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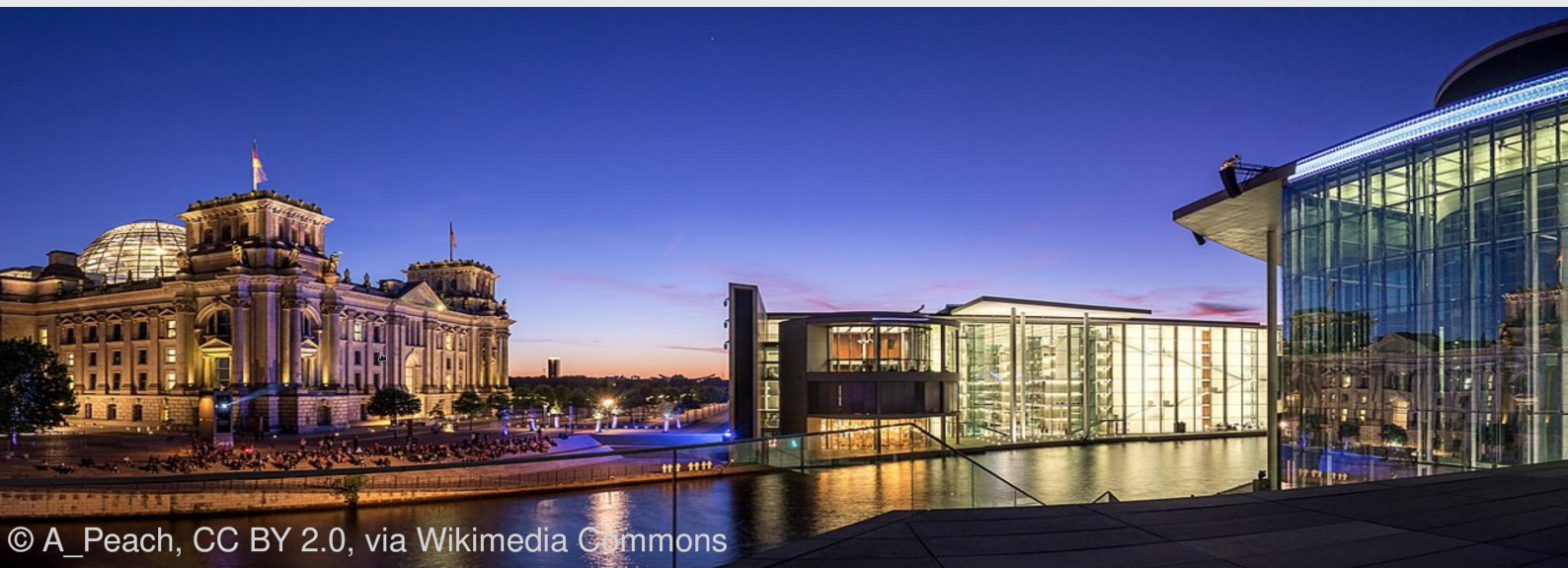
MORe 2022

« Model Reduction and Surrogate Modeling »

September 2022, 19-23, Technische Universität Berlin, Germany

BOOK OF ABSTRACTS



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Content

1 About MORe 2022

The conference **Model Reduction and Surrogate Modeling (MORe)** merges activities of the two independent conference series *MoRePaS* and MODRED. Previous *MoRePaS* editions were held in Münster (2009), Günzburg (2012), Trieste (2015) and Nantes (2018). Previous MODRED editions were held in Berlin (2010), Magdeburg (2013), Odense (2017) and Graz (2019).

1.1 Topics

The goal is to foster an international exchange of new concepts and ideas related to the following topics:

- Parametric model order reduction
- System-theoretic model reduction methods and frequency-domain methods
- Data-driven approaches
- Non-intrusive model order reduction
- Machine learning/deep learning and model order reduction
- Tensor methods
- Kernel methods for nonlinear MOR
- MOR for problems with poor Kolmogorov N-width decay (e.g. transport phenomena)
- Structure-preserving and energy-based MOR (e.g. Hamiltonian or port-Hamiltonian systems)
- Nonlinear model reduction
- Localized MOR and multi-scale problems
- Randomized algorithms
- High dimensional parameter spaces and reduction in parameter space
- Dynamic and adaptive approximations, error estimation
- Multifidelity methods
- MOR for uncertainty quantification
- Model reduction for nonlinear bifurcating PDEs
- Model reduction for optimization, control and inverse problems
- MOR for multiphysics/multiphase problems
- Large-scale applications, digital twins
- MOR for industrial applications
- Emerging computational technologies based on ROM
- Model reduction software and benchmarks

1.2 Venue

The conference will be located at:
Technische Universität Berlin (Google Maps)
Straße des 17. Juni 135
10623 Berlin, GERMANY
Contact : more@sciencesconf.org

1.3 Committees

Executive Committee

Tobias Breiten (TU Berlin, Germany), *Chair*
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1.4 Financial support

The event is financially supported by the German Research Foundation (project number 496449925).

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1.5 Social program

Welcome reception. The welcome reception takes place on **Monday, September 19, 7:30 pm** at the Foyer of the **architecture building (A)** which is located diagonally opposite to the main building on the Straße des 17. Juni.

Conference dinner. The conference dinner (dinner ticket needed) takes place on **Wednesday, September 21, 7:30 pm** at the event location **Wartehalle Berlin, Julie-Wolfthorn-Strasse 1, 10115 Berlin** which can be reached via public transport (S-Bahn S1/S2/S25/S26 to Nordbahnhof or U-Bahn U6 to Naturkundemuseum).

Coffee breaks. Coffee, soft drinks, snacks and fruits are served during the breaks in rooms H 3005 and H 3006 of the main building.

Lunch breaks. Participants might go to one of the many cafés, bistros and small restaurants in the surroundings of the Ernst-Reuter-Platz (e.g., Knesebeckstraße). There is also the possibility to have lunch at the cafeteria of the math building (MA) which is located opposite of the main building on the Straße des 17. Juni. For having lunch at the mensa of TU Berlin, participants are required to have a (guest) mensa card which can be obtained at the information desk of the mensa.

1.6 Internet access

Participants have access if their home university is part of the **eduroam** network. In this case, use your account information from your home university.

1.7 Speaker information

The scheduled time for oral presentations is 25 minutes and includes questions, answers and change of speakers. We will provide laptop computers (with HDMI and VGA connector) and laser pointers for presentations in each room and we strongly advise to use these computers for the presentation in order to avoid delays between presentations and technical difficulties. The presentation laptops run openSUSE Leap 15.3 and provide Okular (pdf reader) and LibreOffice 7.3.3.1 as well as Chromium, Firefox and Google Chrome web browsers and the VLC video player with standard codecs.
Please make sure to copy your slides to the presentation laptop before the start of your session. Technical assistance (wearing a black shirt with a TU Berlin logo) will be present in the lecture rooms 20 minutes before the start of your session.

2 Program

Monday, September 19

Time	Event
12 : 45 - 13 : 30	**Registration (H 3005)**
13 : 30 - 14 : 00	**Opening (H 1012)**
14 : 00 - 14 : 45	**Plenary (H 1012 - Chair : Mario Ohlberger)**
	· *Boris Kramer – Nonlinear balanced truncation : Scalable computation and manifold reduction*
14 : 50 - 16 : 05	**Session 1 (H 1012 - Chair : Mario Ohlberger)**
	· *Marie Billaud Friess – Probabilistic reduced basis method for parameter-dependent problems*
	· *Saskia Dietze – Stability Analysis of Reduced Basis Model Predictive Control for Parametrized Optimal Control Problems*
	· *Constantin Greif – Solving parametric PDEs with an enhanced model reduction method based on Linear/Ridge expansions*
16 : 05 - 16 : 30	**Coffee break (H 3005/3006)**
16 : 30 - 17 : 45	**Parallel Session 1a (H 1012 - Chair : Volker Mehrmann)**
	· *Axel Klawonn – Data-driven learning of coarse basis functions in adaptive FETI-DP*
	· *Linus Ballicki – Data-driven model order reduction with the p-AAA algorithm*
	· *Quirin Aumann – Data-driven reduced-order modeling of thermo-mechanical models of machine tools*
16 : 30 - 17 : 45	**Parallel Session 1b (H 1058 - Chair : Lihong Feng)**
	· *Valentin Resseguier – Stochastic reduced order models for Bayesian estimation problems in fluid mechanics*
	· *Francesco Attilio Bruno Silva – A Reduced Basis Ensemble Kalman Method*
	· *Patrick Héas – Adapting Reduced Models for Importance Sampling*
17 : 45 - 18 : 35	**Parallel Session 2a (H 1012 - Chair : Volker Mehrmann)**
	· *Martin Hess – Data-Driven Enhanced Model Reduction for Bifurcating Models in Computational Fluid Dynamics*
	· *Guillaume Steimer – Data driven reduced modelling of the Vlasov-Poisson equation*
17 : 45 - 19 : 00	**Parallel Session 2b (H 1058 - Chair : Lihong Feng)**
	· *Shuwen Sun – Parametric dynamic mode decomposition for nonlinear parametric dynamical systems*
	· *Igor Pontes Duff – Dominant Subspaces of High-Fidelity Nonlinear Structured Parametric Dynamical Systems and Model Reduction*
	· *Francesca Bonizzoni – A greedy MOR method for the tracking of eigensolutions to parametric PDEs*
19 : 30 - 21 : 30	**Welcome Reception (A Foyer)**

Tuesday, September 20

Time	Event
08 : 30 - 09 : 15	**Plenary (H 1012 - Chair : Peter Benner)**
	· *Laura Grigori – Randomization techniques for solving large scale linear algebra problems*
09 : 20 - 10 : 35	**Session 2 (H 1012 - Chair : Peter Benner)**
	· *Davide Torlo – Model order reduction for Friedrichs' systems : a bridge between elliptic and hyperbolic problems*
	· *Hendrik Kleikamp – Nonlinear model order reduction for hyperbolic conservation laws by means of diffeomorphic transformations of space-time domains*
	· *Angela Monti – Adaptive POD-DEIM correction for Turing pattern approximation in reaction-diffusion PDE systems*
10 : 35 - 11 : 00	**Coffee break (H 3005/3006)**
11 : 00 - 12 : 40	**Parallel Session 3a (H 1058 - Chair : Heike Faßbender)**
	· *Lihong Feng – Matrix-free Transfer Function Prediction using Model Reduction and Machine Learning*
	· *Corbin Foucart – Deep-Reinforcement-Learning-informed Adaptive Refinement for High-order Discontinuous Galerkin Methods*

	· *Björn Liljegren-Sailer – On error estimates for reduced models obtained by balanced truncation*
	· *Jorge Cisneros – Automated model reduction for pharmacology models*
11 : 00 - 12 : 40	**Parallel Session 3b (H 1012 - Chair : Bernard Haasdonk)**
	· *Robin Klein – A structure-preserving DEIM formulation for non-linearly stable hROMs of the incompressible Navier-Stokes equations*
	· *Matthias Heinkenschloss – Model Reduction of Navier-Stokes Equations using the Loewner Framework*
	· *Giovanni Stabile – Model order reduction for turbulent and compressible flows : hybrid approaches in physics and geometry parametrization*
	· *Victor Zucatti – POD-Based Adaptive Model Reduction to Accelerate Computational Fluid Dynamics*
12 : 40 - 14 : 00	**Lunch**
14 : 00 - 15 : 15	**Session 3 (EW 201 - Chair : Michael Hinze)**
	· *Shaimaa Monem Abdelhafez – Model reduction for dynamics on deformable complex surfaces*
	· *Jörg Fehr – Nonlinear Model Order Reduction for Three-dimensional Discretized FE Models using Graph Convolutional Autoencoders*
	· *Francesco Romor – Nonlinear manifold Reduced Order Models with Convolutional Autoencoders and Reduced Over-Collocation method*
15 : 20 - 16 : 05	**Plenary (EW 201 - Chair : Michael Hinze)**
	· *Rachel Ward – Learning to Forecast Dynamical Systems from Streaming Data*
16 : 05 - 16 : 30	**Coffee break (H 3005/3006)**
16 : 30 - 17 : 45	**Parallel Session 4a (H 1012 - Chair : Matthias Heinkenschloss)**
	· *Louis Schuler – Non-intrusive multi-physics PGD-based reduced model for the modeling of power electronic modules*
	· *Maria Strazzullo – Full Order Model and Reduced Order Model Consistency for Evolve-Filter-Relax Regularization*
	· *Theron Guo – Hyper-reduction of geometrically parameterized nonlinear microstructures*
16 : 30 - 17 : 45	**Parallel Session 4b (H 1058 - Chair : Axel Klawonn)**
	· *Stephan Rave – Two-Scale Reduction of LOD Multiscale Models*
	· *Tim Keil – Adaptive Localized Reduced Basis Methods in Multiscale PDE-Constrained Parameter Optimization*
	· *Matthew Zahr – Model reduction of convection-dominated partial differential equations via optimization-based implicit feature tracking*

Wednesday, September 21

Time	Event
08 : 30 - 09 : 15	**Plenary (H 1012 - Chair : Gianluigi Rozza)**
	· *Youssef Marzouk – Simulation-based Bayesian inference and surrogate modeling*
09 : 20 - 10 : 35	**Session 4 (H 1012 - Chair : Gianluigi Rozza)**
	· *Aaron Charous – Deep learning and the dynamical low-rank approximation*
	· *Abhinav Gupta – Generalized Neural Closure Models with Interpretability*
	· *Martin Weiser – Conditional gradient-based Identification of Non-linear Dynamics*
10 : 35 - 11 : 00	**Coffee break (H 3005/3006)**
11 : 00 - 12 : 40	**Parallel Session 5a (H 1058 - Chair : Boris Kramer)**
	· *Jennifer Przybilla – Model reduction of descriptor systems with quadratic output functional*
	· *Pawan Goyal – Learning Quadratic Embeddings for Nonlinear Dynamical Systems using Deep Learning*
	· *Alejandro Diaz – Impact of the Convergence of Series Expansions on Model Reduction of Quadratic-Bilinear Systems*
	· *Christian Himpe – Data-Driven Model Reduction for Gas Network Digital Twins*
11 : 00 - 12 : 40	**Parallel Session 5b (H 1012 - Chair : Anthony Nouy)**
	· *Silke Glas – Symplectic Model Reduction of Hamiltonian Systems on Nonlinear Manifolds*
	· *Volker Mehrmann – Model reduction for port-Hamiltonian descriptor systems*
	· *Jonas Nicodemus – Dynamic Mode Decomposition for Continuous Port-Hamiltonian Systems*
	· *Tommaso Bradde – A non-intrusive algorithm for parameterized model order reduction of LTI systems with guaranteed dissipativity*
12 : 40 - 14 : 00	**Lunch**
14 : 00 - 14 : 45	**Plenary (H 1012 - Chair : Tobias Breiten)**

	· *Cecilia Pagliantini – Structure-preserving and adaptive reduced order models of conservative dynamical systems*
15 : 00 - 16 : 30	**Poster Blitz (H 1012 - Chair : Tobias Breiten)**
	· *Tony Ryu – Neural Closure Model for Dynamic Mode Decomposition Forecasts*
	· *Patrick Buchfink – A Differential Geometric Formulation for Model Order Reduction on Manifolds*
	· *Pierfrancesco Siena - A machine learning-based reduced order model for the investigation of the haemodynamics in coronary artery bypass grafts*
	· *Phillip Semler - Adaptive Gaussian Process Regression for Efficient Building of Surrogate Models in Inverse Problems*
	· *Michele Girfoglio - An efficient computational framework for atmospheric and ocean flows*
	· *Lukas Bürger - Analysis of Hyper Reduction for the Computation of Nonlinear Normal Modes*
	· *Steffen W. R. Werner - Balancing-related model reduction of large-scale sparse systems in MATLAB and Octave with the MORLAB toolbox*
	· *Jonas Nitzler - Bayesian multi-fidelity inverse analysis for computationally demanding models in high stochastic dimensions*
	· *Ulrich Römer - Combining adaptive model order reduction and stochastic collocation for uncertainty quantification of vibroacoustic systems*
	· *Anna Ivagnes - Data enhanced reduced order methods for turbulent flows*
	· *Dimitrios Karachalios - Data-driven nonlinear model discovery*
	· *Giovanni Conni - Data-Driven Linearization of Nonlinear Finite Element Analyses*
	· *Robin Herkert - Dictionary-based Online-adaptive Structure-preserving Model Order Reduction for Parametric Hamiltonian Systems*
	· *Julian Koellermeier - Dynamical low rank approximation and parametric reduced order models for shallow water moment equations*
	· *Johannes Rettberg - Effective A-posteriori Error Estimation for Port-Hamiltonian Systems*
	· *Simon Le Berre - Efficient Hyper-Reduction of contact problems treated by Lagrange multipliers.*
	· *Tobias Ehring - Hermite kernel surrogates for the value function of high-dimensional nonlinear optimal control problems*
	· *Jiahua Jiang - Hybrid Projection Methods with Recycling for Inverse Problems*
	· *Jens Saak - Interpolatory (P)MOR via low-rank (tensor) approximation in general linear matrix equations*
	· *Martin Stoll - Low-rank methods in large scale constrained optimization*
	· *Benjamin Carrel - Low-rank Parareal : a low-rank parallel-in-time integrator*
	· *Jens Saak - M-M.E.S.S. 3.0 - Introducing Krylov-based solvers*
	· *George Drakoulas - Machine learning-based reduced order modelling : Towards intelligent digital twins*
	· *Henrik Rosenberger - Mass-conserving and energy-consistent ROMs for the incompressible Navier-Stokes equations with time-dependent boundary conditions*
	· *Muhammad Hamza Khalid - Model order reduction for wave-type problems with band-limited outputs of interest*
	· *Julia Vettermann - Model order reduction via substructuring for a nonlinear switched differential algebraic machine tool model*
	· *Sebastian Schopper - Multi-fidelity Optimization of an Acoustic Metamaterial using Model Order Reduction and Machine Learning*
	· *Davide Pradovera - Non-intrusive adaptive surrogate modeling of parametric frequency-response problems*
	· *Sean Reiter - On Balanced Truncation Error Bound and Sign Parameters*
	· *Michel-Niklas Senn - On the use of exponential integrators for large-scale Hamiltonian systems*
	· *Yevgeniya Filanova - Operator inference method for mechanical systems*
	· *Eki Agouzal - Parametric model order reduction approach for quasi-static non-linear mechanical problems using an industrial code : application to an elasto-plastic material*
	· *Stephan Rave - pyMOR - Model Order Reduction with Python*
	· *Anna Sanfilippo - Reduced Basis Methods for Time-Harmonic Maxwell's Equations*
	· *Catharina Czech - Reduced order models for efficient uncertainty quantification of wooden structures with inhomogeneous material properties*
	· *Jana Tarhini - Reduction of single phase flow models in porous media using a quantity of interest*
	· *Moaad Khamlich - ROM for Large-scale Modelling of Urban Air Pollution*
	· *Bernhard Höveler - Spectral approximation of Lyapunov operator equations with applications in high dimensional non-linear feedback control*
	· *Harshit Kapadia - Subspace-Distance-Enabled Active Learning for Parametric Model Order Reduction of Dynamical Systems*
	· *Clement Vella - Symplectic formulation of PGD reduced-order models for structural dynamics applications*

	· *Jan Heiland - Tensor Galerkin Proper Orthogonal Decomposition for Uncertainty Quantification of PDEs with Random Parameters*
	· *Pablo Solán-Fustero - Time extrapolation technique applied to POD-based ROM*
	· *Kathryn Lund - Towards a Benchmark Framework for Model Order Reduction in the Mathematical Research Data Initiative (MaRDI)*
16 : 30 - 17 : 00	**Coffee break (H 3005/3006)**
17 : 00 - 18 : 00	**Poster Session (H 3006)**
19 : 30 - 23 : 30	**Conference Dinner (Wartehalle, Julie-Wolfthorn-Straße 1, 10115 Berlin)**

Thursday, September 22

Time	Event
08 : 30 - 09 : 15	**Plenary (H 1012 - Chair : Ralf Zimmermann)**
	· *Jan Hesthaven – Digital Twins through Reduced Order Models and Machine Learning*
09 : 20 - 10 : 35	**Session 5 (H 1012 - Chair : Ralf Zimmermann)**
	· *Martin Redmann – Optimization based model order reduction for stochastic systems*
	· *Elizabeth Qian – Balanced Truncation for Bayesian Inference*
	· *Sebastian Kaltenbach – Semi-supervised Invertible DeepONets for Bayesian Inverse Problems*
10 : 35 - 11 : 00	**Coffee break (H 3005/3006)**
11 : 00 - 12 : 40	**Parallel Session 6a (H 1012 – Chair : Tobias Breiten)**
	· *Ion Victor Gosea – Structured barycentric forms and their application to iterative data-driven model reduction of second-order systems*
	· *Petar Mlinaric – Structured L2-Optimal Parametric Model Order Reduction*
	· *Luka Grubisic – High Order Approximations of the Operator Lyapunov Equation Have Low Rank*
	· *Stefania Fresca – Long-time prediction of nonlinear parametrized dynamical systems by deep learning-based reduced order models*
11 : 00 - 12 : 40	**Parallel Session 6b (H 1058 - Chair : Mario Ohlberger)**
	· *Vince Maes – Hybrid fluid/particle methods for kinetic equations describing neutral particles in nuclear fusion plasma-edge modelling*
	· *Mattia Manucci – Model Order Reduction in Contour Integral Methods for parametric PDEs*
	· *Sridhar Chellappa – Inf-Sup-Constant-Free Error Estimation for Linear Parametric Systems*
	· *Shubhaditya Burela – Parametric reduced order modelling for transport dominated systems via shifted POD deep learning models*
12 : 40 - 14 : 00	**Lunch**
14 : 00 - 14 : 45	**Plenary (H 1012 - Chair : Serkan Gugercin)**
	· *Benjamin Unger – Port-Hamiltonian systems – from a general modelling wishlist to surrogate models with guarantees*
14 : 50 - 16 : 05	**Session 6 (H 1012 - Chair : Serkan Gugercin)**
	· *Tommaso Taddei – Registration-based model reduction of parameterized PDEs with spatio-parameter adaptivity*
	· *Lewin Ernst – A certified wavelet-based physics-informed neural network for nonlinear model reduction of parameterized partial differential equations*
	· *Federico Pichi – Neural networks investigation of bifurcating phenomena in fluid-dynamics*
16 : 05 - 16 : 30	**Coffee break (H 3005/3006)**
16 : 30 - 17 : 45	**Session 7 (H 1012 - Chair : Benjamin Peherstorfer)**
	· *Nicola Franco – Deep Orthogonal Decomposition via Mesh-Informed Neural Networks for Reduced Order Modeling of parametrized PDEs*
	· *Felix Schindler – An adaptive hierarchy of certified machine learning and reduced basis surrogates for parametrized PDEs*
	· *Philipp Diercks – Multiscale modeling of heterogeneous structures based on a localized model order reduction approach*

Friday, September 23

Time	Event
08 : 30 - 09 : 15	**Plenary (H 1012 - Chair : Karsten Urban)**
	· *Andrea Manzoni – Deep learning for reduced order modeling*
09 : 20 - 10 : 35	**Session 8 (H 1012 - Chair : Karsten Urban)**
	· *Julia Schleuß – Generating reduced order models parallel in time via random sampling*
	· *Philipp Trunschke – The local sample complexity of non-linear least squares approximation*
	· *Kathrin Smetana – Randomized local model order reduction for nonlinear PDEs*
10 : 35 - 11 : 00	**Coffee break (H 3005/3006)**
11 : 00 - 11 : 50	**Session 9 (H 1012 - Chair : Sara Grundel)**
	· *Steffen W. R. Werner – Context-aware learning of low-dimensional stabilizing controllers in the scarce data regime*
	· *Feliks Nüske – Slow collective dynamics via data-driven approximation of the Koopman generator*
11 : 55 - 12 : 40	**Plenary (H 1012 - Chair : Sara Grundel)**
	· *Virginie Ehrlacher – Structure-preserving reduced-order models for parametric cross-diffusion systems*
12 : 40 - 12 : 50	**Closing (H 1012)**

3 Abstracts

3.1 Monday, September 19

Nonlinear balanced truncation: Scalable computation and manifold reduction

B. Kramer[1]

[1] *Department of Mechanical and Aerospace Engineering*
University of California San Diego

Nonlinear balanced truncation is a model order reduction technique that reduces the dimension of nonlinear systems in a manner that accounts for either open- or closed-loop observability and controllability aspects of the nonlinear system. Two computational challenges have so far prevented its deployment on large-scale systems: (a) the computation of Hamilton-Jacobi-(Bellman) equations that are needed for characterization of controllability and observability aspects, and (b) efficient model reduction and reduced-order model (ROM) simulation on the resulting nonlinear balanced manifolds. In this talk I will review several existing methods for nonlinear balanced truncation and present a novel unifying and scalable approach to balanced truncation for large-scale systems. We consider a Taylor-series based approach to solve a class of parametrized Hamilton-Jacobi-Bellman equations that are at the core of the balancing approach. Moreover, I will present a nonlinear balance-and-reduce approach that finds a reduced nonlinear state transformation that balances the system properties. The talk will illustrate the strength and scalability of the algorithm on two semi-discretized partial differential equations, namely Burgers' equation and the Kuramoto-Sivashinsky equation.

Probabilistic reduced basis method for parameter-dependent problems

M. Billaud-Friess[1], **A.Macherey**[1,2], **A. Nouy**[1], **and C. Prieur**[2]

[1] *Nantes Université, Centrale Nantes, LMJL, UMR CNRS 6629, France*
[2] *Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, 38 000 Grenoble, France*

In this talk, we consider the approximation of some function $u : \xi \mapsto u(\xi)$, defined on $\Xi \subset \mathbb{R}^p$ and taking its values in some vector space V, by means of a Reduced Basis (RB) method. It aims at constructing an approximation $u_n(\xi)$ of $u(\xi)$ as a projection in a finite dimensional space $V_n \subset V$ generated by snapshots of u selected through a greedy procedure. A practical algorithm is as follows. Given $\{\xi_1, \dots, \xi_{n-1}\}$ and the corresponding subspace $V_{n-1} = \text{span}\{u(\xi_1), \dots, u(\xi_{n-1})\}$, a new parameter value ξ_n is selected as

$$\xi_n \in \arg\max_{\xi \in \tilde{\Xi}} \Delta(u_n(\xi), \xi), \tag{1}$$

with $\Delta(u_n(\xi), \xi)$ a suitable error estimate and $\tilde{\Xi} \subset \Xi$ a finite training set. Recently, probabilistic variants of this algorithm have been considered. In [4], different training sets $\tilde{\Xi} = \Xi_n$ randomly chosen are used at each step. In [2, 3], a control variate using a RB paradigm has been proposed where $\Delta(u_n(\xi), \xi)$ is a Monte Carlo estimate of the variance of the projection error. In the lines of [2, 3], we propose a probabilistic greedy algorithm in which $\Delta(u_n(\xi), \xi)$ is expressed as the expectation of a parameter-dependent random variable $Z_n(\xi)$, i.e.

$$\Delta(u_n(\xi), \xi) = \mathbb{E}(Z_n(\xi)). \tag{2}$$

To solve (1) with (2), a Probably Approximately Correct bandit algorithm [1] is retained. It returns a quasi-optimum in relative precision, with high probability. The resulting greedy algorithm is proven to be a weak greedy algorithm with high probability.

