedback control.

We present numerical tests to illustrate our approach and show the effectiveness of the proposed methods in comparison to existing approaches.

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Reduced Basis Solutions of Parametrized Optimal Control Problems with Non-Affine Source Terms

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We employ the reduced basis method as a surrogate model for the solution of optimal control problems governed by parametrized elliptic partial differential equations [2] with non-affine source terms [3]. The proposed method constructs affine approximations of the non-affine parameter dependent source term by employing the empirical interpolation method (EIM) [1]. We develop online-efficient a posteriori error bounds for the error in the optimal control and present numerical results motivated by the planning of thermal cancer treatments.

In particular we determine the optimal power of the heat source $u \in U \equiv \mathbb{R}$, so that the desired state $y_d \in Y \equiv H^1(\Omega)$ is achieved. The desired state y_d and the u -dependent state $y \in Y$ represent temperature fields over the computational domain Ω . The corresponding optimal control problem can be formulated as follows:

Given parameter μ from the parameter set \mathcal{D} , find

$$\min_{(y,u) \in Y \times U} J(y, u; \mu) := \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\lambda}{2} |u|^2, \quad (1)$$

$$\text{so that } (y, u) \in Y \times U \text{ solves } a(y, v; \mu) = b(v; \mu)u + f(v; \mu), \quad \text{for all } v \in Y. \quad (2)$$

Here both the coercive, continuous bilinear form $a(\cdot, \cdot; \mu) : Y \times Y \rightarrow \mathbb{R}$, and the continuous linear form $f(\cdot; \mu) : Y \rightarrow \mathbb{R}$ are affine parameter dependent. However, the linear bounded functional $b(\cdot; \mu) : Y \rightarrow \mathbb{R}$ is non-affine in μ .

We present real-time efficient error bounds for the control variable u . The proposed error bounds take into account the error introduced by the reduced basis approximation and the error associated with the EIM interpolation error.

The numerical example under consideration relates to thermal cancer treatments, and is parametrized with respect to source placement parameters. For a 2-D model the heat source is described using a Gaussian function, i.e. $b(x; \mu)u = u \exp(-|x - \mu|^2/(2c^2))$, for all x in the computational domain Ω and $\mu \in \mathcal{D}$ and the diffusion of heat in living tissue is described using the Pennes bioheat model [4]. In this case, the placement parameters $\mu \in \mathcal{D} \subset \mathbb{R}^2$ correspond to the center of the Gaussian.

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Accelerating Implicit Integrators for Parametric ODE Systems by Greedy Kernel Approximation.

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In this presentation, we want to demonstrate how kernel-based approximation methods can contribute to a paradigm of “Data-based Numerical Mathematics”. Parametric MOR has intensively focussed on approximately solving parametric high-dimensional PDE and ODE systems during the last decades. We want to widen this view to more general parametric problems in numerical mathematics, that might benefit from the same concept: 1) gathering data from solving some specific problem instantiations, 2) processing this data and obtain a surrogate that can be used for 3) rapidly solving or approximating the original parametric problem.

We will first review some basic tools in kernel approximation for the reconstruction of high-dimensional functions, both in input and output. These methods allow to construct approximants to general target functions defined on arbitrary domains by means of scattered samples, i.e., without requiring any structure on the sampling locations. We will then focus on greedy algorithms, in particular the VKOGA [3], which constructs approximants based on a small subset of the data sites, thus being faster to evaluate, while still providing a good accuracy, which can even be proven to be quasi-optimal in some cases [2]. The proof actually makes elegant use of known results for Reduced Basis Methods. These theoretical and computational features make greedy kernel-based algorithms particularly attractive for the construction of surrogate models.

Then we will exemplify an application in data-driven numerical mathematics, namely acceleration of implicit ODE integrators by forecasting. A set of state trajectories precomputed with a high-accuracy ODE solver is used to train a kernel model which predicts the next point in the trajectory as a function of the previous one. This model is cheap to evaluate, and it is used in the online phase to provide a good initialization point for the nonlinear solver of the implicit integrator. The accuracy of the surrogate model results in a significant reduction of the number of required steps of the solver, thus providing an overall speedup of the full simulation. Despite the acceleration, the method maintains the accuracy of the original model. Although the method can be potentially applied to a large variety of solvers and different ODEs, we will present in detail its use with the implicit Euler method (VKOGA-IE) in the solution of e.g., the Burgers equation, which is an important test case to demonstrate the method’s features [1].

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Fast Estimation of Blood Vessel Cooling Effects in Hepatic Radio-Frequency Ablation using the Reduced Basis Method

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Minimally invasive treatment methods are more appropriate for the treatment of liver cancers because of the presence of multiple tumours, close proximity to large blood vessels or co-existing conditions like cirrhosis. Radio-frequency ablation is a minimally invasive treatment method that has become popular in recent years [1]. In this method, radio-frequency current is passed through the tumour using a probe. This current produces heat which is intended to kill the tumour cells. The drawback of this method is dependence of the outcome of the treatment on the amount of experience possessed by the clinician. One reason for this is the cooling effect of blood vessels [2]. Ideally, the treatment methodology should be such that any clinician can guarantee a high success rate irrespective of the clinician's experience. With this in view, our objective is to develop a mathematical model of RFA, which can predict treatment outcomes in the clinical setting.

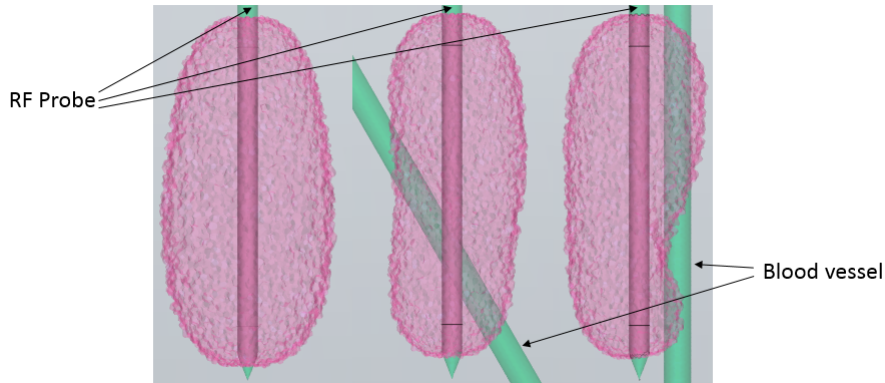


Figure 1: Left: RFA lesion (pink region) unaffected by blood vessel. Center & Right: two views of lesion (pink region) affected by blood vessel.

With the objective of real-time prediction of RFA in mind, we propose the following study. We consider a problem setting with a single tumour and a single blood vessel located in its vicinity. The inputs for the simulation are the parameters related to the size, location and the orientation of the blood vessel, as well as the active region of the RF probe. The output of interest is the temperature distribution at the end of the RFA procedure. Since the output is desired within a short amount of time, the use of model order reduction will be explored.

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Parameter space and model reduction with shape parametrization, by means of active subspace and POD-Galerkin methods for industrial and biomedical applications

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In this work we present both industrial and biomedical applications, focusing on shape parametrization and parameter space reduction by means of active subspaces. In particular we introduce a combined parameter and model reduction methodology using a POD-Galerkin approach, and its application to the efficient numerical estimation of a pressure drop in a set of deformed carotids [2]. The aim is to simulate a wide range of possible occlusions after the bifurcation of the carotid artery. A parametric description of the admissible deformations, based on radial basis functions interpolation technique implemented in the PyGeM python package, is introduced. The use of the reduced order model acting on the reduced parameter space allows significant computational savings and better performances. Moreover we present the reduction of heterogeneous parameter space in a naval engineering problem, that is the hydrodynamic flow past the hull of a ship advancing in calm water [3], considering structural and shape parameters. The geometrical parametrization is done via free form deformation. Some perspectives on a complete shape optimization pipeline by means of Dynamic Mode Decomposition (DMD) and POD with interpolation (PODI) are presented [1], together with the integration of the python packages PyDMD and EZyRB respectively.

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Efficient Therapy Planning via Model Reduction for Laser-Induced Interstitial Thermotherapy

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We investigate the planning of minimally invasive tumor treatments via laser-induced thermotherapy. The goal is to control the laser in order to obtain an optimal treatment, e.g. eradicating the tumor, while leaving as much healthy tissue unharmed as possible. To this end, we define a PDE-constrained optimal control problem. As these problems are usually computationally expensive, we propose a simplified modeling approach using reduced-order models. Numerical results illustrate the viability of our approach.

Localized Reduced Basis Methods for Time Harmonic Maxwell's Equations

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We discuss stable, localized model order reduction of non-coercive but inf-sup stable problems like the one which arises from the discretization of the time-harmonic Maxwell's equations.

Localized model order reduction methods have attracted significant attention during the last years. They have favorable parallelization properties and promise to perform well on cloud architectures, which become more and more commonplace. We introduced ArbiLoMod [1], a localized reduced basis method targeted at the important use case of changing problem definition, wherein the changes are of local nature. This is a common situation in simulation software used by engineers optimizing a CAD model.

An especially interesting application is the simulation of electromagnetic fields in printed circuit boards, which is necessary to design high frequency electronics. The simulation of the electromagnetic fields can be done by solving the time-harmonic Maxwell's equations, which results in a parameterized, inf-sup stable problem which has to be solved for many parameters. In this multi-query setting, the reduced basis method can perform well. Experiments have shown two dimensional time-harmonic Maxwell's to be amenable to localized model reduction [2].

However, Galerkin projection of an inf-sup stable problem is not guaranteed to be stable. Existing stabilization methods for the reduced basis method involve global computations and are thus not applicable in a localized setting. We discuss a stable, localized projection of inf-sup stable problems based on localized a posteriori error estimators. While we use time-harmonic Maxwell's equations as an example, the same techniques could be used for other inf-sup stable problems, like e.g. acoustics.

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Biogeochemical Oceanographic Data Assimilation: Dimensionality Reduced Kalman Filter for Mediterranean Sea Forecasting

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Data Assimilation is a key element to improve the performance of Biogeochemical ocean/marine forecasting systems. Handling the very big dimension of the state vector of the system (often of the order of 10^6) remains an issue, also considering the computational efficiency of operational systems. Indeed, simple product operations involving the covariance matrices are too heavy to be computed for operational forecasting purposes. Various attempts have been made in literature to reduce the complexity of this task, often adding strong hypotheses to simplify the problem and decrease the computational cost.

The MedBFM model system ([2], [3], and referencies thereby), which is responsible for monitoring and forecasting the biogeochemical state of the Mediterranean Sea within the European Copernicus Marine Services (see <http://marine.copernicus.eu/>) assimilate surface chlorophyll data through a 3D Variational algorithm, that decomposes the background error covariance matrix into sequential operators to reduce complexity [3].

In the present work, we compare the variational scheme with a Kalman Filter from a Bayesian point of view showing that the Kalman Filter is able to assimilate data with better accuracy.

Therefore, we aim at developing a novel Kalman Filter for the MedBFM system. The novel Kalman Filter scheme benefits from advanced Principal Component Analysis (PCA, [1]) to reduce the dimension of correlation matrices and improve the computational efficiency.

Finally, we will discuss our results comparing the new Kalman implementation in the MedBFM system and the current variational Data Assimilation system in terms of computational performance and forecast skill assessment.

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Dynamical low rank approximation of random time dependent PDEs

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Partial differential equations with random coefficients and input data arise in many real world applications. What they often have in common is that the data describing the PDE model are subject to uncertainties either due to a lack of knowledge of the system or to its inherent variability. The numerical approximation of statistics of this random solution poses several challenges, in particular when the number of random parameters is large and/or the parameter-to-solution map is complex. Therefore, effective surrogate or reduced models are of great need.

We consider a class of time dependent PDEs with random parameters and search for an approximate solution in a separable form, i.e. at each time instant expressed as a linear combination of linearly independent spatial functions multiplied by linearly independent random variables (low rank approximation) in the spirit of a truncated Karhunen-Loève expansion. Since the optimal deterministic and stochastic modes can significantly change over time, static versions, such as proper orthogonal decomposition or polynomial chaos expansion, may lose their effectiveness. Instead, here we consider a dynamical approach in which those modes are computed on-the-fly as solutions of suitable auxiliary evolution equations. From a geometric point of view, this approach corresponds to constraining the original dynamics to the manifold of fixed rank functions. The original equations are projected onto the tangent space of this manifold along the approximate trajectory.

In this poster we recall the construction of the method introduced in [3] and give some implementation details. The spatial discretization is carried out by the finite element method and the discretization of the random variables relies on an adaptive choice of sparse grid. We will present some numerical test cases including the heat equation with a random diffusion coefficient and initial condition as well as the wave equation with a random wave speed, for which we are applying a dynamical low rank approximation that preserves the symplectic structure of the governing equations [1, 2].

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Reduced Models for Uncertainty Quantification in the Cardiovascular Network via Domain Decomposition

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Reduced 1D models of the cardiovascular system are widely employed to study the propagation of pressure waves induced by the mutual interaction between the fluid and the compliant vessel walls. In particular, the interplay between anomalous pressure waves and pathologies like amputations, stenoses or devices like stents is of great interest from a medical viewpoint. However, the parameters that characterize reduced 1D models are often unknown, and feature variability not only from patient to patient, but also within the same individual, depending on physiological conditions (e.g., rest vs. stress, and young vs. old). This motivated the design of mathematical and numerical techniques to *quantify* the uncertainties in these models. Uncertainty Quantification (UQ) studies on the cardiovascular network entail two major challenges or limitations (see, e.g., [5, 2, 4]): (i) The employment of full 3D models for UQ analysis is extremely costly and requires computational resources that may not be easily accessible by users like hospitals, for financial, privacy or time constraints; (ii) Reduced 1D models may be inaccurate in capturing anomalies of the physiology in presence of cardiovascular pathologies like stenoses or aneurysms. Following the DDUQ approach presented in [1], we enhance the efficiency and parallelism of the solvers by performing UQ at the subsystem level at each time step, and by propagating the information via Domain Decomposition techniques. We plan to enhance accuracy and reliability by replacing the 1D models with *educated* reduced models such as the Transversally Enriched Pipe Element Method [3], capable of retaining the local cross-sectional dynamics, approximately at the same cost of 1D reduced models. Research supported by National Science Foundation grant DMS 1419060.

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A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems

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We investigate new developments of the combined Reduced-Basis and Empirical Interpolation Methods (RB-EIM) for parametrized nonlinear parabolic problems [1, 2]. In many situations, the cost of the EIM in the offline stage turns out to be prohibitive since a significant number of nonlinear time-dependent problems need to be solved using the full-order model.

In the present work, we develop a new methodology, the Progressive RB-EIM (PREIM) method for nonlinear parabolic problems. The purpose is to reduce the offline cost while maintaining the accuracy of the RB approximation in the online stage. The key idea is a progressive enrichment of both the EIM approximation and the RB space, in contrast to the standard approach where the EIM approximation and the RB space are built separately. PREIM uses full-order computations whenever available and RB computations otherwise. Another key feature of PREIM is to select twice the parameter in a greedy fashion, the second selection being made after computing the full-order solution for the firstly-selected value of the parameter. Numerical examples will be presented on nonlinear heat transfer problems.

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An efficient algorithm for Padé-type approximation of the frequency response for the Helmholtz problem

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Given an open bounded Lipschitz domain $D \subset \mathbb{R}^d$ ($d = 1, 2, 3$), whose boundary is partitioned into Γ_D and Γ_N , and $f \in L^2(D)$, we consider the map $\mathcal{S} : \mathbb{C} \rightarrow H_{\Gamma_D}^1(D) = \{v \in H^1(D), v|_{\Gamma_D} = 0\}$, which associates a complex value z with the weak solution of the (complex) Helmholtz problem

$$\text{find } \mathcal{S}(z) \in H_{\Gamma_D}^1(D) : \quad \langle \nabla \mathcal{S}(z), \nabla v \rangle_{L^2(D)} - z \langle \mathcal{S}(z), v \rangle_{L^2(D)} = \langle f, v \rangle_{L^2(D)} \quad \forall v \in H_{\Gamma_D}^1(D).$$

Several results (see e.g. [1]) show that \mathcal{S} is well-defined and meromorphic in $\mathbb{C} \setminus \Lambda$, $\Lambda = \{\lambda_\alpha\}_{\alpha=1}^\infty$ being the (countable, unbounded) set of (real, non-negative) eigenvalues of the Laplace operator (restricted to $H_{\Gamma_D}^1(D)$, with homogeneous Neumann boundary conditions on Γ_N). In particular, it holds

$$\mathcal{S}(z) = \sum_{\alpha=1}^{\infty} \frac{s_\alpha}{\lambda_\alpha - z}, \quad (1)$$

where the elements of $\{s_\alpha\}_{\alpha=1}^\infty \subset H_{\Gamma_D}^1(D)$ are pair-wise orthogonal with respect to the $H_{\Gamma_D}^1(D)$ inner product, and the equality in (1) has to be understood with respect to the $H_{\Gamma_D}^1(D)$ norm.

