UC San Diego
JACOBS SCHOOL OF ENGINEERING
Mechanical and Aerospace Engineering

MORe 2024

« Model Reduction and Surrogate Modeling »

September 9-13, 2024, University of California San Diego

BOOK OF ABSTRACTS

PHOTO CREDITS

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https://more2024.sciencesconf.org/

1 About MORe 2024

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), Graz (2019). Previous **MORe** editions were held in Berlin (2022).

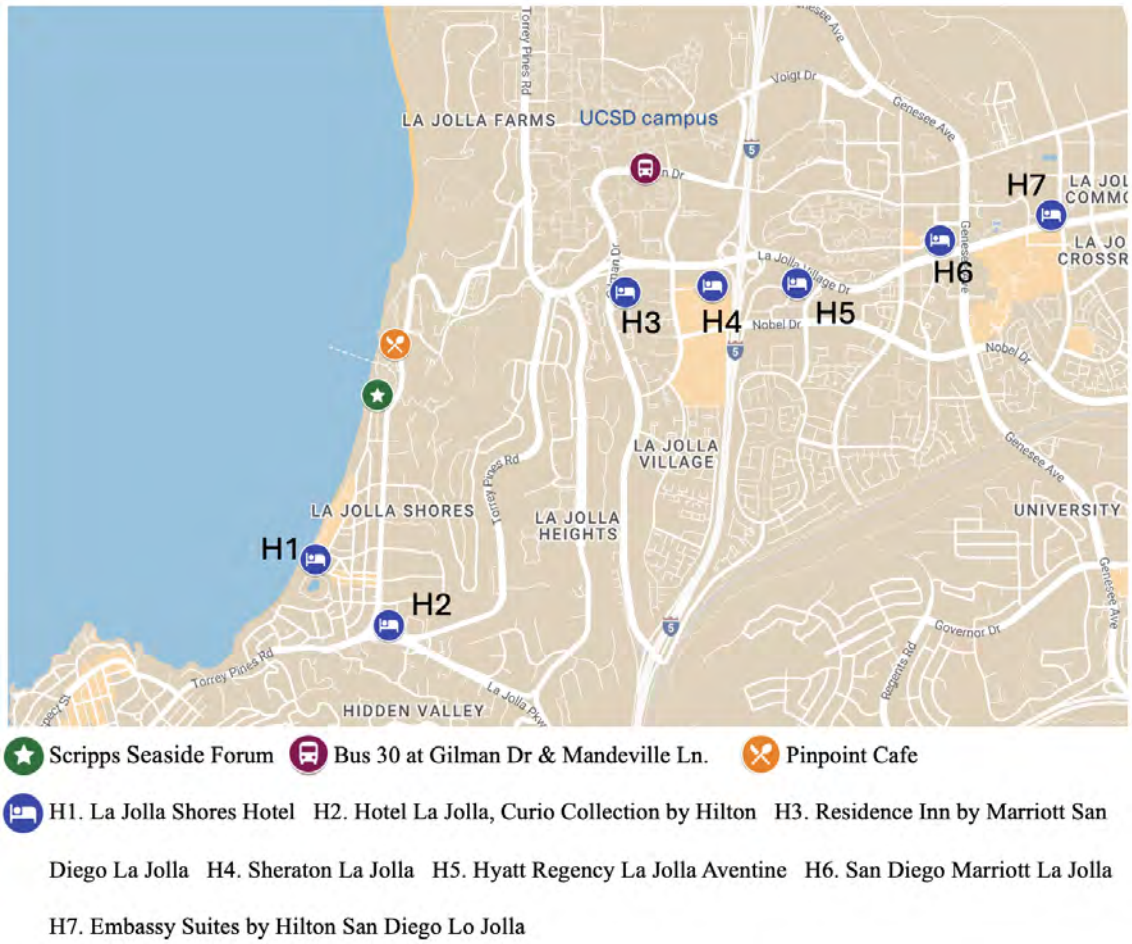
1.1 Topics

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
- Machine learning and model order reduction (in particular when data is sparse)
- Data-driven approaches and hybrid data and physics based model reduction
- Non-intrusive model order reduction
- Tensor methods
- Nonlinear Model Reduction (e.g. geometric approaches on manifolds)
- Kernel methods for nonlinear MOR
- Nonlinear Model Reduction (e.g. on manifolds)
- MOR for problems with poor Kolmogorov N-width decay (e.g. transport phenomena)
- Localized MOR and multi-scale problems
- Randomized methods
- High dimensional parameter spaces, reduction in parameter space, offline stage efficiency
- Dynamic, adaptive and on the fly reduced a approximations, error estimation
- MOR for uncertainty quantification
- Model reduction for optimization, control, inverse problems and data assimilation
- Structure-preserving and energy-based MOR (e.g. Hamiltonian or port-Hamiltonian systems)
- MOR for multiphysics/multiphase problems
- Model reduction for nonlinear bifurcating PDEs
- MOR for industrial applications and sustainable development
- Model order reduction for predictive digital twins
- Model reduction software and benchmarks

1.2 Venue

The conference will be held at the University of California San Diego at the:
Scripps Seaside Forum (Google Maps)
6610 Kennel Way
La Jolla, CA 92037, USA
Contact : more@sciencesconf.org



1.3 Committees

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MATTHIAS MORZFELD (University of California San Diego) matti@ucsd.edu
SERKAN GUGERCIN (Virginia Tech) gugercin@vt.edu

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1.4 Financial support

The event is financially supported by Akselos (akselos.com), ASML, Mitsubishi Electric Research Laboratories (merl.com), and the Air Force Office of Scientific Research under Grant FA9550-24-1-0107 (PMs Dr. Fariba Fahroo and Dr. Frederick Leve). Travel support for US-based students and early career researchers was provided by the National Science Foundation Division of Civil, Mechanical and Manufacturing Innovation under Award No. 2347981 from the program of Dynamics, Control and System Diagnostics.

1.5 Social program