Applications concern the approximation of $u(\xi) : D \to \mathbb{R}$, $D \subset \mathbb{R}^d$, for which we only have access to pointwise evaluations at $(x, \xi) \in D \times \Xi$. For u a costly functional given a priori, the proposed method is applied to compute u_n an interpolant of u in V_n. In that case, it can be seen as a probabilistic empirical interpolation method. Then, we consider a probabilistic RB method for the solution of parameter-dependent partial differential equations on D. Here, as u is not explicitly given, the proposed method relies on pointwise estimates $u(x, \xi)$ obtained through the so-called *Feynman-Kac representation formula*.

References

[1] M. Billaud-Friess, A. Macherey, A. Nouy, and C. Prieur. A PAC algorithm in relative precision for bandit problem with costly sampling. *arXiv:2007.15331*, Jul 2020, (to appear in Math. Methods Oper. Res).

[2] M.-R. Blel, V. Ehrlacher, and T. Lelièvre. Influence of sampling on the convergence rates of greedy algorithms for parameter-dependent random variables. *arXiv:2105.14091*, May 2021.

[3] S. Boyaval and T. Lelièvre. A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm. *Commun. Math. Sci.*, 8(3):735–762, Sep 2010.

[4] A. Cohen, W. Dahmen, R. DeVore, and J. Nichols. Reduced basis greedy selection using random training sets. *ESAIM: Mathematical Modelling and Numerical Analysis*, 54(5):1509–1524, 2020.

Stability Analysis of Reduced Basis Model Predictive Control for Parametrized Optimal Control Problems

Saskia Dietze[1] **and Martin A. Grepl**[1]

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Model Predictive Control (MPC) is a well established approach to solve infinite horizon optimal control problems. Since optimization over an infinite time horizon is, in general, infeasible, the method determines a suboptimal feedback control by repeatedly solving finite time optimal control problems. Although MPC has been successfully used in many applications, applying MPC to large-scale systems – arising, e.g., through discretization of partial differential equations – requires the solution of high-dimensional optimal control problems and thus poses immense computational effort.

We consider systems governed by parametrized parabolic partial differential equations and employ the reduced basis method (RB) as a low-dimensional surrogate model for the finite time optimal control problem. The reduced order optimal control serves as the feedback control for the MPC of the original large-scale system. We analyze the proposed RB-MPC approach by first developing rigorous *a posteriori* error bounds for the errors in the optimal control and the associated cost functional. These bounds can be evaluated efficiently in an offline-online computational procedure and therefore allow us to guarantee asymptotic stability of the closed-loop system using the RB-MPC approach. Furthermore, we propose an adaptive strategy based on the error bounds to choose the optimal horizon length of the finite time optimal control problem. We present numerical results to validate our approach.

Although we can provide rigorous results only for linear-quadratic problems, our approach may also provide a guideline for nonlinear problems. To this end, we compare two methods: First, we consider a (simple) piecewise linearization approach that allows to invoke the theory on linear-quadratic problems. In the second approach, we consider the nonlinear problem and employ the Empirical Interpolation Method (EIM) to efficiently solve the associated optimal control problem. A semilinear parabolic model problem is considered in order to discuss and compare the two proposed approaches.

Solving parametric PDEs with an enhanced model reduction method based on Linear/Ridge expansions

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Classical projection-based model reduction methods, like the reduced basis method [1, 2], are popular tools for getting quickly solvable reduced order models for parametric PDEs. Unfortunately, for some problems the error-decay with respect to the dimension of the projection space is predetermined to be slow, e.g., for transport or wave equations with jump discontinuities [2]. Therefore nonlinear methods are needed that do not project onto a linear space.
Our approach is to build the reduced order model with linear basis functions that are enhanced with some ridge functions [3, 4]. A ridge function consists of a one dimensional profile function as well as a direction that expands the profile to the multivariate domain. For the difficult task of finding the optimal directions, we developed a particle grid algorithm. The Linear/Ridge function space consisting of linear basis functions as well as linear combinations of ridge functions with parameter-dependent directions, is clearly nonlinear.
Offline, we first build the linear basis with known techniques by using snapshots that are solutions of the parametric PDE. If the error does not decay fast enough by adding more basis functions, we enhance the linear space with ridge functions. This is done by iteratively picking a worst parameter, computing the associated snapshot and determining directions with the particle grid algorithm for the profiles to approximate the snapshot at best. Then, extending the ridge function space by adding new profiles to the basis set until the approximation is precise enough for this specific snapshot. This procedure is repeaded until the overall error is sufficient small. Finally with the generated Linear/Ridge function space, the parametric PDE can be solved online-efficient by using interpolation for the directions [3].

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Data-driven learning of coarse basis functions in adaptive FETI-DP

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The convergence rate of FETI-DP domain decomposition methods is generally determined by the eigenvalues of the preconditioned system. For second-order elliptic partial differential equations, coefficient discontinuities with a large contrast can lead to a deterioration of the convergence rate. A remedy can be obtained by enhancing the coarse space with elements, which are often called constraints, that are computed by solving small eigenvalue problems on portions of the interface of the domain decomposition, i.e., edges in two dimensions or faces and edges in three dimensions. This approach is denoted as adaptive FETI-DP. For many elliptic partial differential equations, this leads to a provably robust method.

In general, it is difficult to predict where these constraints have to be computed, i.e., on which edges or faces. Using a machine learning strategy based on neural networks the geometric location of these edges or faces can be predicted in a preprocessing step. This reduces the number of eigenvalue problems that have to be solved. Numerical experiments for model problems and realistic microsections using regular decompositions as well as those from graph partitioners are provided, showing very promising results.

In a further step, using deep learning, we directly learn the constraints and build a surrogate model which replaces the eigenvectors associated with the local eigenvalue problems. Numerical results show the robustness of this approach.

Data-driven model order reduction with the p-AAA algorithm

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Rational approximation represents a powerful tool for accurately capturing complex system dynamics via low-order models. The adaptive Antoulas-Anderson (AAA) algorithm [3] combines the benefits of interpolatory methods and least-squares approximation to compute univariate rational approximants based on a set of function samples. A generalization to the AAA algorithm which enables approximations via multivariate rational functions has been introduced in [1] as the parametric AAA (p-AAA) algorithm. The method has been successfully used in order to obtain low-order surrogate models which precisely capture the behaviour of parametric dynamical systems and stationary models. In this talk, we present recent modifications to p-AAA to increase its viability for practical use cases amongst others by computing real-valued state-space representations of the p-AAA approximant and improving the conditioning of the numerical computations in various steps in the algorithm. Additionally, for the case in which p-AAA interpolates the input data, we introduce a post-processing step which guarantees that the interpolant is of minimal order and thus coincides with the parametric Loewner interpolant [2]. We illustrate these modifications via various benchmark models.

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Data-driven reduced-order modeling of thermo-mechanical models of machine tools

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Thermo-mechanical finite element models predict the dynamic behavior of machine tool systems during the manufacturing process. Such models consist of interconnected substructures, which may or may not be moving relative to each other. The main quantity of interest is the displacement of the tool center point from its desired location due to mechanical deformation, which is mainly caused by the system's constantly changing thermal field. Resulting numerical models are typically very large, and methods to reduce the computational complexity are therefore required for their efficient application in design and control [4, 3].
Machine tool systems typically consist of multiple interconnected substructures which may exhibit different properties, for example local nonlinearities. Maintaining independent (reduced-order) models for the substructures enables a flexible design process, as new machine designs can efficiently be assembled by combining the substructures. However, such models often have a high number of inputs and outputs to correctly model their interconnections and couplings.
In this contribution, we use a data-driven model order reduction method based on the Loewner framework to obtain reduced-order models of thermo-mechanical numerical models of machine tools. The method computes a reduced-order model from transfer function measurements only and does not require direct access to the discretized models. The resulting reduced-order models are required to preserve stability, as they should be used for time domain analysis [2]. A particular challenge for an effective model order reduction are the high number of inputs and outputs of the subsystems [1]. In the considered case, the matrix-valued transfer function is not fully populated, i.e. certain combinations of input and output mappings produce zero outputs.

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Stochastic reduced order models for Bayesian estimation problems in fluid mechanics

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We are interested in Bayesian inverse problem for fluid dynamics in real-time application context. 3D unsteady and turbulent fluid systems encompass poor Kolmogorov N-width decays. Therefore, drastic dimensional reduction – typically from 10^7 to 10 – yields important truncation errors. Furthermore, for long-time integrations, these errors grow possibly without bound. Closures alleviate truncation errors but without preventing divergences in long-time extrapolations. Besides, for Bayesian inverse problems such as ensemble-based data assimilation (DA), a single reduced order model (ROM) solution is not enough. We must generate relevant solution priors instead.
We address this priors emulation problem with an energy-preserving stochastic closure called "Location uncertainty models" (LUM) [3, 4] and new statistical estimators based on stochastic calculus, signal processing and physics [4]. The deterministic ROM coefficients are obtained by a Galerkin projection whereas the correlations of the noises are estimated from the residual velocity, the physical model structure, and the evolution of the resolved modes. Posterior distributions are then easily computed assimilating measurement streams with a particle filter [2].
Whether we consider the priors [4] or the posteriors [2] of the ROM solution, our method greatly exceeds the state of the art, for ROM degrees of freedom smaller than 10 and moderately turbulent 3D flows (Reynolds number up to 300).
Our methodology is now implemented on the OpenFOAM-based ROM library ITHACA-FV [5]. In order to address higher Reynolds numbers, we now consider the hyper-reduction (DEIM) [1] of non-polynomial terms appearing in turbulence models (e.g., large eddy simulation).

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A Reduced Basis Ensemble Kalman Method

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In the process of estimating the state dynamics of distributed-parameter systems, data from physical measurements can be incorporated into the mathematical model to reduce the uncertainty in the parameter estimates and, consequently, improve the state prediction. This process of data assimilation must deal with the data and model misfit arising from experimental noise as well as from model inaccuracies. In our study, we focus on the ensemble Kalman method (EnKM) [1], an iterative Monte Carlo method for the solution of inverse problems. The method is gradient-free and, just like the ensemble Kalman filter, relies on an ensemble of "particles" (here, a sample of parameter values) to identify the state that better reproduces the physical observations, while preserving the physics of the system as described by the model.
In this talk, we show how model order reduction can be combined with the EnKM to greatly accelerate the EnKM solution of inverse problems. In addition, we experimentally study the latter's performance with respect to different levels of noise and model error. Such numerical experiments, e.g., involving unknown distributed parameters in two or more spatial dimensions, can be very expensive and are (here) enabled only by the computational efficiency of the surrogate models. For a physical problem governed by non-linear parabolic partial differential equations, we investigate the role of the ensemble size on the reconstruction error and extend the method by introducing a measurement bias correction to improve the parameter estimate.

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Adapting Reduced Models for Importance Sampling

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We want to compute the probability of a rare event of the form $P(S(X) > L)$, with X a random vector in $\mathbf{R^d}$, with a computable density (up to a normalization constant), and S a real function that is very expensive to compute. We assume that we have a budget, i.e., a fixed number of complete evaluations of S, and that we can also build reduced-order models of S, which can be iteratively refined when new values of S are computed. We propose a fully adaptive algorithm to iteratively build an importance sampling distribution and draw from it, the objective being the evaluation of the probability of the rare event. The importance distribution takes the form of a Gibbs measure based on the current reduced order model, with parameters adjusted to minimize the relative entropy with respect to the target rare event probability distribution. A sequential Monte-Carlo technique generates from this Gibbs measure a swarm of particles, which is used as an empirical approximation of the importance distribution. At each iteration, a sample is drawn from the current empirical measure, the exact value of S calculated, the estimate of the rare event updated, as well as the reduced order model, the Gibbs measure, and the empirical sampling distribution. After the detailed presentation of the algorithm, we will give some heuristics. Some numerical results will also illustrate its relevance.

Data-Driven Enhanced Model Reduction for Bifurcating Models in Computational Fluid Dynamics

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We investigate various data-driven methods to enhance projection-based model reduction techniques with the aim of capturing bifurcating solutions. In particular, we use a three-step procedure of proper orthogonal decomposition (POD), dynamic mode decomposition (DMD) and manifold interpolation [7] to compute parametrized reduced order models for a cavity undergoing Hopf bifurcations with varying Grashof number [3], [6]. The approach can be extended to solution trajectories, which are not necessarily on the limit cycle but start from a common initial state for all trajectories correponding to the considered parameters with the Hankel-DMD [1], [5]. Addtionally, it is possible to resolve multiple solutions for a channel flow undergoing a pitchfork bifurcation [2] using localized model reduction and artificial neural networks [4], [5].

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Data driven reduced modelling of the Vlasov-Poisson equation

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Keywords: *Deep Learning, Hamiltonian systems, Model Order Reduction*

Nowadays, deep learning neural networks are widely deployed and they flourish in many fields of applications. We propose to use them to develop a new Model Order Reduction (MOR) technique for kinetics models. It will be elaborated on the Vlasov-Poisson model. Indeed, this model describes the evolution of a charged particle distribution submitted to an electromagnetic field. The latter may be self-consistent, i.e. generated by the above-mentioned distribution. In consequence dynamics can be strongly non-linear.
There exists symplectic POD (Proper Orthogonal Decomposition) methods for parametric MOR in the self-consistent case [2]. It achieves to preserve the Hamiltonian structure of the model. Nonetheless, this approach seems insufficient in strongly non-linear cases. We propose a new, efficient and scalable process based on neural networks to reduce the ODE derived from Vlasov and learn a reduced model with a preserved Hamiltonian structure. We use Hamiltonian neural networks [4] conjointly with autoencoders neural networks [1]. The latter is being used for MOR as in [3] however we rely on coupled learning for both networks and well-chosen learning constraints to ensure an adequate reduction with good stability properties.

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Parametric dynamic mode decomposition for nonlinear parametric dynamical systems

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A non-intrusive model reduction method which combines features of the dynamic mode decomposition (DMD) and the radial basis function (RBF) as a network, is proposed to predict the dynamics of parametric nonlinear dynamical systems. In lots of applications, the information of the whole system is not accessible, which motivates non-intrusive model reduction. The most complex point is to capture the dynamics of the solution without knowing the physics inside the "black-box" system. DMD is a powerful tool to mimic the dynamics of the system and give a reliable approximation in the time domain using only the dominant DMD modes. However, DMD cannot reproduce the parametric behaviour of the dynamics.
Our contribution focuses on extending DMD to parametric DMD by RBF interpolation. Specifically, a RBF network is first trained using snapshots at limited parameter samples. The snapshot matrix learned by the RBF network at any new parameter is passed to DMD to predict the time patterns of the dynamics corresponding to this new parameter sample. The proposed formulation and algorithm are tested and validated with numerical examples including models with parametrized and time-varying inputs. One of them is a complex and nonlinear Pseudo-two-dimensional (P2D) battery model, which is sequentially excited by a periodic current signal at a defined amplitude $0.77A$ but parametrized with the frequency $\omega \in [10^{-3}, 10^{4}]Hz$. We study the behaviour of the voltage as the output response to the parametrized current. In Figure 1, the time-evolution of the output at a new specific frequency $\omega^* = 3.69Hz$ computed by the proposed parametric DMD is compared with the reference solution obtained from direct numerical simulation as well as the solution computed by the RBF network only. The green lines separate the whole simulation into the training phase and the prediction phase. While the RBF solution cannot commit predictions beyond the training time period $[0, 0.6748s]$, it shows the prediction quality in the parameter domain. The DMD-RBF solution computed by the proposed method demonstrates good predictive performance in both the parameter and the time domain, which shows the flexibility and stability of the proposed parametric DMD.

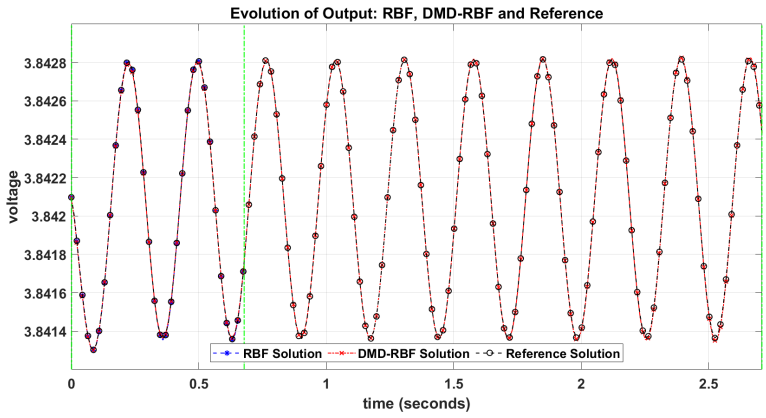

Figure 1: DMD-RBF prediction of the evolution of the voltage in a P2D-battery model

Dominant Subspaces of High-Fidelity Nonlinear Structured Parametric Dynamical Systems and Model Reduction

Peter Benner[1], **Pawan Goyal**[1], **and Igor Pontes Duff**[1]

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In this work, we investigate a model order reduction scheme for high-fidelity nonlinear structured parametric dynamical systems. More specifically, we consider a class of nonlinear dynamical systems whose nonlinear terms are polynomial functions, and the linear part corresponds to a linear structured model, such as second-order, time-delay, or fractional-order systems. Our approach relies on the Volterra series representation of these dynamical systems. Using this representation, we identify the kernels and, thus, the generalized multivariate transfer functions associated with these systems. Based on this, we aim at constructing reduced-order systems interpolating the generalized transfer functions from the original model at a given set of interpolation points. We show that if enough interpolation points are taken, the projection matrices of interpolation-based model reduction encode the reachability and observability subspaces of the system. Moreover, we propose an algorithm that enables the extraction of dominant subspaces from the prescribed interpolation conditions. This allows the construction of reduced-order models that preserve the structure. We demonstrate the efficiency of the proposed method by means of various numerical benchmarks.

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A greedy MOR method for the tracking of eigensolutions to parametric PDEs

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The present talk concerns the numerical solution to eigenvalue problems arising from parametric partial differential equations. Such mathematical models are used to describe various phenomena in engineering and design, statistics, biology and life science. While uncertainty quantification techniques for partial differential equations with parametric/stochastic inputs is an active research field, less attention has been devoted to eigenvalue problems.
Before any reasonable discretization, the regularity of the eigenvalue/eigenfunction solutions with respect to the parameters should be discussed. From this perspective, the main challenge is represented by the eigenvalue/eigenfunction crossings that might happen as the parameter values change. It is then of paramount importance to properly track all correct modes. So far, only few investigations have been carried on, mainly related to isolated eigenvalues [1, 2].
We consider an elliptic eigenvalue problem with a multi parametric dependence and we design an adaptive algorithm which minimizes the number of solves to guarantee the correct matching of the eigenvalues within a prescribed tolerance. The proposed scheme can be interpreted as a greedy model order reduction (MOR) method, where the greedy selection of the parameter values is guided by the a-priori cost functional introduced in [3] combined with a suitable a-posteriori strategy, capable of detecting possible mistakes in the output of the a-priori phase.
Several numerical examples are presented to display the performances and the effectiveness of the method.

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3.2 Tuesday, September 20

Randomization techniques for solving large scale linear algebra problems

L. Grigori[1]

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In this talk we discuss randomization techniques for solving large scale linear algebra problems. We focus in particular on solving linear systems of equations and eigenvalue problems. We first introduce a randomized Gram-Schmidt process for orthogonalizing a set of vectors and its block version. We discuss its efficiency and its numerical stability while also using mixed precision. Further randomized GMRES and randomized FOM methods are discussed for solving linear systems of equations as well as randomized Rayleigh-Ritz procedure for solving eigenvalue problems.

Model order reduction for Friedrichs' systems: a bridge between elliptic and hyperbolic problems

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Friedrichs' systems (FS) [3] are symmetric positive linear systems of first order PDEs that can describe many well known hyperbolic and elliptic problems in a unified framework. This allows, for example, to pass from one regime to another in different areas of the domain. One of the key ingredients of FS is the possibility of rewriting higher order derivative terms of PDEs through additional variables in the system of equations with only first order terms. This leads to a formulation composed by a linear combination of many block-structured fields $\mathcal{A}^k$ applied to the unknown z and its first order derivatives, i.e.,

$$\begin{cases} Az = f, \\ (\mathcal{D} - \mathcal{M})z = 0, \end{cases} \qquad \text{with} \qquad \begin{cases} Az = A_{(0)}z + A_{(1)}z, \\ A_{(0)}z = \mathcal{A}^0 z, \\ A_{(1)}z = \sum_{k=1}^{d} \mathcal{A}^k \partial_{x_k} z, \end{cases}$$

where $\mathcal{D}$ and $\mathcal{M}$ are boundary fields, one given by the problem and the second used to impose the boundary conditions. Under some coercivity assumptions on the fields, the existence, uniqueness and well-posedness of the problem can be proven in different forms (strong, weak, ultraweak).
A series of (linear) discontinuous Galerkin (DG) methods has been proposed [5, 2] to solve FS accurately. Moreover, the error analysis performed in [1] provides an error estimator for the methods.
Now, if one introduces physical parameters in the blocks of the fields defining the system, one obtains very different problems. In order to speed up the computational costs of many-query simulations of FS, one can resort to classical reduced order methods such as POD and greedy algorithms [4]. The error analysis available at the DG level can be used for a sharp error estimator in the reduced order method that certifies the accuracy of the reduced method. Moreover, it leads to an efficient offline phase for the greedy algorithm.
We will show some simulations of various problems passing through different regimes using the same framework for all of them: advection-diffusion-reaction problems, linear elasticity problems, curl-curl problems. The preliminary results show an incredible reduction in computational costs for simulating FS thanks to the reduced order method.

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Nonlinear model order reduction for hyperbolic conservation laws by means of diffeomorphic transformations of space-time domains

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Parametrized hyperbolic conservation laws constitute a severe difficulty for model order reduction due to moving and interacting shock fronts and discontinuities. The solution manifold suffers from a slow decay of the Kolmogorov n-width, see [1] and [4], making it impossible for linear approaches like the reduced basis method to achieve accurate approximations.
We propose a nonlinear approach based on diffeomorphic transformations of space-time domains, allowing to align shocks, and thus, to overcome this drawback of linear methods. By considering solutions depending on space and time, shock interactions are directly incorporated into the snapshots. The transformations are treated as elements from the diffeomorphism group, which forms a Lie group, i.e. it has the structure of a smooth manifold. Associated with the Lie group of diffeomorphisms is the Lie algebra of smooth vector fields that parametrizes parts of the Lie group by geodesic evolution in the diffeomorphism group. The Lie algebra of smooth vector fields forms a vector space. Therefore, we can apply well-known algorithms from linear model order reduction to obtain a reduced model for the vector fields, see for instance [5]. Numerical experiments show the potential of the proposed algorithm for hyperbolic problems like Burgers' equation.
The method uses ideas similar to geodesic shooting in image registration, mainly developed in [2], and shows strong connection to differential geometry and the theory of Lie groups and Lie algebras. Further, the approach is motivated by the method of freezing, discussed in [3], which was restricted to problems without interaction of discontinuities.

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Adaptive POD-DEIM correction for Turing pattern approximation in reaction-diffusion PDE systems

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In this talk we focus on the stabilization of the POD-DEIM technique for the numerical approximation of Turing patterns, that are stationary solutions of reaction-diffusion PDE (RD-PDE) systems. We show that solutions of surrogate models built by classical POD-DEIM (see e.g. [2, 3]) exhibit an unstable error behaviour over the dimension of the reduced space. To overcome this drawback, we add a correction term as for e.g. [5, 4] that provides missing information to the reduced model and we apply the POD-DEIM technique to the corrected model (see [1]). To further improve the computational efficiency, we propose an adaptive version of this algorithm in time that accounts for the peculiar dynamics of the RD-PDE in presence of Turing instability. We show the effectiveness of the proposed methods in terms of accuracy and computational cost for a selection of RD systems, i.e. FitzHugh-Nagumo, Schnackenberg and the morphochemical DIB models, with increasing degree of nonlinearity and more structured patterns.

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Matrix-free Transfer Function Prediction using Model Reduction and Machine Learning

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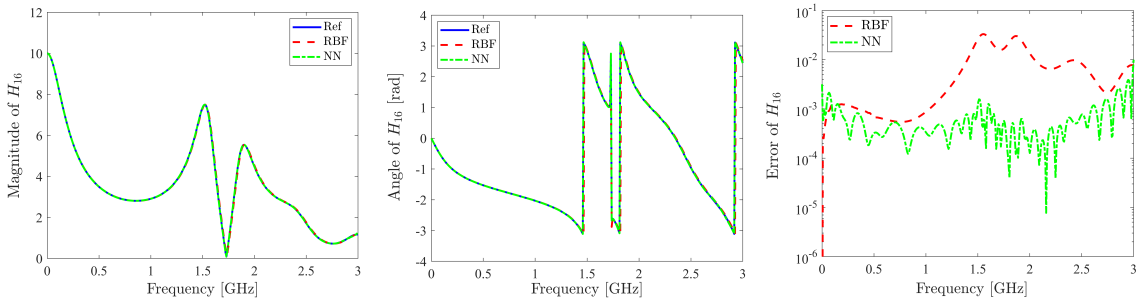
We propose a technique for fast predicting the transfer function of dynamical systems without information of system matrices by combining machine learning with model order reduction. The transfer function of a linear time invariant system can be written as $H(s) = CG(s)^{-1}B$. In some situations, it is difficult to obtain the individual system matrices that are implicitly included in $G(s)$. The only information available is the data of $G(s)$ at samples of frequency s. The proposed method derives a reduced-order model of the transfer function in the form of neural networks using limited data of $G(s)$. Discrete reduced transfer functions at training samples $s_i, i = 1, \ldots, l$, of the frequency are firstly generated based on the data of $G(s)$ at those training samples, i.e. $\hat{H}(s_i) = \hat{C}\hat{G}(s_i)^{-1}\hat{B}$. A reduced-order model of the original transfer function as a continuous function of the frequency is then learned using the data of the discrete reduced transfer functions. The original transfer function at any testing frequencies can then be quickly predicted using either a compact machine learning model or a deep learning model with a few layers. The discrete reduced transfer functions used as training data for machine learning, are guaranteed to be accurate thanks to a cheap and sharp error estimator. If only the data of the original transfer function are available, then the proposed machine/deep learning methods can be directly applied without generating the data of the discrete reduced transfer function. The proposed methods are tested on two PEEC models with many delays, efficiency and accuracy of the reduced-order models are demonstrated.

In the following Figure 1, we show some results for one of the two test examples used in the full paper, a powerbus model. In the figure, "Ref" refers to the original transfer function at 400 testing frequencies. The subscript "16" means the transfer function associated with the input port 6 and output port 1. "RBF" is the transfer function predicted by radial basis function (RBF) networks. "NN" corresponds to the transfer function predicted by deep feed forward neural networks. All the neural networks are trained using 200 training frequencies. It is seen that the neural networks predict the original transfer function accurately. Results for other input ports and output ports are also sufficiently accurate and are with errors below $O(10^{-2})$. The proposed methods have similar performance on the second example.



(a) Magnitude of H_{16}. (b) Angle of H_{16}. (c) Error of H_{16}.

Figure 1: Experimental results for a powerbus example.