It is possible to define a Padé-type approximant of any map (1) around $z_0 \in \mathbb{C}$: given $M, N \in \mathbb{N}$, the exact map is approximated by a rational map $\mathcal{S}_{[M/N]} : \mathbb{C} \setminus \Lambda \rightarrow H_{\Gamma_D}^1(D)$ of the form

$$\mathcal{S}_{[M/N]}(z) = \frac{\mathcal{P}_{[M/N]}(z)}{\mathcal{Q}_{[M/N]}(z)} = \frac{\sum_{j=0}^M P_j (z - z_0)^j}{\sum_{i=0}^N Q_i (z - z_0)^i},$$

with $\{P_j\}_{j=0}^M \subset H_{\Gamma_D}^1(D)$ and $\{Q_i\}_{i=0}^N \subset \mathbb{C}$.

In [1] the authors define such approximant within a Least-Squares framework, through the minimization of a suitable functional which involves $E' \geq M + N$ derivatives of \mathcal{S} in z_0 . This poster introduces a new definition, which relies on a simplified version of the functional, and only requires $E \geq M$ derivatives of the solution map. As such, starting from the same amount of information on \mathcal{S} , it is possible to find a higher order - hence more accurate - approximant.

In particular, the denominator $\mathcal{Q}_{[M/N]}$ is the minimizer (under some normalization constraints) of the $H_{\Gamma_D}^1(D)$ norm of the E -th Taylor coefficient of $Q\mathcal{S}$, as Q varies in the space of polynomials with degree $\leq N$. The numerator is then computed by matching as many terms as possible of the Taylor series of \mathcal{S} with those of $\mathcal{S}_{[M/N]}$, analogously to the classical Padé approach.

The resulting approximant is shown to converge exponentially, as M goes to infinity, to the exact map \mathcal{S} in the $H_{\Gamma_D}^1(D)$ norm within $B_N \setminus \Lambda$, B_N being an open disk centered at z_0 whose boundary includes the $(N + 1)$ -th element of Λ closer to z_0 .

Moreover, it is proven that the roots of the denominator $\mathcal{Q}_{[M/N]}$ converge exponentially (as M goes to infinity) to the N elements of Λ closer to z_0 .

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Multi space reduced basis preconditioners for large-scale parametrized PDEs

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In this talk we present a new two-level preconditioner for the efficient solution of large-scale linear systems arising from the finite element (FE) discretization of parametrized partial differential equations (PDEs). Our preconditioner combines multiplicatively a reduced basis (RB) coarse correction and a nonsingular fine grid preconditioner. The proposed technique hinges upon the construction of a new Multi Space Reduced Basis (MSRB) method proposed in [2], where a RB space is built through proper orthogonal decomposition at each step of the iterative method used to solve the linear system. As a matter of fact, each RB space is tailored to solve a particular iteration and aims at fixing the scales that have not been treated by previous iterations yet. The MSRB preconditioner allows to tune the error decay by properly choosing the accuracies of the RB spaces, providing a very accurate solution of the large-scale finite elements system in very few (often less than 10) iterations. As iterative solver, we employ the flexible GMRES method.

Standard RB methods strongly rely on the affine dependence of the FE matrix and right hand side, in order to gain the maximum efficiency with respect to the FE problem. If such assumption is not satisfied, an approximated affine decomposition must be recovered, e.g. with the Empirical Interpolation Method (EIM). As a matter of fact, an accurate affine representation can however represent a bottleneck and lead to huge offline and online costs. The proposed MSRB preconditioning technique is shown to overcome this limitation thanks to a milder dependence than standard RB methods on such approximated affine decomposition.

Numerical tests are carried out to evaluate the performance of the MSRB preconditioner in different large-scale modeling settings related to elliptic [2, 1], parabolic and saddle-point [4, 3] parametrized PDEs. As relevant application, we employ the aforementioned technique to deal with cardiovascular simulations, where the problem is nonaffinely parametrized with respect to physical data and the deformation of the computational domain.

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Certified POD-Based Multiobjective Optimal Control of Time-Variant Heat Phenomena

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Many optimization problems in applications can be formulated using several objective functions, which are conflicting with each other. This leads to the notion of multiobjective or multicriterial optimization problems; cf. [4].

This talk discusses the application of the reference point method in combination with model-order reduction to multiobjective optimal control problems with up to four cost functions.

As an example an optimal control problem arising in the energy efficient heating, ventilation and air-conditioning (HVAC) operation of a building with the conflicting objectives of energy consumption and comfort is suggested. Since the reference point method transforms the multiobjective optimal control problem into a series of scalar optimization problems, the method of proper orthogonal decomposition (POD) is introduced as an approach for model-order reduction. Due to the lack of a-priori analysis for the POD method, a-posteriori estimates are important to be able to ensure a good approximation quality. To this end, an a-posteriori estimate for the problem at hand (cf. [1, 2]) is introduced and used for developing new strategies for efficiently updating the POD basis in the optimization process (cf. [3]).

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REDUCED BASIS METHOD FOR PARAMETER FUNCTIONS

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The Reduced Basis (RB) method is a well-known model order reduction technique that proves extremely valuable in the multi-query and real-time context of parametrized partial differential equations (PPDE) [1, 2, 5, 6]. Here, efficiency is guaranteed by splitting the solution into an offline and an online phase. While in the, possibly time and resource consuming, offline phase a RB solution space is built up, the online phase is used to rapidly compute a solution in this RB space for each incoming parameter. Typically, the parameter space is given by a finite-dimensional subset $\mathcal{P} \subset \mathbb{R}^P$, $P \in \mathbb{N}$. However, one could also think of applications where the parameter space is infinite-dimensional. Consider for example the following problem: Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $f \in H^{-1}(\Omega)$. Find $u \in H_0^1(\Omega)$ such that

$$-\operatorname{div}(\mu \nabla u) + u = f \quad \text{in } H^{-1}(\Omega), \quad (1)$$

where the diffusion coefficient $\mu \in L_\infty(\Omega)$ is interpreted as a parameter function. While finite-dimensional parameter spaces have been extensively studied in recent decades, there has been done little work on the infinite-dimensional setting so far. First progress in this direction has been made by [3] where the initial condition of a parabolic partial differential equation is interpreted as a parameter function.

We propose an ansatz to deal with problems of the form (1) that follows [3, 4]. In particular, the idea is to capture the main features of μ in terms of a truncated wavelet decomposition up to a certain level. This approach has two advantages: Firstly, the infinite-dimensional parameter space is discretized to a finite-dimensional one spanned by the wavelets. Secondly, the locality of wavelets can be exploited to adaptively enrich the RB spaces by local updates during the online phase.

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Singular Value Decomposition on Intersection Spaces

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A well known result from linear algebra states that any matrix admits a singular value decomposition (SVD). SVD is a prominent tool in computational science for both analysis and approximation of matrices or tensors of order two. Specifically for model order reduction SVD can be used for constructing a reduced basis via the proper orthogonal decomposition or to truncate a tensor of order $d = 2$ to a tensor with a pre-specified fixed rank or a fixed error tolerance. For more general tensors of order $d > 2$ there are several versions of higher order SVD, see [1].

The singular value decomposition can be generalized to any Hilbert tensor space $H = H_1 \otimes H_2$ equipped with the canonical inner product

$$\langle x_1 \otimes y_1, x_2 \otimes y_2 \rangle_H = \langle x_1, x_2 \rangle_{H_1} \langle y_1, y_2 \rangle_{H_2}, \quad (1)$$

Then a tensor $u \in H$, which can be identified with a Hilbert Schmidt operator from H_1 to H_2 (or vice versa), admits a SVD: $u = \sum_{k=1}^{\infty} \sigma_k x_k \otimes y_k$. A truncation of this decomposition by retaining the first r terms provides an optimal rank- r approximation with respect to the canonical norm defined by (1). A prominent example is the space $H = L_2(\Omega_1 \times \Omega_2) = L_2(\Omega_1) \otimes L_2(\Omega_2)$, where $u \in H$ can be identified with the kernel of an integral operator and decomposed as above. As in the finite dimensional case, it can be extended to tensors of order $d > 2$.

We are interested in applying SVD to more general spaces, the motivating example being the Sobolev space $H^1(\Omega)$ of weakly differentiable functions over a domain $\Omega \subset \mathbb{R}^d$. Controlling the truncation error in the energy norm is particularly interesting for PDE applications. To this end, one can apply SVD to tensors in $H^1(\Omega_1) \otimes H^1(\Omega_2)$ equipped with the canonical inner product. However, the resulting space is not $H^1(\Omega_1 \times \Omega_2)$ but is instead the space $H_{\text{mix}}^1(\Omega_1 \times \Omega_2)$ of functions with mixed regularity. For large $d > 2$ this poses a restrictive regularity requirement on $u \in H^1(\Omega)$. On the other hand, the space $H^1(\Omega)$ is a Hilbert tensor space equipped with a norm $\|\cdot\|_{H^1}$ which is not stronger than the injective norm. Thus, we can not identify $H^1(\Omega)$ with a space of compact operators and apply SVD.

However, it is known that $H^1(\Omega)$ is isomorphic (here written for $d = 2$) to the intersection tensor space

$$H^1(\Omega_1 \times \Omega_2) = (H^1(\Omega_1) \otimes L_2(\Omega_2)) \cap (L_2(\Omega_1) \otimes H^1(\Omega_2))$$

with equivalent norms. Each of the spaces in the intersection is a Hilbert tensor space equipped with the canonical inner product for which SVD applies. We want to exploit this information for defining SVD of $u \in H^1(\Omega)$ and construct low-rank approximations with error control in $\|\cdot\|_{H^1}$. Thus, we investigate generalizations of SVD to such intersection spaces. We consider truncating u in both $H^1(\Omega_1) \otimes L_2(\Omega_2)$ and $L_2(\Omega_1) \otimes H^1(\Omega_2)$, as well as in generalized spaces of mixed smoothness. Under certain conditions, we can bound the truncation error in $\|\cdot\|_{H^1}$. Furthermore, we propose generalizations for $d > 2$.

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A HIERARCHICAL A-POSTERIORI ERROR ESTIMATOR FOR THE REDUCED BASIS METHOD

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In context of parametrized partial differential equations (PPDE) a well-known method for dealing with the high-dimensionality arising from a multi-query and/or real-time situation is the Reduced Basis Method (RBM), see for example [5]. A-posteriori error estimators are a crucial part in the theory of RB. They are used both for constructing the RB space X_N in the offline-phase and then verifying the reduced approximation after its computation in the online phase. In this context, an a-posteriori error estimator has at least two important requirements: (i) The error estimator has to be sharp in order to yield a reliable estimate of the error; (ii) Its evaluation has to be at least as efficient as the computation of the reduced approximation to yield online efficiency.

A fairly standard way for constructing such an error estimator is based on the residual in combination with the inverse of the inf-sup constant. A well-known method for yielding a lower bound of the inf-sup constant is the Successive Constraint Method (SCM), see for example [2, 3]. Although such a residual-based error estimator works well in many applications, we are interested in those cases, where the conditions (i) and (ii) are not fulfilled. This could be the case if the dual norm of the residual can not be computed efficiently in the online phase and/or the computational complexity of the SCM is too high in the online phase and/or the inf-sup constant is very small or even vanishes numerically.

From the theory of adaptive finite element methods hierarchical error estimators are well-known, see for example [1, 4]. In analogy to such hierarchical error estimators we want to present a hierarchical a-posteriori error estimator for the RBM which uses the difference $\|u_N(\mu) - u_M(\mu)\|$ of two RB solutions of different accuracy. We want to investigate the effectivity as well as the performance of the hierarchical error estimator, especially for those cases where the inf-sup constant is hard to compute numerically or behaves badly.

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Combining POD Model Order Reduction with Adaptivity

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A crucial challenge within snapshot-based POD model order reduction for time-dependent systems lies in the input dependency. In the 'offline phase', the POD basis is computed from snapshot data obtained by solving the high-fidelity model at several time instances. If a dynamical structure is not captured by the snapshots, this feature will be missing in the ROM solution. Thus, the quality of the POD approximation can only ever be as good as the input material. In this sense, the accuracy of the POD surrogate solution is restricted by how well the snapshots represent the underlying dynamical system.

If one restricts the snapshot sampling process to uniform and static discretizations, this may lead to very fine resolutions and thus large-scale systems which are expensive to solve or even can not be realized numerically. Therefore, offline adaptation strategies are introduced which aim to filter out the key dynamics. On the one hand, snapshot location strategies detect suitable time instances at which the snapshots shall be generated. On the other hand, adaptivity with respect to space enables us to resolve important structures within the spatial domain. Motivated from an infinite-dimensional perspective, we explain how POD in Hilbert spaces can be implemented. The advantage of this approach is that it only requires the snapshots to lie in a common Hilbert space. This results in a great flexibility concerning the actual discretization technique, such that we even can consider r-adaptive snapshots or a blend of snapshots stemming from different discretization methods. Moreover, in the context of optimal control problems adaptive strategies are crucial in order to adjust the POD model according to the current optimization iterate.

In this talk, recent results in this direction are discussed and illustrated by numerical experiments.

Parametric Model Order Reduction for Gas Flow Models

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Planning the dispatch of contracted gas denominations requires various simulations of the involved gas transport infrastructure. Furthermore, due to the growing interplay of traditional gas transport and fluctuating demands related to renewable energies, the number of necessary simulations vastly increases.

Mathematically, a system of Euler equations, which are coupled according to the underlying gas network topology, embodies an associated model [2]. A numerical simulation of such a gas flow model is itself challenging, as the model is nonlinear and hyperbolic [1]. Thus, the repeated simulation of large networks for varying supply and demand scenarios often necessitates model order reduction. Yet, beyond these variable boundary conditions, further attributes of the network may be uncertain or need to be kept variable throughout simulations, which motivates parametric model order reduction.

Since the boundary conditions together with the quantities of interest form a square input-output system, the empirical cross Gramian [3] method for parametric systems [4] is applicable. We present the construction of a global reduced order model for this parametric model and demonstrate its application on a set of benchmark networks, as well as extensions to this approach.

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Parametric model order reduction for large-scale and complex systems using Krylov subspace methods

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Numerical simulations of complex dynamical systems are an indispensable tool in studying thermodynamic phenomena. However, for complex thermal systems where ultra-high precision simulations are required, the finite element method (FEM) commonly yields large-scale models. These models demand considerable computational resources. Therefore, model order reduction techniques are employed to reduce the computational complexity by replacing the high-order dynamic model with a low-order one.

For systems with uncertain or time-varying parameters there is a persistent need of novel reduction techniques. Since creating a new reduced model for every parameter value is inefficient and computationally costly, there is a strong need for parametric model order reduction (pMOR) techniques as introduced by [1]. We distinguish among reduction techniques in which both the state dimension and parameter vector dimension are reduced, and techniques in which state dimension is reduced while the parameter vector keeps its physical relevance. In addition, we distinguish among time-varying and time-invariant parametric dependence of high-fidelity models.

In this work, we propose a method for reduced order models that preserve the physical parameters and therefore enable the optimization of the design parameters, material properties or geometries. More specifically, for an arbitrary rational transfer function $G(s, p)$ in the complex variables s and parameter p , we aim to find a low order rational $G_r(s, p)$ that matches the moments in both frequencies and design parameters at dedicated points $\mathcal{S} := \{s_1, \dots, s_k\} \subset \mathbb{C}$ and $\mathcal{P} := \{p_1, \dots, p_\ell\} \subset \mathbb{R}$. We construct the projection matrices along these two sets.

An a-priori error bound has been derived that represents the local accuracy of the reduced model's transfer function nearby the points $\mathcal{S} \times \mathcal{P}$ [3]. Furthermore, this error bound allows for finding the optimal expansion points and truncation order. Simulation results show that both time domain and frequency domain indicate that the proposed method delivers good matching and outperforms the previous work such as [2].

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Parametric space-frequency reduction for second-order system models

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In many mechanical applications, a design optimization is performed on the transfer function of the mechanical system in order to limit the vibrational, sound, ... transmission. In general, this transfer function $\mathbf{H}(\mathbf{p}, \omega)$ is obtained as:

$$\mathbf{H}(\mathbf{p}, \omega) = (-\mathbf{M}(\mathbf{p}, \omega)\omega^2 + i\mathbf{C}(\mathbf{p}, \omega)\omega + \mathbf{K}(\mathbf{p}, \omega))^{-1} = \mathbf{D}(\mathbf{p}, \omega)^{-1}, \quad (1)$$

where \mathbf{M} , \mathbf{C} and \mathbf{K} are parameter and frequency dependent mass, damping and stiffness matrices, respectively, and a dynamic impedance \mathbf{D} . During manual and automatic design studies, the evaluation of this transfer function leads to high computational loads due to a large number n of degrees-of-freedom in the underlying finite element models for these problems and the large number n_ω of frequency lines to evaluate.