Welcome reception. The welcome reception takes place on **Monday, September 9, 2024 from 4:15–6:15 pm** outside the conference venue.

Conference dinner. The conference dinner takes place on **Wednesday, September 11, 2024 from 6:00–10:00 pm** at the La Jolla Shores Hotel **8110 Camino Del Oro, La Jolla, CA 92037**. The first hour 6:00–7:00 pm will be a cocktail hour at the Shores Lawn of the hotel, and the dinner will be served buffet style from 7:00-9:00 pm at the Garden Patio. The La Jolla Shores hotel can be reached from the conference venue by a 15 minute walk (0.7m/1km), a 4-min drive (parking available for pay) and a limited shuttle service will run at 5:45pm, 6:00pm, 6:15pm and 6:30pm.

Coffee breaks. Coffee, soft drinks, pastries and fruits are served during the breaks outside the conference venue.

Lunch breaks. Catered lunch by UCSD Catering Services will be provided every day during the lunch break from 12:30 - 2:00pm, which is included in the registration fee.

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 20 minutes and includes questions, answers and change of speakers.
We will provide laser pointers for presentations and encourage the speakers to use their own laptops to avoid transfer and software issues. We strongly advise test your presentation and connection during the break before your talk in order to avoid delays between presentations and technical difficulties.
Technical assistance will be present in the lecture rooms 20 minutes before the start of your session.

1.8 Code of Conduct

This event is supported all or in part by the NSF under Award No. 2347981 from the program of Dynamics, Control and System Diagnostics and is governed by the NSF PAPPG which became effective January 30, 2023. Note that Chapter II.F.9 of this guide requires that we provide all event participants with information on the University's policy on sexual harassment, other forms of harassment and sexual assault as well as information about how to report any violations of such policy. For purposes of this requirement, "other forms of harassment" is defined as "Non-gender or non-sex-based harassment of individuals protected under federal civil rights laws, as set forth in organizational policies or codes of conduct, statutes, regulations, or executive orders."

The University of California is committed to creating and maintaining a community dedicated to the advancement, application, and transmission of knowledge and creative endeavors through academic excellence, where all individuals who participate in University programs and activities can work and learn together in an atmosphere free of harassment, exploitation, or intimidation.