Deep-Reinforcement-Learning-informed Adaptive Refinement for High-order Discontinuous Galerkin Methods

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Discontinuous Galerkin (DG) finite element methods have enjoyed considerable success as a flexible and robust technique for the numerical solution of partial differential equations [3]. One of the advantageous features of DG methods is its element-locality and weak element-to-element coupling, which allow for straightforward adaptive refinement, given an error estimator. The discontinuous nature of the DG polynomial spaces in which the numerical solution is sought additionally provide a natural error estimator, the so-called non-conformity (NCF) indicator [5]. The NCF estimator is based on the assumption that the exact solution is physically continuous, implying that jumps in the numerical solution can be seen as a measure of error. However, despite the generality of this estimator, it is unable to take into account temporal or non-local patterns and remains a relatively uninformed heuristic. On the other hand, deep reinforcement learning provides a very general framework for learning action policies in complicated settings by rewarding good strategies and penalizing undesirable ones through trial and error [1]. Recent work to incorporate deep learning into finite element methods is in its infancy, and has focused on either on only classical continuous Galerkin schemes or on other aspects of DG-FEM unrelated to adaptive refinement [6, 2, 4]. We investigate the application of deep reinforcement learning as an approach to augment or replace the state-of-the-art error estimators such as the NCF and heuristic adaptive refinement strategies. We demonstrate the methodology on test cases in computational physics.

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On error estimates for reduced models obtained by balanced truncation

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A priori error bounds have been derived for different balancing-related model reduction methods. The most classical result is a bound for balanced truncation and singular perturbation approximation that is applicable for asymptotically stable linear time-invariant systems with homogeneous initial conditions. Recently, there have been a few attempts to generalize the balancing-related reduction methods to the case with inhomogeneous initial conditions [1, 2], but the existing error bounds for these generalizations are quite restrictive. Particularly, it is required to restrict the initial conditions to a low-dimensional subspace, which has to be chosen before the reduced model is constructed. In the contribution [3], we propose an estimator that circumvents this hard constraint completely. Our estimator is applicable to a large class of reduction methods, whereas the former results were only derived for certain specific methods. Moreover, our approach yields to significantly more effective error estimation, as also will be demonstrated numerically.
If time permits, we point towards the treatment of differential-algebraic equations and other potential extensions and implications of the new estimator.

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Automated model reduction for pharmacology models

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Quantitative systems pharmacology (QSP) and physiologically-based PK (PBPK) models are often too complex for population analysis in a clinical setting [5]. Developing an automatic and robust workflow for model reduction may help fill this gap [2, 6, 7, 8]. We constructed a computational pipeline in MATLAB that loads SimBiology models and allows users to define constraints (species of interest). We symbolically prepare nonlinear models to avoid linearizations and associated errors. Reduced-order models are automatically determined for a given model through proper lumping, where simulated annealing searches for the best lumping matrices for a given model order and a selection criterion determines the best reduced model [1, 3, 4]. This pipeline is applied to reduce the number of species and parameters, either separately or together. Then, the robustness of the selected reduced model is assessed at various doses and parameter values. The pipeline was applied to several nonlinear models, where predefined species of interest from the reduced models minimally deviated from the full models. Most notably, one model is reduced from 14 to 12 species and 38 to 22 parameters, while another is reduced from 17 to 11 species and 33 to 7 parameters. Our novel approach allows for automatic reduction of several types of models, while retaining high accuracy. The simplified models will be better suited for future population analyses.

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A structure-preserving DEIM formulation for non-linearly stable hROMs of the incompressible Navier-Stokes equations

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An issue of increasing interest in projection-based reduced order modeling of conservation laws is the preservation of the conservative structure underlying such equations at the reduced level ([2], [3]). A non-linearly stable POD-Galerkin ROM of the incompressible Navier-Stokes equations that globally conserves kinetic energy (in the inviscid limit), momentum and mass on periodic domains was constructed in [2]. The quadratic nonlinearity in the convection operator was dealt with using an exact tensor decomposition to eliminate the dependence of the computational scaling of the ROM on the FOM dimensions. However, such a cubic tensor decomposition is not always feasible: in case many POD modes are required (cases with slow Kolmogorov N-width decay), the exact decomposition becomes prohibitively expensive. One possible solution is the use of hyper-reduction methods such as the discrete empirical interpolation method (DEIM) [1]. The DEIM generally does not retain the conservative structure of the ROM to which it is applied and, as a consequence, non-linear stability of the ROM of the incompressible Navier-Stokes equations proposed in [2] is no longer guaranteed.

In this work we propose a novel DEIM formulation that allows us to construct a non-linearly stable hyper-reduced order model (hROM) of the incompressible Navier-Stokes equations. The hROM has the same mass, momentum and energy conservation properties as the ROM proposed in [2], but does not suffer of prohibitive computational scaling when the number of POD modes is increased. In detail, the proposed structure-preserving DEIM formulation is a rank-one correction of the conventional DEIM method which can be calculated efficiently with the Sherman-Morrison inverse formula. This results in a structure-preserving DEIM formulation that has equivalent computational scaling as the conventional DEIM, but provides provably stable, structure-preserving hROMs.

We implement the structure-preserving DEIM formulation in a hROM of the incompressible Navier-Stokes equations based on the ROM proposed in [2]. The computational cost associated with the hROM is compared to the ROM employing the cubic tensor decomposition for several convection-dominated flow configurations with slow Kolmogorov N-width decay, for example: turbulent channel flow, shear-layer instabilities, and the Taylor-Green vortex.

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Model Reduction of Navier-Stokes Equations using the Loewner Framework

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The Loewner framework is extended to compute reduced order models (ROMs) for systems governed by the incompressible Navier-Stokes (NS) equations. For quadratic ordinary differential equations (ODEs) it constructs a ROM directly from measurements of transfer function components derived from an expansion of the system's input-to-output map. Given measurements, no explicit access to the system is required to construct the ROM. To extend the Loewner framework, the NS equations are transformed into ODEs by projecting onto the subspace defined by the incompressibility condition, as in e.g., [1, 3, 5]. This projection is used theoretically, but avoided computationally.
A number of extensions over [1, 5] are presented. Specifically, system outputs involving the pressure lead to quadratic terms in the output of the projected system. These quadratic terms are systematically included. In addition, a number of computational issues are addressed that allow implementation of the approach using the trilinear form for the Navier-Stokes equations, rather than expressing it using the Kronecker product typically used to derive the ROM.
The straight forward application of the Loewner approach to the incompressible NS equations can lead to unstable ROMs [5]. This was already observed for Burgers' equation in [2] and in [4] for a related interpolation based ROM. Following [2, 5] a possible approach, which currently requires access to the NS system, to deal with these instabilities is outlined, and studied for specific systems.

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Model order reduction for turbulent and compressible flows: hybrid approaches in physics and geometry parametrization

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In this talk we will review recent developments on reduced order models for turbulent compressible flows.
In order to have an accurate turbulent model, we merge projection-based methods and data-driven techniques. The model utilizes classical Galerkin-projection method to solve for the reduced degrees of freedom approximating velocity and pressure. Instead, a data-driven technique for the approximation of the eddy viscosity solution manifold is employed.
As regards pressure stabilization, it is a matter that occurs both at the Full Order and at the Reduced Order levels, thus several different strategies have been developed in order to overtake the obstacle.
In this work the idea is to follow the segregated algorithms employed at the full order level also at the reduced level so that it is possible to have both a stable pressure recovery and a coherent reduced procedure at the same time. These type of segregated approaches are quite widespread in almost all finite volume solvers. The methodology is introduced for laminar incompressible flows and extended [1] to turbulent [2] and turbulent-compressible flows [3]
We show some results obtained by its application on problems with both physical and geometrical parametrization.

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POD-Based Adaptive Model Reduction to Accelerate Computational Fluid Dynamics

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Reduced order modeling is a popular approach that generates surrogate models [1] by using data generated by high-dimensional models (HDMs). Unfortunately, stability issues and failure to generalize beyond training make reduced order models (ROMs) unreliable in an industrial setting [1]. This is particularly the case when modeling time-dependent nonlinear problems such as those usually found in viscous or high-speed CFD problems. Generating enough training data to make ROMs generalize is often infeasible. Taking this shortcoming into consideration, adaptive reduced order methods (AROMs) [3] improve predictive capabilities by frequently updating the reduced basis with local spatial-temporal HDM data. However, AROMs have several issues still to be addressed. The computational cost of AROMs also needs to be carefully examined given that the HDM needs to be frequently locally solved.

Our work relies on several techniques to improve AROMs capabilities. First, we developed implicit HDM local surrogates with good accuracy and stability properties. The implicit time marching methods required by some problems (e.g., viscous flow) cannot provide the local solutions needed by adaptive ROMs because the numerical domain of dependence is the entire computational grid. Second, literature results [3] rely on the adaptive discrete empirical interpolation method (ADEIM) to update the reduced basis. Preliminary results show that updating the basis through proper orthogonal decomposition (POD) is superior in regards to sampling size, stability and accuracy. Third, initial results show that AROMs can go unstable. In fact, combining local HDM and ROM solutions without any further consideration leads to spurious oscillations which in turn lead to unstable solutions. Therefore, these methods benefit from explicit filtering techniques [2] used by HDMs. Additionally, we propose a residual-based adaptive sampling algorithm as opposed to a fixed-size sampling procedure. Finally, our methodology is successfully applied to two-dimensional unsteady flow problems with shock waves.

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Model reduction for dynamics on deformable complex surfaces.

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Dynamics of deforming surfaces, 2-dimensional objects embedded in 3D spaces, are governed by Newton's law of motion for mechanical systems under internal and external forces, $\mathbf{M}\ddot{q}(t) = f_{int}(q(t)) + f_{ext}$. Simulating such structures is very expensive, especially under real time changing internal forces acting on vertices and/or their connected faces, particularly when the meshes under consideration include hundreds of thousands of vertices.

Exploiting the variational formulation of the system, positions $q(t) \in \mathbb{R}^{N\times 3}$ of vertices at different time steps, can be written as a minimizer that compromises between both associated momentum and potential energies. The computations then divided into many parallel local nonlinear solves and one linear global solve; this is known as the projective dynamics scheme [2].

The nonlinear internal forces, such as bending and strain, express and control the material behavior of the surface as a geometrical object and they require re-computation at every time step. External forces typically remain constant during computations. We explore different model reduction techniques to tackle the computational complexity of simulating deformable surfaces. To find a low dimensional subspace, we consider different candidate methods, namely localized sparse-PCA [4] and localized quaternion-PCA [1]. We also compare to skinning subspaces which have been earlier used [3]. Figure 1 bellow shows the first 8 sparse localized PCA components extracted using a simple simulation for the bunny mesh falling under gravitational forces.

(a) Original object

Figure 1: First 8 sparse-PCA components under gravitational force simulation for a bunny object. Each component is localized around the vertex that shows the largest change. Normalized weights associated to different components are shown in blue.

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Nonlinear Model Order Reduction for Three-dimensional Discretized FE Models using Graph Convolutional Autoencoders

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Besides classical data-driven dimensionality reduction techniques like proper orthogonal decomposition (POD), autoencoders (AEs) have been established as a nonlinear alternative in the field of model order reduction (MOR) as in [1]. They are well-suited to find low-dimensional representations of high-dimensional systems by incorporating a "bottleneck" in their architecture. Compared to classical approaches, AEs relying on fully connected layers have disproportionately more adjustable parameters resulting in an expensive offline trainings-phase that requires vast amounts of resources.
An often used remedy are convolutional neural networks (CNNs) [2, 3]. They can exploit geometric patterns in the data and construct complex patterns from small and basic patterns that are stored in their filters. Often, they are used in Euclidean domains with grid-based structured data. Unfortunately, data obtained from finite element (FE) models are usually not spatially discretized in a grid-like structure but in a complex three-dimensional shape. Hence, the generalization of CNNs to such models is not trivial.
FE models, however, can be represented in a graph-like structure enabling the usage of graph convolutions. They share with the conventional version the property of recognizing local patterns but lack the feature of dimensionality reduction. Hence, graph convolution autoencoders (GCA) must be combined with mesh reduction techniques to be successfully applied in the context of MOR similar as it already has been done in computer vision [4].
This enables the efficient identification of low-dimensional coordinates with which the system can be described. With these coordinates, the connection between simulation parameters and system behavior can be learned efficiently within the autoencoder itself or with any other regression algorithm.
We demonstrate the capabilities of this approach on high-dimensional static as well as dynamic problems, including human body models and crash simulations [5]. Furthermore, the methodology is compared to more widespread approaches like POD-based data-driven model reduction.

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Nonlinear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method

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Non-affine parametric dependencies, nonlinearities and advection-dominated regimes of the model of interest can result in a slow Kolmogorov n-width decay, which precludes the realization of efficient reduced-order models based on linear subspace approximations. Among the possible solutions, there are purely data-driven methods that leverage autoencoders and their variants to learn a latent representation of the dynamical system, and then evolve it in time with another architecture. Despite their success in many applications where standard linear techniques fail, more has to be done to increase the interpretability of the results, especially outside the training range and not in regimes characterized by an abundance of data. Not to mention that none of the knowledge on the physics of the model is exploited during the predictive phase. In order to overcome these weaknesses, we implement the nonlinear manifold method introduced by Carlberg et al [2, 1] with hyper-reduction achieved through reduced over-collocation and teacher-student training of a reduced decoder [3]. A scheme of the new procedure is shown in Figure 1 [1]. We test the methodology on a 2d nonlinear conservation law and a 2d shallow water models, and compare the results obtained with a purely data-driven method for which the dynamics is evolved in time with a long-short term memory network.

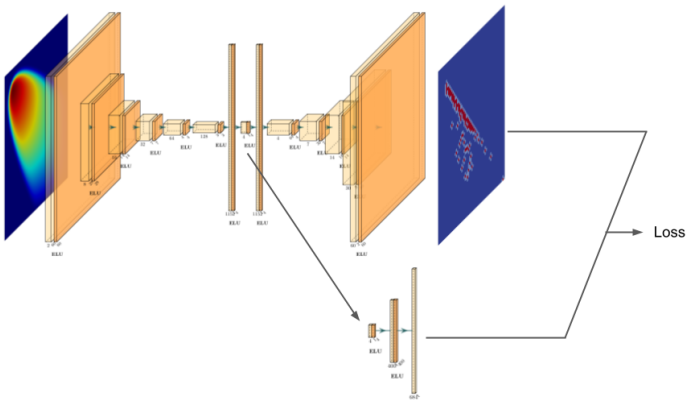

Figure 1: Teacher-student training of the compressed decoder for the 2d non-linear conservation law test case. The magic points, which the snapshots are restricted to, are shown in red over the domain.

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Learning to Forecast Dynamical Systems from Streaming Data

R. Ward[1]

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Kernel analog forecasting (KAF) is a powerful methodology for data-driven, non-parametric forecasting of dynamically generated time series data. This approach has a rigorous foundation in Koopman operator theory and it produces good forecasts in practice, but it suffers from the heavy computational costs common to kernel methods. In this talk, we will discuss a streaming algorithm for KAF that only requires a single pass over the training data. This algorithm dramatically reduces the costs of training and prediction without sacrificing forecasting quality. Computational experiments demonstrate that the streaming KAF method can successfully forecast several classes of dynamical systems. The overall methodology may have wider interest as a new template for streaming kernel regression.

This is joint work with Dimitris Giannakis, Amelia Henriksen, and Joel Tropp.

Non-intrusive multi-physics PGD-based reduced model for the modeling of power electronic modules

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Power electronic modules transform the electrical grid current with respect to the need of the motor, and are key components of numerous electrical systems. Power modules are made of an assembly of multiple materials with different constitutive properties (Fig. 1). The self-heating of the chip by Joule's effect and the difference of thermal expansion coefficients generate thermal stresses leading to crack propagation. In return, the crack modifies the module behavior by increasing electrical and thermal resistances. Cracks ultimately lead to module failure [1]. The accurate modeling of the electro-thermo-mechanical module behavior is of paramount importance to predicting the module lifetime. However, multiple uncertainty sources decrease the reliability of lifetime models. Uncertainty quantification studies need to evaluate the lifetime model a high number of times and thus require a reduced model.

In this work, we developed a reduced-order model based on the Proper Generalized Decomposition (PGD) [2, 3] to obtain an explicit representation of the solution with respect to space, time, and design parameters. The considered types of design parameters are material properties and geometric parameters. The studied model is a realistic industrial model that requires commercial finite element software, ANSYS. PyAnsys python packages are used to work interactively with ANSYS and to develop a non-intrusive approach to build the reduced model. To solve the multi-physics problem, a specific method has been developed. First, a strongly coupled electro-thermal problem is solved using an iterative method in which the crack length is parametrized. Then, the mechanical problem is solved in which the temperature field is the input. The crack length evolution, modeled with a cohesive zone model, is then obtained from the mechanical solution.

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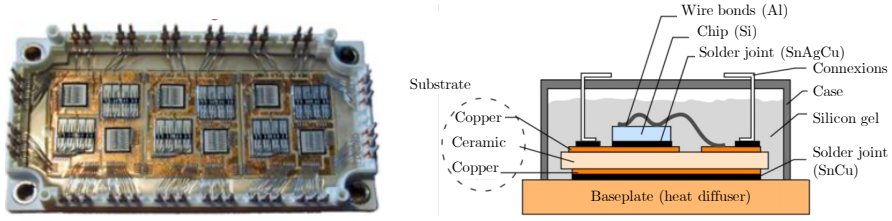

Figure 1: IGBT power electronic module and schematic representation of its components.

Full Order Model and Reduced Order Model Consistency for Evolve-Filter-Relax Regularization

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The goal of this talk is to provide a recipe to alleviate the spurious oscillations generally produced by full order models (FOMs) in marginally-resolved simulations of convection-dominated incompressible flows. In a parametric setting (in our case for time-dependent and physical parametric problems), these simulations can be unbearable in terms of computational time and resources.
We propose Proper Orthogonal Decomposition-based reduced order models (ROMs) to solve them in a smaller amount of time. Specifically, we investigate whether the evolve-filter-relax (EFR) numerical stabilization is needed both at the FOM and the ROM level.
Indeed, we present two ROM strategies:

(i) the EFR-noEFR, in which the EFR stabilization is used at the FOM level and not at the ROM level.

(ii) The EFR-EFR, in which the EFR stabilization is used both at the FOM and at the ROM level.

We perform the reduction in terms with respect to both time and Reynolds number for a 2D incompressible flow past a circular cylinder. The results are both reconstructive and predictive and they suggest that FOM-ROM consistency is beneficial in the proposed setting [1].

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Hyper-reduction of geometrically parameterized nonlinear microstructures

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To study the effect of microstructures onto effective macroscopic properties, two-scale simulations are often employed, where the macroscopic constitutive model is replaced by a microscopic partial differential equation (PDE) that is defined on a representative volume element (RVE), and which needs to be solved at every macroscopic quadrature point. Such simulations are typically expensive and therefore infeasible in multi-query contexts such as material design or optimization. To overcome this issue, the microscopic PDE needs to be replaced by a fast-to-evaluate surrogate model. Since the final goal is to employ the surrogate model for two-scale shape optimization, it must be accurate for a wide range of loading and geometrical parameters.
One popular method for parametric model order reduction is the Reduced Basis (RB) method [3], in which one finds a reduced solution space from pre-computed solution snapshots, for example using a proper orthogonal decomposition (POD). However, to achieve a high speed up for non-linear problems, a further reduction, termed hyper-reduction, is required. Hyper-reduction deals with finding a reduced set of integration points and corresponding weights. One possible approach is the Empirical Cubature Method (ECM) [1]. Geometrical parameters are typically dealt with by mapping the snapshots onto a parent domain. When the transformation map is known, the problem can then be solved on the parent domain. In the context of RB, related works often find these transformations using either free-form deformations or radial basis functions (see, e.g., [4]). However, these transformations are rather inflexible.
In this contribution, we obtain the transformation map by solving an auxiliary linear PDE (see, e.g., [2]). With the transformations available for all snapshots, we utilize POD to find a reduced basis on the parent domain, and, by using an adapted version of ECM, we then obtain a reduced set of integration points and weights that is accurate for a wide range of geometries.
To validate the methodology, several composite microstructures are tested, consisting of hyperelastic and elasto-plastic materials, and considering rotations and shape variations of the inclusions. At last, the surrogate model is tested in a full two-scale example, where, compared with the full simulation, a high accuracy in both local and global quantities as well as a high speed up is achieved.

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Two-Scale Reduction of LOD Multiscale Models

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The Localized Orthogonal Decomposition (LOD) method is a successful recent approach for the numerical solution of multiscale PDE problems with or without scale separation (see [3] and references therein). The LOD is based on the idea of splitting the solution space into a negligible fine-scale space, given by the kernel of a coarse-mesh interpolation operator, and an energy-orthogonal multiscale space, in which the solution is sought. To obtain the multiscale space, fine-scale corrector problems need to be solved for each basis function of the coarse-mesh finite element space. Due to the fast decay of the corrector functions, the corrector problems can be approximated by restricting the domain to a patch of coarse-elements around the support of the respective basis function. Thus, similar to other numerical multiscale methods, the computational effort is split into the solution of many small local fine-scale problems and the solution of a globally coupled effective coarse-scale problem.
To accelerate the solution of large parameterized multiscale problems in a multi-query context, a natural approach is to combine the LOD with Reduced Basis (RB) methods. In [1] an RB-LOD scheme was introduced in which the corrector problems are replaced by corresponding RB surrogate models. However, for very large problems also the solution of the coarse-scale problem requires relevant work, which is not addressed by this approach. Also, the error in the LOD solution induced by the RB approximation of the corrector problems is not rigorously controlled.
In this contribution we present an efficient two-stage two-scale model reduction approach for the LOD which takes both the fine and coarse scale of the problem into account [2]. It is based on a new two-scale formulation of the LOD for which we show well-posedness and stability. By applying the RB method to this formulation, we obtain a surrogate model of small dimension independent of the size of the coarse- and fine-scale meshes. Rigorous a priori and a posteriori bounds control the model reduction error. Numerical experiments yield speedup factors of up to 1000 over an approach similar to [1] where only the corrector problems are reduced.

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Adaptive Localized Reduced Basis Methods in Multiscale PDE-Constrained Parameter Optimization

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PDE-constrained parameter optimization problems with large- or multiscale applications easily exceed computational resources if standard approximation methods are employed for the underlying forward problem. For the involved parameterized partial differential equations, the reduced basis (RB) method is a model order reduction (MOR) method allowing for an efficient and certified approximation of the solution manifold. Admittedly, for problems with a slow convergence of the Kolmogorov n-width, e.g., with a high-dimensional parameter space, the offline phase for constructing a sufficiently accurate surrogate model can be prohibitively large.
To remedy this, we discuss more recent approaches that go beyond the classical offline-online splitting of MOR methods and adaptively build a surrogate model along the optimization path. The design of error-aware trust-region reduced basis (TR-RB) methods [1, 4] allows for localizing the reduction with respect to the parameter space and enables a certified optimization method with a high convergence rate. On the other hand, localized model order reduction techniques can replace the high-dimensional full-order model in scenarios where standard approximation schemes fail. A recently proposed approach in the context of multiscale problems is the two-scale reduced basis localized orthogonal decomposition method (TSRBLOD) [3], which is particularly suitable for the design of localized TR-RB methods [2]. In addition, we can use a relaxation of the outer trust-region optimization loop, also proposed in [2], allowing for a rigorous convergence result but converges much faster due to larger step sizes in the initial phase of the iterative algorithm.
In this talk, we present many different aspects of the TR-(L)RB algorithm with particular emphasis on a posteriori error estimation, the convergence of the overall optimization method, and numerical experiments that demonstrate the applicability of our approach. To this end, we focus on several different aspects of the algorithm in both the optimization loop as well as the full- and reduced-order models.

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Model reduction of convection-dominated partial differential equations via optimization-based implicit feature tracking

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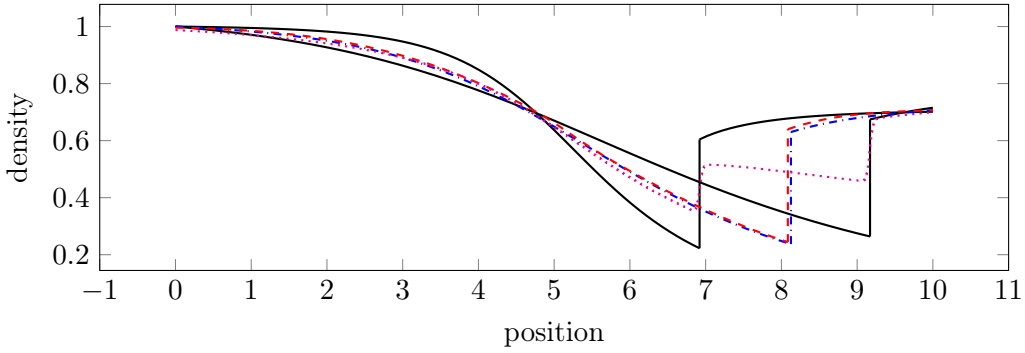
Partial differential equations (PDEs) that model convection-dominated phenomena often arise in engineering practice and scientific applications, ranging from the study of high-speed, turbulent flow over vehicles to wave propagation through solid media. The solutions of these equations are characterized by local features or disturbances that propagate throughout the domain as time evolves or a system parameter varies. Numerical methods to approximate these solutions require stabilization and fine, usually adaptive, grids to adequately resolve the local features, which lead to expensive discretizations with a large number of degrees of freedom. Projection-based model reduction methods tend to be ineffective in reducing the computational cost of such problems due to a slowly decaying Kolmogorov n-width of the solution manifold.

To avoid the fundamental linear reducibility limitation associated with convection-dominated problems, we construct a nonlinear approximation by composing a low-dimensional linear space with a parametrized domain mapping [1, 2]. The linear space is constructed using the method of snapshots and POD; prior to compression, each snapshot is composed with a mapping that causes its local features to align (same spatial location) with the corresponding features in all other snapshots. The parametrized domain mapping is chosen such that the local features present in the linear space deform to the corresponding features in the solution being approximated, effectively removing the convection-dominated nature of the problem. The domain mapping is determined implicitly through the solution of a residual minimization problem, rather than relying on explicit sensing/detection. We provide numerous numerical experiments to demonstrate the effectivity of the proposed method on benchmark problems from computational fluid dynamics.



Comparison of the HDM, L^2 projection (without snapshot alignment), and ROM-IFT on a nozzle flow problem with two training parameters. Legend: training snapshots (——), HDM solution at test parameter (-·-·-), L^2 projection of test parameter onto reduced basis (·····), and ROM-IFT solution at test parameter (- - -).

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3.3 Wednesday, September 21

Simulation-based Bayesian inference and surrogate modeling

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Many practical Bayesian inference problems fall into the simulation-based or "likelihood-free" setting, where evaluations of the likelihood function or prior density are unavailable or intractable; instead one can only draw samples from the joint parameter-data prior. Learning conditional distributions is essential to the solution of these problems. To this end, I will discuss a powerful class of methods for conditional density estimation and conditional simulation based on transportation of measure, and elucidate links between these methods and surrogate modeling. An important application for these methods lies in data assimilation for dynamical systems, where transport enables new approaches to nonlinear filtering and smoothing. I will also present new results on the joint dimension reduction of data and parameters in data assimilation and other non-Gaussian inference problems.

This is joint work with Ricardo Baptista, Max Ramgraber, Alessio Spantini, and Olivier Zahm.