In this work, we are exploring a novel model reduction technique for parametric analysis of these systems of equations. The approach revolves around two main aspects:

- A first aspect is the definition of a local reduced order basis (LROB) in the frequency range. In classical approaches, a computed reduced order basis (ROB) which accounts for the parameter variations is exploited over the full frequency range. However, for systems with high modal densities, this often leads to a limited reduction ratio. In this work, we propose to exploit a number of training responses at each frequency line to set up an ROB which is only employed at that specific frequency line \mathbf{V}_ω . As each basis only has to hold at a specific frequency, this basis can be drastically smaller compared to the general case.
- A second aspect is a hyper-reduction through sampling in the frequency range. In order to reduce the total number of frequency line evaluations, a greedy sampling algorithm is deployed in order to determine a limited set of dominant frequency lines for the considered parametric variations. A corresponding interpolation matrix \mathbf{P} is then defined to reconstruct the full frequency range from the obtained samples.

This approach leads to an approximation over the frequency range from ω_1 to ω_{n_f} as:

$$\begin{bmatrix} \mathbf{D}(\mathbf{p}, \omega_1)^{-1} \\ \vdots \\ \mathbf{D}(\mathbf{p}, \omega_{n_f})^{-1} \end{bmatrix} \approx \sum_{k=1}^{n_s} \mathbf{P}_k (\mathbf{V}_{\omega_k}^T \mathbf{D}(\mathbf{p}, \omega_k) \mathbf{V}_{\omega_k})^{-1}, \quad (2)$$

for n_s frequency samples and where \mathbf{P}_k corresponds to the interpolation matrix for the sample k .

In order to limit the setup cost of the reduced order model, the LROB setup and hyper-reduction steps are reversed in the practical implementation, such that the LROBs only need to be computed for the retained frequency lines. The non-intrusive property of the proposed hyper-reduction scheme is an important benefit, since it allows the usage of existing finite-element software for which interfaces are typically available to extract system matrices for different frequencies.

The proposed approach is validated on an academic parameterized mass-spring damper system and on a parameterized vibro-acoustic model.

Parametric state-time reduction for the transient analysis of multi-physical systems

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In a model based design process, a system-level design optimization on a low-dimensional model is typically performed at an early stage to compare different topologies and obtain good initial design parameters. This system-level parametric, time-continuous system-level model

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}; \mathbf{p}), \quad (1)$$

with state $\mathbf{x} \in \mathbb{R}^{n_s}$, input $\mathbf{u} \in \mathbb{R}^{n_u}$ and parameter set $\mathbf{p} \in \mathbb{R}^{n_p}$ is typically a lumped parameter model. The dimension of the state vector n_s of a lumped parameter model is considerably smaller compared to the dimension of distributed parameter models (typically $n_s < 50$). However, the time discretization of the low-dimensional system can lead to a high temporal dimension n_t due to: (i) high-frequency behavior in the system which influences the stability of the numerical integration or (ii) simulations over a large time interval. Hence, transient simulations of low-dimensional models in many-query applications can be computationally expensive, yet the low order n_s of the model does not lend itself to typical model order reduction.

The proposed state-time reduction method addresses this type of problems by reducing the time-discretized algebraic system

$$\mathbf{D}\chi = \mathbf{s}(\chi, \mathbf{x}_0, \mathbf{p}), \quad (2)$$

with the state-time unknown $\chi = \{\mathbf{x}^T[1], \dots, \mathbf{x}^T[n_t]\}^T \in \mathbb{R}^{(n_s \cdot n_t)}$, the initial condition $\mathbf{x}_0 \in \mathbb{R}^{n_s}$ and the state difference $\mathbf{D} \in \mathbb{R}^{n_s \cdot n_t \times n_s \cdot n_t}$ and system specific $\mathbf{s} \in \mathbb{R}^{n_s \cdot n_t}$ contribution of the time discretization. The state-time reduction encompasses:

- The computation of a reduced order basis (ROB) $\mathbf{V} \in \mathbb{R}^{n_s \cdot n_t \times n_{st}}$, which spans a manifold containing an approximation $\mathbf{V}\mathbf{q}$ of the solution χ . The ROB consists of the left singular vectors of the singular value decomposition (SVD) on training data.
- A Galerkin projection of the time-discretized algebraic system (2) with the ROB.
- Hyper-reduction of the non-linear term $\mathbf{V}^T \mathbf{s}(\mathbf{V}\mathbf{q}, \mathbf{x}_0, \mathbf{p})$ with the Discrete Empirical Interpolation Method (DEIM).

The state-time reduction method leads to a low-dimensional, non-linear reduced order model (ROM)

$$\mathbf{r}(\mathbf{q}, \mathbf{p}) = \epsilon, \quad (3)$$

which is solved by

$$\mathbf{q} = \underset{\mathbf{q} \in \mathbb{R}^{n_{st}}}{\operatorname{argmin}} \|\mathbf{r}(\mathbf{q}, \mathbf{p})\|_2^2. \quad (4)$$

The developed reduction is relatively non-intrusive such that existing modeling software can be utilized to evaluate the system equations (1) at certain time instances. Moreover, the single timestep integration at the selected time instances allows for a fully parallelized evaluation of the the different timesteps.

The developed state-time reduction method is validated on a non-linear, mechatronic drivetrain model containing an induction motor and a cardanic shaft.

3.3 Thursday, April 12

Laura Iapichino, Eindhoven University of Technology (TU/e) (09 :15-09 :40)	71
<i>Greedy Controllability of Reduced-Order Linear Dynamical Systems</i>	
Igor Pontes Duff, Max Planck Institute for Dynamics of Complex Technical Systems (09 :40-10 :05)	72
<i>Balanced truncation model reduction for polynomial control systems</i>	
Felix Schindler, University of Münster (10 :05-10 :30)	73
<i>True error control for localized model reduction with online enrichment in PDE constrained optimization</i>	
Markus Bachmayr, University of Bonn (11 :00-11 :45)	74
<i>Reduced Bases and Low-Rank Methods</i>	
Reinhold Schneider, Technische Universität Berlin (11 :45-12 :10)	75
<i>Variational Monte Carlo for the Hierarchical Tensor Representation</i>	
Asma Toumi, Ecole Polytechnique (12 :10-12 :35)	76
<i>Tensor Empirical Interpolation Method for multivariate functions</i>	
Kevin Carlberg, Sandia National Laboratories [Livermore] (14 :00-14 :25)	77
<i>Space-time least-squares Petrov-Galerkin projection for nonlinear model reduction</i>	
Giovanni Stabile, International School for Advanced Studies (14 :25-14 :50)	78
<i>Stabilised finite volume POD-Galerkin ROMs of the incompressible Navier-Stokes equations</i>	
Cédric Herzet, Institut National de Recherche en Informatique et en Automatique (14 :50-15 :15)	79
<i>Beyond Petrov-Galerkin projection by using “multi-space” priors</i>	
Julia Brunken, Applied Mathematics, University of Münster (15 :15-15 :40)	80
<i>Model reduction based on optimally stable variational formulations of parametrized transport equations</i>	
Silke Glas, Ulm University (15 :40-15 :45)	81
<i>Model Reduction for Hamilton-Jacobi-Bellman Equations resulting from Intraday Trading of Electricity</i>	
Patrick Héas, Institut National de Recherche en Informatique et en Automatique (15 :40-15 :45)	82
<i>Optimal Kernel-Based Dynamic Mode Decomposition</i>	
Sebastian Ullmann, Graduate School of Computational Engineering, Technische Universität Darmstadt, Department of Mathematics, Technische Universität Darmstadt (15 :40-15 :45)	83
<i>Stochastic Galerkin reduced basis methods for parametrized elliptic PDEs with random data</i>	
Ion Gosea, Data-Driven System Reduction and Identification Group, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg (15 :45-15 :50)	84
<i>Data-driven model reduction of descriptor linear systems in the Loewner framework</i>	
Olena Burkovska, Department of Scientific Computing, Florida State University (15 :45-15 :50)	85
<i>Model order reduction for parametrized nonlocal variational inequalities</i>	
Dominik Garmatter, Goethe-University Frankfurt am Main (15 :45-15 :50)	86
<i>Reduced basis methods for MREIT</i>	
Denise Degen, Computational Geosciences and Reservoir Engineering [RWTH Aachen University], Aachen Institute for Advanced Study in Computational Engineering Science [RWTH Aachen University] (15 :50-15 :55)	87
<i>A Geoscientific Application of the Certified Reduced Basis Method</i>	

Y. Yue, Max Planck Institute for Dynamics of Complex Technical Systems (15 :50-15 :55)	88
<i>On the Interpolation of Reduced Order Models</i>	
Maria Cruz Varona, Chair of Automatic Control, Technical University of Munich (15 :50-15 :55)	89
<i>Some Aspects of Systems Theory and Model Order Reduction for Nonlinear Systems</i>	
Fabrizio Di Donfrancesco, ONERA - The French Aerospace Lab, Institut d'Alembert - UPMC (15 :55-16 :00)	90
<i>A CFD supported Reduced Order Model using a goal-oriented domain restriction</i>	
Steffen W. R. Werner, Max Planck Institute for Dynamics of Complex Technical Systems (15 :55-16 :00)	91
<i>Computing the Hankel-Norm Approximation of Large-Scale Descriptor Systems</i>	
Sébastien Riffaud, Inria Bordeaux - Sud-Ouest, Institut de Mathématiques de Bordeaux (15 :55-16 :00)	92
<i>Reduced-order model approximating the BGK model based on Proper Orthogonal Decomposition</i>	
Stefano Grivet-Talocia, Politecnico di Torino (16 :30-16 :35)	93
<i>Data-driven parameterized modeling of LTI systems with guaranteed stability</i>	
Christopher Bach, BMW Group Research and Innovation Centre, Technische Universität München (16 :30-16 :35)	94
<i>Reduced-order model assisted optimization of automotive structures with nonlinearities</i>	
Nicolas Montes, University CEU Cardenal Herrera - Lucia Hilario, University CEU Cardenal Herrera (16 :35-16 :40)	95
<i>PGD Variational vademecum for robot motion planning. A dynamic obstacle case</i>	
Benjamin Fröhlich, Institute of Engineering and Computational Mechanics (16 :35-16 :40)	96
<i>Shape Finding in Structural Optimization with Parametrically Reduced Finite-Element Models</i>	
Fahad Alsayyari, Delft University of Technology (16 :40-16 :45)	97
<i>A Reduced Order Modeling Approach for Reactor Physics Problems Using Locally Adaptive Sparse Grids</i>	
Sara Grundel, Max Planck Institute for Dynamics of Complex Technical Systems (16 :40-16 :45)	98
<i>Clustering Model Order Reduction for Water Networks</i>	
Mikel Balmaseda, ONERA, The French Aerospace Lab, Université de Lyon, CNRS INSA-Lyon, LaMCoS UMR5259 (16 :40-16 :45)	99
<i>Geometrically nonlinear autonomous reduced order model for rotating structures</i>	
Harshit Bansal, Department of Mathematics and Computer Science, Eindhoven University of Technology (16 :45-16 :50)	100
<i>Model Order Reduction for convection dominated problems</i>	
Zoran Tomljanovic, Department of Mathematics University of Osijek (16 :45-16 :50)	101
<i>Sampling-free parametric model reduction of systems with structured parameter variation</i>	
Babak Maboudi Afkham, Computational Mathematics and Simulation Science (16 :45-16 :50)	102
<i>Symplectic Model Reduction with respect to Energy Inner Product</i>	
Sridhar Chellappa, Max Planck Institute for Dynamics of Complex Technical Systems (16 :50-16 :55) .	103
<i>Adaptive POD-DEIM model reduction based on an improved error estimator</i>	
Lyes Nechak, Laboratoire de Tribologie et Dynamique des Systèmes (16 :50-16 :55)	104
<i>On the reducibility of linear dynamic systems with hybrid uncertainties</i>	

Romain Hild, IRMA (16 :50-16 :55)	105
<i>Towards real time computation of 3D magnetic field in parametrized Polyhelix magnets using a reduced basis Biot-Savart model</i>	
Felipe Galarce, Inria de Paris, Laboratoire Jacques-Louis Lions (16 :55-17 :00)	106
<i>Enhancing Hemodynamics Measurements with Mathematical Modeling</i>	
Cleophas Kweyu, Max Planck Institute for Dynamics of Complex Technical Systems (16 :55-17 :00) ...	107
<i>Fast Solution of the Nonlinear Poisson-Boltzmann Equation using the Reduced Basis Method and Range-Separated Tensor Format</i>	
Dennis Grunert, Institute of Engineering and Computational Mechanics, University of Stuttgart (16 :55-17 :00)	108
<i>Faster A-posteriori Error Estimation for Second Order Mechanical Systems</i>	

Greedy Controllability of Reduced-Order Linear Dynamical Systems

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Often a dynamical system is characterized by one or more parameters describing physical features of the problem or geometrical configurations of the computational domain. As a consequence, by assuming that the system is controllable, a range of optimal controls exists corresponding to different parameter values. The goal of the proposed approach is to avoid the computation of a control function for any instance of the parameters. The greedy controllability [2] consists in the selection of the most representative values of the parameter set that allows a rapid approximation of the control function for any desired new parameter value, ensuring that the system is steered to the target within a certain accuracy. By proposing the reduced basis method [1] in this framework, we are able to consider linear parametrized partial differential equations (PDEs) in our setting. The computational costs are drastically reduced and the efficiency of the greedy controllability approach is significantly improved. As a numerical example a heat equation with convection is studied to illustrate our proposed RB greedy controllability strategy.

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Balanced truncation model reduction for polynomial control systems

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Balanced truncation is one of the most common model order reduction techniques. This method mainly relies on reachability and observability energy functionals. For linear systems, these functionals are encoded by the reachability and observability Gramians. Later, the concept of balanced truncation and energy functionals was proposed for nonlinear systems in [5]. Therein, it was shown that energy functionals for nonlinear systems are the solutions of state-dependent nonlinear Hamilton-Jacobi equations. Thus, they are not only difficult to compute for large-scale systems but also hard to utilize in the model reduction framework. To overcome this, algebraic Gramians were proposed for a class of nonlinear systems, namely bilinear [1] and quadratic-bilinear systems [3], and their connections to energy functionals were also studied [2, 3]. As a result, these algebraic Gramians allow us to compute reduced-order systems.

In this talk, we propose an extension of balanced truncation for model reduction of continuous time polynomial control systems, whose dynamics are governed by

$$\begin{aligned}\dot{x}(t) &= Ax(t) + \sum_{j=2}^{n_p} H_j x_j^{\otimes}(t) + \sum_{j=1}^{n_p} \sum_{k=1}^m N_j^k x_j^{\otimes}(t) u_k(t) + Bu(t), \\ y(t) &= Cx(t), \quad x(0) = 0,\end{aligned}$$

where n_p is the degree of the polynomial part of the system, $x(t) \in \mathbb{R}^n$, $x_j^{\otimes}(t) = \underbrace{x(t) \otimes \cdots \otimes x(t)}_{j\text{-times}}$,

$A \in \mathbb{R}^{n \times n}$, $H_j, N_j^k \in \mathbb{R}^{n \times n^j}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{p \times n}$. This class of systems has a variety of applications in science and engineering, *e.g.*, neuronal dynamics [4]. By following [3], we propose algebraic Gramians for polynomial systems based on the underlying Volterra series of those systems and their Hilbert adjoint. We then show their relations with a certain type of generalized polynomial Lyapunov equations. Furthermore, we present how these algebraic Gramians and energy functionals relate to each other. This allows us to find those states that are hard to control and hard to observe via an appropriate transformation based on the proposed Gramians. Truncating such states yields reduced-order systems. The efficiency of the reduced systems obtained by the proposed method is demonstrated by means of various semi-discretized nonlinear partial differential equations and compared with the most commonly used model reduction techniques, proper orthogonal decomposition.

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True error control for localized model reduction with online enrichment in PDE constrained optimization

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The computational demand of PDE constrained optimal control or inverse problems easily exceeds existing resources, if standard approximation methods are employed for the underlying forward problem. Model order reduction (MOR) methods for parameterized partial differential equation (pPDEs), such as the Reduced Basis (RB) method, allow to quickly explore the solution space by a decomposition of the computation into an expensive offline and a cheap online part. If employed as a surrogate approximation for the forward problem, MOR methods have the potential to significantly speed up outer-loop algorithms, or even allow to study hitherto off-limits large scale problems. However, standard global (in a spatial as well as parametric sense) MOR methods that construct a single reduced space for the whole parameter range of the underlying pPDE may still induce a tremendous offline computational burden for multi-scale or large scale problems.

A possible remedy is to consider localized methods, both in parameter- as well as physical space. In the context of the latter, localized RB methods combine ideas from domain decomposition and RB methods to obtain a (parameter) global surrogate model spanned by spatially localized reduced spaces. As a particular example, the localized RB multi-scale method equipped with error control w.r.t. the true solution allows to adaptively enrich these local reduced spaces [2]. In the context of optimization or inverse problems, such adaptive localized MOR methods have the potential to evolve the reduced model during the outer-loop algorithm (see also [3, 1]).