The University has policies, which prohibit discrimination, harassment, and sexual violence and address how to report such violations. These policies include the University of California Policy on Discrimination, Harassment, and Affirmative Action in the Workplace, the University of California Policy on Sexual Violence and Sexual Harassment and the UC San Diego Procedures for Discrimination and Harassment Complaint Resolution. These policies cover admission, employment, access, and treatment in University programs and activities.

The UC Policy on Sexual Violence and Sexual Harassment addresses sexual violence, sexual harassment, and retaliation ("Prohibited Conduct"). This Policy outlines the University's responsibilities and procedures related to Prohibited Conduct in order to ensure an equitable and inclusive education and employment environment free of sexual violence

and sexual harassment. UC San Diego Guidelines cover discrimination and harassment on the basis of race, color, national origin, religion, sex, gender, gender expression, gender identity, gender transition status, pregnancy, physical or mental disability, medical condition (cancer-related or genetic characteristics), genetic information (including family medical history), ancestry, marital status, age, sexual orientation, citizenship, or service in the uniformed services. The Policies applies to all University faculty, staff, and students (undergraduates, graduates, and professional students), and third parties.

The Policy applies at all University campuses, University programs and activities, the Lawrence Berkeley National Laboratory, Medical Centers, the Office of the President, and Agriculture and Natural Resources.

The full text of the Policy can be reviewed on the UCSD Sexual Violence Prevention & Response website or the UC Office of the President website. UCI will respond promptly and effectively to reports of Prohibited Conduct and will take appropriate action to prevent, stop, and remedy conduct violates the Policy.

Confidential resources, including CARE at the Sexual Assault Resource Center, are available to those who have experienced sexual harassment or sexual violence. CARE is on-call 24 hours a day and on weekends throughout the year. Those in need of urgent support during non-business hours, weekends, or holidays, may reach CARE at (858) 534-5793. A survivor can make use of confidential resources at any time, regardless of whether the event has been reported to the Title IX office or other authorities. For more information about UCSD CARE and other support services at UC San Diego, see the CARE at SARC website.

Any person may report incidents of sexual harassment, discrimination or sexual violence to the campus Title IX office, which is named The Office for the Prevention of Harassment and Discrimination (OPHD). Contact OPHD by visiting `https://ophd.ucsd.edu/` or by calling (858) 534-8298.

Reports to law enforcement can be made to UC San Diego Police Department for on-campus incidents or to the local department where the crime occurred. A confidential advocate from the UCSD CARE Office or UCSD Police Department staff can help determine which police department to contact. In an emergency, dial 911, or call (858) 534-HELP (4357) to reach the non-emergency phone. Reports to the UCSD Police Department can be made in person at the Campus Services Complex, Building B (map).

2 Program

Monday, September 9

Time	Event
8 : 45 - 9 : 00	**Opening Remarks**
9 : 00 - 9 : 10	**Opening Remarks : Dean Al Pisano**
9 : 10 - 10 : 00	**Plenary 1 (Chair : Serkan Gugercin)**
	· *Nicole Aretz – Exploiting structure via nested operator inference in physics-based learning*
10 : 00 - 10 : 40	**Session 1 : Nonlinear MOR (Chair : Serkan Gugercin)**
	· *Paul Schwerdtner – Greedy construction of quadratic manifolds for nonlinear dimensionality reduction and nonlinear model reduction*
	· *Moritz Feuerle – Model reduction for the wave equation beyond the limitations of the Kolmogorov N-width*
10 : 40 - 11 : 10	**Coffee**
11 : 10 - 12 : 30	**Session 2 : Nonlinear MOR (Chair : Boris Kramer)**
	· *Samuel Otto – On the role and computation of the fiber in model reduction*
	· *Charles Beall – Randomized local model order reduction for p-Laplacian problems*
	· *Alejandro Diaz – Domain decomposition least-squares Petrov-Galerkin model reduction for time-dependent problems*
	· *Christopher Wentland – Accelerated simulation of advection-dominated flows with automated multifidelity modeling and domain decomposition*
12 : 30 - 14 : 00	**Lunch**
14 : 00 - 14 : 50	**Plenary 2 (Chair : Ionut Farcas)**
	· *Youngsoo Choi – Latent space dynamics identification*
14 : 50 - 16 : 10	**Session 3 : Adaptive MOR (Chair : Ionut Farcas)**
	· *Sridhar Chellappa – Tensor-based adaptive sampling strategies for the reduced basis method with application to full-state approximation*
	· *Robert Van Heyningen – Adaptive reduced-order models for high-speed flow via optimally transported meshes*
	· *Jonathan Cangelosi – An adaptive surrogate model refinement framework for trajectory simulation and optimization*
	· *Xianmin Xu – Transformed model reduction for partial differential equations with sharp inner layers*
16 : 15 - 18 : 15	**Welcome Reception**