Deep learning and the dynamical low-rank approximation

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The dynamical low-rank approximation [4, 6] is a reduced-order modeling technique that evolves a low-rank matrix or tensor approximation of a PDE or data-driven dynamics. It may be applied to high-dimensional deterministic problems where a fine mesh or large domain is required, or to stochastic problems, where a reduced-order Monte Carlo system is evolved, enabling inference on non-Gaussian distributions for uncertainty quantification. Recently, rank-adaptive integration schemes have been developed [5, 2, 1]. However, the proposed criteria for when and how to augment or decrease the rank of the solution are either computationally costly or heuristic and greedy; they usually only evaluate the system its current state in a Markov sense without regard for past or future states. Furthermore, the rank of the system is highly sensitive to the system's parameterization, particularly the choice of coordinates, which can be relatively arbitrary. We investigate deep learning techniques such as reinforcement learning and neural delayed equations [3] as alternative approaches to these heuristics choices. In learning how to better augment and parameterize our system, we develop schemes that adapt the subspace as we integrate in time, which better captures the dynamic, high-order curvature of the low-rank manifold. Because we combine techniques from numerical mathematics and machine learning, we preserve convergence guarantees and interpretability while improving accuracy and computational efficiency. We demonstrate this methodology on test cases in computational ocean acoustics.

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Generalized Neural Closure Models with Interpretability

Abhinav Gupta[1] **and Pierre F.J. Lermusiaux**[1]

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Complex dynamical systems are used for predictions in many domains. Because of computational costs, models are truncated, coarsened, or aggregated. As the neglected and unresolved terms become important, the utility of model predictions diminishes. In our recently published work [1], we developed a novel neural delay differential equations (nDDEs) based framework to learn closure parameterizations for known-physics/low-fidelity models using data from high-fidelity simulations or high-resolution data, and increase the long-term predictive capabilities of the original models. The need for the time-delays in these *neural closure models* is rooted in the presence of inherent delays in real-world systems and justified by the Mori-Zwanzig formulation. In the present study, we develop the unified neural partial delay differential equations (nPDDEs) theory which augments low-fidelity models in their partial differential equation (PDE) forms with both Markovian and non-Markovian closure parameterized with neural networks (NNs). The amalgamation of low-fidelity model and NNs in the continuous spatio-temporal space followed with numerical discretization, automatically allows for generalizability to computational grid resolution, boundary conditions, initial conditions, and provide interpretability. We provide adjoint PDE derivations in the continuous form, thus allowing one to implement across differentiable and non-differentiable computational physics codes, different machine learning frameworks, and also allowing for nonuniformly-spaced spatio-temporal training data. We demonstrate the ability of our new framework to discriminate and learn model ambiguity in the advecting shock problem governed by the KdV-Burgers PDE and a biogeochemical-physical ocean acidification model in an interpretable fashion. We also learn the subgrid-scale processes and augment model simplification in those models, respectively. Finally, we analyze computational advantages associated with our new framework.

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Conditional gradient-based Identification of Non-linear Dynamics

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Sparsity of nonlinear dynamical models extracted from data is an attractive feature for the numerical efficiency of surrogate models as well as for the inference of interpretable governing laws from observations. Symbolic regression approaches like *Sparse Identification of Nonlinear Dynamics* (SINDy) [1] solve a data-fitting problem such as

$$\min_{\xi\in\mathbb{R}^n} \sum_{i=1}^{k} \left\| \dot{x}_i - \sum_{j=1}^{n} \xi_j f_j(x_i) \right\|^2$$

for coefficients ξ_j for a potentially huge library of n atoms f_j, subject to some sparsity-enhancing constraint or penalization such as the *Least Absolute Shrinkage and Selection Operator* [4] leading to a ℓ^1 constraint $\|\xi\|_1 \le \alpha$.
A large variety of methods are available for solving the resulting optimization problem. We propose the efficient first-order Conditional Gradient [3] algorithm CINDy (named as an hommage to SINDy) for its solution [2]. In comparison to the most prominent alternative algorithms, the new algorithm shows significantly improved performance on several essential issues like sparsity induction, structure preservation, noise robustness, sample efficiency, and predictive power. We demonstrate these advantages on several dynamics from the field of synchronization (Fig. 1), particle dynamics, and enzyme chemistry.

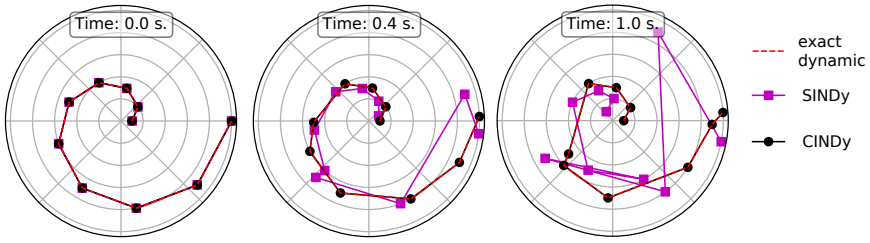

Figure 1: Trajectory comparison of a Kuamoto model identified with SINDy and CINDy.

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Model reduction of descriptor systems with quadratic output functional

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This work is dedicated to the model reduction of differential-algebraic systems with quadratic output (`DAE_QO`) functional of the form

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \qquad x(0) = 0, \\ y(t) &= x(t)^T M x(t). \end{aligned}$$

Under some mild conditions, these systems can be transformed into a Weierstraß canonical form and thus decouple into a differential equation and an algebraic equation, and the corresponding proper and improper states. In contrast to the case of differential-algebraic systems with linear output (`DAE_LO`), the system `DAE_QO` presents a coupling of the proper and improper states in the output signal. Our goal is to determine the dominant subspaces of the differential and algebraic states and then reduce the system accordingly.

To this end, we propose new Gramians that encode the suitable subspaces and demonstrate their relationship with energy functions. Firstly, we show that reachability is encoded by the proper and improper reachability Gramians, similarly as in the `DAE_LO` case. For the observability, we decompose the system output into four subsystems, two of those associated with proper states and the other two with improper states. Hence, based on this subsystem decomposition, we derive new observability Gramians for the proper and improper state vectors. They can again be determined by solving continuous-time and discrete-time Lyapunov equations. Finally, the proper reachability and observability Gramians are then used to derive a reduced differential state-space model using balanced truncation. Additionally, the improper Gramians are used to truncate uncontrollable and unobservable algebraic states. Furthermore, we derive an error estimator, which is used to evaluate the quality of the reduced surrogate model. Finally, we illustrate the effectiveness of our method by applying it to example problems.

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Learning Quadratic Embeddings for Nonlinear Dynamical Systems using Deep Learning

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Dynamical modeling of a process is essential to study its dynamical behavior and perform engineering studies such as control and optimization. With the ease of accessibility of data, learning models directly from the data have recently drawn much attention. It is also desirable to construct simple and compact models describing complex nonlinear high-fidelity dynamics for efficient simulations and engineering studies on modest computer hardware. To achieve our goal, we merge two important ingredients. These are–(a) high-fidelity dynamics often evolve in a low-dimensional manifold, and (b) sufficiently smooth nonlinear systems can be rewritten as quadratic models in an appropriate coordinate system, conferring to the McCormick relaxation idea in non-convex optimization. Therefore, we focus on identifying low-dimensional embeddings for high-fidelity dynamical models such that a quadratic model can describe the dynamics of the embeddings. To determine such embeddings, we leverage the powerful expressive capabilities of deep learning, particularly autoencoders. We illustrate the methodologies to learn low-dimensional quadratic embeddings for high-fidelity dynamical models by a couple of examples.

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Impact of the Convergence of Series Expansions on Model Reduction of Quadratic-Bilinear Systems

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Quadratic-bilinear (QB) systems arise naturally from a large class of problems, including semi - discretizations of fluid flow systems governed by Burgers' equation or by the Navier-Stokes equations. Consequently, the model order reduction (MOR) of QB systems has been studied extensively in the literature [1, 3, 5]. Several MOR approaches for QB systems are based on so-called moment-matching, in which one expands the state in an infinite series, truncates the expansion after k (typically $k = 2$) terms, computes the generalized transfer functions of these terms, and computes a reduced order model (ROM) whose first k transfer functions interpolate the corresponding transfer functions of the full order model (FOM). While this approach has been successful in several cases, the impact of the truncation of the series on the quality of the resulting ROM has received little attention. The papers [2, 4] report that the ROMs computed using a straight forward application of the so-called Loewner framework for systems governed by Burgers' equation or the Navier-Stokes equations exhibit instabilities. This raises the question whether the convergence of the series, and its early truncation, contributes to these poor ROMs. In this talk, it is shown that the convergence of the series expansion indeed plays a critical role in the quality of the ROM. In particular, for systems governed by Burgers' equation, numerical experiments indicate that when the series expansion does not converge, the ROM is unstable, whereas when the series does converge, the resulting ROM is stable. Theoretical results on the convergence of the series expansion, which are tailored to systems governed by Burgers' equation and which expose the impact of viscosity, a critical parameter in Burgers' equation, are also provided.

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Data-Driven Model Reduction for Gas Network Digital Twins

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Spanning across and beyond the European continent, the gas transport network is a large-scale industrial application with critical relevance not only for current daily supply of natural gas, but also for the green energy transition namely through biogas and hydrogen. Therefore, dynamic gas network simulations are increasingly important for an interconnected smart energy grid, to compensate renewable energy production shortfalls and surpluses on short notice, since gas can be converted promptly into power, and excess renewable power can be converted back into gas.
Gas network models are typically based on the Euler equations for pipes, which lead to a system of nonlinear, parametric and hyperbolic partial differential-algebraic equations for pipeline networks. Using a port-Hamiltonian formulation along-side an analytic index reduction and spatial discretization yields a state-space input-output ordinary differential equation system:

$$\overbrace{\begin{pmatrix} E_p(\theta) & 0 \\ 0 & E_q \end{pmatrix}}^{E(\theta)} \overbrace{\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix}}^{\dot{x}} = \overbrace{\begin{pmatrix} 0 & A_{pq} \\ A_{qp} & 0 \end{pmatrix}}^{A} \overbrace{\begin{pmatrix} p \\ q \end{pmatrix}}^{x} + \overbrace{\begin{pmatrix} 0 & B_{pd} \\ B_{qs} & 0 \end{pmatrix}}^{B} \overbrace{\begin{pmatrix} s_p \\ d_q \end{pmatrix}}^{u} + \overbrace{\begin{pmatrix} 0 \\ F_c \end{pmatrix} + \begin{pmatrix} 0 \\ f_q(p,q,\theta) \end{pmatrix}}^{f(x,\theta)}$$

$$\underbrace{\begin{pmatrix} s_q \\ d_p \end{pmatrix}}_{y} = \underbrace{\begin{pmatrix} 0 & C_{sq} \\ C_{dp} & 0 \end{pmatrix}}_{C} \underbrace{\begin{pmatrix} p \\ q \end{pmatrix}}_{x}.$$

Due to the large-scale nature and manifold complexities of realistic gas network models, as well as the many-query setting of the practical application, model reduction can be used to reduce the order of the system, accelerating simulations, and hence, enable more scenarios to be evaluated prior to actual dispatch of denominations. Yet, the amalgamation of challenging features in gas transmission models makes the selection of suitable model reduction methods inherently difficult.
Given the model's hyperbolicity, non-smooth nonlinearity and parameter-dependence, we adapt, apply and compare data-driven system-theoretic model reduction methods [1], discuss model properties and algorithmic aspects affecting the reduced order system, and lay out extensibility to water networks, district heating networks and power networks. Furthermore, heuristic comparability of reduced order models is discussed [2].
Computationally, our open-source "morgen" (Model Order Reduction for Gas and Energy Networks) research software [3], a modular transient gas network simulation and model reduction prototyping stack, tests, compares and benchmarks model-solver-reductor ensembles for gas network digital twin development and model reduction research, which we demonstrate in numerical experiments.

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Symplectic Model Reduction of Hamiltonian Systems on Nonlinear Manifolds

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Classical model reduction techniques project the governing equations onto linear subspaces of the high-dimensional state-space. However, for problems with slowly decaying Kolmogorov-n-widths such as certain transport-dominated problems [6], classical linear-subspace reduced order models (ROMs) of low dimension might yield inaccurate results. Thus, the reduced space needs to be extended to more general nonlinear manifolds. Moreover, as we are dealing with Hamiltonian systems, it is crucial that the underlying symplectic structure is preserved in the reduced model, see [5, 7].

To the best of our knowledge, existing literatures addresses either model reduction on manifolds, see e.g. [4], or symplectic model reduction for Hamiltonian systems, but not their combination. In this talk, we bridge the two aforementioned approaches by providing a novel projection technique called *symplectic manifold Galerkin*, which projects the Hamiltonian system onto a nonlinear symplectic trial manifold such that the reduced model is again a Hamiltonian system, see [1]. We derive analytical results such as stability, energy-preservation and a rigorous a-posteriori error bound. Moreover, we construct a weakly symplectic convolutional autoencoder in order to computationally approximate the nonlinear symplectic trial manifold. We numerically demonstrate the ability of the method to outperform structure-preserving linear subspace ROMs results for a linear wave equation for which a slow decay of the Kolmogorov-n-width can be observed, see e.g. [2, 3].

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Model reduction for port-Hamiltonian descriptor systems

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We analyze model reduction methods and their use in treating large scale port-Hamiltonian differential-algebraic systems in a way that is able to preserve and take advantage of the underlying structural features of the system. We introduce approaches that incorporate regularization. We focus on linear time-invariant systems and present a systematic treatment of a variety of model classes that include combinations of index-1 and index-2 systems, describing in particular how constraints may be represented in the transfer function so that the polynomial part can be preserved with interpolatory methods.

Dynamic Mode Decomposition for Continuous Port-Hamiltonian Systems

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We present a novel physics-informed system identification method to construct a passive linear time-invariant system. In more detail, for a given quadratic energy functional, measurements of the input, state, and output of a system in the time domain, we find a realization that approximates the data well while guaranteeing that the energy functional satisfies a dissipation inequality. One of the main advantages of requiring the learned model to satisfy a dissipation inequality is that whenever the model is coupled with another passive model via a powerconserving or dissipative interconnection, then the coupled model is also passive. To this end, we use the framework of port-Hamiltonian (pH) systems [5] and modify the dynamic mode decomposition (DMD) [3] to be feasible for continuous-time pH systems. We propose an iterative numerical method, to solve the corresponding least-squares minimization problem of the form

$$\min \left\| \mathcal{Z} - (\widetilde{\mathcal{J}} - \widetilde{\mathcal{R}})\mathcal{T} \right\|_{\mathrm{F}} \qquad \text{s. t. } \widetilde{\mathcal{J}} = -\widetilde{\mathcal{J}}^T \text{ and } \widetilde{\mathcal{R}} \succeq 0, \tag{1}$$

where $\mathcal{Z}$ and $\mathcal{T}$ correspond to the discrete-time data and $\widetilde{\mathcal{J}}$ and $\widetilde{\mathcal{R}}$ to the matrices of the continuous-time pH system. The proposed method divides the original problem into two subproblems, by alternately fixing $\widetilde{\mathcal{J}}$ respectively $\widetilde{\mathcal{R}}$ and optimizing solely over the remaining matrix. The resulting subproblems are a skew-symmetric and a symmetric positive semi-definite Procrustes problem. The skew-symmetric Procrustes problem can be solved analytically [1] and algorithmic solutions are available for the symmetric positive semi-definite Procrustes problem [2]. We present a modification of the proposed Fast Gradient Method, based on [4], with which it is possible to use the solution of the skew-symmetric Procrustes problem iteratively. For an effective initialization we analyze the least-squares problem in a weighted norm,

$$\min \left\| \mathcal{T}^T\mathcal{Z} - \mathcal{T}^T(\widetilde{\mathcal{J}} - \widetilde{\mathcal{R}})\mathcal{T} \right\|_{\mathrm{F}} \qquad \text{s.t. } \widetilde{\mathcal{J}} = -\widetilde{\mathcal{J}}^T \text{ and } \widetilde{\mathcal{R}} \succeq 0, \tag{2}$$

for which we present the analytical minimum-norm solution. The efficiency of the proposed method is demonstrated with several numerical examples.

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A non-intrusive algorithm for parameterized model order reduction of LTI systems with guaranteed dissipativity

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We present a non-intrusive approach for generating LTI parameterized reduced-order models (PROMs) that are dissipative by construction. The approach is based on a convex formulation and enforcement of the dissipativity constraints, thus avoiding potentially unreliable heuristic post-processing schemes. Let $\boldsymbol{\vartheta} \in \Theta \subset \mathbb{R}^d$ be a vector of external parameters and s the Laplace variable. We assume that the frequency response of the underlying system $\breve{H}(s, \boldsymbol{\vartheta}) \in \mathbb{C}^{P \times P}$ is available at discrete frequency $s_k = j\omega_k,\ k = 1 \dots K$ and parameter samples $\boldsymbol{\vartheta}_m,\ m = 1 \dots M$ through some measurement or first-principle solver. The PROM is generated by enforcing a fitting condition $\mathsf{H}(j\omega_k, \boldsymbol{\vartheta}_m) \approx \breve{H}(j\omega_k, \boldsymbol{\vartheta}_m)$, assuming the following parameterized rational model structure

$$\mathsf{H}(s, \boldsymbol{\vartheta}) = \frac{\mathsf{N}(s, \boldsymbol{\vartheta})}{\mathsf{D}(s, \boldsymbol{\vartheta})} = \frac{\sum_{i=0}^{\bar{n}} \sum_{\boldsymbol{\ell} \in \mathcal{I}_{\bar{\boldsymbol{\ell}}}} R_{i,\boldsymbol{\ell}}\, b_{\boldsymbol{\ell}}^{\bar{\boldsymbol{\ell}}}(\boldsymbol{\vartheta})\, \varphi_i(s)}{\sum_{i=0}^{\bar{n}} \sum_{\boldsymbol{\ell} \in \mathcal{I}_{\bar{\boldsymbol{\ell}}}} r_{i,\boldsymbol{\ell}}\, b_{\boldsymbol{\ell}}^{\bar{\boldsymbol{\ell}}}(\boldsymbol{\vartheta})\, \varphi_i(s)} \tag{1}$$

where $R_{i,\boldsymbol{\ell}}$, $r_{i,\boldsymbol{\ell}}$ are unknown coefficients, and $\varphi_i(s) = (s - q_i)^{-1}$ with $\mathrm{Re}\{q_i\} < 0$ are partial fraction frequency-dependent basis functions, as in Vector Fitting schemes [2]. Parameterization is induced by multivariate Bernstein polynomials $b_{\boldsymbol{\ell}}^{\bar{\boldsymbol{\ell}}}(\boldsymbol{\vartheta})$ with degree $\bar{\boldsymbol{\ell}} = (\bar{\ell}_1, \dots, \bar{\ell}_d)$, where $\mathcal{I}_{\bar{\boldsymbol{\ell}}}$ denotes the set of admissible multi-indices. Due to the presence of unknowns at both numerator and denominator in (1), determination of model coefficients is performed through an iteratively re-weighted linearized least squares process known as PSK iteration [3].

Both asymptotic stability and dissipativity are enforced uniformly $\forall \boldsymbol{\vartheta} \in \Theta$ by exploiting the uniform positivity and partition of unity properties of Bernstein polynomials. On one hand, stability is implied by the denominator $\mathsf{D}(s, \boldsymbol{\vartheta})$ being a uniformly Positive Real function, whereas dissipativity is implied by $\mathsf{H}(s, \boldsymbol{\vartheta})$ being a uniformly Bounded Real function, assuming a scattering representation. Both conditions are formulated algebraically through the appropriate Kalman-Yakubovich-Popov lemmas, which lead to parameter-dependent Linear Matrix Inequality (LMI) conditions, to be enforced uniformly $\forall \boldsymbol{\vartheta} \in \Theta$. All terms in these LMIs are then represented as truncated Bernstein polynomial expansions, including also the energy storage function. The result is a finite set of independent LMIs in the model coefficients, which are enforced concurrently with the model-data fitting. Exploiting the degree elevation property of Bernstein polynomials is shown to effectively reduce the conservativity of the LMI discretization, leading to certified uniformly stable and dissipative models, with controlled accuracy. Technical derivations and proofs are available in [1]. Application examples in the area of electronic CAD will be presented.

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Structure-preserving and adaptive reduced order models of conservative dynamical systems

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Conservative systems describe reversible processes with no dissipative effects in a broad variety of phenomena of scientific and industrial interest. Examples of such systems are the n-body problem, the Lotka-Volterra equation of population dynamics, wave-type problems (e.g. the KdV equation, the Schrödinger equation, the shallow water equations, ...), conservation laws in fluid dynamics, and kinetic plasma models. In this talk we consider parametric conservative problems by resorting to their (semi-discrete) formulation as Hamiltonian dynamical systems. The development of reduced order models of such systems is challenged by several factors: (i) failing to preserve the geometric structure encoding the physical properties of the dynamics, such as invariants of motion or symmetries, might lead to instabilities and unphysical behaviors of the resulting approximate solutions; (ii) the slowly decaying Kolmogorov n-width of transport-dominated and non-dissipative phenomena demands large reduced spaces to achieve sufficiently accurate approximations; and (iii) nonlinear operators require hyper-reduction techniques that preserve the gradient structure of the flow velocity. We will discuss how to address these aspects via a nonlinear model order reduction approach based on evolving low-dimensional surrogate models on a phase space that adapts in time while being endowed with the geometric structure of the full model. To deal with nonlinear operators we propose a gradient-preserving strategy that consists in a sparse decomposition of the Hamiltonian gradient projected into the reduced space, followed by a discrete empirical interpolation of the resulting nonlinear factors. We will demonstrate the efficiency of the proposed techniques on a set of numerical tests.

This work is in collaboration with J. S. Hesthaven (EPFL Lausanne), N. Ripamonti (EPFL Lausanne), and F. Vismara (TU/e Eindhoven).

Neural Closure Model for Dynamic Mode Decomposition Forecasts

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Dynamic Mode Decomposition (DMD) is a data-driven, equation-free dimensionality reduction algorithm [4, 5, 7] that constructs an approximate linear operator for a sequential data set. It has been demonstrated that DMD can serve as a computationally efficient forward model to provide forecasts in a wide variety of applications. However, DMD forecast suffer from three key issues. First, the absence of truncated modes and lack of adaptation may lead to drastically different forecasts [4], especially due to the linear approximation of possibly highly nonlinear dynamics [6]. Second, as the standard DMD formulation is steady in time, it may become irrelevant in evolving systems [9, 3, 6, 1]. Third, uncertainties are not commonly represented and sub-DMD (closure) models not commonly utilized [3, 2, 8]. To address these issues, we investigate augmenting the stochastic DMD model with a closure model parameterized using neural networks. We demonstrate our new results on several test cases in high-dimensional computational multivariate ocean dynamics and modeling.

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A Differential Geometric Formulation for Model Order Reduction on Manifolds

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Differential geometric formulations are central in multiple classes of dynamical systems like e.g. Lagrangian systems. In classical Model Order Reduction (MOR) these underlying differential geometric formulations are typically not reflected. This becomes especially problematic for recent MOR approaches which use nonlinear techniques to approximate the state [1, 2, 3] (in the following referred to as MOR on manifolds) since inconsistent projections of the full-order model might be used, see [2, Remark 3.5 (Alternative Galerkin projection)]. In this work, we present how MOR (on manifolds) can be formulated for basic differential geometric objects like vector fields and covector fields. This rigorous formulation has the advantage that it clearly shows how to project the full-order system and thereby inherently prevents inconsistent projections. Sparked by the insights of the new differential geometric formulation, we discuss extensions to the training of nonlinear autoencoders $(\boldsymbol{d}(\cdot,\boldsymbol{\theta}), \boldsymbol{e}(\cdot,\boldsymbol{\theta}))$ based on a dataset $X := \{\boldsymbol{x}_i\}_{i=1}^{n_\mathrm{s}} \subset \mathbb{R}^N$

$$\begin{aligned} &\boldsymbol{d}(\cdot,\boldsymbol{\theta}) : \mathbb{R}^n \to \mathbb{R}^N, \\ &\boldsymbol{e}(\cdot,\boldsymbol{\theta}) : \mathbb{R}^N \to \mathbb{R}^n, \end{aligned} \qquad \text{choose } \boldsymbol{\theta} \in \mathbb{R}^{n_\mathrm{p}} \text{ such that} \qquad (\boldsymbol{d}(\cdot,\boldsymbol{\theta}) \circ \boldsymbol{e}(\cdot,\boldsymbol{\theta}))(\boldsymbol{x}_i) \approx \boldsymbol{x}_i \quad \text{for } 1 \leq i \leq n_\mathrm{s}.$$

These extensions include two ideas: (i) The modification for exact reproduction of initial values from [2, Section 5.3] is adopted in the formalism and respected in the training procedure. This guarantees that the same coordinates are used in the training and the evaluation of the autoencoder and results in a modified loss function

$$\mathcal{L}_\mathrm{D}(\boldsymbol{\theta}) := \sum_{i=1}^{n_\mathrm{s}} \left\| (\boldsymbol{d}(\cdot,\boldsymbol{\theta}) \circ \boldsymbol{e}(\cdot,\boldsymbol{\theta}))(\boldsymbol{x}_i) - (\boldsymbol{d}(\cdot,\boldsymbol{\theta}) \circ \boldsymbol{e}(\cdot,\boldsymbol{\theta}))(\boldsymbol{0}) - \boldsymbol{x}_i \right\|^2. \tag{1}$$

As a second extension, (ii) snapshots of the right-hand side $X_{\boldsymbol{f}} := \{\boldsymbol{f}_i\}_{i=1}^{n_\mathrm{s}}$ are included in the training by introducing an additional loss function

$$\mathcal{L}_{\boldsymbol{f}}(\boldsymbol{\theta}) := \sum_{i=1}^{n_\mathrm{s}} \left\| \left(\boldsymbol{I}_N - \mathrm{D}_{\boldsymbol{x}}(\boldsymbol{d}(\cdot,\boldsymbol{\theta}) \circ \boldsymbol{e}(\cdot,\boldsymbol{\theta}))\big|_{\boldsymbol{x}_i} \right) \boldsymbol{f}_i \right\|^2. \tag{2}$$

Appropriate balancing of the both losses, (1) and (2), is discussed. In the numerical experiment, we consider the reduction of the one-dimensional Burgers' equation via a so-called deep convolutional autoencoder from [2] and investigate how the suggested extensions can improve the approximation quality.

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A machine learning-based reduced order model for the investigation of the haemodynamics in coronary artery bypass grafts

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The diffusion of coronary artery diseases and the increasing demand from the medical community for quantitative and patient-specific investigations are the main motivations which gave a strong impulse in recent time to the development of fast and accurate numerical models. The final goal is a better understanding of the blood flow behaviour in grafts and graft junctions so as to aid in surgical planning of grafting and improve the lifetime of grafts.
In this work, a machine learning Reduced Order Model (ROM) is employed in order to ensure rapid computations of the blood flow patterns in patient-specific configurations of Coronary Artery Bypass Grafts (CABGs) for variable physical and geometrical parameters of clinical interest. An expensive and time consuming offline phase performs a large number of parameter and time dependent high-fidelity solutions and generates the reduced basis from them. Then, during an online stage, the behaviour of the system in the parameter space can be investigated at a considerable reduced time.
In this scenario, we consider two different applications:

- Firstly, the ROM is implemented and its performance is tested for the reconstruction of pressure, velocity and wall shear stress computed by the Navier-Stokes equations for a patient-specific geometry, where the bypass is performed with the left internal thoracic artery on the Left Anterior Descending artery (LAD). The inlet flow rate and the severity of the stenosis are considered as parameters in the reduced framework [2].