In this contribution, we demonstrate recent advances of localized RB methods in the context of PDE constrained optimization and inverse problems. In particular, we will present localized true error estimates for the optimization problem, including a posteriori error estimates for the objective functional and the optimal parameters or parameter functions, and numerical experiments to demonstrate the potential of our approach.

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Reduced Bases and Low-Rank Methods

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In this talk, we consider the connections and differences between reduced basis methods and SVD-based low-rank approximations for solutions of parameter-dependent elliptic PDEs, and we discuss some recent findings concerning the respective approximability properties of solutions that determine the potential performance of these methods.

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Variational Monte Carlo for the Hierarchical Tensor Representation

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In Variational Monte Carlo we aim at optimizing a function from a hypothesis space with respect to an objective functional. But instead of using the, possibly unknown, exact objective functional we rely on a sample based *empirical objective functional*. This idea is closely related to the risk minimization in statistical learning. For the optimization we only require the gradients at the sample points to be computable. For this empirical optimization problem, we can show *convergence in probability*, i.e. that error estimates hold with high probability, given a sufficient amount of samples. The analysis is carried out in the framework introduced Cucker and Smale [1].

For the hypothesis space we use tensors in the Hierarchical Tucker format, introduced by Professor Dr. Wolfgang Hackbusch et al [2] and its special case the Tensor Train (TT) format [3]. Both formats have proven to be very efficient for approximating very high dimensional problems. For example these multi-linear parametrization can be applied to solve high-dimensional PDE in a variational framework, restricted to tensor low rank classes. However for non-linear or more complex problems this direct approach becomes very difficult due to required tensor product approximations of the operators. The proposed variational Monte Carlo approach on the other hand can be carried out relatively easy for parametric problems in uncertainty quantification and can be formally extended to approximate the meta-stable eigenfunctions of the corresponding Backward Kolmogorov operator by numerical approximation of the transfer operator (also known as Koopman operator) and vice versa the Fokker Planck operator.

This is joint work with F. Nüske and F. Noé from FU Berlin.

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Tensor Empirical Interpolation Method for multivariate functions

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Several problems of practical interest in physical, chemical, biological or mathematical applications naturally lead to multivariate approximation problems. Such problems are often composed of multiple simpler systems and models. Therefore, in order to better understand the behavior and properties of multi-dimensional models, tensor-based modeling is a natural choice in these cases. We thus derive a Tensor Empirical Interpolation Method (TEIM) for multivariate functions (the case of bivariate functions have already been treated in [1]). This method relies on the classical Empirical Interpolation Method (EIM) where the greedy procedure is used to compute the interpolation points and the basis functions "direction-by-direction". The algorithm returns interpolation functions that directly fulfill the Lagrange property. The TEIM provides an approximate representation of a given function f in separate form. As any tensor decomposition procedure, the TEIM leads to a computational complexity for highly multivariate functions. We then propose two strategies to reduce the complexity due to the use of the TEIM. The first one is the mixed EIM-SVD tensor decomposition. It consists in applying the Singular Value Decomposition (SVD) with low-rank truncation to the separate form of f resulting from the TEIM decomposition. As a second strategy, we develop an interpolation method by sparse collocation point set. This method is also based on EIM greedy procedure and it returns basis functions that satisfy the Lagrange property. Error estimates of the developed TEIM, the truncated SVD decomposition and the sparse collocation interpolation are derived. To validate the performance of the proposed algorithms, several numerical experiments are proposed. We apply the algorithms first to a regular bivariate function then to a non regular bivariate function and finally to a multivariate regular function (5D function). Numerical experiments confirm that each of the three methods has a very good behavior in terms of stability and accuracy.

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Space–time least-squares Petrov–Galerkin projection for nonlinear model reduction

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Reduced-order models (ROMs) of nonlinear dynamical systems are typically characterized by *low spatial dimensionality* but *high temporal dimensionality*: the spatial dimensionality (i.e., number of degrees of freedom) is reduced via projection, but the temporal dimensionality (i.e., number of time instances) remains unchanged from the high-fidelity model. This limits the realizable computational savings of such ROMs, especially for problems requiring long-time integration. Several attempts have been made to address this temporal-complexity bottleneck. At the two previous MoRePaS meetings, we presented a ‘forecasting’ approach that employs time-domain data to produce online forecasts of the ROM solution via gappy POD. We proposed to use these forecasts (1) as initial guesses for the Newton solver at each time instance [2], or (2) as a coarse propagator for time-parallel methods [1]. While both approaches reduce the computational cost incurred by time integration, neither directly reduces the temporal dimension of the ROM. Alternatively, space–time reduced-basis methods have been proposed [4, 5]. While these pioneering approaches reduce the temporal dimension and are equipped with error bounds that grow only linearly in time, they exhibit several drawbacks. For example, they require a space–time variational interpretation of the high-fidelity model, they provide no mechanism for hyper-reduction, and they compute only one space–time basis vector per training simulation. To this end, we present a space–time least-squares Petrov–Galerkin (ST-LSPG) method [3] that (1) reduces both the spatial and temporal dimensions of the dynamical system; (2) is equipped with error bounds that grow sub-quadratically in time; (3) is applicable to general nonlinear dynamical-system models; (4) is equipped with hyper-reduction; and (5) can extract multiple space–time basis vectors from each training simulation via tensor decomposition.

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Stabilised finite volume POD-Galerkin ROMs of the incompressible Navier-Stokes equations.

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It is crucial in the development of Reduced Order Methods (ROMs) to preserve the stability properties of the original system. It is well known that Reduced Order Methods Techniques for the incompressible Stokes and Navier-Stokes equations, obtained with Galerkin projection methods, are prone to several instability issues. In this talk the attention will be devoted to the treatment of inf-sup pressure instabilities due to spurious pressure modes when the equivalent inf-sup condition for the reduced system is not fulfilled. In particular we will focus the attention on ROMs generated starting from full order finite volume approximations [1, 3, 2]. Although this discretisation technique is particularly widespread for industrial applications, with respect to the finite element method, it has received less attention in the reduced order modelling community. We will present and compare two different stabilisation approaches based on a supremizer stabilisation technique and on a pressure Poisson equation approach. Moreover, some relevant challenges concerning the use of the finite volume method, in view of more advanced applications of ROMs in several industrial contexts, are presented and discussed. The efficiency of the proposed method is verified with benchmark classic test cases.

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Beyond Petrov-Galerkin projection by using “multi-space” priors

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Let \mathcal{H} be some Hilbert space with induced norm $\|\cdot\|$. We consider the problem of approximating the solutions of a parametric partial differential equation (PPDE), say $\mathcal{M} = \{\mathbf{h} : \text{PDE}(\mathbf{h}, \theta) = 0 \text{ for some } \theta \in \Theta\}$, within a N -dimensional subspace $V_N \subset \mathcal{H}$. We consider a PPDE whose weak formulation takes the following form:

$$\text{find } \mathbf{h} \in \mathcal{H} \text{ such that } a_\theta(\mathbf{h}, \mathbf{h}') = b_\theta(\mathbf{h}') \quad \text{for } \mathbf{h}' \in \mathcal{H},$$

where $a_\theta(\cdot, \cdot)$ and $b_\theta(\cdot)$ are respectively some bilinear and linear forms.

The orthogonal projection (with respect to $\|\cdot\|$) of the elements of \mathcal{M} onto V_N being usually too computationally-demanding, one standard option is to resort to Galerkin projection:

$$\text{find } \mathbf{h} \in V_N \text{ such that } a_\theta(\mathbf{h}, \mathbf{h}') = b_\theta(\mathbf{h}') \quad \text{for } \mathbf{h}' \in V_N.$$

The “quality” of the Galerkin approximation (its closeness to the true orthogonal projection) depends on the “conditioning” of the operator $a_\theta(\cdot, \cdot)$ and $b_\theta(\cdot)$ (e.g., via their coercivity and continuity constants [2]). In some difficult case, Galerkin projection may thus leads to poor approximation results. In our work, we propose a simple way to improve Galerkin projections.

We consider the setup where V_N corresponds to the N -dimensional subspace computed via a reduced-basis method [2]. Now, while computing the subspace V_N , this type of methodology also generates a sequence of subspaces $\{V_i\}_{i=0}^N$ and some positive scalars $\{\epsilon_i\}_{i=0}^N$ such that

$$V_0 \subset V_1 \subset \dots \subset V_N,$$

and

$$\sup_{\mathbf{h} \in \mathcal{M}} \text{dist}(\mathbf{h}, V_i) \leq \epsilon_i.$$

The last inequality provides some information about \mathcal{M} since it implies that the latter is included in the intersection of N (degenerate) ellipsoids, i.e., $\mathcal{M} \subseteq \bigcap_{i=0}^N \{\mathbf{h} : \sup_{\mathbf{h} \in \mathcal{M}} \text{dist}(\mathbf{h}, V_i) \leq \epsilon_i\}$.

In our work, we propose a new suboptimal projection method exploiting the fact that \mathcal{M} is included in the intersection of a set of *known* ellipsoids. The proposed methodology boils down to the standard Galerkin projection when one single ellipsoid is considered. We provide both theoretical and empirical results showing that the proposed methodology clearly outperforms the standard Galerkin projection in some situations. Our derivations are based on the recent work by Binev *et al.* [1]

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Model reduction based on optimally stable variational formulations of parametrized transport equations

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Motivated by high-dimensional kinetic transport equations we consider in this talk stable variational formulations and model reduction techniques for possibly time-dependent transport equations.

Kinetic equations describe densities in phase space consisting of independent space, time, and velocity variables. To tackle the high-dimensionality we employ the Reduced Basis-Hierarchical Model Reduction approach where we use a problem-adapted basis in the velocity variable to arrive at a hyperbolic system in the space-time domain [1].

In this context, stable discretizations and efficient error estimators are desirable both for the construction of the reduced basis and the validation of reduced solutions.

To derive such stable variational formulations for general transport equations we use, similar to [2], an ultraweak approach to find an L_2 approximation of the solution. We introduce new pairs of optimally stable trial and test spaces: By first choosing a suitable test space and then defining the trial space by the application of the adjoint operator, we obtain optimally stable spaces with an inf-sup constant of one in the continuous as well as in the discrete case.

The setting allows for an easy implementation of the solution procedure and is especially beneficial in the context of model reduction for parametrized transport equations: We apply the Reduced Basis method to parametrized equations within this framework. In contrast to previous works, due to the optimally inf-sup-stable setting we do not need any further stabilization for the reduced spaces. Hence, also the reduced models can be constructed easily and efficiently.

We exemplify the approach by presenting numerical results for full order and reduced order models for the first order transport equation in space or space and time and compare our new framework to existing works [2, 3].

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Model Reduction for Hamilton-Jacobi-Bellman Equations resulting from Intraday Trading of Electricity

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Due to the growth of renewable energy, the future perspective of energy markets is seen in short-term trading markets. In this talk, we consider the intraday trading of electricity and derive a Hamilton-Jacobi-Bellman (HJB) equation for this setting, extending the work of [1]. A recent change in regularity constraints even allows that the participants of the intraday market can trade every 15 minutes instead of every hour.

Our aim is to find an optimal trading strategy within 15 minutes/an hour using the most recent information of the market. As solving the HJB equation is a nonlinear and nonsmooth problem, fine discretizations, that are needed, can resolve in long computation times. Therefore, we use the reduced basis method (RBM) [2, 3] to derive a reduced model.

The RBM is a well-known technique to efficiently reduce the numerical efforts for many parametrized problems. We introduce the parametric formulation of our HJB equation, in which the parameter is the incoming data of the market and analyze the reducability of this problem. We comment on the (to our knowledge) only existing approach for this problem by [4] and provide numerical investigations for our method.

This is joint work with N. von Luckner and R. Kiesel, Chair for Energy Trading and Finance, University Duisburg-Essen.

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Optimal Kernel-Based Dynamic Mode Decomposition

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This work is concerned with the approximation of high-dimensional dynamical systems of the form:

$$\begin{cases} x_t(\theta) = f_t(x_{t-1}(\theta)), & t = 1, \dots, T, \\ x_1(\theta) = \theta, \end{cases} \quad (1)$$

where $x_t \in \mathbb{R}^p$ is the state variable, $f_t : \mathbb{R}^p \rightarrow \mathbb{R}^p$, and $\theta \in \mathbb{R}^p$ denotes an initial condition. We consider a data-driven approach relying on representative trajectories $\{x_t(\theta_i)\}_{t=1}^T$, $i = 1, \dots, N$, obtained by running (1) for N different initial conditions $\{\theta_i\}_{i=1}^N$ in a given set Θ . Assume the knowledge of a vector-valued function $\Psi \in (\mathcal{L}^2(\mathbb{R}^p))^n$ with $p \leq n$, admitting the inverse Ψ^{-1} , such that its image is an invariant vector space of the Koopman operator. Then, it can be shown that a finite approximation of the Koopman operator of rank $k \leq p$ leads to approximating $x_t(\theta)$ in (1) by

$$\tilde{x}_t(\theta) = \Psi^{-1}\left(\sum_{i=1}^k \lambda_i^{t-1} \xi_i^\top \Psi(\theta) \zeta_i\right), \quad (2)$$

where $\xi_i \in \mathbb{C}^n$ and $\zeta_i \in \mathbb{C}^n$ are the left and right eigen-vectors associated to the eigen-value $\lambda_i \in \mathbb{C}$ of an (assumed diagonalisable) matrix

$$A_k^* \in \arg \min_{A: \text{rank}(A) \leq k} \sum_{t=2, i=1}^{T, N} \|\Psi(x_t(\theta_i)) - A\Psi(x_{t-1}(\theta_i))\|_2^2. \quad (3)$$

Kernel-based dynamic mode decomposition (k-DMD) is a state-of-the-art algorithm estimating the ξ_i 's, ζ_i 's and λ_i 's in reduced-model (2) from the representative trajectories and then computing $\tilde{x}_t(\theta)$ [3]. It presents an advantageous complexity scaling linearly in p and independent of n , which is crucial in the case $p \ll n$. However, k-DMD relies on crude approximations and on restrictive assumptions, making this algorithm generally sub-optimal.

The purpose of this work is to propose an upgraded version of the k-DMD algorithm, able to compute reduced model (2) exactly for any $\theta \in \Theta$, with a similar complexity. The proposed algorithm relies on an optimal solution of (3) given in [1] and on kernel-based computation. Details on this work can be found in [2].

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Stochastic Galerkin Reduced Basis Methods for Parametrized Elliptic PDEs with Random Data

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We study reduced basis methods derived from stochastic Galerkin finite element discretizations of parametrized elliptic boundary value problems with random data. The approach is based on a Galerkin projection of a spatial-stochastic weak solution onto a subspace spanned by spatial-stochastic reduced basis functions, which is similar to the concept of space-time reduced basis methods [3]. The idea of stochastic Galerkin reduced basis methods was posed in [4, section 8.2.1] and formulated for linear dynamical systems in [2].

Stochastic Galerkin reduced basis methods are online-efficient in the sense that the cost of estimating the expected value of some output functional does not depend on the number of stochastic Galerkin finite element degrees of freedom. Moreover, the statistical estimation requires only a single solution of the reduced basis model for any given deterministic parameter value. In contrast, conventional sampling-based reduced basis methods require multiple evaluations of a reduced basis model to estimate output statistics [1].

The reduced basis theory equips stochastic Galerkin reduced basis methods with computable a posteriori error bounds regarding the expectation of parameter-dependent linear outputs. It is assumed that the underlying stochastic Galerkin finite element discretization is sufficiently accurate. This is similar to conventional sampling-based reduced basis methods, which require that the underlying finite element discretizations are sufficiently accurate and that sufficiently many stochastic samples are used in the online phase.

We illustrate the efficiency and accuracy of our approach with numerical tests for a reaction-diffusion problem, where the reaction coefficient acts as a deterministic parameter and a Karhunen-Loève decomposed random diffusion field acts as random data. The results show that a parameter-dependent statistical estimation with a stochastic Galerkin reduced basis method can be much more efficient compared to a Monte Carlo reduced basis method, because the former does not suffer from the overhead imposed by computing random samples of the reduced basis solution in the online phase.

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Data-driven model reduction of descriptor linear systems in the Loewner framework

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We study linear descriptor systems described by DAE's (differential algebraic equations) characterized by $\Sigma : \{\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) \text{ where } \mathbf{E}, \mathbf{A} \in \mathbb{C}^{n \times n}, \mathbf{B} \in \mathbb{C}^{n \times m}, \mathbf{C} \in \mathbb{C}^{p \times n}, \mathbf{x} \in \mathbb{C}^n, \mathbf{u} \in \mathbb{C}^m \text{ and } \mathbf{y} \in \mathbb{C}^p\}$. The transfer function $\mathbf{H}(s) = \mathbf{C}(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{B}$ includes a strictly proper part, i.e. $\tilde{\mathbf{H}}(s)$ and also a polynomial part, i.e. $\mathbf{H}(s) = \tilde{\mathbf{H}}(s) + \sum_{\ell=0}^{\eta-1} c_\ell s^\ell$. Here, the dimension of Σ is $n \in \mathbb{N}$ while the index of Σ is denoted with $\eta \in \mathbb{N}$.