Tuesday, September 10

Time	Event
8 : 30 - 9 : 20	**Plenary 3 (Chair : Tobias Breiten)**
	· *Tamara Kolda – Tensor decomposition meets reproducing kernel Hilbert spaces*
9 : 20 - 10 : 40	**Session 4 : System-theoretic Model Reduction (Chair : Tobias Breiten)**
	· *Thanos Antoulas – The Loewner framework for parametric systems and the curse of dimensionality. Part I : Theory*
	· *Ion Victor Gosea – The Loewner framework for parametric systems and the curse of dimensionality. Part II : Applications*
	· *Petar Mlinarić – Riemannian optimization over the manifold of rational functions*
	· *Mattia Manucci – Certified model order reduction for large-scale switched differential-algebraic equations*
10 : 40 - 11 : 10	**Coffee**
11 : 10 - 12 : 30	**Session 5 : System-theoretic Model Reduction (Chair : Christopher Beattie)**
	· *Nicholas Corbin – Progress towards scalable nonlinear balancing algorithms*
	· *Tobias Breiten – Nonlinear balanced truncation via infinite-dimensional Koopman lifting*
	· *Reetish Padhi – Balanced truncation for bilinear systems with quadratic outputs*
	· *Sean Reiter – Interpolatory $\mathcal{H}_2$ model order reduction of linear systems with quadratic output functions*
12 : 30 - 14 : 00	**Lunch**
14 : 00 - 15 : 20	**Session 6 : Structure-preserving Model Reduction (Chair : Benjamin Unger)**
	· *Robin Klein – Entropy-stable non-linear manifold ROMs for hyperbolic conservation laws*
	· *Gruber Anthony – Flexible and variationally consistent Hamiltonian model reduction*
	· *Harsh Sharma – Lagrangian operator inference enhanced with structure-preserving machine learning for nonintrusive model reduction of mechanical systems*
	· *Jonas Nicodemus – Learning passive dynamical systems via spectral factorization*
15 : 20 - 16 : 20	**Posters & Coffee**
	· *Steffen W. R. Werner – Model reduction of large-scale sparse systems in MATLAB and octave with the MORLAB toolbox*
	· *Sam Bender – Reduction of periodic systems with partial floquet transforms*
	· *Robin Herkert – Randomized symplectic model order reduction for Hamiltonian systems*
	· *Ray Qu – Entropy stable reduced order modeling of nonlinear conservation laws using discontinuous Galerkin methods*
	· *Albani Olivieri – Discovering quadratic representations of PDEs : Algorithms and software*
	· *Opal Issan – Conservative reduced order modeling of the plasma kinetic equations*
	· *Yingda Cheng – Robust implicit adaptive low rank time-stepping methods for matrix differential equations*
	· *Alessandro Alla, Agnese Pacifico – An online algorithm to identify and control unknown partial differential equations*
	· *Martin Alexander Reinhold – Model order reduction for parabolic PDE constrained optimization in a space time variational setting*
	· *Sebastiaan Van Schie – Parametric proper orthogonal decomposition approaches for high-dimensional design optimization problems*
	· *Jannis Marquardt – Optimal control based reformulation of a data assimilation problem as a new approach for applying model order reduction methods*
	· *Julie Pham – Real-time aerodynamic load estimation for hypersonics via strain-based inverse maps*
	· *Francisco-Javier Granados-Ortiz – Surrogate model generation in CFD with Machine Learning-Aided Design Optimization Method (MLADO)*
	· *Yilin Zhuang – Physically consistent score-based diffusion models for PDE-based inverse problems*
16 : 20 - 17 : 40	**Session 7 : Structure-preserving Model Reduction (Chair : Steffen Werner)**
	· *Johannes Rettberg – Data-driven identification of reduced port-Hamiltonian systems*
	· *Riccardo Morandin – Structure-preserving model order reduction of linear time-varying port-Hamiltonian systems*
	· *Benjamin Unger – Beyond linear - a differential geometric framework for nonlinear projections*
	· *Silke Glas – Structure-preserving model reduction : From the formulation on manifolds to data-driven realizations*