- Then, the ROM approach is used within an optimal control problem in order to match measured clinical data with numerical outcomes at varying of the Reynolds number. This approach is introduced to overcome the issues arising from unrealistic outlet boundary conditions, which can lead to doubtful predictions. Here, we consider a bypass performed with the right internal thoracic artery on the LAD.

In both cases, we show that the data-driven ROM is able to provide a computational speed-up significantly greater than the one provided by classic projection-based strategies [1, 3].

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Adaptive Gaussian Process Regression for Efficient Building of Surrogate Models in Inverse Problems

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Given a task where many similar inverse problems need to be solved, evaluating costly simulations is infeasible, such that replacing the model y with a fast to evaluate surrogate model y_s results in a significant speed up. The approximation quality of the surrogate model depends highly on the number, position and accuracy of the sample points. Given an additional finite computational budget hence leads to a design of (computer) experiment problem. In contrast to the selection of sample points, the accuracy-effort trade off has so fast barely been investigated systematically e.g., [1]. We therefore propose an adaptive algorithm for finding an optimal design in terms of position *and* accuracies. Following a sequential design by incrementally spending computational budget, leads to a convex and constrained optimization problem. As surrogate we construct a Gaussian process regression model. We measure the global approximation error by its impaxt on the accuracy of the identified parameter, and aim at a uniform absolute tolerance, assuming y_s being calculated by finite element computation. A priori error estimates and a coarse estimate of the computational work relates the expected improvement of the surrogate model error the computational work, which leads to the most efficient combination of sample point and evaluation tolerance. We also allow for improving the accuracy of already existing sample points by continuing previously truncated finite element solution procedures.

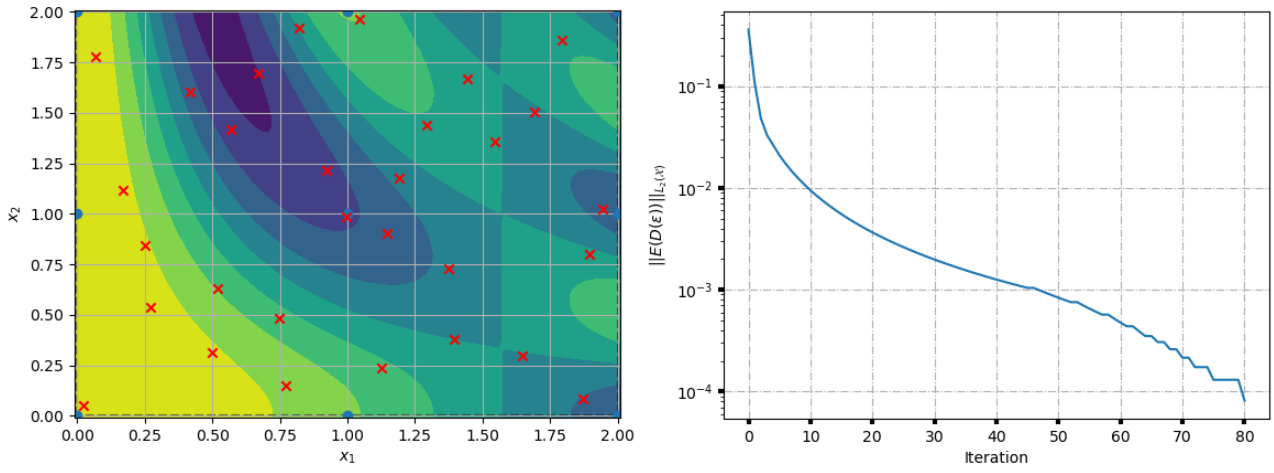

Figure 1: Left: Initial data points are indicated with blue dots. Red crosses are adaptively added data points. The color mapping indicates the isolines of y. Right: Log-plot of global error estimator over number of iterations.

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An efficient computational framework for atmospheric and ocean flows

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Numerical simulations of geophysical flows are an essential tool for ocean and weather forecast. Moreover, they could also provide insights on the mechanisms governing climate change. However, often long time intervals have to be simulated, making the computational cost prohibitive. We propose two different strategies to reduce such computational cost:

(i) The development of a Reduced Order Model (ROM) with the aim to lower the computational cost of the numerical simulations without a significant loss in terms of accuracy. In this context, we consider the 2D Navier-Stokes equations in terms of stream function and vorticity as Full Order Model, which represents an attractive alternative to the model in primitive variables for geophysical fluid dynamics applications. We present a novel POD-Galerkin ROM where different reduced coefficients for the vorticity and stream function fields are considered. A global POD basis space obtained from a database of time dependent full order snapshots related to sample points in the parameter space. The performance of our ROM strategy is tested against the classical vortex merger benchmark [2].

(ii) The development of a Large Eddy Simulation (LES) approach that allows to use a coarser mesh than the one required by a Direct Numerical Simulation by modeling the effect of the small scales that do not get resolved. Here, we refer to the Quasi-Geostrophic equations, which is a toy problem describing the main features of geophysical flows under certain simplifying assumption. We propose a novel variant of the so-called BV-α model [3] that introduces nonlinear indicator function to identify the regions of the domain where the flow needs regularization [1]. In order to assess the performance of the proposed LES approach, we consider the double-gyre wind forcing benchmark.

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Analysis of Hyper Reduction for the Computation of Nonlinear Normal Modes

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Nonlinear Normal Modes(NNMs) are defined as the invariant manifolds that correspond to the Lyapunov subcenter manifolds for nonlinear structural dynamic systems. In case of conservative systems, an NNM reduces to a periodic solution of the system and is the extension of the concept of linear eigenmodes for nonlinear systems. The variety of nonlinear phenomena e.g. bifurcation, chaos and internal resonances poses a challenge in the setup of reduced order models (ROMs)[2].

The Galerkin projection of the system into a significantly smaller subspace is commonly employed in Model Order Reduction (MOR) of nonlinear Finite Element(FE) models [4]. As a consequence of nonlinear phenomena, the a-priori selection of adequate basis vectors presents a difficulty. Additionally, a computational bottleneck is created in the computation of the nonlinear force vector as it needs to be evaluated in the full model space.

To remove this bottleneck, hyper reduction methods are used to compute the nonlinear forces in the reduced subspace. The Energy Conserving Sampling and Weighting (ECSW) method selects a limited subset of elements and assigns them a weighting factor to reduce the computational effort of the nonlinear force evaluation by then only evaluating that limited subset [1]. A direct computation of the nonlinear force in the reduced subspace is enabled by the Stiffness Evaluation Procedure (STEP) that sets up a reduced stiffness tensor [3].

This work consists of the computation of NNMs for a doubly clamped beam by using the Multi Harmonic Balance method in combination with a continuation algorithm. Different reduction bases are created by using modal derivatives and linear eigenmodes. The major novelty is the application of HR with ECSW and STEP to the computation of NNMs. A qualitative analysis of the NNMs of the reduced system in comparison to the full system is presented. Furthermore, the computational effort needed to compute the NNMs is analyzed for different ROMs.

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Balancing-related model reduction of large-scale sparse systems in MATLAB and Octave with the MORLAB toolbox

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The modeling of real-world applications often results in linear dynamical systems of the form

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

with $E, A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$ and $D \in \mathbb{R}^{p\times m}$, described by a large number n of differential and algebraic equations. Model order reduction is the remedy to construct cheap-to-evaluate surrogates of similar structure to (1) by reducing the number of describing equations to $r \ll n$.
For the use of model reduction methods in practice, potentially by users who may have never been introduced to the underlying theory, efficient implementations of these methods with intuitive interfaces are needed. The MORLAB, Model Order Reduction LABoratory, toolbox [1] has been providing such implementations in MATLAB and Octave mainly for balancing-related model reduction, e.g., balanced truncation, for the case of medium-scale ($n \in \mathcal{O}(10^3)$), dense systems (1). The underlying spectral projection methods allow for fast and accurate computations, even able to handle general cases of differential-algebraic equations describing (1). The toolbox is open source and freely available, has a unified framework for all implemented methods that allows for quick exchanges of routines and easy comparisons between methods, and it is portable to all different operating systems on which bare MATLAB and Octave installations are available. However, in many applications, especially in the context of discretized partial differential equations, the coefficient matrices in (1) are of large scale ($n \in \mathcal{O}(10^5)$ and larger) and sparsely populated. Efficient large-scale sparse matrix equations solvers, such as those provided in the Matrix Equation Sparse Solvers (M-M.E.S.S.) library [2], are the key to extend the balancing-related model reduction MORLAB routines to this system case.
This poster describes the latest release, version 6.0, of the MORLAB toolbox. It features new implementations of balancing-related model reduction methods for large-scale sparse, linear systems, using the Lyapunov and Riccati equation solvers from the M-M.E.S.S. library as their backbone.

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Bayesian multi-fidelity inverse analysis for computationally demanding models in high stochastic dimensions

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The biggest challenges in (Bayesian) inverse analysis of large-scale numerical models are posed by the high computational demands in combination with a high stochastic dimension. The latter is often caused by inverse problems that involve random fields, i.e., in the case of unknown boundary conditions, elastography problems, unknown microstructure distributions or geometric quantities, to name a few examples. The solution process is further impeded when model derivatives are inaccessible as it is often the case in legacy codes and coupled problems.
We propose *Bayesian multi-fidelity inverse analysis (BMFIA)* which overcomes the aforementioned difficulties by employing computationally inexpensive, lower-fidelity models and constructing a multi-fidelity likelihood function. The approach builds upon previous developments of the authors in the field of uncertainty quantification [1, 2, 3, 4]. The multi-fidelity likelihood is learned robustly from a small number of high-fidelity simulations and reflects the uncertainty, not only in the original inverse problem, but also due to the (small) training data employed. We specifically address challenges imposed by the *small data regime* and demonstrate how the the multi-fidelity dependency can be learned with higher accuracy in an extended space that is equipped with low-dimensional, informative features of the input. *BMFIA* is independent of the problem's stochastic dimension as it primarily relies on the dependence between the outputs of models of varying fidelities and not on the input.
Furthermore, improved efficiency is attained since the inference process, which can be performed using state-of-the-art sampling-based or variational methods, requires solely evaluations of the low-fidelity model(s). The latter can be chosen or constructed such that they provide model derivatives (e.g., from adjoint formulations) which further expedite inference. The performance can be even further increased when the low-fidelity model is given by a physics-informed surrogate model or physical knowledge is incorporated directly in the multi-fidelity likelihood function.
We demonstrate our approach on large-scale biomechanical and coupled multi-physics problems and compare them with state-of-the-art single- and multi-fidelity methods.

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Combining adaptive model order reduction and stochastic collocation for uncertainty quantification of vibroacoustic systems

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We address vibroacoustic problems, which are simulated with the finite element method and where material properties exhibit uncertainties. Modeling all uncertain parameters with a jointly distributed random vector leads to a high-dimensional reformulation of the problem, where both frequency and random material parameters need to be considered. In realistic applications, multi-query simulations are hardly possible due to the size of the system and the size of the parameter space. To overcome this problem, we propose to combine model order reduction (MOR) and stochastic collocation in a fully adaptive way [2].
The model problem reads

$$(-\omega^2 M(p) + i\omega D(p) + K(p))x(\omega, p) = F, \tag{1}$$

where $p \in \Gamma \subset \mathbb{R}^P$ denotes a parameter vector with an underlying probability distribution, ω the angular frequency and $M(p), D(p), K(p) \in \mathbb{C}^{n\times n}$. We are interested in computing moments of an output quantity, i.e. the quantity of interest

$$\mathbb{E}_p[y(\omega, \cdot)] = \mathbb{E}_p[\Psi(x(\omega, \cdot))], \tag{2}$$

for all $\omega \in [\underline{\omega}, \overline{\omega}]$, with a manageable computational effort. To that end, we apply a dimension-adaptive stochastic collocation method with Leja nodes. At each collocation node $\{p^{(i)}\}_{i=1}^{I}$ we build a reduced order model with the rational Arnoldi method and an adaptive selection of frequency expansion points $\{\omega_i^{(j)}\}_{j=1}^{J_i}$. The parametric output quantity is then obtained by interpolating the frequency response.
A major ingredient is the selection of adaptive expansion and collocation points, which we base on dual error indicators. In particular, we require the adjoint of both the full and reduced order model to estimate the error contributions from collocation and MOR separately. Both adjoints can be computed efficiently, if sparse direct solution methods are used for the linear systems. The resulting algorithm only requires a target accuracy and automatically generates and interpolates local adaptive ROMs.
We will demonstrate the accuracy of the estimators and the efficiency of the method with several simple examples and examples from vibroacoustics. We also discuss the advantages and limitations of the method related to other available approaches, which are based on pole matching [3, 1].

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Data enhanced reduced order methods for turbulent flows

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The focus of the present contribution is on Reduced Order Methods (ROMs) applied to the study of turbulent flows. To ensure a low ROM computational cost, relatively few basis functions are usually considered to build the model. However, when a *marginally-resolved* modal regime is adopted, the number of modes is enough to capture the underlying dynamics of the system, but the standard Galerkin-ROM yields inaccurate results. In order to improve the results in terms of accuracy, the ROM approach is combined with stabilization and data-driven techniques. Specifically, we propose the first pressure-based data-driven variational multiscale ROM (P-DD-VMS-ROM) [3], in which the available data are used to construct the so-called *correction* terms appearing in both the momentum and the continuity equations.
Such terms are aimed at reintroducing the contribution of the neglected modes in the reduced equations. As investigated in [4], they are computed by solving an optimization problem between the exact correction term and a postulated ansatz chosen to model it.
The case study considered in our numerical investigation is that of the two-dimensional flow past a circular cylinder. Two different velocity-pressure coupling approaches are used, following the lead of [1]. In the first one, additional supremizer modes are added to the velocity POD space to ensure the fulfillment of the inf-sup condition. In the second approach, the continuity equation is replaced by the Pressure Poisson Equation, leading to the formulation of novel pressure correction terms.
A different type of data-driven technique is combined with the VMS-ROM formulation in order to include the turbulence treatment at the reduced order level. A reduced eddy viscosity field is modelled with *regression* techniques starting from the velocity field making use of *machine learning* tools [1, 2]. The techniques we discuss yield significantly more accurate results than the standard ROM and, more importantly, than the original data-driven variational multiscale ROM (i.e., without pressure components). In particular, our numerical results show that adding the correction term in the momentum equation significantly improves both the velocity and the pressure approximations. On the other hand, adding the novel pressure correction terms only improves the pressure approximation.

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Data-driven approaches for system identification and reduction

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We discuss different ways of constructing nonlinear models from input-output data. We formally present the model order reduction (MOR) problem and comment on conventional intrusive methods that offer solutions. In this context, having access to the original model's operators usually results in dealing with a large-scale system [1]. Therefore, intrusive MOR techniques provide reduced models capable of capturing the original system's response with high accuracy and accelerating the simulation time for efficient design and control.
When the underlying model is unknown or complicated to construct, non-intrusive methods (i.e., interpolation-based) can provide solutions based purely on data [2]. Typically, non-intrusive methods have two aims. The first aim is to identify an embedded model into the general assumed model structure, and the second aim is to construct a reduced model. We present non-intrusive methods for achieving the above two goals based on the Hankel and Loewner frameworks. Both frameworks can identify linear and nonlinear systems from input-output measurements and provide robust interpretable models [3, 4, 5]. We present challenges in handling different data types (e.g., time and frequency) and challenges related to missing data. Finally, we offer solutions to theoretical benchmarks and real engineering problems.

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Data-Driven Linearization of Nonlinear Finite Element Analyses

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Nonlinear finite element analysis is gaining attention for the modeling of complex mechanical assets. The nonlinear nature of these systems is another issue that complicates their analysis. This can be seen, e.g., for system identification and Kalman filtering. In this talk, we propose a method that approximates the output of a nonlinear dynamical system by a linear one. Moreover, the second order nature of the nonlinear system is conserved by the linear approximation.
The Full Order Models (FOMs) we consider should be treated as a black box, since knowledge of the underlying dynamical system may not be available. Instead of looking for a linearization of the whole FOM, we focus on the response of the system at a specific input. Given the input signal $u(t)$, we therefore look for an approximation of the system's response $y_u(t)$. To this end we define a new data-driven system-theoretic method, which we call tLS-AAA. This method is able to find a linear Reduced Order Model (ROM) whose impulse response accurately approximates $y_u(t)$.
The base of tLS-AAA is the AAA algorithm [2], and in particular its Least Squares form introduced in [1]. This form is useful to delete possible unstable poles obtained in the AAA procedure. The ROM generated by tLS-AAA is the linear second order system

$$\Sigma_r : \quad \begin{cases} M_r \ddot{\boldsymbol{x}}_r(t) + E_r \dot{\boldsymbol{x}}_r(t) + A_r \boldsymbol{x}_r(t) = B_r \delta(t) \\ y_r(t) = \varepsilon_0 \delta(t) + \varepsilon_1 + \boldsymbol{\alpha}^T \boldsymbol{x}_r(t) + \boldsymbol{\beta}^T \dot{\boldsymbol{x}}_r(t) \end{cases}, \tag{1}$$

where the coefficients ε_0, ε_1, $\boldsymbol{\alpha}$, and $\boldsymbol{\beta}$ can be found by solving the LS problem

$$\min \|y_u - y_r\|_2. \tag{2}$$

Since this method focuses on the time domain, we call it Time LS-AAA (tLS-AAA). Even though the ROM (1) is generated for the specific input $u(t)$, we show that it can easily deal with a larger set of input signals. We consider different test cases, and we demonstrate the accuracy and flexibility of this method.

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

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

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

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

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Dynamical low rank approximation and parametric reduced order models for shallow water moment equations

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Standard shallow water models assume a constant horizontal velocity over the water height. This nonphysical assumption is overcome by recently developed shallow water moment equations (SWME) [3, 4], which model a varying velocity profile using a potentially high-order polynomial. However, this leads to a large system of coupled PDEs for the evolution of the polynomial coefficients, even though the solution might evolve on a lower-order manifold.
In this work, we investigate two different approaches to reduce the complexity of the SWME. Firstly, we apply a dynamical low-rank approximation [2], which represents the solution as a low-rank factorization, e.g. with help of the Proper Orthogonal Decomposition (POD). The dynamical low-rank approximation framework provides time evolution equations for the individual factors, which can be solved with significantly reduced computational cost. Consequently, the method can be interpreted as a Galerkin method that updates basis functions according to the solution dynamics. Secondly, we introduce intrusive and non-intrusive parametric reduced order models [1] using POD-Galerkin and POD deep-learning methods. In this approach we set up the POD-basis a priori by computing snapshots of the SWME for different time-parameter instances. Predictions of the resulting Galerkin or deep-learning reduced order model are compared to the dynamical low-rank approximation concerning accuracy and runtime.

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Effective A-posteriori Error Estimation for Port-Hamiltonian Systems

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The modeling of modern technical systems typically includes the consideration of different physical domains to represent a realistic behavior. The method of port-Hamiltonian (pH) systems manages to describe such systems in a unified framework by defining the energy as the *lingua franca* between the involved subsystems [1]. High-dimensional systems result from the spatial discretization of these models, leading to computationally demanding simulations and making model order reduction (MOR) techniques indispensable to allow for real-time scenarios or multi-query simulations.

Typically structure-preserving MOR techniques are used to preserve the pH structure and with it some of its advantages, such as passivity or modularity. The control of the introduced approximation error requires the usage of an error estimator. Error estimation approaches help to build confidence in the reduced model and can be used to work on adaptive basis generation, e.g. greedy algorithms, to improve the projection basis iteratively.

Based on the knowledge of different (non-)structure-preserving basis generation and projection techniques from our previous work [2, 3], the current work aims at developing an a-posteriori error estimator based on residuals for port-Hamiltonian systems by taking advantage of the specific pH-structure. One problem of current mathematical error estimators like [4] is the overestimation for large realistic systems retained from commercial FE which makes these unsuitable for instance in uncertainty quantification (UQ) in parameter identification. This problem is eased by introducing a so-called auxiliary linear problem (ALP), which provides an approximation for the residual, that helps to increase the effectivity of the error bound [5]. The obtained results are illustrated by a sophisticated example from the field of fluid-structure interaction.

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Efficient Hyper-Reduction of contact problems treated by Lagrange multipliers.

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Keywords: Hyper-Reduction; contact mechanics; Lagrange multipliers; solvability condition; condition number; clustering; local reduced order models

The resolution of contact mechanics problems is often time consuming because of the non-linearity of the contact constraints. For contact problems treated by Lagrange multipliers (ensuring the Signorini contact conditions to be respected), applying reduced-order modeling remains challenging due in particular to the non-negativity constraint on the Lagrange multipliers [1]. We focus here on the Hybrid Hyper-Reduction (HHR) of contact problems proposed in [3], based on a reduced integration domain (RID). Hence a reliable reduced dual basis is obtained by restricting the full order dual basis to the RID. The HHR model is then a saddle-point problem that must respect the necessary solvability condition associated to the well-posedness of the reduced problem. In the discrete setting, this condition imposes the projected contact rigidity matrix to be of full row rank. This may lead to an extension of the primal POD reduced basis [3]. By highlighting the strong link between the condition number of the projected contact rigidity matrix and the precision of the dual reduced solutions, we propose two enrichment methods aiming at respecting the solvability condition and controlling the size of the primal reduced basis with respect to the required precision on the dual solutions [4]. For large parametric variation of the contact zone, the reachable dual precision may remain limited due to the high nonlinearity of the dual solutions. We then propose a clustering strategy (derived from [2]) on the parametric space in order to circumvent this issue through piecewise low-rank approximations. On each cluster, a local accurate HHR model is built thanks to the enrichment strategies. The overall solutions is then deeply improved while preserving an interesting compression of both primal and dual bases.

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

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Optimal feedback control is required in many modern applications such as autonomous driving to ensure safety and also to keep energy consumption to a minimum. An optimal feedback rule is based on an optimal control problem (OCP), which shall be of the following form

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

The value function (VF) v provides due to Bellman's principle of optimality (BPOO) the optimal feedback law, which maps the current state to the optimal signal, via its gradient, i.e. $u(x) = -\frac{1}{2}g^\top(x)R^{-1}g(x)\nabla v(x)$. Obtaining the VF for nonlinear, high-dimensional OCPs by solving the Hamilton-Jacobi-Bellman equation arising from the BPOO is not possible with classical numerical algorithms for PDEs for dimensions $N > 6$ because of the the curse of dimensionality (COD). Since the dynamics are often high-dimensional when originating from semi-discretized PDEs, extensive research efforts have been spent in recent years to find strategies to overcome this difficulty.
Exploiting the well-known relation between the BPOO and the Pontryagin's maximum principle (PMP), which are the first-order necessary conditions of the OCP and lead to a two-point boundary value problem, it is possible to generate information about the VF and its gradient along optimal trajectories. Thus, a data-driven strategy is to solve the PMP for many initial states and build a surrogate for the VF on top of that in an offline phase. Then, it can be used to obtain an approximate optimal feedback rule in an online phase. In our approach based on [1], the domain of interest is explored through optimal trajectories starting from a problem-dependent set of initial states. This avoids having to specify a domain of possible states. In addition, in our data generation process, the selected initial states are chosen using a greedy strategy with the advantage that already computed data can be taken into account in order to find new, promising initial states. Then Hermite kernel interpolation techniques are applied to this data set to obtain a surrogate that exploits all the available information of the VF. Here a vectorial kernel orthogonal greedy algorithm (VKOGA) [2] is used to select the centers. Generally, kernel techniques are typically robust against the COD as they are grid-free. One difficulty when considering Hermite kernel interpolation are very large system matrices, impossible to store or work with. We overcome this with a matrix-free strategy using a specific class of kernels. Furthermore, under the assumption that the VF belongs to the reproducing kernel Hilbert space of the considered kernel, the convergence of the surrogate to the VF as well as the convergence of the surrogate-controlled solution to the optimal solution can be proven. With the whole procedure we can overcome the COD and still receive a very precise, robust and real-time capable feedback control.

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Hybrid Projection Methods with Recycling for Inverse Problems

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Abstract: Iterative hybrid projection methods have proven to be very effective for solving large linear inverse problems due to their inherent regularizing properties as well as the added flexibility to select regularization parameters adaptively. In this work, we develop Golub-Kahan-based hybrid projection methods that can exploit compression and recycling techniques in order to solve a broad class of inverse problems where memory requirements or high computational cost may otherwise be prohibitive. For problems that have many unknown parameters and require many iterations, hybrid projection methods with recycling can be used to compress and recycle the solution basis vectors to reduce the number of solution basis vectors that must be stored, while obtaining a solution accuracy that is comparable to that of standard methods. If reorthogonalization is required, this may also reduce computational cost substantially. In other scenarios, such as streaming data problems or inverse problems with multiple datasets, hybrid projection methods with recycling can be used to efficiently integrate previously computed information for faster and better reconstruction. Additional benefits of the proposed methods are that various subspace selection and compression techniques can be incorporated, standard techniques for automatic regularization parameter selection can be used, and the methods can be applied multiple times in an iterative fashion. Theoretical results show that, under reasonable conditions, regularized solutions for our proposed recycling hybrid method remain close to regularized solutions for standard hybrid methods and reveal important connections among the resulting projection matrices. Numerical examples from image processing show the potential benefits of combining recycling with hybrid projection methods.

Interpolatory (P)MOR via low-rank (tensor) approximation in general linear matrix equations

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It is a well known fact that interpolation of the transfer function

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

in certain points $s_j = \mathrm{i}\omega_j \in \mathrm{i}\mathbb{R}$, in projection-based model order reduction, can be achieved via projection to rational Krylov subspaces [1]. Further it has been shown that the solutions X and Y of the Sylvester equations

$$-AX + EXS = BL, \tag{2}$$
$$-A^{\mathsf{T}}Y + E^{\mathsf{T}}YS = C^{\mathsf{T}}L, \tag{3}$$

with the spectrum of S equal to the set of all s_j, span these exact Krylov subspaces, as long as none of the s_j is a pole of H and (S, L) is controllable. It is a well observed fact that the low rank of the right hand sides often transfers to a low (numerical) rank of the solutions X and Y. This is especially true when many interpolation points are used, i.e. S gets large. Our solvers aim to exploit this fact to automatically decide about the reduced orders after massive oversampling.
When H additionally depends on parameters, i.e. there are parameter dependencies in E, A, B, or C, we derive tensor versions of (2), (3) and suggest low-rank tensor solvers to compute the truncation matrices.

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Low-rank methods in large scale constrained optimization

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Many challenging problems in computational science and engineering are formulated as constrained optimization problems. In particular, the constraint is often a partial differential equation (PDE) or a system of PDEs. When discretizing such optimization problems in both space and time the resulting linear or nonlinear systems are of very large scale. Adding parameters or uncertainties to this makes the dimensionality even larger. This poses a significant challenge to the numerical algorithms and storage availability. But we are often in luck as the systems come with an inherent Kronecker product structure where we will show in this talk is amenable to employing low-rank optimization techniques based on matrix or tensor factorisations. We start reviewing the basic technique on a simple PDE-constrained optimization problem and then illustrate how this technique can be carried over to more challenging examples coming from fractional PDEs, discretizations via isogeometric analysis, or uncertainty quantification.