The Loewner framework, first introduced in [3], is an effective data-driven model reduction method, that constructs reduced order models for which the transfer function matches that of the original system at selected interpolation points in the frequency domain. Directly applying this method to systems with polynomial transfer function will yield a large approximation error in the high frequency band. This is due to the mismatch between the polynomial part of the original system's transfer function and of the reduced system's transfer function.

To remedy this mismatch, we propose the following procedure; start by constructing a raw Loewner model Σ_L of dimension $N > n$ based on sampled data composed of sample points and values $\{(s, \mathbf{H}(s)) | s = j\omega_k, k = \overline{1, 2N}\}$. We decompose the system Σ_L into a strictly proper and a polynomial part, by means of the ADTF algorithms in [2]. The estimated polynomial coefficients are denoted with \tilde{c}_ℓ , for $\ell = \overline{1, \eta}$.

Next, construct a Loewner model $\tilde{\Sigma}_L$ of dimension N based on the original data from which we subtract the polynomial part, i.e. $\{(s, \mathbf{H}(s) - \sum_{\ell=0}^{\eta-1} \tilde{c}_\ell s^\ell) | s = j\omega_k, k = \overline{1, 2N}\}$. Reduce the model $\tilde{\Sigma}_L$ (by projection) to a much smaller model $\tilde{\Sigma}_L^r$ of dimension $r \ll N$. This latter system will have a strictly proper transfer function. Finally, reattach the polynomial part given by $\{\tilde{c}_\ell | \ell = \overline{1, \eta}\}$ to $\tilde{\Sigma}_L^r$ and obtain the final Loewner model denoted with $\hat{\Sigma}_L$. This system will capture the behavior of the original system Σ both for low and high frequency ranges. The proposed procedure is tested for several index 2 or 3 problems from the literature, i.e.

1. The constrained damped mass-spring system (of index 3) from [4];
2. The semidiscrete Oseen equations (of index 2) from [1];
3. The first MNA system (of index 3) from the SLICOT benchmark examples in <http://slicot.org/20-site/126-benchmark-examples-for-model-reduction>.

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Model order reduction for parametrized nonlocal variational inequalities

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We consider a parametrized obstacle problem driven by a nonlocal diffusion operator, which, in a special case, reduces to a fractional Laplace operator. By means of the nonlocal vector calculus [1] and a Lagrange multiplier approach we cast the problem in a variational saddle point form. A regularity study for the nonlocal problem is conducted and a higher regularity of the Lagrange multiplier is proven.

The lack of sparsity of the corresponding discrete problem increases the computational cost of solving it. To reduce the computational complexity we apply the reduced basis method (RBM) to the nonlocal model. To certify the method and provide a reliable estimate of the approximation error, a posteriori estimators for the solution and Lagrange multiplier are derived. Here we can generalize existing results from the local setting [2]. Numerical results are provided to illustrate the theoretical findings.

Furthermore, an extension of the reduced basis method to variational inequalities parametrized by random input data is also presented. Here, we incorporate the reduced basis approach to speed-up the computational procedure and compare it with some existing stochastic approximation methods.

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Reduced basis methods for MREIT

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The numerical solution of parameter identification problems in a partial differential equation (PDE) setting from (noisy) measurements usually requires numerous amounts of forward solutions of the respective PDE. One way to speed up the solution process therefore is to reduce the computational time of the forward solution, e.g. via the reduced basis method.

The reduced basis method is a model order reduction technique which constructs a low-dimensional subspace of the solution space. Galerkin projection onto that space allows for an approximative solution. An efficient offline/online decomposition enables the rapid computation of the approximative solution for many different parameters.

This talk will focus on the problem of magnet resonance electrical impedance tomography (MREIT), where the main objective is the acceleration of the well-known Harmonic B_z Algorithm [2] using the adaptive reduced basis framework developed in [1] that is able to handle very high-dimensional parameter spaces. The general idea of the framework is to adaptively construct a small, problem-oriented reduced basis space instead of constructing a global reduced basis space like it is usually the case in reduced basis methods. This will be done in an iterative procedure: the Harmonic B_z Algorithm is projected onto the current reduced basis space and iterated until certain termination criteria are reached. The resulting parameter then is utilized to enrich the reduced basis space and therefore fit it to the given problem. This process is repeated until an iterate is accepted as the solution of the inverse problem. Numerical results will demonstrate the usefulness of the approach.

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A Geoscientific Application of the Certified Reduced Basis Method

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The field of Geosciences aims at obtaining an accurate understanding of the spatial distribution of the earth's subsurface properties and of the involved physical processes to provide meaningful predictions concerning a sustainable use of the subsurface as a valuable resource. Most of the geoscientific applications face the challenge of how to address high-dimensional problems. The high-dimensional character is caused by a complex coupling of different physics as, for instance, heat transport, chemical transport and mechanical interactions and by the highly heterogeneous character of the earth's subsurface. Additionally, we face the problem of limited access resulting in data associated with high uncertainties. To overcome or address this problem it is obviously necessary to perform uncertainty quantifications, which is often prohibitively expensive using the standard finite element method. Therefore, we are presenting the reduced basis (RB) method, being a model order reduction (MOR) technique, that constructs low-order approximations to, for instance, the finite element (FE) space. We use the RB method to address this computationally challenging simulations because this method significantly reduces the degrees of freedom. The RB method is based on a decomposable implementation of an offline and online stage. This allows performing all the expensive pre-computations beforehand to get real-time results during the online stage, which can be, for instance, directly used during field measurements. Generally, the RB approach is most beneficial in the many-query and real-time context [3],[2]. We will illustrate the advantages of the RB method for the field of Geosciences through a Darcy flow problem, which emphasizes the benefits of parabolic partial differential equations. We will provide a quality evaluation of the approximations and we will compare the runtimes for both the FE and the RB simulations. Furthermore, we are going to highlight the advantages of this method for repetitive simulations by showing the speed-up for the RB solution in contrast to the FE solution. Also, we will demonstrate how the method can be used in repetitive forward simulations as, for instances, parameter studies, by taking advantage of the in our example coupled MOOSE [4] and Dakota framework [1].

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On the Interpolation of Reduced Order Models

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During the last decades, Model Order Reduction (MOR) has attracted much research attention and many different techniques have been proposed. When we conduct parametric studies such as optimization and uncertainty quantification, it is desired to preserve the parameters in the reduced-order model (ROM). Therefore, many Parametric MOR (PMOR) methods have been developed. In this talk, we consider an alternative approach, which uses pre-computed nonparametric ROMs at sampled parameters p_1, \dots, p_k to build a ROM at a parameter value of interest, say p_* . The motivation of this study is twofold. First, in the most general case, the original large-scale Full-Order Model (FOM) may be unknown and the ROMs corresponding to samples of parameters can be built by different types of MOR methods. An example is the Loewner Framework [2], which is a data-driven method that constructs a ROM completely from the samples and does not assume the availability of the FOM. Second, the popular projection-based PMOR methods can suffer from a possibly large dimension of the ROM, especially when the dimension of the parameter space is large.

Several research efforts have been directed towards the interpolation of nonparametric ROMs. In [3], the authors pointed out that interpolating ROMs directly performs poorly in general, and proposed a method that “reprojects” all ROMs onto a common subspace. However, this method applies only to projection-based MOR methods and requires that the bases used to build all ROMs have been stored, which is often not the case. In [1], a method that builds a ROM at p_* by interpolating the pre-computed ROMs (at sampled parameters p_1, \dots, p_k) on a manifold is proposed. In our numerical experiments, the method works when the order of the ROM is low. However, we often fail to increase the accuracy of the ROM by using a higher order because the ROM can diverge.

In this talk, we will show that the accuracy of ROM interpolation depends heavily on the realization of the systems. As an extreme example, interpolating two ROMs built by the Loewner Framework is equivalent to interpolating frequency response functions, which leads to fixed poles. Therefore, instead of a moving peak, this interpolation may result in wax and wane of two peaks, the positions of which depend on the choice of the interpolation points, which makes no physical sense. The method proposed first converts all ROMs, which may be built by different algorithms and of different properties, into a modified “modal” realization. Interpolating the modified modal realization is equivalent to interpolating the positions and amplitudes of all poles, respectively, and therefore, has a clear physical meaning and gives accurate parametric ROMs. Another merit of the proposed method is that the order of the parametric ROM does not increase with the dimension of the parameter space. It can be used as a post-processing method for any MOR method to build ROMs that can be readily interpolated.

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Some Aspects of Systems Theory and Model Order Reduction for Nonlinear Systems

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In recent years, model order reduction for nonlinear dynamic systems has gained a lot of attention due to the existence of many applications (e.g. aerospace, automotive, biomechanical, circuit simulation, etc.), where large-scale systems of *nonlinear* differential(-algebraic) equations arise. The most general nonlinear model reduction approach is given by the simulation-based Proper Orthogonal Decomposition (POD), along with a subsequent hyperreduction with e.g. the Discrete Empirical Interpolation Method (DEIM). For special, rather weakly nonlinear system classes – such as bilinear and quadratic bilinear systems – model reduction techniques have been developed in the past years [1, 5, 2, 4, 3]. The drive for the extension and generalization of many well-known linear system-theoretic concepts (e.g. transfer functions, Gramians, \mathcal{H}_2 -norm) and reduction methods (e.g. balanced truncation, Krylov subspaces) to these special system classes has been the prominent Volterra theory [7], which allows to represent a nonlinear system by an infinite series of coupled subsystems and multivariate kernels.

In this talk, new insights and perspectives concerning the system theory (i.e. Volterra representation, impulse response, eigenfunctions) and model order reduction (specially through Krylov subspaces/Moment Matching) for nonlinear systems will be presented and discussed. Initial attempts regarding bilinear systems [6] as well as current developments and findings towards system-theoretic and simulation-free nonlinear model reduction approaches by Moment Matching will be exposed.

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A CFD supported Reduced Order Model using a goal-oriented domain restriction

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Reduced-order models (ROMs) of nonlinear dynamical systems are essential for enabling high-fidelity non linear CFD design optimization or aeroelastic investigation. In fluid mechanics, the wide variety of ROMs reported in literature shares the aim of reducing the dimensionality of dynamical systems by performing a projection of the governing equations. Unfortunately, the performance of available ROMs are still unsatisfactory in terms of real-life applications. For instance, parameter changes imply projection basis interpolation or several rebuilds of the ROM that could result in a lack of robustness or efficiency.

Moreover, in aeroelastic investigations, a wide range of parameters has to be taken into account resulting in a time performance issue. Nevertheless, for such practical fluid mechanics investigations the results of interest are limited to the aerodynamics loads, therefore it would be sufficient to compute only the aerodynamic field close to the wall.

To this end, the approach used in the present work relies to the classical Galerkin projection onto a basis constructed via the proper orthogonal decomposition (POD). The discrete empirical interpolation method (DEIM) is adopted in order to deal with the compressible Navier-Stokes non-linearities [3]. In particular, we propose to perform the POD and the on-line time integration on a restricted spatial domain which contains the wall boundary points used to compute the aerodynamics loads. In line with the concept of Sampled Mesh introduced by Carlberg et al.[2], such a sub-mesh plays a crucial role in the interface between the reduced and the full order model. In this work, we deal with the ROM sensitivity to the sub-mesh dimension and to the boundary conditions implementation.

Numerical tests have been carried out to evaluate the performance of the model. First, we validate the classical POD-DEIM technique for a time dependent flow around a cylinder. Then, we apply the sub-mesh technique to two time dependent problems (i.e. slightly compressible flow around a NACA-0012 airfoil with high incidence and a complete 3D realistic wing configuration). Numerical results show that the proposed technique enables additional computational savings without penalizing the accuracy. Finally, on the basis of the achieved result, we outline how to extend the proposed technique to a parametric and an aeroelastic problem [1].

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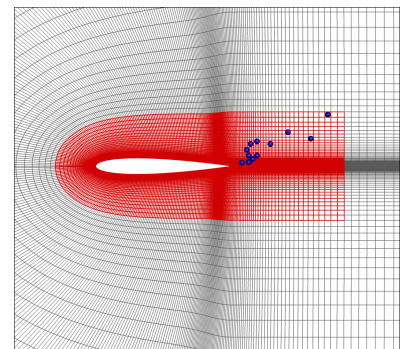


Figure 1: An example of sub-mesh in red, and the related DEIM points in blue.

Computing the Hankel-Norm Approximation of Large-Scale Descriptor Systems

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The modeling of many applications, like mechanical systems and fluid dynamics, results in linear time-invariant continuous-time descriptor systems

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{1}$$

with $E, A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$ and $D \in \mathbb{R}^{p \times m}$. Additionally, the descriptor matrix E is assumed to be singular. The aim of model reduction is to approximate the original system (1) by a surrogate model of order $r \ll n$. For a system (1) with transfer function G , the Hankel semi-norm is defined as

$$\|G\|_H = \sup_{u_- \in \mathcal{L}_2} \frac{\|y_+\|_{\mathcal{L}_2}}{\|u_-\|_{\mathcal{L}_2}}, \tag{2}$$

where u_- are the past inputs and y_+ the future outputs of the system.

The Hankel-norm approximation method is a model reduction approach that minimizes the approximation error in the Hankel semi-norm (2). Based on the work of Adamjan, Arov, and Krein, a model reduction method finding a reduced model with minimal error measured in the Hankel semi-norm for the standard system case $E = I_n$ was developed by Glover in [2]. One approach for the generalization of the Hankel-norm approximation to the case of descriptor systems (1) can be found in [1]. Therein, the Weierstrass canonical form of the matrix pencil $\lambda E - A$ is computed explicitly and transformation formulas, based on this, are given. This method is problematic due to the numerically unstable and costly computation of the Weierstrass canonical form. This comes already into account for small systems and makes the approach unapplicable for the large-scale sparse system case.

Using the generalized balanced truncation method [3], a much more efficient and numerically stable method can be formulated. Using different techniques, the new approach can also be applied to the case of large-scale sparse systems; see [4]. We will demonstrate this using some examples of large-scale descriptor systems from the literature.

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Reduced-order model approximating the BGK model based on Proper Orthogonal Decomposition

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We present a reduced-order model approximating the BGK model in order to decrease the computational cost of the simulations. The BGK model describes the dynamic of a rarefied gaz flow, and the density distribution function f of the gaz follows :

$$\frac{\partial f}{\partial t}(\mathbf{x}, \xi, t) + \xi \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \xi, t) = \frac{M_f(\mathbf{x}, \xi, t) - f(\mathbf{x}, \xi, t)}{\tau} \quad (1)$$

In the reduced-order model, the density distribution function is approximated in velocity space by a small number of basis functions $\Phi_n(\xi)$ which reduce significantly the degrees of freedom :

$$\tilde{f}(\mathbf{x}, \xi, t) = \sum_{n=1}^N a_n(\mathbf{x}, t) \Phi_n(\xi) \quad (2)$$

This basis functions $\Phi_n(\xi)$ are computed by Proper Orthogonal Decomposition and the reduced-order model is obtained by Galerkin projection. The resulting system of partial differential equations is hyperbolic by construction and an appropriate projection of the Maxwellian distribution function M_f ensures the positivity of the approximate distribution function \tilde{f} . The system of PDE is then solved by an IMEX Runge-Kutta in time and a finite-volume scheme in space. The different test cases show that we can reduce significantly the computational cost and have an accurate approximate solution. Moreover, optimal transport is used to predict distribution function in velocity space and leads to even better approximation.

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Data-driven parameterized modeling of LTI systems with guaranteed stability

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We consider the problem of extracting a parameterized reduced-order model from a set of measurements of some underlying LTI system with (unknown) transfer function $\check{H}(s; \vartheta) \in \mathbb{C}^{P \times P}$, where s is the Laplace variable and $\vartheta \in \Theta \subset \mathbb{R}^\rho$ is a vector of external parameters. The model is constructed using a data-driven approach starting from frequency response samples $\check{H}_{k,m} = \check{H}(j\omega_k; \vartheta_m)$ at discrete frequency $s_k = j\omega_k$ and parameter values ϑ_m for $k = 1, \dots, \bar{k}$ and $m = 1, \dots, \bar{m}$.