Low-rank Parareal: a low-rank parallel-in-time integrator

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University of Geneva

The Parareal algorithm of Lions, Maday, and Turinici is a well-known time parallel algorithm for evolution problems. It is based on a Newton-like iteration, with cheap coarse corrections performed sequentially, and expensive fine solves performed in parallel. In this work, we apply Parareal to evolution problems that admit good low-rank approximations and for which the dynamical low-rank approximation (DLRA), proposed by Koch and Lubich, can be used as time stepper. Many discrete integrators for DLRA have recently been proposed, based on splitting the projected vector field or by applying projected Runge–Kutta methods. The cost and accuracy of these methods are mostly governed by the rank chosen for the approximation. We want to use these properties in a new method, that we call low-rank Parareal, in order to obtain a time-parallel DLRA solver for evolution problems. We propose an analysis of the algorithm on affine linear problems and illustrate our results numerically.

M-M.E.S.S. 3.0 - Introducing Krylov-based solvers

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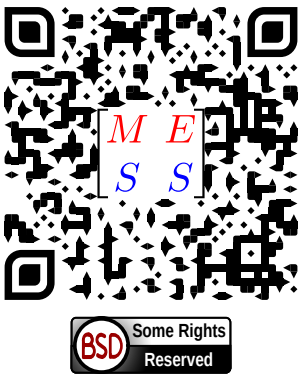
Matrix equations have many important applications in Model Order Reduction (MOR). Lyapunov and Riccati equations are the central ingredients in balancing based methods and Sylvester equations are related to eigenvalue problems in modal approximations, and in certain cases their solutions span the rational Krylov subspaces sought in interpolatory MOR. Especially when large-scale dynamical systems are treated, the coefficients become large, and are usually sparse. In these settings, the solutions to the equations are observed to often have low (numerical) rank and, thus, low-rank approximations to the solution are of central interest. M-M.E.S.S. [2] provides solvers that iterate directly on the low-rank factors of the solutions.

Classically, the solvers in M-M.E.S.S. have been centered around the low-rank ADI iteration. The latest version additionally supports methods based on projection to extended and rational Krylov subspaces [3, 4]. Moreover, a specialized method for Sylvester equations with tall and skinny solutions [1] was added.

On the poster, we show how these benefit MOR and embed in the general structure of the toolbox.



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Machine learning-based reduced order modelling: Towards intelligent digital twins

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Reduced Order Modeling (ROM) is a mathematical technique that reduces the time and cost of static or dynamic numerical simulations while preserving the dominant effects of the high fidelity model. The combination of physics-based models with artificial intelligence enables the construction of Non-Intrusive ROMs (NIROMs) that constitute the backbone of real-time digital twin systems [1]. Machine Learning (ML) methods along with linear algebra techniques have proven an efficient way to construct NIROMs [2]. Motivated by this approach, in this work we present a newly developed ROM network, that combines a Singular Value Decomposition (SVD) update methodology with deep learning models. Our innovative framework, which we refer to as *FastSDV-ML-ROM* can handle large-scale full order models, predict and forecast the spatiotemporal solutions for a given parameter set in a limited amount of time. *FastSDV-ML-ROM* can be very effective for real-time monitoring driving the decisions of an active control system through a feedback process.

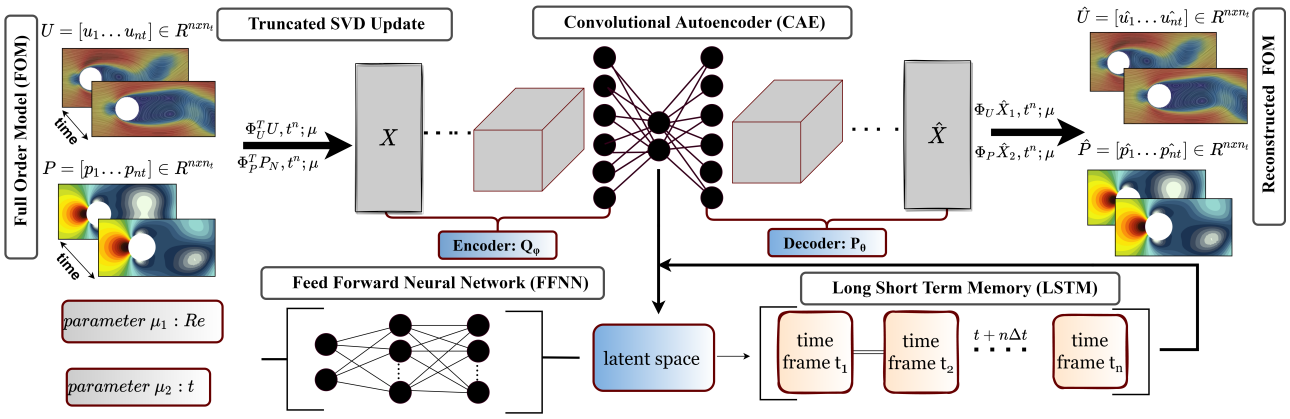

Figure 1: *FastSDV-ML-ROM* framework during the online and offline phase for the fluid flow past a cylinder case simulated in Simcenter STAR-CCM+. i) SVD is used to identify a low-rank approximation of the multi-fidelity model, ii) convolutional autoencoders for non-linear dimensionality reduction, iii) feed forward neural networks map the input parameters to the latent spaces and long short-term memory models to identify the dynamics of the system.

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Mass-conserving and energy-consistent ROMs for the incompressible Navier-Stokes equations with time-dependent boundary conditions

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Keywords: *Structure preservation, incompressible Navier-Stokes equations, time-dependent boundary conditions, finite volume method*

In the reduced order modeling of the incompressible Navier-Stokes equations, significant interest is paid to the preservation of fundamental physical structures such as the mass conservation and the energy balance. However, many existing methods are limited to fluid flows with homogeneous or inhomogeneous, but time-independent boundary conditions [3, 4]. In this work, we propose a mass-conserving and energy-consistent reduced order model (ROM) for fluid flows with time-dependent boundary conditions.

We consider an energy-conserving finite volume discretization on a staggered grid [4] and decompose the velocity field into a component satisfying homogeneous boundary conditions and a time-dependent lifting function. Other works involving such lifting functions require that the boundary conditions are parametrized by a small number of time-dependent coefficients [2]. On the contrary, we allow arbitrary boundary conditions and apply Proper Orthogonal Decomposition to snapshots of the boundary conditions to obtain an approximation of the boundary conditions. The resulting ROM satisfies the mass conservation equation exactly with respect to these approximated boundary conditions. Moreover, the ROM is velocity-only, i. e. the velocity field can be computed without knowledge of the pressure field. Thereby, we avoid additional computational costs and pressure-related inf-sup-instabilities. Furthermore, due to our choice of the lifting function, which is inspired by the Helmholtz-Hodge decomposition [1], the ROM satisfies an kinetic energy evolution which matches corresponding evolutions of the full order model and the continuous model. As a consequence, the ROM is observed to be more accurate and stable compared to ROMs which violate this kinetic energy evolution.

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Model order reduction for wave-type problems with band-limited outputs of interest

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In this talk, we present a goal-oriented model order reduction (MOR) technique targeting wave-type problems. Constructing reduced order models for wave-type problems poses various challenges, such as, potentially slow Kolmogorov n-width decay [1] in contrast to exponential decay for certain linear elliptic coercive problems, the inability to preserve properties of the original model, and potentially weak stability properties. We propose constructing reduced order models in the frequency domain, where the parametric partial differential equation is an elliptic problem. In many applications the output of interest is band-limited. Therefore, the input-to-output map for these applications is amenable to reduction. Inspired by the time domain POD-greedy algorithm [2], we propose a POD-Greedy algorithm driven by a goal-oriented error estimator in the frequency domain to generate reduced basis functions. In each greedy iteration, we apply a POD-based compression technique to iteratively enrich the basis and benefit from the band-limited output of interest to guarantee rapid convergence of the reduced basis approximation. Moreover, targeting the basis generation to the considered output further helps to obtain a reduced order model of small dimension. The reduced basis functions preserve the structure of the full-scale problem during projection and generate stable reduced order models. In addition, the resulting reduced order models do not jeopardize the time domain accuracy after numerical Laplace inversion of the frequency domain approximation. The proposed algorithms are widely applicable to various seismological applications with a seismogram as output of interest, and to structural health monitoring applications with damping. Numerical experiments for a 2D seismic wave equation with semi-realistic data functions demonstrate an exponentially converging reduced basis approximation and stable reduced order models.

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Model order reduction via substructuring for a nonlinear, switched, differential-algebraic machine tool model

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Machine tools are permanently exposed to complex loads, induced by static, dynamic and thermal effects. This often results in an undesired displacement of the tool center point (TCP), causing additional errors in the production process and thus limiting the achievable workpiece quality. To counter these effects, profound knowledge in modeling and simulation techniques is required. Also, current research impulses in the context of model-based data analytics strive for process-parallel solutions utilizing machine internal data.
In order to combine existing modeling capabilities with modern data-driven approaches, a massive reduction of calculation times is a fundamental requirement. At this point, model order reduction (MOR) becomes crucial. Sophisticated MOR strategies enable the computation of compact low-dimensional models for the fast simulation of entire machine tool models while preserving the model accuracy. The resulting low-dimensional models are required for various applications, e.g., in digital twins, the correction of thermally induced errors at the TCP during the production process as well as for lifetime calculations in predictive maintenance.
In this contribution, we investigate advanced modeling of thermo-mechanical effects in machine tools with nonlinear machine components using the example of a feed axis. We present strategies of MOR for this coupled thermo-mechanical model with nonlinear subsystem and moving loads. Applying tailored substructuring techniques, we are able to separate the linear and nonlinear system components. This allows to apply classic linear MOR methods, to the, in our case much larger, linear parts, and thus enables drastically reduced computing times. Transient thermo-mechanical interactions of the feed axis are calculated in a final investigation, comparing the performance of the resulting reduced-order model and the original one.

Multi-fidelity Optimization of an Acoustic Metamaterial using Model Order Reduction and Machine Learning

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Metamaterials are structures that are designed to show properties which cannot be observed in conventional materials [3]. One of those properties is the generation of a stop band, a frequency range in which vibrations are strongly attenuated. Metamaterials that show a stop band are often generated by a periodic repetition of a so-called unit cell. To assess the stop band behavior, a single unit cell is first discretized by means of the Finite Element Method. By applying periodic boundary conditions, the discretized undamped equation of motion turns into a dispersion eigenvalue problem with respect to the frequency and the wavenumbers. Since the quantity of interest are stop bands in the frequency range, real values for the wavenumbers are prescribed and the eigenvalue problem is solved for the frequency. Consequently, the eigenvalue problem has to be solved repeatedly for all possible values of the wavenumbers. Since the involved matrices are obtained by means of the Finite Element Method and thus can become very large, the stop band calculation for a single parameter point is computationally very expensive. [4]
In order to reduce the computational effort, models of lower fidelity, i.e. models that approximate the same output compared to the full order model but with a lower accuracy and a lower computational complexity, can be derived. For the stop band calculation, three different models of lower fidelity are used: (i) Model Order Reduction using the Generalized Bloch Mode Synthesis [2], which is a modal reduction method based on the Component Mode Synthesis. Furthermore, (ii) surrogate modeling is applied in order to estimate the objective function value without performing any Finite Element simulation. The surrogate model is thereby used via a surrogate-based adaptive optimization strategy [1]. Finally, the characteristics of the stop band computation are exploited: Since we are not interested in the relationship between frequencies and wavenumbers for all possible wavenumbers but only in a band in the frequency range, (iii) it is sufficient to solve the eigenvalue problem of the full order model for the two points in the wavenumber-space, for which the upper and the lower bound of the stop band occur. In order to learn these relevant values of the wavenumbers, machine learning methods, namely neural networks and polynomial regression, are used. The three models of lower fidelity are combined in a multi-fidelity optimization strategy to exploit the properties of each.

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Non-intrusive adaptive surrogate modeling of parametric frequency-response problems

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Numerical methods for time-harmonic wave propagation phenomena are often computationally intensive, especially in mid- and high-frequency regimes, making a direct frequency response analysis prohibitively expensive. In this framework, starting from few expensive solves of the problem, model order reduction (MOR) methods can provide a reliable and cheap-to-evaluate approximation of the frequency response of the system. In this talk, we describe an MOR approach for parametric frequency-response problems, where the high-fidelity problem

$$\begin{cases} zE(\mathbf{p})\mathbf{x}(z,\mathbf{p}) = A(\mathbf{p})\mathbf{x}(z,\mathbf{p}) + \mathbf{b}(z,\mathbf{p}) \\ \mathbf{y}(z,\mathbf{p}) = C(\mathbf{p})\mathbf{x}(z,\mathbf{p}) + \mathbf{d}(z,\mathbf{p}) \end{cases}$$

models not only the impact of the frequency z on the system response, but also that of additional design and/or uncertain parameters $\mathbf{p}$. Our approach is non-intrusive, i.e., we do not require access to the matrices/operators defining the underlying high-fidelity problem.
Our proposed method relies on *minimal rational interpolation* [2] for the surrogate modeling of the frequency dependence, for few fixed values of the parameters $\mathbf{p} \in \{\mathbf{p}_j\}_{j=1}^T$. In this step, only the dependence on z is taken into account, and the T resulting surrogates $\{\widetilde{\mathbf{y}}_j\}_{j=1}^T$ (with $\widetilde{\mathbf{y}}_j(z) \approx \mathbf{y}(z,\mathbf{p}_j)$ for all j) are rational functions of z. We describe how an adaptive selection of the frequency sample points can be carried out even in a non-intrusive framework.
Then, the T different z-surrogates, properly converted to a modal form

$$\left\{ \widetilde{\mathbf{y}}_j \ : \ z \ \mapsto \ \sum_i \frac{r_i^j}{z - \lambda_i^j} \right\}_{j=1}^T,$$

are combined to obtain a global approximation with respect to both frequency and parameters [1]. We also describe how locally adaptive sparse grids can be applied over $\mathbf{p}$-space to (i) weaken the curse of dimension and (ii) perform non-intrusively an adaptive sampling of the parameters.
Numerical examples in modeling of electrical circuits and elasto-dynamic systems will also be presented, providing evidence of the approximation quality and computational efficiency of the surrogate models obtained with the proposed technique.

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On Balanced Truncation Error Bound and Sign Parameters

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Balanced truncation model reduction [2, 3] is a powerful tool for reducing linear time-invariant (LTI) dynamical systems, yielding reduced-order models that satisfy a simple *a priori* error bound in terms of the system's Hankel singular values. Consider the single-input, single-output (SISO) system

$$\mathcal{G}: \begin{cases} x'(t) = Ax(t) + bu(t), & y(t) = cx(t), \end{cases} \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^{n\times 1}$, and $c \in \mathbb{R}^{1\times n}$. We assume (1) is asymptotically stable and minimal. Such a system is called *principal-axis balanced* if the unique solutions $\mathcal{P}$ and $\mathcal{Q}$ to the Lyapunov equations

$$A\mathcal{P} + \mathcal{P}A^\top + bb^\top = 0 \quad \text{and} \quad A^\top\mathcal{Q} + \mathcal{Q}A + c^\top c = 0$$

satisfy $\mathcal{P} = \mathcal{Q} = \Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_n)$, where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n > 0$ are the *Hankel singular values* of $\mathcal{G}$. In this balanced realization, $\mathcal{G}$ satisfies the sign-symmetry condition

$$A = SA^\top S, \quad b = (cS)^\top,$$

where $S = \operatorname{diag}(s_1, \ldots, s_n)$ and $\{s_i\}_{i=1}^n \subset \{\pm 1\}$ are the *sign parameters* corresponding to the Hankel singular values. Balanced truncation reduces the model order by removing components of the state space that correspond to small Hankel singular values, resulting in a reduced-order model $\mathcal{G}_r$ satisfying the $\mathcal{H}_\infty$ error bound [1]:

$$\|\mathcal{G} - \mathcal{G}_r\|_{\mathcal{H}_\infty} \leq 2(\sigma_{r+1} + \cdots + \sigma_n), \tag{2}$$

assuming the neglected Hankel singular values are distinct. First, we show that the balanced truncation error bound (2) holds with equality for SISO systems when sign parameters corresponding to the *truncated* Hankel singular values are consistent, that is $s_i = +1$ or -1 for $i = r+1, \ldots, n$. Second, we show how to determine these sign parameters for systems having *arrowhead realizations* of the form

$$A = \begin{bmatrix} d_1 & \alpha_2 & \cdots & \alpha_n \\ \beta_2 & d_2 & & \\ \vdots & & \ddots & \\ \beta_n & & & d_n \end{bmatrix}, \quad b = \gamma e_1, \quad \text{and} \quad c = e_1^\top,$$

where $\gamma \in \mathbb{R}$ and $e_1 \in \mathbb{R}^n$ is the first canonical basis vector. We prove that the sign parameters s_i are determined, up to a permutation, by the signs of the off-diagonal entries of the corresponding arrowhead realization: Namely, there exists a permutation $\{\pi_1, \pi_2, \ldots, \pi_n\}$ of $\{1, 2, \ldots, n\}$ such that

$$s_{\pi_1} = \operatorname{sign}(\gamma), \quad s_{\pi_i} = \operatorname{sign}(\gamma\alpha_i\beta_i), \quad i = 2, \ldots, n.$$

We illustrate these results with an arrowhead system arising in power systems modeling.

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On the use of exponential integrators for large-scale Hamiltonian systems

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

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

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

Operator inference method for mechanical systems

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Mechanical systems are typically modeled by second-order differential equations.

$$\boldsymbol{M}\ddot{\mathbf{x}}(t) + \mathbf{E}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) = \mathbf{B}\mathbf{u}(t) \tag{1}$$

Whenever the system realization is known, model reduction using projection methods can be performed. However, in many setups, mechanical systems are modeled using legacy codes, and the dynamical equations are not accessible.
The remedy for this is non-intrusive MOR, which allows constructing low-dimensional surrogate models directly from simulated or experimental data. One recent non-intrusive approach, known as operator inference [1], consists of inferring the reduced operators by solving least-squares optimization problems using the trajectories and inputs of the original system.

In this talk, the application of operator inference for mechanical systems preserving the original system structure and properties will be discussed. The results for different benchmarks will be presented.

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Parametric model order reduction approach for quasi-static non-linear mechanical problems using an industrial code: application to an elasto-plastic material

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We present our work on parametric model order reduction (pROM) for a generic class of parametric mechanical problems with internal variables in a non-linear quasi-static framework. This work is the result of a collaboration between the MEMPHIS team of Inria Bordeaux Sud-Ouest and the R&D departments of EDF. Within the engineering studies performed by EDF, engineerqs might have to run simulations repeatedly for slightly different configurations, which are associated with different physical or geometric model parameters (parametric study). However, successive evaluations for non-linear mechanical problems can lead to prohibitive computational costs.

We implement an hyper-reduced reduced-order model (ROM) based on an industrial FEM code (Code Aster). We develop an adaptive algorithm based on a POD-Greedy strategy [2]. Since the differential operator is nonlinear, we develop an hyper-reduction strategy based on empirical quadrature (EQ): our approach relies on the construction of a reduced quadrature to speed up online assembly costs of the ROM. This strategy relies on recasting the EQ problem ([1], [3]) as a sparse representation problem over all integration points, or elements. Moreover, we introduce an error indicator correlated to the approximation error, whose evaluation is cost-efficient in terms of computational time.

As an illustration and validation of our methodology, we present numerical results for a plate with a hole under traction with a elastoplastic behaviour, with physical variable parameters (strain hardening or elasticity coefficients).

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pyMOR – Model Order Reduction with Python

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pyMOR (`https://pymor.org`) is a free and open source model reduction software library for the Python programming language. Originally created with the application of Reduced Basis methods to large-scale problems in mind [4], it has been designed from the ground up for seamless integration with external PDE solvers by expressing all algorithms in terms of operations on `VectorArray`, `Operator` and `Model` interface classes [2]. Since its inception in 2012, pyMOR has grown significantly beyond its original scope and now offers a wide selection of both Reduced Basis and system-theoretic algorithms, being maintained by an open group of developers from both fields [1, 3]. Recent additions include data-driven algorithms such as Dynamic Mode Decomposition or neural-network based approaches, structure-preserving methods as well as randomized numerical linear algebra algorithms.
With this poster we will give an overview on pyMOR's design and features. We will also discuss our current and future development goals.

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Reduced Basis Methods for Time-Harmonic Maxwell's Equations

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One of the main practical difficulties concerning the solution of parametrized problems derived from Maxwell's equations is the required running time. These problems often use edge, or Nédélec, finite elements for the approximation of the main unknown that belongs to the space $H(\text{curl}, \Omega)$ properly modified according to the boundary conditions. The aim of this work is to study the performance of Reduced Basis (RB) methods when the first family of Nédélec finite elements, see [2], is used. For all the tests we employ the RBniCSx software [1], that is the new version of RBniCS, based on FEniCSx where complex numbers are available. Thus, our studies are focused on applying Reduced Basis (RB) methods to edge finite elements and verifying their effectiveness in the RBniCSx environment, since in our knowledge it is the first time that edge elements are use in a RBniCS software. In particular, we use both Proper Orthogonal Decomposition (POD) and greedy sampling as strategy to generate the RB space.
We use time harmonic Maxwell's equations with impedance boundary conditions parametrized in terms of the frequency ω, see [3], i.e.

$$\begin{aligned} \nabla \times (\mu^{-1} \nabla \times \boldsymbol{E}) - (\omega^2 \varepsilon + i\omega\sigma)\boldsymbol{E} &= \boldsymbol{F} && \text{in} \quad \Omega, \\ \boldsymbol{n} \times \boldsymbol{E} &= \boldsymbol{0} && \text{on} \quad \Gamma_{int}, \\ (\mu^{-1} \nabla \times \boldsymbol{E}) \times \boldsymbol{n} - i\omega\lambda(\varepsilon_0 \mu_0^{-1})^{1/2} \boldsymbol{E}_T &= \boldsymbol{g} && \text{on} \quad \Gamma_{out}, \end{aligned} \tag{1}$$

where $\boldsymbol{E}_T := (\boldsymbol{n} \times \boldsymbol{E}|_{\Gamma_{out}}) \times \boldsymbol{n}$ and the domain Ω is a cube with a cubical cavity, i.e. $\Omega := (-1,1)^3 \setminus (-1/2, 1/2)^3$.
For this problem it can be proved that the sesquilinear form is coercive on the Hilbert space $X := \{\boldsymbol{u} \in H(\text{curl}, \Omega) \mid \boldsymbol{n} \times \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_{int};\ \boldsymbol{u}_T \in L^2(\Gamma_{out}, \mathbb{C}^3) \text{ on } \Gamma_{out}\}$. Thus, the complex valued Lax-Milgram lemma holds and it is possible to determine explicitly the *a-posteriori* error bound for the greedy procedure through the coercivity constant, rather than with a lower bound of the the inf-sup constant as done in [2]. The numerical results have attained the theoretical expectations and we observed that the speedup numbers for time harmonic Maxwell's equations are very significant.

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Reduced order models for efficient uncertainty quantification of wooden structures with inhomogeneous material properties

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Simulating natural fiber-based structures is not a trivial task as - in addition to the inherent geometrical complexity - environmental conditions influence the material properties significantly. Especially knots and fiber deviation of wooden components are decisive for the quantification of the material behavior [3]. To achieve better quantification of the material properties, the spatial heterogeneous properties can e.g. be modeled by the theory of random fields within a simulation workflow. However, such detailed and complex FE analysis are computationally costly and impractical for uncertainty studies with multiple analysis iterations. Hence, a low-fidelity model is developed here to enable an efficient multi-query scheme. For nonlinear problems, a widely used approach is the Model Order Reduction (MOR) technique, which combines data-based and physical knowledge. The MOR scheme assumes that the combination of a few basis vectors approximates the system sufficiently well with a reduced number of unknowns. For this study the idea is modified and transferred to applications for wood structures.

In general, the MOR workflow can be divided into an online and an offline phase. The offline phase is a preparation step, where full-order model results, called snapshots, are exploited to derive the main deformation modes. Besides a conventional singular value decomposition of the snapshot matrix, the proposed training of intrusive MOR schemes includes here an additional hyper-reduction step to approximate the nonlinear terms [1, 2]. Moreover, a suitable approach for inhomogeneous material properties is developed to create a low-fidelity model predestined for the uncertainty studies, conducted in the online phase. Within this contribution, an efficient analysis of the anisotropic and heterogeneous material behavior is proposed. The material properties of a natural fiber-based material are modeled by the theory of random fields and a statistical analysis is conducted. Therefore, an intrusive MOR model is created to efficiently evaluate the nonlinear, transient problems within the multi-query analysis.

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Reduction of single phase flow models in porous media using a quantity of interest

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In hydrogeology, the calibration of the inputs of flow models is based on in-situ measurements such as well or seismic data. However, these calibration workflows usually require several runs of a flow simulator leading to a large computational effort. In this context, the reduced basis (RB) technique may be a solution to lower the overall simulation cost. In this work, we consider a porous rock saturated with a slightly compressible fluid. Writing the mass balance equation along with Darcy's law gives:

$$\Phi \rho c_t \frac{\partial p}{\partial t} - \nabla.(\frac{\rho \mathbf{k}}{\mu}(\nabla p + \rho g \nabla z)) = q \text{ in } \Omega \times (0,T) \tag{1}$$

where ϕ is the rock porosity, p the pressure, c_t the total compressibility, $\mathbf{k}$ the rock permeability, ρ the density, μ the viscosity, g the gravity constant and q the well source term. Equation (1) is closed by imposing the following boundary and initial conditions over $\partial\Omega = \Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}}$:

$$p = p_{\mathrm{D}} \text{ on } \Gamma_{\mathrm{D}} \times (0,T), \tag{2}$$

$$\frac{\rho \mathbf{k}}{\mu}(\nabla p + \rho g \nabla z) \cdot \mathbf{n} = h_{\mathrm{N}} \text{ on } \Gamma_{\mathrm{N}} \times (0,T), \tag{3}$$

$$p(x, t=0) = p^0(x) \text{ in } \Omega. \tag{4}$$

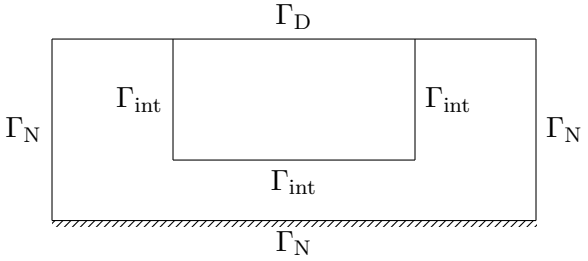

Figure 1: Boundaries of the domain

In practice, we have to solve (1)–(4) at all time steps for many values of $\mathbf{k}$ and several depths of the geological horizons. This work aims at being predictive on the time evolution of the flux $\mathbf{s}$ defined by

$$\mathbf{s} = \int_{\Gamma_{\mathrm{int}}} \frac{\rho \mathbf{k}}{\mu}(\nabla p + \rho g \nabla z).\mathbf{n}\, \mathrm{ds}$$

over the interior boundary Γ_{int} represented on figure 1. To avoid the induced computational cost, we construct a reduced model by using a Greedy-POD algorithm. The greedy basis generation process relies on a posteriori error estimate of the output of interest $\mathbf{s}$, which requires a construction of reduced bases for both the primal and dual problems. Numerical results are presented to illustrate the methodology for the aforementioned parameters, the convergence of the greedy algorithm and the efficiency of the a posteriori error estimate.