We adopt a Generalized Sanathanan-Koerner (GSK) framework [3] by representing the model as

$$H(s; \vartheta) = \frac{N(s, \vartheta)}{D(s, \vartheta)} = \frac{\sum_{n=0}^{\bar{n}} \sum_{\ell=1}^{\bar{\ell}} R_{n,\ell} \xi_\ell(\vartheta) \varphi_n(s)}{\sum_{n=0}^{\bar{n}} \sum_{\ell=1}^{\bar{\ell}} r_{n,\ell} \xi_\ell(\vartheta) \varphi_n(s)}, \quad (1)$$

where $R_{n,\ell} \in \mathbb{R}^{P \times P}$ and $r_{n,\ell} \in \mathbb{R}$ are the model coefficients, and where $\varphi_n(s)$, $\xi_\ell(\vartheta)$ are suitable basis functions. In particular, we use partial fractions $\varphi_n(s) = (s - q_n)^{-1}$ associated to a set of predetermined stable poles q_n (as in the well-known Vector Fitting scheme [2]) and tensor products of Chebychev polynomials $\xi_\ell(\vartheta)$ for frequency and parameter dependence, respectively. Model coefficients are computed through a Sanathanan-Koerner iteration [3] by setting $D^0(j\omega, \vartheta) = 1$ and solving

$$\min_{k,m} \sum |D^{\mu-1}(j\omega_k, \vartheta_m)|^{-1} \|N^\mu(j\omega_k, \vartheta_m) - D^\mu(j\omega_k, \vartheta_m) \check{H}_{k,m}\|_F^2 \quad \text{for } \mu = 1, 2, \dots \quad (2)$$

Our main result is a sufficient condition and an associated algorithm for enforcing uniform stability of the model $H(s; \vartheta)$ throughout the parameter domain $\vartheta \in \Theta$. This condition requires constraining the model denominator $D(s, \vartheta)$ to be a Positive Real (PR) function (see [1] for the sketch of a proof).

Based on the model structure (1), the PR-ness of $D(s, \vartheta)$ is guaranteed when $\Re\{D(j\omega, \vartheta)\} \geq 0, \forall \vartheta \in \Theta$ and $\forall \omega \in \mathbb{R}$. This is achieved by an adaptive sampling process in the parameter space Θ . At GSK iteration μ and for any given ϑ_* , the imaginary eigenvalues of the Hamiltonian matrix associated to a state-space realization of $D^{\mu-1}$ are used to determine the frequency bands where $\Re\{D^{\mu-1}(j\omega, \vartheta_*)\} < 0$, and a first-order perturbation analysis of the non-imaginary Hamiltonian eigenvalues is used to determine which directions need to be searched in the parameter space to find local minima of $\Re\{D^{\mu-1}\}$. The result is an automatically determined set of discrete points (ω_i, ϑ_i) where the constraint $\Re\{D^\mu(j\omega_i, \vartheta_i)\} > 0$ is formulated and embedded in the GSK iteration (2). When the residual of (2) stabilizes, the model poles $p_n(\vartheta)$ (i.e., the zeros of $D(s, \vartheta)$) result uniformly stable $\forall \vartheta \in \Theta$.

Several examples from Electronic Design Automation applications are provided, demonstrating the robustness and the efficiency of proposed approach. For a preview of these examples, see [1].

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Reduced-order model assisted optimization of automotive structures with nonlinearities

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Numerical optimization methods are a popular means of improving concepts and designs, and are widely used across many disciplines. Nonetheless, the optimization of complex and detailed finite element (FE) models, as typically encountered in the automotive industry, can easily become cumbersome due to the large number of degrees of freedom of the FE discretization, and the large number of design parameters involved [4].

Nonlinear model order reduction methods aim to reduce the computation times associated with each simulation, and thus each evaluation of the objective function. We discuss particularities and challenges of reduced-order model (ROM) assisted optimization for the design optimization of car body structures, more specifically with respect to crashworthiness, noise and vibration requirements. We then make use of a nonlinear model order reduction procedure based on the Proper Orthogonal Decomposition (POD) snapshot method [6]. It is equipped with a hyper-reduction technique based on the Discrete Empirical Interpolation Method (DEIM) [1, 3], as well as the Gauss-Newton with Approximated Tensors (GNAT) [2], and the Energy-Conserving Sampling and Weighting (ECSW) methods [5]. The method is then applied to an example problem. We discuss the occurring nonlinearities and analyse the accuracy and resulting speed-ups of the ROM-based optimisation compared to the high-dimensional model. Results indicate that significant simulation speed-ups can be achieved and that reduced-order modelling can be used to reduce the computation times of optimization studies for car body structures, although the application to larger and more complex models still needs to be investigated in future studies.

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PGD Variational vademecum for robot motion planning. A dynamic obstacle case

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A fundamental robotics task is to plan collision-free motions for complex bodies from a start to a goal position among a set of static and dynamic obstacles. This problem is well known in the literature as motion planning (or the piano mover's problem). The complexity of the problem has motivated many works in the field of robot path planning. One of the most popular algorithms is the Artificial Potential Field technique (APF), [4]. This method defines an artificial potential field in the configuration space (C-space) that produces a robot path from a start to a goal position. This technique is very fast for RT applications. However, the robot could be trapped in a deadlock (local minima of the potential function). The solution of this problem lies in the use of harmonic functions in the generation of the potential field, which satisfy the Laplace equation, [2]. Unfortunately, this technique requires a numerical simulation in a discrete mesh, making useless for RT applications. In our previous work, [3], [1], was presented for the first time, the Proper Generalized Decomposition method to solve the motion planning problem. In that work, the PGD was designed just for static obstacles and computed as a vademecum for all Start and goal combinations. This work demonstrates that the PGD could be a solution for the motion planning problem. However, in a realistic scenario, it is necessary to take into account more parameters like for instance, dynamic obstacles. The goal of the present paper is to introduce a diffusion term into the Laplace equation in order to take into account dynamic obstacles as an extra parameter. Both cases, isotropic and non-isotropic cases are taken into account in order to generalize the solution.

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Shape Finding in Structural Optimization with Parametrically Reduced Finite-Element Models

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The demand for energy efficient technical products leads to an increased usage of lightweight components. One way to realize lightweight components is to apply structural optimization and to optimize the shape of the components for a particular load case, e.g. to minimize a displacement due to external forces. Shape optimizations in structural mechanics are usually done numerically based on the Finite-Element method in an iterative optimization procedure where the design parameters of the optimization problem describe the shape of the component. As a first step of this procedure the geometry of the component is discretized according to the current design parameters. The equations of motion

$$\mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{D}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) = \mathbf{f}(t), \quad \mathbf{x}(t) \in \mathbb{R}^N \quad (1)$$

are then derived for the current discretized geometry. The cost function is evaluated and passed to the optimization algorithm to derive new design parameters. This procedure is then repeated until the optimization problem converges. However, this procedure shows some drawbacks. First, as complex shaped components require fine discretizations, the number of degrees of freedom N can easily exceed hundreds of thousands. Second, the equations of motion are only derived for a fixed discretization and therefore for a fixed shape of the component. A parametric formulation of the equations of motion for a variable shape does not exist. This means that the equations of motion have to be derived in every iteration of the optimization procedure again including the Finite-Element method preprocessing. Furthermore, it means that Parametric Model Order Reduction (PMOR), see [2], cannot be applied directly as there is no parametric formulation of the equations of motion. It is indeed possible to use Model Order Reduction for linear time-invariant systems. However, this is also not satisfying since it still requires to apply the Finite-Element method and to perform the reduction in every iteration of the optimization. This contribution introduces an approach where the components are modeled with a variable discretization. This variable discretization allows to derive a parametric formulation of the equations of motion for a variable shape. The parametric system matrices are derived in an affine representation such that for example the parametric stiffness matrix becomes

$$\mathbf{K}(\mathbf{p}) = \mathbf{K}_0 + \sum_{i=1}^k w_i(\mathbf{p})\mathbf{K}_i, \quad \mathbf{K}(\mathbf{p}) \in \mathbb{R}^{N \times N}. \quad (2)$$

The representation according to Eq. (2) allows then an efficient application of PMOR. Here, interpolatory methods from [1] are applied since they allow to match the parametric transfer function of the reduced parametric system and its gradient to the transfer function of the original parametric system which is advantageous in an optimization. The proposed combination of a variable discretization and PMOR enables a significant speedup compared to conventional approaches. The approach is not limited to academic examples, but will be presented for an industrial structural optimization problem.

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A Reduced Order Modeling Approach for Reactor Physics Problems Using Locally Adaptive Sparse Grids

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While high-fidelity complex models are often used to model nuclear reactors, these models are extremely expensive for parametric study applications. To reduce the computational burden of such large-scale nonlinear systems, a Reduced Order Model (ROM) using Proper Orthogonal Decomposition (POD) can be built. However, projection-based POD methods are code intrusive, which is a major limitation when access to the governing equations is unattainable. Moreover, problems parametrized on high dimensional spaces are prone to the curse of dimensionality. Nevertheless, POD can be applied in a non-intrusive manner by building surrogate models for the POD coefficients. Smolyak's sparse grids can alleviate the curse of dimensionality. We propose the use of locally adaptive sparse grids to refine the POD sampling space only around regions of high interest. This iterative algorithm exploits the hierarchical nature of sparse grids to only add points from the next sparse grid level that are neighbours to points identified with errors above a certain threshold. We introduce an L_2 norm error based measure to guide the adaptive algorithm. The quality of exploring the parameter space is increased by adding not only neighbouring points from the next level (children) but also all neighbouring points from the previous level (parents). The algorithm has been tested on several analytical functions to determine its robustness and performance. Subsequently, the algorithm was used to build a ROM model for a reactor physics problem test. This problem was a finite difference, 1D, two-group, neutron diffusion problem parametrized by two input variables, corresponding to the positions of two control rods in the reactor. The considered output was the neutron thermal flux at 780 mesh points. The built ROM was highly effective in reducing the online runtime while providing acceptable accuracy. Moreover, the developed algorithm reduced the number of model evaluations in the offline phase by a factor of 25 compared to classical sparse grids sampling. Figure 1 shows the L_2 norm error as result of testing the ROM on 961 points that were not part of the sampling space. The POD sampled points generated by the developed algorithm are also marked on the figure.

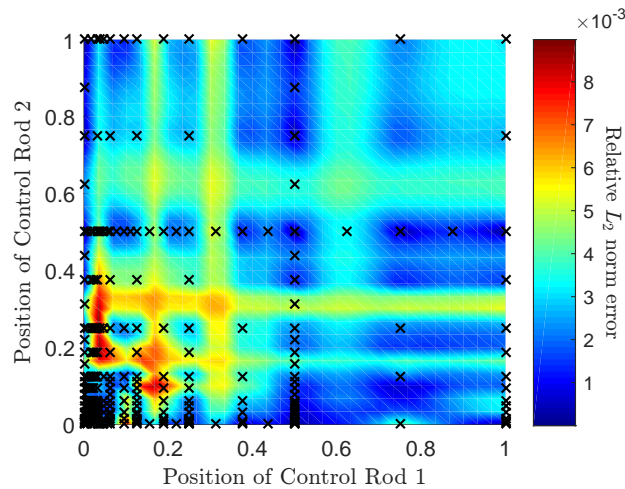


Figure 1: Map of the L_2 norm error resulted from testing the ROM of the reactor physics problem on 961 points. The black crosses mark the sampled points generated by the developed algorithm.

Clustering Model Order Reduction for Water Networks

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In the minimum cost operative planning of pressurized water supply networks the underlying model is a Differential Algebraic Equation [1]. The structure of that equation depends on the topology of the distribution network. If the network gets complicated a clustering is done manually. We use clustering based model order reduction techniques as in [2] to create such clusters automatically. The methods presented there are extended to create an edge projection matrix R as well as the node projection matrix P which is defined as

$$P_{ki} = \begin{cases} \alpha_{ki}, & \pi(k) = i \text{ (node } k \text{ is in cluster } i), \\ 0, & \pi(k) \neq i \text{ (node } k \text{ is not in cluster } i), \end{cases} \quad (1)$$

for a given clustering π . In the standard version of the model order reduction clustering algorithm all the α_{ki} are 1. In order to create a consistent reduced network the projection matrix R has to come from an edge clustering and

$$R^T EP = \hat{E},$$

where E and \hat{E} are the incidence matrix of the original and the reduced graph.

We will show how to compute such matrices and what properties they have. We furthermore compare the manual clusters with the automatically generated ones.

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Geometrically nonlinear autonomous reduced order model for rotating structures

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Rotating structures are widely used in industrial applications such as turbo-machinery, helicopter blades and wind turbines. The design tendency to create more slender, more flexible and lighter structural components under greater excitations increases the nonlinear behaviour of these components. Thus, the need to accurately predict the dynamic response of geometrically nonlinear structures becomes essential for the designer. Many researchers have studied the geometrically nonlinear reduced order models for non rotating structures, geometrically nonlinear formulations of beam type finite elements, the dynamic behaviour of rotating geometrically nonlinear beams and the classical geometrically nonlinear finite element (FE) formulation that considers a nonlinear static equilibrium state induced by the effect of rotation.

In the present work, as an extension to [3], an autonomous geometrically nonlinear reduced order model for the study of dynamic solutions of complex rotating structures is developed. In opposition to the classical FE formulation for geometrically nonlinear rotating structures that considers small linear vibrations around the static equilibrium, nonlinear vibrations around the pre-stressed equilibrium are now considered. For that purpose, the linear normal modes are used as a reduced basis for the construction of the reduced order model. The stiffness evaluation procedure method (STEP) [5] is applied to compute the nonlinear forces induced by the displacements around the static equilibrium. This approach enhances the classical linearised small perturbations hypothesis to the cases of large displacements around the static pre-stressed equilibrium. Furthermore, a comparison between the steady solution given by HHT- α [2] and the Harmonic Balance Method (HBM) [4] is carried out. The STEP method has been integrated in frequency domain in order to increase the time performances of the nonlinear HBM and avoid the time consuming Alternating Time-Frequency (AFT) technique [1] for the computation of the nonlinear forces.

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Model Order Reduction for convection dominated problems

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Model Order Reduction (MOR) of systems of non-linear (parameterized) Hyperbolic Partial Differential Equations (PDEs) is still an uncharted territory in the scientific community. Moving discontinuities are representative features of this class of problems and pose a major hindrance to obtain effective reduced-order model representations, since typically bases with high spatial frequency are needed to accurately capture these moving discontinuities. We will discuss a MOR framework to efficiently capture the travelling dynamics of such systems. The motivation of this work is to enable the usage of multi-phase hydraulic models, such as the Drift Flux Model (DFM) [2], in developing drilling automation strategies for real-time down-hole pressure management.

The DFM is a system of multiscale non-linear PDEs, whose convective subset is conditionally hyperbolic. Convection dominated problems, such as the DFM, admit solutions, which possess a diagonal structure in space-time diagram and high solution variability. As a first step, we apply standard MOR approaches [4] to obtain a reduced-order representation of the DFM for a representative multi-phase shock tube test case. We capture the dynamics in an essentially non-oscillatory manner but we obtain a small dimensionality reduction. Since the dimension of the reduced model is still too large, we develop new techniques for deriving more efficient alternative reduced-order models for this class of problems.

We invoke the idea of the method of freezing [1] and combine it with non-linear reduced basis approximations [3] to develop an efficient reduced-order model representation, which we demonstrate for several benchmark problems. These benchmark problems embody the challenges faced in the reduced-order representation of the DFM. However, the existing MOR framework [3] lacks consideration of boundary conditions and multiple fronts. The main novelty of this work is to mathematically incorporate boundary conditions into the formalism of the method of freezing and then investigate their impact on the MOR framework. We also demonstrate the necessity of establishing multiple co-moving frames. Finally, we present numerical experiments and discuss the efficacy of above mentioned approach in terms of computational speed up and computational accuracy compared with standard numerical techniques.

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Sampling-free parametric model reduction of systems with structured parameter variation

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We consider a parametric linear time invariant dynamical systems represented in state-space form as

$$E\dot{x}(t) = A(p)x(t) + Bu(t), \quad (1)$$

$$y(t) = Cx(t), \quad (2)$$

where $E, A(p) \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{l \times n}$. Here $x(t) \in \mathbb{R}^n$ denotes the state variable, while $u(t) \in \mathbb{R}^m$ and $y(t) \in \mathbb{R}^l$ represent, respectively, the inputs and outputs of the system.

We assume that $A(p)$ depends on $k \ll n$ parameters $p = (p_1, p_2, \dots, p_k)$ such that we may write

$$A(p) = A_0 + U \operatorname{diag}(p_1, p_2, \dots, p_k) V^T,$$

where $U, V \in \mathbb{R}^{n \times k}$ are given fixed matrices.

We propose an approach for approximating the full-order transfer function $H(s; p) = C(sE - A(p))^{-1}B$ with a reduced-order model that retains the structure of parametric dependence and (typically) offers uniformly high fidelity across the full parameter range. Remarkably, the proposed reduction process removes the need for parameter sampling and thus does not depend on identifying particular parameter values of interest. Our approach is based on the classic Sherman-Morrison-Woodbury formula and allows us to construct a parameterized reduced order model from transfer functions of four subsystems that do not depend on parameters, allowing one to apply well-established model reduction techniques for non-parametric systems. The overall process is well suited for computationally efficient parameter optimization and the study of important system properties.

One of the main applications of our approach is for damping optimization: we consider a vibrational system described by

$$\begin{aligned} M\ddot{q}(t) + (C_{int} + C_{ext})\dot{q}(t) + Kq(t) &= Ew(t), \\ z(t) &= Hq(t), \end{aligned} \quad (3)$$

where the mass matrix, M , and stiffness matrix, K , are real, symmetric positive-definite matrices of order n . Here, $q(t)$ is a vector of displacements and rotations, while $w(t)$ and $z(t)$ represent, respectively, the inputs (typically viewed as potentially disruptive) and outputs of the system. Damping in the structure is modeled as viscous damping determined by $C_{int} + C_{ext}$ where C_{int} and C_{ext} represent contributions from internal and external damping, respectively. Information regarding damper geometry and positioning as well as the corresponding damping viscosities are encoded in $C_{ext} = U \operatorname{diag}(p_1, p_2, \dots, p_k) U^T$ where $U \in \mathbb{R}^{n \times k}$ determines the placement and geometry of the external dampers.

The main problem is to determine the best damping matrix that is able to minimize influence of the disturbances, w , on the output of the system z . We use a minimization criteria based on the \mathcal{H}_2 system norm. In realistic settings, damping optimization is a very demanding problem. We find that the parametric model reduction approach described here offers a new tool with significant advantages for the efficient optimization of damping in such problems.

Symplectic Model Reduction with respect to Energy Inner Product

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Over the past decade, reduced basis methods have emerged as a powerful tool to reduce the computational complexity of large-scale and parametric systems of partial differential equations. However, in problems with strong advective terms, conventional model reduction methods do not generally preserve the stability of the original system. Conservation laws, symmetries, and intrinsic structures are often destroyed over the course of model reduction which result in a qualitatively wrong, and ultimately in an unstable solution.

Recently, a considerable attention has been paid to preserving physical and geometric structures, in order to recover stability in the reduced system. In the context of Lagrangian and Hamiltonian systems, recent developments suggest constructing a reduced-order configuration space with approximated conservation laws [2, 3, 1]. This results in a physically meaningful reduced system and can help recover stability in the reduced system. However, these methods are only suited for a standard inner product on a Euclidean space and are not compatible with a more general inner product.

Weak formulations and inner-products defined on a Hilbert space are at the core of the error analysis of many numerical methods for solving partial differential equations. Therefore, it is natural to seek for model reduction methods that consider such features. Many works have been conducted to make conventional model reduction techniques compatible with various norms defined on a Hilbert space [4]. However, a model reduction method that simultaneously preserves the symplectic symmetry of Hamiltonian systems is still unknown.

We have developed a model reduction technique that minimizes the projection error with respect to some energy norm (weighted norm) while preserving the symplectic symmetry of the original system. This is obtained by projecting the full order Hamiltonian system onto a generalized symplectic subspace. The choice of the symplectic subspace and the energy projection operator depends on the choice of the energy norm. This allows the reduced system to be constructed with respect to the norms, most appropriate to the problem. A natural extension of the greedy basis generation proposed in [2] is developed for constructing a generalized symplectic reduced basis.

Numerical experiments show that the new method preserves the Hamiltonian over time. Also while conventional model reduction methods with respect to energy norm do not yield a stable reduced system, the new method preserves stability over long time-integration.

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Adaptive POD-DEIM model reduction based on an improved error estimator

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We consider adaptive model order reduction using the Proper Orthogonal Decomposition (*POD*) method combined with Discrete Empirical Interpolation method (*DEIM*) for general nonlinear problems of the form

$$\begin{aligned}\dot{x}(t) &= A x(t) + g(x(t)) + B u(t), \\ y(t) &= C x(t),\end{aligned}$$

where, $x(t) \in \mathbb{R}^N$ is the state vector; A, B, C are system matrices obtained after spatial discretization; the function $g(\cdot)$ represents the nonlinear term. $y(t)$ and $u(t)$ are the output and input, respectively.

In [2], an adaptive scheme was proposed to increase the number of *POD-DEIM* basis vectors, if the initial number of basis vectors is too small to produce an accurate reduced-order model (ROM). In this work, we have extended the adaptive scheme to a two-way process, i.e., it can also adaptively decrease the number of basis vectors, so as to obtain a ROM as small as possible for a given error tolerance. Also, a simple heuristic strategy is proposed to avoid oscillation which may arise during the adaptive process. Using the proposed scheme, the *POD-DEIM* basis can be adaptively adjusted in order to derive a ROM with both sufficient accuracy and minimal reduced order. Furthermore, possible instability of the ROM produced by the standard *POD-DEIM* can also be avoided with the adaptive algorithm. In fact, the efficiency of the adaptive process highly depends on efficient error estimation of the ROM. We propose a modified error estimator based on the *primal-dual* error estimation in [2]. Here, instead of reducing the dual system using the projection matrix for the primal system as done in [2], we use a Krylov-subspace method (GMRES) to estimate the solution to the dual system. Moreover, the modified reduced output, $\bar{y} = C u - (\hat{u})_{du}^T r_{pr}$ is introduced to get the proposed error estimator

$$\left\| y^{n+1} - \bar{y}^{n+1} \right\| \leq \left(S \|(A^n)^{-T}\| \|r_{du}^{n+1}\| + \|\hat{u}_{du}^{n+1}\| |1 - S| \right) \|r_{pr}^{n+1}\|,$$

where the superscript n refers to the n -th time step; S is an empirically determined constant; r_{pr}, r_{du} are the primal and dual system residuals, respectively, while \hat{u}_{du} is the estimated dual state vector, obtained via GMRES. Unlike for linear systems [1], the second part of the error estimator involving (\hat{u}_{du}^{n+1}) can not be completely removed. The error estimator has been tested for the benchmark examples of a viscous Burger's equation and a fluidized bed crystallizer (FBC) model. It is seen that it offers a tighter bound in comparison to the error estimator in [2]. The future work would be extending the adaptive process to parametric systems.

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On the reducibility of linear dynamic systems with hybrid uncertainties

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This study focuses on the analysis of the ability of uncertain linear time-invariant (LTI) systems to be reduced. In deterministic LTI systems, the reducibility can be decided by the analysis of Hankel singular values [1]. These invariant quantities defined from the controllability and observability gramians that are solutions of linear Lyapunov equations for controllability and observability, measure how state variables are simultaneously controllable and observable. From energy view point, Hankel singular values quantify the controllability and observability energies involved in the input/output transfer of a system. Hence, it can be stated that the system is reducible if it possesses state variables with small Hankel singular values which indicate the weak controllability and observability of the state variables [1]. Although the determining of Hankel singular values and thus the reducibility analysis in the deterministic case are relatively well mastered, they remain challenging issues in LTI uncertain systems [2, 5]. This study is interested by the analysis of the reducibility of LTI systems with two kinds of uncertain parameters namely random parameters defined by their probability density functions and interval parameters. In this perspective, an hybrid approach is proposed to approximate parameter-dependent Hankel singular values. It consists in a meta-model constructed from the mixing of the Wiener-Haar and Chebychev polynomial expansions. The first one was proposed to deal with propagation and quantification of random uncertainties [3] and have shown interesting efficiency in numerous applications [4] while the second has shown a suitable accuracy in propagating and quantifying interval uncertainties [6]. As a result, the proposed approach is shown to be suitable for the analysis of the controllability and observability degrees and thus for the reducibility analysis of LTI systems with hybrid parameter uncertainty. Moreover, the proposed approach has shown an interesting potential to be an alternative to the prohibitive scanning/Monte Carlo method conventionally used.

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Towards real time computation of 3D magnetic field in parametrized Polyhelix magnets using a reduced basis Biot-Savart model

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We present in this talk our work on model reduction for the computation of 3D magnetic field, as part of the Hifimagnet project. The model involves a thermoelectric problem which has already been reduced, and we want to benefit from it to be able to compute the magnetic field using the Biot-Savart law.

In practice, we need to compute the electric potential from a non-linear thermoelectric problem. To keep the computational cost reasonable, we use the well-known Empirical Interpolation Method (EIM) [1, 3] within the Simultaneous EIM Reduced basis (SER) [2] algorithm.

From this, we implemented a strategy to use the reduced potential directly into the Biot-Savart law. This allows, in the case of physical parameters, conductivity, current intensity, etc., to compute in real time the magnetic field in a zone of interest, perform uncertainty quantification, sensitivity analysis or optimization.

In the case of geometrical parameters, the nature of the Biot-Savart law implies to use the Discrete variation of the Empirical Interpolation Method [4]. This method provides a way to recover an affine decomposition from a potentially complex geometrical transformation. Although this method reduces the time needed for the computation of the magnetic field, it does not allow to achieve real time computation.

As an illustration, we present two applications from the Laboratoire National des Champs Magnétiques Intenses (LNCMI): the geometrical optimization of a real magnet, with respect to the homogeneity of the magnetic field, and the identification of cooling parameters to be as close as possible as the experiments.

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Enhancing Hemodynamics Measurements with Mathematical Modeling

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In current medical practice, the risk estimation of vascular accidents in children with sickle cell disease¹ is based on a threshold of the average velocity measured with Doppler ultrasound in the zone of the carotid siphon. This threshold is based on statistical studies that involve strong assumptions and do not take into account any sophisticated physical modeling. As a result, it is desirable to build finer methods to run an accurate risk estimation, which are also more patient-specific.

We propose to build a new risk estimator by taking into account both the Doppler measurements and the knowledge we have about the mathematical modeling of blood flows (a.k.a. hemodynamics) based on classical mechanics equations. We will keep our attention on the carotid artery and base the risk estimator upon a reconstruction of the blood flow with the Parametrized Background Data-Weak approach ([1], [2]). The method makes use of a reduced basis and measurement information (Doppler measurements in our case). The major challenge to face is the use of real Doppler measurements in the PBDW scheme, due to the presence of noise and some artifacts intrinsic to the measures.

In summary, proceeding as was described above, we end up with an algorithm capable of take very poor one-dimensional Doppler measurements (currently only noise-free ones) and then *reconstruct* a 3D velocity field over a realistic human carotid geometry, a first step to build a risk estimator of vascular accident for kids with sickle cell disease.

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¹a genetic disease of major public health concern, according to data compiled by Centers for Disease Control and Prevention (CDC), USA

Fast Solution of the Nonlinear Poisson-Boltzmann Equation using the Reduced Basis Method and Range-Separated Tensor Format

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The Poisson-Boltzmann equation (PBE) is a nonlinear elliptic parametrized partial differential equation that is ubiquitous in biomolecular modeling. It determines a dimensionless electrostatic potential around a biomolecule immersed in an ionic solution [2]. For a monovalent electrolyte (i.e. a symmetric 1:1 ionic solution) it is given by

$$-\vec{\nabla} \cdot (\epsilon(x) \vec{\nabla} u(x)) + \bar{\kappa}^2(x) \sinh(u(x)) = \frac{4\pi e^2}{k_B T} \sum_{i=1}^{N_m} z_i \delta(x - x_i) \quad \text{in } \Omega \in \mathbb{R}^3, \quad (1)$$

$$u(x) = g(x) \quad \text{on } \partial\Omega, \quad (2)$$

where $\epsilon(x)$ and $\bar{\kappa}^2(x)$ are discontinuous functions at the interface between the charged biomolecule and the solvent, respectively. $\delta(x - x_i)$ is the Dirac delta distribution at point x_i . In this study, we treat the PBE as an interface problem by employing the recently developed range-separated tensor format as a solution decomposition technique [1]. This is aimed at separating efficiently the singular part of the solution, which is associated with $\delta(x - x_i)$, from the regular (or smooth) part. It avoids building numerical approximations to the highly singular part because its analytical solution, in the form of $u_s(x) = \alpha \sum_{i=1}^{N_m} z_i / |x - x_i|$ exists, hence increasing the overall accuracy of the PBE solution.

On the other hand, numerical computation of (1) yields a high-fidelity full order model (FOM) with dimension of $\mathcal{O}(10^5) \sim \mathcal{O}(10^6)$, which is computationally expensive to solve on modern computer architectures for parameters with varying values, for example, the ionic strength, $I \in \bar{\kappa}^2(x)$. Reduced basis methods are able to circumvent this issue by constructing a highly accurate yet small-sized reduced order model (ROM) which inherits all of the parametric properties of the original FOM [3]. This greatly reduces the computational complexity of the system, thereby enabling fast simulations in a many-query context. We show numerical results where the RBM reduces the model order by a factor of approximately 350,000 and computational time by 7,000 at an accuracy of $\mathcal{O}(10^{-8})$. This shows the potential of the RBM to be incorporated in the available software packages, for example, the adaptive Poisson-Boltzmann software (APBS).

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Faster A-posteriori Error Estimation for Second Order Mechanical Systems

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A-posteriori error estimation is important for the quality assessment of a particular reduced model. In this work, we improve an existing a-posteriori error estimator for linear second order mechanical systems to scale with large system dimensions and implement it in practice. The main result consists in fast computable analytical terms of constants in the undamped case which need the inversion of a large matrix if computed numerically.

We consider the undamped second order mechanical system

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{B}\mathbf{u}(t)$$

stemming, e.g., from a large scale FE model with symmetric, positive definite mass and stiffness matrices \mathbf{M} and \mathbf{K} . The error estimator from [1]

$$\Delta_{\mathbf{q}}(t) = C_{11}(t)\|\mathbf{e}_{m,0}\|_{\mathbf{G}} + C_{12}(t)\|\dot{\mathbf{e}}_{m,0}\|_{\mathbf{G}} + \int_0^t C_{12}(t-\tau)\|\tilde{\mathbf{R}}_m(\tau)\|_{\mathbf{G}}d\tau$$

of the error \mathbf{e}_m in the position \mathbf{q} has several ingredients: The initial errors $\mathbf{e}_{m,0}$ and $\dot{\mathbf{e}}_{m,0}$, the residual $\tilde{\mathbf{R}}_m$ of the reduced solution, a weighted norm $\|\cdot\|_{\mathbf{G}}$ with weighting matrix $\mathbf{G} := \mathbf{M}$ in our case, and certain constants $C_{11}(t)$ and $C_{12}(t)$. These constants have a major influence on the performance of the error estimator. As described in [1], they are calculated as weighted norms of certain parts $\Phi_{ij}(t)$ of the fundamental matrix $\Phi(t) := e^{\mathbf{A}t}$ of \mathbf{A} which is the system matrix of the equivalent first order system. Calculation of \mathbf{A} involves the inversion of the mass matrix \mathbf{M} . Even though the calculation of the constants $C_{11}(t)$ and $C_{12}(t)$ belong to the offline step, it is unfeasible to calculate the inverse of \mathbf{M} for large systems due to practical restrictions in computation time and memory consumption.

Here, we proof that the constant $C_{11}(t)$ can be chosen to be 1 and $C_{12}(t)$ has a more complex upper bound which can be computed with only a few eigenvalues of a generalized eigenvalue problem. Therefore, no more inversion of the mass matrix is needed and upper bounds of the constants can be calculated very quickly. The proofs involve rewriting the weighted norm $\|\cdot\|_{\mathbf{G}}$ as solution of a generalized eigenvalue problem, a series expansion of $\Phi_{ij}(t)$, the spectral theorem, and several trigonometric identities. The main results states that

$$\|\Phi_{12}(t)\|_{\mathbf{G}} \leq \max \left\{ \frac{|\sin(\mu_1 t)|}{\mu_1}, \frac{|\sin(\mu_2 t)|}{\mu_2}, \dots, \frac{|\sin(\mu_{m-1} t)|}{\mu_{m-1}}, \frac{1}{\mu_m} \right\} \quad (1)$$

for $\mu_1 \leq \mu_2 \leq \dots \leq \mu_N$ being the first N ordered square roots of the generalized eigenvalues of the problem $\mathbf{K}\mathbf{x} = \lambda\mathbf{M}\mathbf{x}$ which can be efficiently computed with an Arnoldi / Lancosz algorithm. The more eigenvalues N the user chooses, the better is the approximation to $C_{12}(t)$. In practice, only a hand full of eigenvalues are needed for a good bound.

In order to be of practical use, we describe a way to add the error estimator in a non-intrusive way to existing simulation code like the elastic multibody software Neweul-M². The error estimator is now calculated in parallel during the solution of the reduced system allowing to influence the simulation by stopping it due to a too large error or by refining the projection basis for improved simulation results.