ROM for Large-scale Modelling of Urban Air Pollution

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Urban air pollution is a major global challenge that is responsible for damage to climate, ecosystems, and health. Recent research conducted by the World Health Organization (WHO) has shown that 9 out of 10 people breathe polluted air and this indirectly translates into a human life cost (over 3 million deaths per year) and an economic cost (estimated at 5 trillion dollars per year). For these reasons, air quality management is listed as one of the UN Sustainable Growth Goals, and a directive by the EU Commission has prescribed to assess air quality through monitoring stations that can be supported by appropriate mathematical modeling tools. In particular, a framework that can combine direct measurements and computational modeling techniques is an important analytical tool, able to extract various insights from the collected statistics and open new strategies for decision support and scenario forecasting at different scales.
Since at the urban level, pollutant dispersion depends on daily weather conditions, CFD models with low time scales, repeated evaluation, and fine mesh discretization must be used. The former requirements translate into huge memory requirements, making it essential to use HPC facilities to get results in reasonable time frames [1]. However, the problem is suitable for the employment of Reduced Order Models (ROMs) to achieve fast converged solutions with limited loss of accuracy. For this reason, the present work consists of the exploration of a Proper Orthogonal Decomposition (POD) coupled with the Galerkin projection approach for the acceleration of external environmental flow problems.
The evolution of the pollutant is described through the transport equation, where the convective field is given by the solution of the Navier-Stokes equation, while the source term consists of an empirical time series. We studied two different options for the reduced order model, namely extracting a POD basis onto which the FOM field is projected, or using the DEIM as a hyper-reduction strategy. Both these approaches are proven to be effective, even when the basis for the source term is extracted on a subset of the time series, and then used for future state prediction. We then tackled the parametrized convective field case, by changing the direction and intensity of the inlet velocity. This modeling choice is in agreement with the aforementioned assumption of coupling the use of our model to experimental measurements. Here we propose a data-driven approach based on a POD-NN reconstruction of the flux field, which is used to recover in a non-intrusive fashion the reduced-order operators required for the online evaluation. Our framework is validated on different scales and using both real traffic measurements and traffic emission models. We first tackled the problem on a small scale using as computational domain the main campus of the University of Bologna, modeled using a mesh with about 40k cells. Then we solved the problem on a mesh representing the whole city of Györ, with 3 million cells, and a resolution of about 2 meters at street level. In the latter case, we also made use of real-world traffic counts obtained with cameras and loop detectors.

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Spectral approximation of Lyapunov operator equations with applications in high dimensional non-linear feedback control

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Solving the infinite horizon Hamilton-Jacobi-Bellman equation in high dimensions is a difficult task that appears in many applications. Instead of calculating the value function directly we present a new approach that will use a spectral decomposition of the solution to an operator Lyapunov equation with respect to a finite rank infinite-time admissible observation operator. Denoting by A the generator of the semigroup of the underlying dynamics and a bilinear form $\langle \cdot, \cdot \rangle_g$ representing the cost, we focus on the operator Lyapunov equation:

$$\langle A^*\phi, \psi \rangle_P + \langle \phi, A^*\psi \rangle_P + \langle \phi, \psi \rangle_g = 0 \qquad \forall \phi, \psi \in \mathcal{D}(A)$$

We will show that the solution P admits a spectral decomposition with rapidly decaying eigenvalues, which makes a finite rank approximation feasible. In the simple case of a linear quadratic problem this approach is equivalent to finding the best low-rank solution of an ordinary Lyapunov equation and will lead to linear eigenfunctions. Motivated by this, we then also reformulate the problem as an optimization problem over the manifold of all fixed rank operators. Two main benefits of this approach can be expected: For once, the representations in terms of a tensor train (TT), which we will use for discretization, have lower ranks. Secondly we will use Riemannian optimization to perform a simultaneous update for both the control and the value function. This will significantly speed up the computation. We show numerical results for simple, but non-linear, systems without control, which prove the concept viable.

Subspace-Distance-Enabled Active Learning for Parametric Model Order Reduction of Dynamical Systems

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In scenarios where repeated evaluations for varying parameter configuration of a high-fidelity physical model are required, surrogate modeling techniques based on model order reduction are used. The reduced basis method [1], equipped with a residual-based error estimator, is one possible methodological choice. There, snapshots at new parameter samples are generated and the reduced basis space is greedily updated via an iterative procedure. However, when the governing equations of the dynamics are not accessible, we need to construct the parametric reduced-order model (ROM) in a non-intrusive fashion. In this setting, the residual-based error estimate for optimal parameter sampling is not available. Our work intends to provide an alternative optimality criterion to efficiently populate the parameter snapshots, thereby, enabling us to efficiently construct a parametric ROM.

In contrast to the reduced basis method, we consider separate parameter-specific proper orthogonal decomposition (POD) subspaces. We design several metrics based on the subspace distance which can be used to extract the most important parameter values. One approach is to first generate low-accuracy (on a coarse grid for fast computation) snapshots for a preliminary fine parameter set. Then using the metrics, we pick the most important parameter locations for which high-accuracy snapshots are generated. An alternate approach is to first start with high-accuracy snapshots for a preliminary coarse parameter set. We then sample new parameter locations by progressively subdividing the farthest subspaces, in an iterative fashion, based on the metrics. We also present heuristically sound strategies to perform this subdivision between any two selected subspaces. Ultimately, a parametric ROM based on kernel-based shallow neural networks is actively learned with the proposed framework.

To demonstrate the validity of our proposed ideas, we present numerical experiments using several physical models. For instance, consider the parametric viscous Burgers' equation. Figure 1 shows the first 35 parameter selections and their corresponding POD dimension when using the subspace-distance-enabled active learning (SDE-ActLearn) procedure. And figure 2 shows the performance of the ROM at out-of-training time instances t for an out-of-training viscosity value of 10^{-3}.

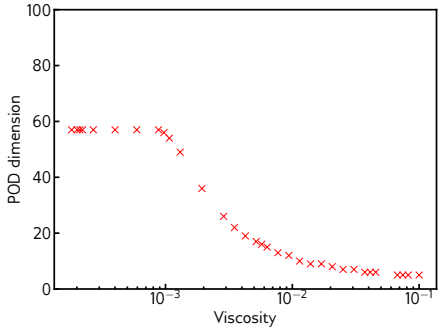

Figure 1: Selected parameters and corresponding POD subspace dimension for Burgers' equation.

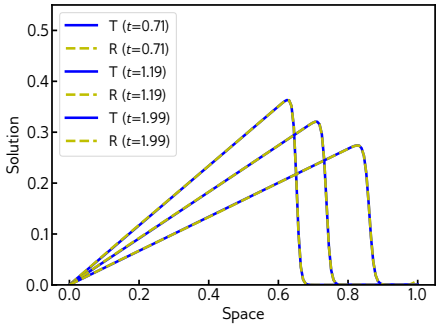

Figure 2: Comparison of ROM (R) and true (T) solutions for Burgers' equation with viscosity 10^{-3}.

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Symplectic formulation of PGD reduced-order models for structural dynamics applications

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Keywords: *Model Reduction, Proper-Generalized Decomposition, Hamiltonian Formulation, Symplectic Schemes*

The talk is concerned with the construction of proper-generalized decomposition formulations that preserve the structure and stability, such as the symplectic properties, of the original systems. The formulations are derived from the Hamiltonian formalism and will be shown to be more stable than classical approaches, e.g. [1]. The framework also allows one to define an optimization problem with constraints on the error in goal functionals in order to construct reduced models capable of delivering accurate approximation of quantities of interest [2]. Numerical examples dealing with the dynamical behavior of beam structures will be presented in order to demonstrate the efficiency of the proposed approach.

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Tensor Galerkin Proper Orthogonal Decomposition for Uncertainty Quantification of PDEs with Random Parameters

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The statistically sound treatment of modelled uncertainties in simulations comes with significant additional computational costs. Since a deterministic model can already be arbitrarily complex, running statistics for general problems may soon become infeasible unless some kind of model reduction is involved.
In this talk, we present a multidimensional Galerkin Proper Orthogonal Decomposition (POD) that simultaneously reduces the physical dimensions of the model and the dimensions related to the uncertainties; see [2] for details.
Using basic tensor calculus we extend our recent work of space-time Galerkin POD [1] to arbitrary dimensions and apply it to PDEs with multivariate uncertainties. By means of a numerical example we illustrate the procedure, how it outperforms POD based on random snapshots and how it compares to statistics informed greedy sampling strategies as proposed in [3].

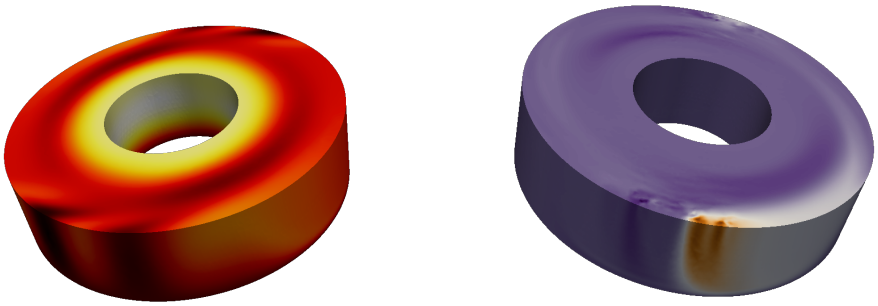

Figure 1: Illustration of the state of an example convection-diffusion simulation and the spatially distributed error in the expected value of the solution under a multivariate uncertainty in the diffusion parameter.

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Time extrapolation technique applied to POD-based ROM

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Reduced-order models (ROMs) based on the proper orthogonal decomposition (POD, [3]) are frequently used to solve partial differential equations more efficiently. The ROM must be trained off-line following the snapshots method [2]: a set of solutions is computed up to the training time, t_{train}, by means of the full-order model (FOM), the name given to the discretization of the equation of interest. POD-based ROMs are not able to compute solutions of advection-dominated problems beyond t_{train}. In this work, a novel method based on a coordinate transformation [1], called CT-ROM, is presented to allow for the extrapolation of solutions beyond the training time.
Figure 1 shows the difference between the standard ROM (left) and the CT-ROM (right) applied to the linear advection-diffusion equation $\partial_t u + a\partial_x = \nu\partial_{xx} u$, with $a = 0.5$ and $\nu = 0.001$. The initial Gaussian profile, the computed solution at t_{train} and $T > t_{\text{train}}$ are plotted together in a case where the Peclet number is $Pe = 5$.

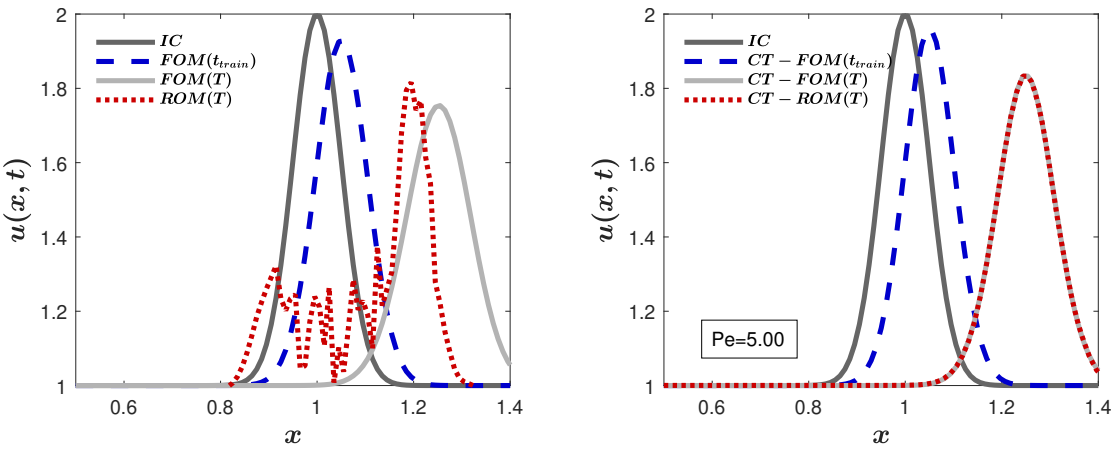

Figure 1: Solutions computed with the FOM/ROM (left) and with the CT-FOM/CT-ROM (right).

The CT-ROM strategy shows promising results in different scenarios, such as 1D linear advective equation with diffusion source term. This method has been applied to more examples: linear advective equation with reaction source term, systems of coupled linear equations and the non-linear inviscid Burgers' equation [3].

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Towards a Benchmark Framework for Model Order Reduction in the Mathematical Research Data Initiative (MaRDI)

Peter Benner[1], René Fritze[2], Jan Heiland[1], Christian Himpe[2], Hendrik Kleikamp[2], Kathryn Lund[1], Tim Mitchell[1], Mario Ohlberger[2], Stephan Rave[2], and Jens Saak[1]

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The race for the most efficient, accurate, and universal algorithm in scientific computing drives innovation. Yet, this healthy competition is only beneficial if the research output is actually comparable to prior results. Fairly comparing algorithms can be a complex endeavor, as the implementation, configuration, compute environment, and test problems need to be well defined. Due to the increase in computer-based experiments, new infrastructure for facilitating the exchange and comparison of new algorithms is also needed. To this end, we propose a benchmark framework, which is a generic toolkit for comparing implementations of algorithms using test problems native to a community. Its value lies in its ability to fairly compare and validate existing methods for new applications, as well as compare newly developed methods with existing ones.

As a prototype for a more general framework, we have begun building a benchmark tool for the Model Order Reduction Wiki (MORWiki) [4]. The wiki features three main categories: benchmarks [2, 3], methods, and software. An editorial board curates submissions and edits entries. Data sets for linear and parametric-linear models are already well represented in the existing collection. Data sets for non-linear or procedural models, for which only evaluation data, rather than equations, are available, are being added and extended. Properties and interesting characteristics used for benchmark selection and later assessments are recorded in the model metadata.

The MORWiki collection will be the data basis for our model reduction benchmark tool. To this end, experiences from [1] serve as a prototype and will be extended to the remaining model classes and methods. The MORWiki will serve as a proof-of-concept for a living-document progress-tracker of a field, while also facilitating fair comparisons of new findings and methods. Its core information will be mirrored in the MaRDI-Portal, which is concurrently under development.

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3.4 Thursday, September 22

Digital Twins through Reduced Order Models and Machine Learning

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The vision of building digital twins for complex infrastructure and systems is old. However, realizing it remains very challenging due to the need to combine advanced computational modeling, reduced order models, data infusion for calibration, updating and uncertainty management, and sensor integration to obtain models with true predictive value for decision support. Nevertheless, the perspectives of using digital twins for predictive maintenance, operational optimization, and risk analysis are very substantial and the potential for impact significant, from safety, planning, and financial points of view. In this talk we shall first discuss the importance of reduced models in the development of digital twin technologies and continue by discussing different aspects of the challenges associated with developing digital twins through a few examples, combining advanced model and data driven technologies, e.g., classifiers, Gaussian regression and neural networks, to enable failure analysis, optimal sensor placement and, time permitting, multi-fidelity methods and risk analysis for rare events.
These are all elements of the workflow that needs to be realized to address the challenge of building predictive digital twins and we shall demonstrated the value of such technologies through a number of different examples of increasing complexity.

Optimization based model order reduction for stochastic systems

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[2]*Institute for Mathematics, University of Halle-Wittenberg, 06099 Halle (Saale) Germany*

In this talk, we will connect ideas from model order reduction for stochastic linear systems and $\mathcal{H}_2$-optimal model order reduction for deterministic systems. In particular, we supplement and complete the theory of error bounds for model order reduction of stochastic differential equations. With these error bounds, we establish a link between the output error for stochastic systems (with additive and multiplicative noise) and modified versions of the $\mathcal{H}_2$-norm for both linear and bilinear deterministic systems. When deriving the respective optimality conditions for minimizing the error bounds, we will see that model order reduction techniques related to iterative rational Krylov algorithms (IRKA) are very natural and effective methods for reducing the dimension of large-scale stochastic systems with additive and/or multiplicative noise. We apply modified versions of (linear and bilinear) IRKA to stochastic linear systems and show their efficiency in numerical experiments.

Balanced Truncation for Bayesian Inference

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[2] *University of Edinburgh*
[3] *Virginia Tech*
[4] *ShanghaiTech University*
[5] *Rensselaer Polytechnic Institute*
[6] *University of Utah*

We consider the Bayesian inverse problem of inferring the initial condition of a linear dynamical system from noisy output measurements taken after the initial time. In practical applications, the large dimension of the dynamical system state poses a computational obstacle to computing the exact posterior distribution. Balanced truncation is a system-theoretic method for model reduction which obtains an efficient reduced-dimension dynamical system by projecting the system operators onto state directions which simultaneously maximize energies defined by reachability and observability Gramians. We show that in our inference setting, the prior covariance and Fisher information matrices can be naturally interpreted as reachability and observability Gramians, respectively. We use these connections to propose a balancing approach to model reduction for the inference setting. The resulting reduced model then inherits stability properties and error bounds from system theory, and yields an optimal posterior covariance approximation.

Semi-supervised Invertible DeepONets for Bayesian Inverse Problems

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[2]*Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia*
[3]*Munich Data Science Institute (MDSI - Core Member), www.mdsi.tum.de*

Deep Operator Networks (DeepONets) [2] offer a powerful, data-driven tool for solving parametric PDEs by learning operators, i.e. maps between infinite-dimensional function spaces. Recently proposed physics-informed versions have made use of governing law residuals in the loss function in order to significantly reduce requirements for expensive, labeled training data (i.e. input-output pairs), as well as to improve predictive accuracy under extrapolative conditions [3]. In this work, we employ physics-informed DeepONets in the context of high-dimensional, Bayesian inverse problems. Traditional solution strategies necessitate an enormous, and frequently infeasible, number of forward model solves, as well as the computation of parametric derivatives. In order to enable efficient solutions, we extend DeepONets by employing a realNVP architecture [1] which yields an invertible and differentiable map between the parametric input and the branch net output. This allows us to construct accurate approximations of the full posterior which can be readily adapted irrespective of the number of observations and the magnitude of the observation noise. As a result, no additional forward solves are required, nor is there any need for costly sampling procedures. We demonstrate the efficacy and accuracy of the proposed methodology in the context of inverse problems based on a reaction-diffusion and a Darcy-flow equation.

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Structured barycentric forms and their application to iterative data-driven model reduction of second-order systems

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Data-driven and reduced-order modeling are essential tools for computing high-fidelity compact dynamical models that approximate real-world physical phenomena. Here, data are represented by frequency response measurements, i.e., samples of the transfer function of the unknown model. There are many methods available to tackle this problem in the unstructured standard case; see, e.g., [1]. In particular, we mention here the vector fitting (VF) algorithm from [2] and the AAA algorithm [3], which both iteratively fit transfer functions to data by means of solving linear(ized) least-squares problems.
The key ingredient of these data-driven approaches is the *barycentric form* of the system's rational transfer function. This is an advantageous representation of general rational functions, that:

- provides an easy transition between rational functions and the matrix representation of (linear time-invariant) systems;
- directly imposes interpolation conditions at selected support points.

In this work, we present extensions of the classical barycentric form to the case of mechanical systems described by second-order differential equations:

$$\begin{aligned} M\ddot{x}(t) + D\dot{x}(t) + Kx(t) &= B_{\mathrm{u}}u(t), \\ y(t) &= C_{\mathrm{p}}x(t), \end{aligned} \tag{1}$$

with the transfer function $H(s) = C_{\mathrm{p}}(s^2M + sD + K)^{-1}B_{\mathrm{u}}$. In particular, we make use of these barycentric forms to develop various new structure-preserving reduced-order modeling approaches to obtain systems of the form (1) from given frequency domain data. We present the following approaches:

- an extension of the VF algorithm for fitting modally damped mechanical systems (1) in [4];
- extensions of the AAA for (1) by imposing one-sided interpolation conditions, and by fitting other conditions in a least-squares manner.

For the latter, we show that by carefully choosing the interpolation points (in a greedy manner, inspired by classical AAA), structured reduced models (1) can be constructed to enforce reliable approximations.

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Structured $\mathcal{L}_2$-Optimal Parametric Model Order Reduction

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Consider the full-order model (FOM) and reduced-order model (ROM)

$$\text{FOM: } \begin{cases} \mathcal{A}(\mathsf{p})x(\mathsf{p}) = \mathcal{B}(\mathsf{p}), \\ y(\mathsf{p}) = \mathcal{C}(\mathsf{p})x(\mathsf{p}), \end{cases} \quad (1) \qquad \text{and} \qquad \text{ROM: } \begin{cases} \widehat{\mathcal{A}}(\mathsf{p})\widehat{x}(\mathsf{p}) = \widehat{\mathcal{B}}(\mathsf{p}), \\ \widehat{y}(\mathsf{p}) = \widehat{\mathcal{C}}(\mathsf{p})\widehat{x}(\mathsf{p}), \end{cases} \quad (2)$$

where $\mathsf{p} \in \mathcal{P} \subseteq \mathbb{C}^d$ is the parameter, $x(\mathsf{p}) \in \mathbb{C}^{n \times n_i}$ is the state, $y(\mathsf{p}) \in \mathbb{C}^{n_o \times n_i}$ is the output, $\widehat{x}(\mathsf{p}) \in \mathbb{C}^{r \times n_i}$ is the reduced state for some $r \ll n$, and $\widehat{y}(\mathsf{p}) \in \mathbb{C}^{n_o \times n_i}$ is the approximate output. Therefore, $\mathcal{A}(\mathsf{p}) \in \mathbb{C}^{n \times n}$, $\mathcal{B}(\mathsf{p}) \in \mathbb{C}^{n \times n_i}$, $\mathcal{C}(\mathsf{p}) \in \mathbb{C}^{n_o \times n}$, $\widehat{\mathcal{A}}(\mathsf{p}) \in \mathbb{C}^{r \times r}$, $\widehat{\mathcal{B}}(\mathsf{p}) \in \mathbb{C}^{r \times n_i}$, and $\widehat{\mathcal{C}}(\mathsf{p}) \in \mathbb{C}^{n_o \times r}$. Our goal is to find a ROM (2) that is an $\mathcal{L}_2$-optimal approximation of the form

$$\widehat{\mathcal{A}}(\mathsf{p}) = \sum_{i=1}^{q_{\widehat{\mathcal{A}}}} \widehat{\alpha}_i(\mathsf{p})\widehat{A}_i, \quad \widehat{\mathcal{B}}(\mathsf{p}) = \sum_{j=1}^{q_{\widehat{\mathcal{B}}}} \widehat{\beta}_j(\mathsf{p})\widehat{B}_j, \quad \widehat{\mathcal{C}}(\mathsf{p}) = \sum_{k=1}^{q_{\widehat{\mathcal{C}}}} \widehat{\gamma}_k(\mathsf{p})\widehat{C}_k, \quad (3)$$

where $q_{\widehat{\mathcal{A}}}, q_{\widehat{\mathcal{B}}}, q_{\widehat{\mathcal{C}}}$ are positive integers; $\widehat{\alpha}_i, \widehat{\beta}_j, \widehat{\gamma}_k \colon \mathcal{P} \to \mathbb{C}$ are given measurable functions; and $\widehat{A}_i \in \mathbb{R}^{r \times r}$, $\widehat{B}_j \in \mathbb{R}^{r \times n_i}$, and $\widehat{C}_k \in \mathbb{R}^{n_o \times r}$. By "$\mathcal{L}_2$-optimality", we mean that we seek a ROM that minimizes

$$\mathcal{J}(\widehat{y}) = \|y - \widehat{y}\|^2_{\mathcal{L}_2(\mathcal{P},\mu)} = \int_{\mathcal{P}} \|y(\mathsf{p}) - \widehat{y}(\mathsf{p})\|^2_{\mathrm{F}} \,\mathrm{d}\mu(\mathsf{p}), \quad (4)$$

where μ is a measure over the parameter set $\mathcal{P}$.

We first derive the gradients $\nabla_{\widehat{A}_i}\mathcal{J}$, $\nabla_{\widehat{B}_j}\mathcal{J}$, and $\nabla_{\widehat{C}_k}\mathcal{J}$ of the squared $\mathcal{L}_2$ error (4) (with respect to the reduced-order matrices), which then leads to a gradient-based optimization method for structured model order reduction (MOR) of parametric problems. We illustrate that these gradients can be computed using only output values, and thus the optimization algorithm can be performed purely in a data-driven manner based on the samples of the output without access to full-order operators.

We show that by appropriately defining the measure μ and the parameter set $\mathcal{P}$, our formulation in (1)–(4) covers a wide range of problems such as parametric stationary problems, e.g., arising from discretization of parametric partial differential equations, as well as (parametric) linear-time invariant systems and discretized least-squares fitting.

We also show that this unifying framework recovers the well-known optimality conditions for $\mathcal{H}_2$ and $\mathcal{H}_2 \otimes \mathcal{L}_2$-optimal MOR for dynamical systems. Furthermore, we develop interpolatory necessary conditions for $\mathcal{L}_2$-optimal MOR of a class of parametric stationary problems; more precisely, we show that if $\widehat{y}(\mathsf{p}) = \sum_{i=1}^{r} \frac{c_i b_i^{\mathrm{T}}}{\mathsf{p}-\lambda_i}$ is an $\mathcal{L}_2$-optimal ROM (with some additional assumptions), then we have

$$Y(\lambda_i)b_i = \widehat{Y}(\lambda_i)b_i, \quad c_i^{\mathrm{T}}Y(\lambda_i) = c_i^{\mathrm{T}}\widehat{Y}(\lambda_i), \quad c_i^{\mathrm{T}}Y'(\lambda_i)b_i = c_i^{\mathrm{T}}\widehat{Y}'(\lambda_i)b_i,$$

for $i = 1, 2, \ldots, r$, where Y and $\widehat{Y}$ are transformed outputs related to y and $\widehat{y}$. Finally, we discuss MOR methods based on (Petrov-)Galerkin projection and whether $\mathcal{L}_2$-optimal ROMs are necessarily of such type.

We illustrate the theory via various numerical examples and compare our framework to standard projection-based approaches.

High Order Approximations of the Operator Lyapunov Equation Have Low Rank

Luka Grubišić[1] **and Harri Hakula**[2]

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We present a low-rank greedily adapted *hp*-finite element algorithm for computing an approximation to the solution of the Lyapunov operator equation. We present a model for analyzing the regularity in eigenfunctions of the solution of the Lyapunov equation which we utilize to justify the use of high order finite element spaces. We also present an a posteriori error estimator and show its effectiveness on the model problem. We use a spectral theoretic setting in order to define the error estimator as well as to define measures of the approximation error. On the example of the Laplace operator on the dumbbell domain we achieve eight figures of accuracy for computing the trace of the solution of the Lyapunov equation using a finite element space of dimension of only 10^4 degrees of freedom. Even more surprising is the observation that *hp*-refinement has an effect of reducing the rank of the approximation of the solution.