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3.4 Friday, April 13

Volker Mehrmann, Technische Universität Berlin (08 :30-09 :15)	110
<i>Reduced order energy based modeling in energy transport networks</i>	
Manuela Hund, Max Planck Institute for Dynamics of Complex Technical Systems (09 :15-09 :40)	111
<i>H₂xL₂-optimal model order reduction of parametric linear time-invariant systems</i>	
Petar Mlinaric, Max Planck Institute for Dynamics of Complex Technical Systems (09 :40-10 :05)	112
<i>H₂-optimal structure-preserving model order reduction for second-order systems</i>	
Xingang Cao, Department of Mathematics and Computer Science [Eindhoven] (10 :05-10 :30)	113
<i>A Bilinear H₂ Model Order Reduction Approach to Linear Parameter-Varying Systems</i>	
Masayuki Yano, University of Toronto (11 :00-11 :25)	114
<i>Model reduction of parametrized aerodynamic flows : discontinuous Galerkin reduced basis empirical quadrature procedure</i>	
Michael Schneier, Florida State University (11 :25-11 :50)	115
<i>A Leray Regularized Ensemble-Proper Orthogonal Decomposition Method for Parameterized Convection-Dominated Flows</i>	
Jean-Baptiste Wahl, Université de Strasbourg (11 :50-12 :15)	117
<i>High Reynolds Aerothermal Simulations and Reduced Basis</i>	
Gerrit Welper, University of Southern California (12 :15-12 :40)	118
<i>h and hp Adaptive Interpolation of Transformed Snapshots for Parametric Functions with Jumps</i>	

Reduced order energy based modeling in energy transport networks

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We discuss an energy based modeling approach to deal with coupled systems from different physical domains that act on widely different scales. Each physical system is modeled via a model hierarchy (ranging from detailed models for simulation to reduced models for control and optimization) of port-Hamiltonian differential algebraic systems [1]. The systems are coupled via a network of submodel hierarchies coupled via power conserving interconnections so that the full system stays port-Hamiltonian. Using this very flexible approach, it is possible to control the accuracy of each component separately and to the need of the application [2, 6]. Error controlled model reduction of the submodels as well as the whole model and Galerkin projection as in Finite Element Modeling work in an analogous way. We will demonstrate the approach with real world examples from gas transport optimization [3, 7], power grid modeling [5], and the analysis of disk brake squeal [4].

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$\mathcal{H}_2 \otimes \mathcal{L}_2$ -optimal model order reduction of parametric linear time-invariant systems

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In our framework, we consider parametric linear time-invariant (LTI) systems

$$\begin{aligned} E(\mu)\dot{x}(t) &= A(\mu)x(t) + B(\mu)u(t), \\ y(t) &= C(\mu)x(t), \end{aligned} \tag{1}$$

assuming the system to be asymptotically stable and the system matrix $E(\mu)$ to be invertible for all parameters $\mu \in \Xi \subset \mathbb{R}^d$. Further, we assume all matrices to be affine decomposable.

Our aim is to reduce (1), while preserving the affine decomposition, in the $\mathcal{H}_2 \otimes \mathcal{L}_2$ -optimal sense meaning that the reduced order model (ROM) minimizes an error measure consisting of the \mathcal{L}_2 -error with respect to the parameters and the \mathcal{H}_2 -error with respect to the system response:

$$\|H - H_r\|_{\mathcal{H}_2 \otimes \mathcal{L}_2}^2 := \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{\Xi} \|H(i\omega, \mu) - H_r(i\omega, \mu)\|_F^2 d\mu d\omega,$$

where H and H_r denote the transfer functions of the full order model and the ROM, respectively.

One way to derive such an $\mathcal{H}_2 \otimes \mathcal{L}_2$ -optimal ROM for (1), where only the input and output matrices $B(\mu)$ and $C(\mu)$ are parametrized, is an interpolatory projection method described in [1], that is based on the Iterative Rational Krylov Algorithm (IRKA) (see [2]).

In contrast to this approach, we present a more general approach picking up the idea of the Two-Sided Iteration Algorithm (TSIA) for non-parametric LTI systems (see [4]). The Wilson conditions (see [3]), given as matrix equations, are necessary conditions for the \mathcal{H}_2 -optimal model order reduction problem. In the parametric setting, Wilson-type necessary optimality conditions are now given as integral matrix-valued equations.

In our contribution, we will show how these Wilson-type conditions can be derived for parametric systems (1). Further, we present a way to solve these conditions analytically if only the input and output matrices are parametrized as in [1]. If time permits, we will show possible extensions of this analysis to more general systems (1).

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\mathcal{H}_2 -optimal structure-preserving model order reduction for second-order systems

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We consider second-order systems of the form

$$\begin{aligned} M\ddot{x}(t) + D\dot{x}(t) + Kx(t) &= Bu(t), \\ y(t) &= C_px(t) + C_v\dot{x}(t), \end{aligned}$$

where M is invertible and $\lambda^2 M + \lambda D + K$ is asymptotically stable. Our objective is finding (locally) \mathcal{H}_2 -optimal reduced order models of the same form

$$\begin{aligned} \widehat{M}\ddot{\hat{x}}(t) + \widehat{D}\dot{\hat{x}}(t) + \widehat{K}\hat{x}(t) &= \widehat{B}u(t), \\ \widehat{y}(t) &= \widehat{C}_p\hat{x}(t) + \widehat{C}_v\dot{\hat{x}}(t). \end{aligned}$$

For first-order systems, the Iterative Rational Krylov Algorithm (IRKA) [2] can find locally \mathcal{H}_2 -optimal reduced order models. It is based on interpolation-based necessary optimality conditions. Several methods for second-order systems based on IRKA were proposed in [4] which attempt to satisfy the necessary optimality conditions for first-order systems as closely as possible. It is not clear if these methods satisfy any necessary optimality conditions for second-order systems.

Interpolation-based necessary optimality conditions for second-order systems were derived for second-order systems [1], but with the assumption that \widehat{M} , \widehat{D} , and \widehat{K} are simultaneously diagonalizable. Additionally, no algorithm was proposed so far to satisfy these interpolation conditions.

We take the approach of a related \mathcal{H}_2 -optimal model order reduction method for first-order systems, the Two-Sided Iteration Algorithm (TSIA) [5]. This method is based on Gramian-based necessary optimality conditions, the Wilson conditions [3]. Following the derivation of Wilson conditions, we find the necessary conditions for a reduced second-order system to be \mathcal{H}_2 -optimal. From this, we propose an algorithm, analogous to TSIA, for structure-preserving \mathcal{H}_2 -optimal model order reduction of second-order systems. We also discuss preservation of symmetry and positive-definiteness of M , D , and K in the reduced model.

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A Bilinear \mathcal{H}_2 Model Order Reduction Approach to Linear Parameter-Varying Systems

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Rigorous models of industrial systems often involve parameter-dependent dynamical processes. For example, in the heat transfer process, the material properties and the external environment often have influences on the heat capacity. In order to study these phenomena, many simulations of large-scale finite element models are necessary, which is a very costly or even prohibitive computational task. As a result, model order reduction techniques are required to capture the parameter-varying behavior of the original model. If the parameter variation is piece-wise constant, several interpolation-based methods can be applied, we refer to [1] and the references therein. However, for time-varying parameters, how to find an efficient reduction method is still an open problem.

In this paper, we consider the linear parameter-varying (LPV) system which has the following form

$$\Sigma_{\text{lpv}} : \begin{cases} \dot{x}(t) &= Ax(t) + \sum_{i=1}^{n_p} p_i(t) A_i x(t) + Bu(t) \\ y(t) &= Cx(t) \end{cases}, \quad (1)$$

where $A, A_i \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{p \times n}$. The number of parameters is n_p . Under the assumption that the system Σ_{lpv} given by (1) is bounded-input bounded-output (BIBO) stable, the system can be reconsidered as a bilinear control system,

$$\Sigma_{\text{bl}} : \begin{cases} \dot{x}(t) &= Ax(t) + \sum_{j=1}^{n_p+m} N_j x(t) u_j(t) + \tilde{B}u(t) \\ y(t) &= Cx(t) \end{cases}, \quad (2)$$

where $N_j = 0, j \leq m$, $N_j = A_i, m < j \leq n_p + m$ and $\tilde{B} = [B \ 0 \ \dots \ 0] \in \mathbb{R}^{n \times (n_p+m)}$.

The aim is to find a reduced-order bilinear control system $\hat{\Sigma}_{\text{bl}}$ such that the \mathcal{H}_2 norm

$$\left\| \Sigma_{\text{bl}} - \hat{\Sigma}_{\text{bl}} \right\|_{\mathcal{H}_2}$$

is minimized. To achieve the above goal, we formulate the model order reduction problem as an optimization problem on the Grassmann manifold and solve it by applying a gradient-based algorithm. Based on the work for LTI systems [2], upper bounds of the line search step size in the algorithm are proposed to guarantee the convergence of the algorithm. Numerical examples are used to demonstrate the performance of the proposed method.

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Model reduction of parametrized aerodynamic flows: discontinuous Galerkin reduced basis empirical quadrature procedure

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We present a model reduction formulation for parametrized nonlinear partial differential equations (PDEs) with emphasis on the compressible Reynolds-averaged Navier-Stokes (RANS) equations. The approach builds on four key ingredients: the discontinuous Galerkin (DG) method which provides high-order accuracy and stability for convection-dominated flows; anisotropic adaptive mesh refinement which quantifies and efficiently controls the spatial discretization error; reduced basis (RB) spaces which provides rapidly convergent approximations to the parametric manifold; sparse empirical quadrature rules which provide “hyperreduction” to enable rapid evaluation of the nonlinear DG residual and output forms associated with the RB spaces. The quadrature rules are identified by a linear program (LP) empirical quadrature procedure (EQP) [1] which (i) admits efficient solution by a simplex method and (ii) directly controls the solution error induced by the approximate quadrature. The errors associated with the spatial discretization, reduced basis approximation, and hyperreduction are simultaneously controlled in a systematic manner by a greedy algorithm in the offline stage.

We demonstrate the approach for combined model and discretization uncertainty quantification (UQ) of the RANS equations with the Spalart-Allmaras (SA) turbulence model. The model error arises from the uncertainty in SA model parameters. The DG-RB-EQP method achieves significant computational savings while tightly controlling the discretization error associated with the spatial, reduced basis, and quadrature approximations; see Table 1 for the control of the latter two. The rapid predictions provided by the DG-RB-EQP method also enables control of the Monte Carlo (MC) sampling error in the context of UQ.

N	$ \mathcal{T}^\nu $	$ \Sigma^\nu $	$\max_{\mu \in \Xi^{\text{trial}}} \ r^h(u_N^\nu(\mu), \cdot; \mu)\ _{(\mathcal{V}^h)^\nu}$	$\max_{\mu \in \Xi^{\text{test}}} \frac{ J^h(\mu) - J_N^\nu(\mu) }{ J^h(\mu) }$
1	6	3	2.2×10^{-1}	2.2×10^{-2}
4	28	15	1.1×10^{-1}	4.4×10^{-3}
8	50	35	6.7×10^{-2}	2.4×10^{-3}

Table 1: Convergence of the DG-RB-EQP method for RANS-SA flow over an RAE2822 airfoil for $M_\infty = 0.3$, $Re_c = 6.5 \times 10^6$ and $\alpha = 2.79^\circ$. The table reports the dimension of the RB space (N), the number of reduced elements ($|\mathcal{T}^\nu|$), the number of reduced facets ($|\Sigma^\nu|$), the maximum dual norm of the residual over a training set, and the maximum relative output error over a test set. The model contains four parameters: the turbulent Prandtl number, Kármán constant, and two near-wall destruction constants. The “truth” approximation obtained by an adaptive DG method contains $|\mathcal{T}^h| = 1315$ elements, $|\Sigma^h| = 2850$ facets, and $\mathcal{N} \equiv 39450$ degrees of freedom; the speedup relative to the adaptive DG method is ≈ 25 , and the speedup relative to a typical second-order method on a “best-practice” mesh is ≈ 500 . The estimated mean drag coefficient is 90.4 counts with the following error decomposition: 0.3% due to spatial (FE) error; 0.24% due to reduced-basis and hyperreduction (RB-EQP) error; and 0.04% due to MC sampling error.

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A Leray Regularized Ensemble-Proper Orthogonal Decomposition Method for Parameterized Convection-Dominated Flows

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Partial differential equations (PDE) are often dependent on input quantities which are inherently uncertain. To quantify this uncertainty these PDEs must be solved over a large ensemble of parameters. Even for a single realization this can be a computationally intensive process. In the case of flows governed by the Navier-Stokes equation, a method has been devised for computing an ensemble of solutions. Recently a reduced order model derived from a proper orthogonal decomposition (POD) was incorporated into a newly developed ensemble algorithm [1]. Although the ensemble-POD method was successful in the numerical simulation of laminar flows, it yields numerical inaccuracies for convection-dominated flows. In this work we put forth a regularized model, the Leray ensemble-POD model, for the numerical simulation of convection-dominated flows. The Leray ensemble-POD model employs spatial filtering to smooth (regularize) the convection term in the Navier-Stokes. For the new Leray ensemble-POD algorithm, we also propose a numerical discretization with better stability properties than those of the numerical scheme for the standard ensemble-POD method. For this new numerical discretization, we prove its stability and convergence. Furthermore, we show that the Leray ensemble-POD method is more accurate than the standard ensemble-POD method in the numerical simulation of a two-dimensional flow between two offset circles.

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High Reynolds Aerothermal Simulations and Reduced Basis

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We present in this talk our work on model order reduction for aerothermal simulations. The model involves the resolution of coupled non-linear parametrized partial differential equations in which affine decomposition is not obtained. We consider the coupling between the incompressible Navier-Stokes equations and an advection diffusion equation for the temperature. This coupling can be either in one or two ways depending if we do consider only forced or both natural and forced convections.

Since the physical parameters induce high Reynolds and Peclet numbers, we have to introduce stabilisation operators in the discrete formulation in order to deal with the well known numerical stability issue. The chosen stabilization, applied to both fluid and heat equations, is the usual Streamline-Upwind/Petrov-Galerkin (SUPG) which adds artificial diffusivity in the direction of the convection field. However this method often produces non physical undershoots or overshoots in the edge of discontinuities, which can be critical when you want to ensure, for instance, the positiveness of certain fields.

To tackle this discontinuity problem, we add in our model a new operator, known in the literature as shock capturing method. This new operator is non-linear and adds artificial diffusivity in the region of the discontinuities in order to treat under/overshoots. Although this method is particularly efficient, it induces a new difficulty, because the system becomes fully non-linear.

We present in this talk our order reduction strategy for this model, based on Reduced Basis Method (RBM). In order to recover a affine decomposition for this complex model, we implemented a discrete variation of the Empirical Interpolation Method (EIM) [1, 3] which is a discrete version of the original EIM. This variant allows to build a approximated affine decomposition for complex operators such as in the case of SUPG [4]. We also use this method for the non-linear operators induced by the shock capturing method.

The construction of a EIM basis for non-linear operators, involves a potentially huge numbers of non-linear FEM resolutions - depending of the size of the sampling. Even if this basis is built during an offline phase, we usually cannot afford such expensive computational cost. We took advantage of the recent development of the Simultaneous EIM Reduced basis algorithm (SER) [2] to tackle this issue. Enjoying the efficiency offered by reduced basis approximation, this method provides a huge computational gain and can require as little as $N + 1$ finite element solves where N is the dimension of the RB approximation. As an illustration we present a application of a cooling system of a printed circuit board with different heat sources. The model is parametrized with different physical and geometrical parameters.

This SER variant is now available in the generic and seamlessly parallel reduced basis framework of the opensource library Feel++ (Finite Element method Embedded Language in C++, <http://www.feelpp.org>).

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h and hp Adaptive Interpolation of Transformed Snapshots for Parametric Functions with Jumps

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In comparison to elliptic and parabolic problems, our abilities to simulate parametric or stochastic hyperbolic PDEs is still fairly limited. Among several challenges, the efficient approximation of the PDE's solution is largely an open problem: They typically contain parameter dependent jumps and kinks, which diminish the convergence rates of established methods, including reduced basis methods, POD or polynomial chaos expansions. However, if the jump locations were independent of the parameters, they would be “invisible” in parameter direction and pose no further difficulty for the approximation. Therefore, we propose to reduce these parameter dependent jumps to this favorable situation, by introducing transformations of the physical domain. They are computed in an offline phase together with the snapshots and align the jump sets of the snapshots with the jumps at an arbitrary target parameter. After alignment, in the online phase, we are in the favorable situation described above and apply a simple polynomial interpolation of the transformed snapshots. In order to calculate the transforms, we minimize the L_1 -error of the transformed interpolation on a training sample of parameters with respect to the transform itself. Although this appears to be a complicated optimization problem, we can split the transform into a series of local contributions that allow us to “localize” the optimization problem and avoid unsatisfactory local minima.

The above outlined method works well if we can align all discontinuities, which is not always the case. For example, if the number of jumps changes in parameter, a proper alignment is not possible. In contrast to the parameter dependent movement of the jumps, which induce singularities for every parameter, changes of the number of jumps (and similar non-align-able cases) are local in parameter space. Therefore, we propose an additional h or hp adaption in parameter space to handle these cases. To make this idea practical, one has to overcome two difficulties:

1. Changes in the shock structure are usually located on a surface in parameter space, which is not resolved with high order by common h refinement strategies.
2. Local adaptations are questionable in high parameter dimensions.

Both difficulties are approached by a “tensor” construction: We first construct h or hp adaptive interpolations with transformed snapshots for low parameter dimensions and then use a tensor product like construction for higher parameter dimensions. In general, tensor products of h adaptive approximations are only reasonable if the singularities are aligned with the coordinate axes. This is rarely the case but automatically accounted for by the transforms in our approximation method. The tensor construction is susceptible to the curse of dimensionality but it is designed to be used with tensor based methods for high dimensions in the future.

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