Long-time prediction of nonlinear parametrized dynamical systems by deep learning-based reduced order models

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Conventional reduced order models (ROMs) anchored to the assumption of modal linear superimposition, such as proper orthogonal decomposition (POD), may reveal inefficient when dealing with nonlinear time-dependent parametrized PDEs, especially for problems featuring coherent structures propagating over time. To enhance ROM efficiency, we propose a nonlinear approach to set ROMs by exploiting deep learning (DL) algorithms, such as convolutional neural networks. In the resulting DL-ROM [2, 5], both the nonlinear trial manifold and the nonlinear reduced dynamics are learned in a non-intrusive way by relying on DL algorithms trained on a set of full order model (FOM) snapshots, obtained for different parameter values. Performing then a former dimensionality reduction on FOM snapshots through POD enables, when dealing with large-scale FOMs, to speedup training times, and decrease the network complexity, substantially [4].
A further step has led us to introduce LSTM neural networks instead of convolutional autoencoders, thus obtaining the μt-POD-LSTM-ROM technique that better grasps the time evolution of the PDE system [1]. This framework allows us to perform extrapolation of the PDE solution forward in time, that is, on a (much) larger time domain than the one used to train the neural network, for unseen values of the input parameters - a task often missed by traditional projection-based ROMs. Accuracy and efficiency of the resulting μt-POD-LSTM-ROM are assessed on several examples, ranging from low-dimensional, nonperiodic systems to applications in structural mechanics dealing with MEMS [3], obtaining faster than real-time simulations that are able to preserve a remarkable accuracy.

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Hybrid fluid/particle methods for kinetic equations describing neutral particles in nuclear fusion plasma-edge modelling

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In nuclear fusion reactors, neutral particles play an important role in shielding the reactor walls and in particular the divertor targets from the hot plasma in which the fusion reactions take place. The neutral particle behaviour is governed by a kinetic equation that is difficult to solve due to the high dimensionality of the phase space and the high collisionality between the neutral particles and the plasma. High dimensionality is typically resolved by resorting to Monte Carlo methods, but in high collisional regimes a pure Monte Carlo solver becomes very expensive. To alleviate the computational cost, recent research focuses on hybrid fluid/particle methods that exploit the high-collisionality of the system [1].
In this talk we will elaborate on a new hybrid fluid/particle method that splits the particle distribution in two phases: a fluid phase and a particle phase. The particle phase is solved using a Monte Carlo scheme, the fluid phase follows a reduced fluid model that is derived from the kinetic equation in the high collisional limit. The two phases co-exist in the whole domain, but the amount of mass in each phase is determined by the local collisionality. This way the amount of particles treated with Monte Carlo is reduced in high collisional regimes, where the cost of Monte Carlo is high, but the reduced fluid model is accurate [2]. In low collisional regimes where the reduced fluid model is not accurate, but Monte Carlo is cheap, most of the mass is in the particle phase.
We anticipate that the new hybrid fluid/particle method enables fast and accurate plasma edge simulations, paving the way towards applications in uncertainty quantification, data assimilation, and ultimately plasma edge code validation.

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Model Order Reduction in Contour Integral Methods for parametric PDEs

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We discuss a projection model order reduction method for linear evolution PDEs, which is based on the application of the Laplace transform. The main advantage of this approach consists in the fact that, differently from time stepping methods, like Runge-Kutta integrators, the Laplace transform allows to compute the solution directly at a given instant, which can be done by approximating the contour integral associated to the inverse Laplace transform by a suitable quadrature formula [2, 1]. In terms of the reduced basis methodology, this determines a significant improvement in the reduction phase, like the one based on the classical proper orthogonal decomposition (POD), since the number of vectors to which the decomposition applies is drastically reduced as it does not contain all intermediate solutions generated along an integration grid by a time stepping method. We show by some illustrative parabolic PDEs arising from finance the effectiveness of the method and also provide some evidence that the method we propose, when applied to a simple advection equation, does not suffer the problem of slow decay of singular values which instead affects methods based on time integration of the Cauchy problem.

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Inf-Sup-Constant-Free Error Estimation for Linear Parametric Systems

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Standard *a posteriori* state error estimation for model order reduction relies on the inf-sup constant [3]. The *a posteriori* error estimation for systems with very small or vanishing inf-sup constant poses a challenge, since the estimator is inversely proportional to the inf-sup constant, resulting in pessimistic error estimation. Such systems appear in electromagnetics where the inf-sup constant values are zero or close to zero, at or near resonant frequencies. In this work, we introduce two efficient *a posteriori* error estimators that are independent of the inf-sup constant.

The first error estimator [1] (called Est1 hereafter) is a state error estimator targeted towards general linear parametric systems. Its derivation is detailed and the associated computational strategies are discussed. Est1 is integrated within an adaptive greedy algorithm that is used to iteratively build the reduced-order model (ROM). The performance of Est1 is compared with the standard error estimator and a recently proposed one from [4]. It is shown that Est1 outperforms both existing estimators. Numerical experiments are performed on real-life microwave devices such as narrowband and wideband antennas, as well as a dual-mode waveguide filter. These examples show the capabilities and efficiency of the proposed methodology.

A modification of Est1, called Est2, is targeted specifically at electromagnetic systems [2]. Est2 makes use of the *Helmholtz decomposition* to significantly reduce the offline computational cost. A greedy ROM generation procedure is also proposed using Est2. The beneficial performance of this new error estimator for electromagnetic systems is illustrated through numerical experiments on real-life microwave devices and filters.

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Parametric reduced order modelling for transport dominated systems via shifted POD deep learning models

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Model reduction for transport dominated phenomena using conventional linear ROM techniques suffers from a very low convergence rate, theoretically quantified by Kolmogorov n-width, which renders these methods practically infeasible for these class of problems. So far, several methods have emerged for such problems one such being shifted POD [4, 3] which was introduced to speed up the convergence. This method essentially decomposes transport fields by shifting the data field in a so-called co-moving frame, in which the travelling wave is stationary and can be described with very few spatial basis functions given by POD. Reduced order modelling for the parametrized PDEs rely on offline-online computational splitting. The expensive task of building the low dimensional subspace out of the FOM snapshots is performed once in the so called offline stage and the ROM approximation corresponding to any new parameter value is computed in the online stage. Besides the linear PDEs for which these methods work well, the problem arises when the dimension of the linear trial subspace becomes very large or when the hyper-reduction strategy scales with the dimension of the FOM. These are often recurrent issues when dealing with non-linear time dependent parametrized PDEs. As a parallel alternative, research on non-intrusive methods have picked up pace in recent years. These methods are purely data driven and feature an offline (training) phase and an online (testing/prediction) phase [1, 2]. Usually these methods employ deep learning frameworks to efficiently learn the nonlinear trial manifold corresponding to the training data and then predicts the solutions for unseen parameter values in the testing phase. In this talk, we address a possible way to extend such non-intrusive methods based on shifted POD. The idea is to learn the low dimensional dynamics created by the frames of the shifted POD using artificial neural networks. With the obtained description we are then able to predict states for unseen parameter values efficiently. The proposed method is tested on one- and two-dimensional examples, including combustion systems and incompressible flows around moving geometries to show the generality of the concept and the appropriate computational savings.

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Port-Hamiltonian systems – from a general modelling wishlist to surrogate models with guarantees

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The framework of port-Hamiltonian (pH) systems is a powerful modeling paradigm in computational science and engineering. It follows a bottom-up philosophy, where each component of a complex system can be modeled separately and then, afterward, combined with the other components through well-defined interaction ports. One of the many advantages of pH systems is that properties like stability and passivity are directly encoded in the system structure. It is thus easy to maintain these properties in surrogate models whenever we are able to preserve the pH structure in the surrogate.
In this talk, I will first discuss how pH systems satisfy a broad range of modern modeling requirements, ranging from their analytical properties to structure-preserving numerical methods [2]. After this general introduction to pH systems, we discuss different aspects of surrogate modeling for pH systems. We start by pointing out the impact of the energy functional on the approximation quality [1], discuss the correct norms to compare pH systems, and explain how we can use the Hamiltonian to learn pH systems from data [3].

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Registration-based model reduction of parameterized PDEs with spatio-parameter adaptivity

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We present a nonlinear registration-based model reduction procedure for rapid and reliable solution of parameterized two-dimensional steady conservation laws [1]. This class of problems is challenging for model reduction techniques due to the presence of nonlinear terms in the equations and also due to the presence of parameter-dependent sharp gradient regions that cannot be adequately represented through linear approximation spaces. Our approach builds on the following ingredients: (i) a general (i.e., independent of the underlying equation) registration procedure for the computation of a parametric mapping that tracks moving features of the solution field [2]; (ii) an hyper-reduced least-squares Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the solution field; (iii) a greedy procedure driven by a residual-based error indicator for efficient exploration of the parameter domain; and (iv) an adaptive mesh refinement technique for the definition of an accurate discretization for all parameter values. We present results for several nonlinear problems in continuum mechanics to demonstrate the effectiveness and the mathematical soundness of our approach.

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A certified wavelet-based physics-informed neural network for nonlinear model reduction of parameterized partial differential equations

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Parameterized partial differential equations (PPDEs)

$$B_\mu : X \to Y', f_\mu \in Y', \mu \in \mathcal{P} \subset \mathbb{R}^p : \quad B_\mu u_\mu = f_\mu \tag{1}$$

arise to describe physical phenomena. These equations often have to be solved either in a multi-query or in a real-time context for different parameters μ resulting in the need for model order reduction. For linear, coercive and affine elliptic as well as parabolic PPDEs it is known that linear projection-based methods, e.g. the reduced basis method [7] are working well. Whereas, for transport- or wave-type problems it has been proven that the Kolmogorov N-width decay is poor ([6], [4]), such that linear model reduction techniques are bound to fail and nonlinear methods are needed.
The recent success in solving various PDEs with neural networks (NNs), particularly with physics-informed NNs (PINNs) (see e.g. [8] [1]) suggests that they are a natural candidate for nonlinear model order reduction (MOR) techniques, although an a-posteriori error control is lacking. Usually the solution of a PPDE is unknown, such that the training of a physics-informed NN exploits the strong-form residual of (1) as a loss function and a penalty term is added to enforce boundary and/or initial conditions. With that at hand, a target function is defined to determine the parameters of the NN during an optimization phase. But to train a quantity which is an upper bound for the error, one has to rely on certain variational formulations of (1).
Our method faces the aforementioned problems for the parameterized transport and wave equation by using the ultra-weak variational formulation ([3], [2], [5]), which involves equality of error and residual. Therefore, the dual norm of the residual

$$\|r_\mu\|_{Y'} := \|f_\mu - B_\mu u_\mu\|_{Y'} \tag{2}$$

gives us not only a-posteriori information about the error of an approximation, but also a loss function to train the PINN. To evaluate the dual norm of (2) we expand the residual in a wavelet basis and exploit the norm equivalences of these. The target function to train the PINN is then defined as a sum of dual norms for a finite sample set $\mathcal{S} \subset \mathcal{P}$ of parameters μ. Due to the fact, that the boundary and initial conditions are encoded in the residual as a part of f_μ we do not need a penalty term. As a result of the training process, the PINN is a nonlinear approximation of the mapping $\mu \mapsto u_\mu$. The application of the method is shown in numerical experiments.

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Neural networks investigation of bifurcating phenomena in fluid-dynamics

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Bifurcating phenomena, i.e. sudden changes in the qualitative behavior of the system linked to the non-uniqueness of the solution naturally arise in several fields. Since the reconstruction of bifurcation diagrams requires a many-query context, which is usually unaffordable using high fidelity simulations, we propose a combination of Reduced Order Models (ROMs) and Machine Learning techniques to reduce the computational burden associated with the investigation of such complex phenomena.
This work aims to show the applicability of the Reduced Basis (RB) model reduction and Artificial Neural Network (ANN), utilizing the POD-NN approach and its physics-informed variant [2, 1], to analyze multi-parameter bifurcating applications in fluid-dynamics.
We considered the Navier-Stokes equations for a viscous, steady, and incompressible flow: (i) in a planar straight channel with a narrow inlet of varying width and (ii) in a triangular parametrized lid-driven cavity. Within this context, we present a new empirical strategy to employ the RB and ANN coefficients for a non-intrusive detection of the bifurcation points [3].
Finally, we introduce a newly developed ROM methodology based on Graph Neural Network, with powerful applications to general parametrized PDEs and branches classification when dealing with bifurcating phenomena [4].

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Deep Orthogonal Decomposition via Mesh-Informed Neural Networks for Reduced Order Modeling of parametrized PDEs

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In the context of parametrized PDEs, Reduced Order Models (ROMs) allow for an efficient approximation of the parameter-to-solution map, which is extremely useful whenever dealing with expensive many-query routines such as constrained optimization, sensitivity analysis and uncertainty quantification. Recently, motivated by the limitations of classical approaches such as the Reduced Basis method, many authors have been considering the use of Deep Learning techniques for building non-intrusive ROMs, e.g. [1, 3, 5, 4]. Within this framework, we propose a novel approach, Deep Orthogonal Decomposition (DOD), where a Deep Neural Network (DNN) yields a representation of the solution manifold in terms of an adaptive local basis. In principle, due to the very high-dimensions involved, designing and training such DNN models can be a challenging task. As a remedy, we exploit Mesh-Informed Neural Networks (MINNs), a novel class of architectures that was recently introduced in [2]. MINNs embed their hidden layers into discrete functional spaces of increasing complexity, obtained through a sequence of meshes defined over the underlying PDE domain. This results in sparse models that are computationally less demanding and thus better suited for implementing the DOD. We assess the robustness of the proposed approach by running different numerical experiments, including domains that feature an involved geometrical shape, and high-dimensional parameter spaces. The method is also compared with other state-of-the-art approaches, such as those involving Principal Orthogonal Decomposition and Autoencoders.

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An adaptive hierarchy of certified machine learning and reduced basis surrogates for parametrized PDEs*

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In the context of parametrized partial differential equations (PDE)s, we are interested in efficiently and accurately approximating time-dependent quantities of interest $f_h \colon \mathcal{P} \to L^2([0,T])$ (for an end time $T > 0$), which are given by applying an output operator to state-trajectories obtained from solving an underlying PDE. We assume we are given a full order model (FOM) to evaluate f_h (e.g., stemming from a spatio-temporal discretization of the PDE), that is however costly to evaluate in the sense that while we may compute $f_h(\mu)$ for few parameters $\mu \in \mathcal{P} \subset \mathbb{R}^p$, for $p > 0$, it is computationally infeasible to evaluate f_h in the context of uncertainty quantification or PDE-constrained optimization. We are in particular interested in the case where this cost does not only stem from a high spatial resolution, but where in addition a high temporal resolution or long-time integration $T \gg 1$ is required.

In our earlier work [1], we used model order reduction by reduced basis (RB) methods to generate an RB-reduced order model (ROM) approximation f_{rb} of f_h by means of the method of snapshots, to generate enough certified data to train a machine learning (ML) based model f_{ml} as an efficient surrogate for f_h. The need for an additional ML surrogate stems from the fact that, while the RB-ROM evaluations might be orders of magnitudes faster than the FOM evaluations, they are still inherently iterative in time, limiting their use in aforementioned scenarios. While demonstrated to perform well, the approach in [1] has two main systematic drawbacks: (i) the a-priori choice of training sets and accuracies for the RB-ROM as well as the ML model (yielding models of fixed size and accuracy) and (ii) more critically, as with most ML surrogates, there is no bound on the prediction error $\|f_h(\mu) - f_{\mathrm{ml}}(\mu)\| \leq ?$ available.

This contribution addresses both shortcomings: (ii) by learning the RB coefficients of the intermediate state, instead of learning the output directly, we propose a certified ML-ROM which combines approximation quality and certification of RB-ROMs with the online efficiency of ML predictions. This allows to certify ML-ROM predictions a posteriori and helps to address (i): we propose an adaptive model hierarchy of FOM, RB-ROM and ML-ROM, where (starting from trivial RB-ROM and ML-ROM) each model is used to generate training data for the next, but only if the online certification indicates a need for enrichment, which we demonstrate in the context of PDE-constrained minimization.

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Multiscale modeling of heterogeneous structures based on a localized model order reduction approach

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Many of today's problems in engineering demand reliable and accurate prediction of failure mechanisms of mechanical structures. Thus, it is necessary to take into account the heterogeneous structure on the smaller scale, to capture the underlying physical phenomena. However, this poses a great challenge to the numerical solution since the computational cost is significantly increased by resolving the smaller scale in the model. Moreover, in applications where scale separation as the basis of classical homogenization schemes does not hold, the influence of the smaller scale on the larger scale has to be modelled directly.
This work aims to develop an efficient concurrent methodology to model heterogeneous structures combining the variational multiscale method (VMM) [4] and model order reduction techniques (e. g. [2]). First, the influence of the smaller scale on the larger scale can be taken into account following the additive split of the displacement field as in the VMM. Here, also a decomposition of the global domain into subdomains, each containing a fine grid discretization of the smaller scale, is introduced. Second, local reduced approximation spaces for the smaller scale solution are constructed by exploring possible solutions for each subdomain based on the concept of oversampling [3] and the solution of the associated transfer operator problem [1]. Herein, we propose to choose the training data based on the solution of a reduced global problem to incorporate the actual physical behaviour of the structure of interest and to extend it by random samples to ensure sufficient approximation capabilities in general. The local reduced spaces are designed such that local contributions of each subdomain can be coupled in a conforming way. Thus, the resulting global system is sparse and reduced in size compared to the direct numerical simulation, leading to a faster solution of the problem.

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Deep learning for reduced order modeling

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Reduced order modeling (ROM) techniques, such as the reduced basis method, provide nowadays an essential toolbox for the efficient approximation of parametrized differential problems, whenever they must be solved either in real-time, or in several different scenarios. These tasks arise in several contexts like, e.g., uncertainty quantification, control and monitoring, as well as data assimilation, ultimately representing key aspects in view of designing predictive digital twins in engineering or medicine. On the other hand, in the last decade deep learning algorithms have witnessed a dramatic blossoming in several fields, ranging from image and signal processing to predictive data-driven models. More recently, deep neural networks have also been exploited for the numerical approximation of differential problems yielding powerful physics-informed surrogate models.

In this talk we will explore different contexts in which deep neural networks can enhance the efficiency of ROM techniques, ultimately allowing the real-time simulation of large-scale nonlinear time-dependent problems. We show how to exploit deep neural networks (and a set of FOM snapshots) to build ROMs for parametrized PDEs in a fully non-intrusive way [3, 2], exploiting deep neural networks as main building block, ultimately yielding deep learning-based ROMs (DL-ROMs) and their further extension [4] to POD-enhanced DL-ROMs (POD-DL-ROMs). Moreover, we show a novel strategy for learning nonlinear ROM operators using deep neural networks [1], thus yielding hyper-reduced order models enhanced by deep neural networks (Deep-HyROMnets), where operator approximation is much more efficient in a projection-based ROM can be performed in an extremely efficient, yet accurate, way. Furthermore, we will also show how to improve a low-fidelity ROM through a multi-fidelity neural network regression technique that allows to merge low- and high-fidelity data, to enhance the ROM accuracy for the sake of input/output evaluations [5].
Through a set of applications from engineering including, e.g., structural mechanics and fluid dynamics problems, we will highlight the opportunities provided by deep learning in the context of ROMs for parametrized PDEs, as well as those challenges that are still open.

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Generating reduced order models parallel in time via random sampling

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

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The local sample complexity of non-linear least squares approximation

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We consider the problem of approximating a function in general nonlinear subsets of L^2 when only a weighted Monte Carlo estimate of the L^2-norm can be computed. Standard concentration of measure arguments can be used to provide a worst-case bound for the probability that a certain error is achieved with a prescribed number of sample points. For model classes of tensor networks, however, this bound depends exponentially on the order of the networks and is independent of the regularity of the sought function. This behaviour is not observed in many practical applications but can indeed be demonstrated in numerical experiments. Restricting the model class to a neighborhood of the best approximation, we can derive a new bound that is able to utilize the regularity and thereby reduce the number of samples that are required to reach a prescribed accuracy.

Randomized local model order reduction for nonlinear PDEs

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We present a localized model order reduction (LMOR) approach for nonlinear (elliptic) partial differential equations (PDEs). LMOR methods are designed to deal with large-scale problems for which full order solves are not affordable in a reasonable time frame and problems with (local) topology changes that prevent the application of monolithic model order reduction techniques.
For linear problems optimal local approximation spaces in the sense of Kolmogorov are spanned by the left singular vectors of a transfer operator [1, 2]. The latter maps unknown Dirichlet boundary data on the boundary of an oversampling domain to the corresponding solution of the local PDE restricted to the subdomain or interface for which one wishes to generate a local reduced space; the boundary of the oversampling domain has to have a certain distance to the target subdomain or interface.
For nonlinear problems we again consider a transfer operator that maps unknown boundary data on the boundary of the oversampling domain to the corresponding local solution of the nonlinear PDE restricted to the target subdomain. Thanks to Caccioppoli's inequality, at the core of the analysis for linear problems, the range of this transfer operator and thus the (nonlinear) set of local solutions of the PDE on the target subdomain is compact. We then use the proper orthogonal decomposition (POD) to optimally approximate this compact set of solutions to a PDE dependent on parameters; the latter is here the unknown boundary data on the boundary of the oversampling domain. However, due to the high-dimensional parameter space, the POD suffers from the curse of dimensionality. To break the curse of dimensionality, we propose a randomized POD [3]. In detail, we consider random boundary conditions of controlled smoothness on the boundary of the oversampling domain, therefore introducing a probability distribution in parameter space. We also derive probabilistic a priori and a posteriori error bounds for the approximation error. Numerical experiments for a nonlinear diffusion problem demonstrate that already a local reduced space of low dimension yields a very accurate approximation.

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Context-aware learning of low-dimensional stabilizing controllers in the scarce data regime

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Stabilizing dynamical systems in science and engineering is challenging, especially in edge cases and limit states where typically little data are available. In this work, we propose a data-driven approach that guarantees finding stabilizing controllers from as few data samples as the dimension of the unstable dynamics, which typically is orders of magnitude lower than the state dimension of systems. The key is learning stabilizing controllers directly from data without learning (reduced) models of the systems, which would require larger numbers of data points.

The starting point for us is the concept of data informativity, which states that the direct construction of stabilizing state-feedback controllers without an intermediate model describing the dynamics is possible using as many data samples as the dimension of the observed states. We sharpened the result in [1] such that the sample complexity scales with the intrinsic (minimal) dimension of the system, rather than the dimension of the observed states, which reduces the sample complexity by several orders of magnitude. In this presentation, we build on the previous findings but go a step further by proposing a data-driven approach that guarantees finding stabilizing controllers from as few data samples as the dimension of the unstable dynamics, which typically is orders of magnitude lower than the dimension of the system. Numerical experiments with systems from chemical reactors (Figure 1) to power systems to fluid dynamics behind obstacles demonstrate that the proposed approach stabilizes systems after observing fewer than five data samples even though the dimension of observed states of the systems is up to several tens of thousands, and learning the corresponding models as well as model-free reinforcement learning with policy gradient methods requires orders of magnitude more data points.

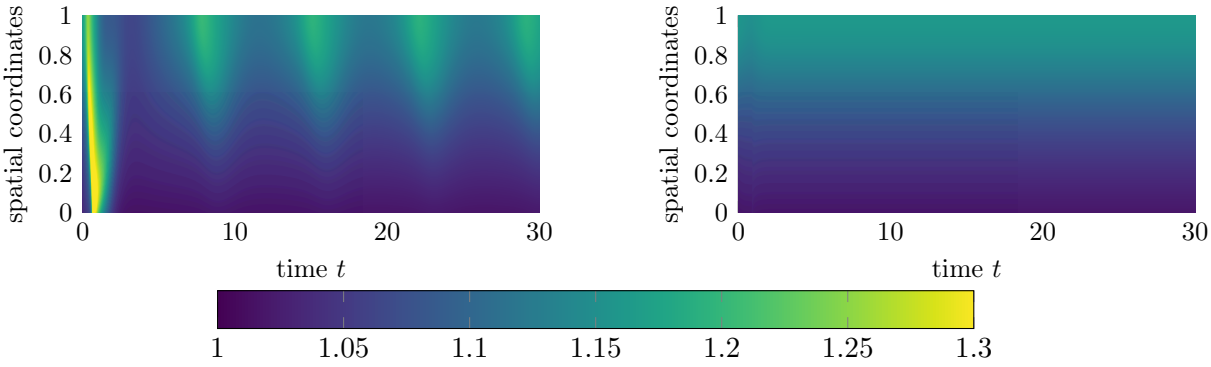

Figure 1: Temperature profiles of a tubular reactor model with unstable oscillations after perturbation of the initial state (right) and the desired steady state behavior (left). Our approach stabilizes the reactor after observing three data samples, which is a three orders of magnitude lower number of samples than required for learning a model of the dynamics.

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Slow collective dynamics via data-driven approximation of the Koopman generator

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The determination of low-dimensional collective variables (CVs) is a critical problem in various application areas, including molecular dynamics simulations. However, finding good CVs, for example in the sense of retaining slow dynamical time scales of the full system, is highly non-trivial and requires the use of state-of-the art data analysis techniques.
In this talk, I will present recent theoretical and algorithmic progress on the determination of CVs and their associated effective dynamics using the projection formalism for stochastic dynamics as developed by Legoll and Lelièvre in [2]. In [6], it was shown that the projection formalism amounts to applying an orthogonal projection to the Koopman generator of the full system. The generator is projected onto the (still infinite-dimensional) space of functions which only depend on the CV space. The first result I will show is an error estimate comparing the slow time scales of the projected system to those of the full one. We arrive at a Galerkin-type estimate, bounding the time scale error in terms of the projection error for dominant eigenfunctions [4].
Then, I will move on to show how a data-driven matrix approximation of the projected generator can be obtained by a technique called generator extended dynamic mode decomposition (gEDMD) [1]. This method can also be formulated if a tensor product basis is used as Galerkin subspace [3], enabling the use of rich approximation spaces and potentially high-dimensional CVs. Finally, I will discuss bounds for the estimation error of the gEDMD method in terms of the amount of simulation data used to learn the Koopman generator [5].

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Structure-preserving reduced-order models for parametric cross-diffusion systems

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Cross-diffusion systems are mathematical models which are used in order to account for complex diffusion phenomena in multi-species mixtures. For instance, these are used to model diffusion of various chemical species in alloys, or to model gaseous mixtures used for medical applications, in particular for respiratory assistance. They read as coupled nonlinear possibly degenerate parabolic systems and their mathematical understanding has only recently attracted the attention of mathematicians. It has recently been understood that some of these systems own a so-called entropic structure, in other words that a particular entropy functional can be seen as a Lyapunov function for such systems. The entropy-entropy dissipation relationship of this system is the key tool in understanding the long-time behaviour of the solutions of these systems. High fidelity structure-preserving finite volume numerical schemes have been developed for the simulation of such systems, but their resolution is very costly from a computational point of view, especially when parametric studies have to be performed. When it comes to model-reduction, it holds that standard Galerkin-POD reduced-order models do not preserve the mathematical properties of the system, in particular its entropic structure. The aim of this talk is to present a new Galerkin-POD type of reduced-order model for these systems, which enable to preserve all the desired mathematical properties of these cross-diffusion systems, and which is based on the choice of a particular nonlinear map specifically adapted to the entropy functional of the system. Numerical results to illustrate the behaviour, the performance and the advantages of this nonlinear structure-preserving reduced-order model will be presented.

This is joint work with Jad Dabaghi.

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