Wednesday, September 11

Time	Event
8 : 30 - 9 : 20	**Plenary 4 (Chair : Mario Ohlberger)**
	· *Tommaso Taddei – Registration in bounded domains for model reduction of parametric conservation laws*
9 : 20 - 10 : 40	**Session 8 : Parametric MOR (Chair : Mario Ohlberger)**
	· *Filip Belik – Greedy frequency domain model reduction for parametric systems : New theory and algorithms*
	· *Karim Cherifi – Snapshot-based modeling of parametric linear systems*
	· *Niklas Reich – A parallel batch greedy algorithm in reduced basis methods : Convergence rates and numerical results*
	· *Chenzi Wang, Page Yu – An iterative active subspace approach for model order reduction of parametric systems with high-dimensional parameter spaces*
10 : 40 - 11 : 10	**Coffee**
11 : 10 - 12 : 30	**Session 9 : Nonintrusive ROMs (not ML) (Chair : Silke Glas)**
	· *Mario Ohlberger – Multi-fidelity learning of reduced order models*
	· *Andrea Manzoni – Multi-fidelity reduced-order surrogate modelling*
	· *Shane McQuarrie – Learning Bayesian reduced-order operators with Gaussian processes*
	· *Mai Peng – Building dynamical stability into data-driven quadratic ROMs*
12 : 30 - 14 : 00	**Lunch**
14 : 00 - 15 : 20	**Session 10 : Nonintrusive ROMs (not ML) (Chair : Mario Ohlberger)**
	· *Antonio Carlucci – Data-driven approximation of linear switched systems*
	· *Ionut Farcas – Distributed computing for physics-based data-driven reduced modeling at scale*
	· *Tomoki Koike – Stability guarantees of non-intrusive data-driven model reduction for nonlinear systems*
	· *Hannah Lu – Data-driven models of nonautonomous systems*
15 : 20 - 16 : 20	**Posters & Coffee**
	· *Nuojin Cheng – Stochastic subspace descent with surrogate-adjusted line search*
	· *Sandeep Reddy Bukka – Physics-informed neural networks assisted operator inference framework for noisy data*
	· *John Rekoske – Rapid 3D Green's functions using reduced-order models of physics-based seismic wave propagation simulations*
	· *Dimitrios Xylogiannis – Construction of nonlinear models from input-output data for atmospheric pollution simulations*
	· *Benjamin Zastrow – Data-driven model reduction via block-structured operator inference for coupled aeroelastic flutter*
	· *Dave May – Non-intrusive reduced order models for geophysics applications : Adaptive sampling for the small data regime*
	· *Cankat Tilki – Wavelet-based dynamic mode decomposition in the context of extended dynamic mode decomposition and Koopman theory*
	· *Vignesh Sella – Surrogate modeling for data-scarce applications using projection-based multifidelity linear regression*
	· *Ion Victor Gosea – Reduced-order modeling as a catalyst and enabler for digital twinning in process and chemical engineering*
	· *Steven Rodriguez – Enabling model reduction of meshless nonlocal methods via modal reference spaces*
	· *Hossein Naderi – Oblique projection for scalable rank-adaptive reduced-order modeling of nonlinear stochastic PDEs with time-dependent bases*
	· *Marissa Whitby – Randomized local model order reduction for nonlinear partial differential equations*
	· *Noé Stauffer – Extracting Markovian description of high-dimensional dynamics via Mori-Zwanzig formalism*
	· *Amirpasha Hedayat – Linear and non-linear reduced dimensional manifolds for global weather predictions*
16 : 20 - 17 : 40	**Session 11 : Nonintrusive ROMs (not ML) (Chair : Alessandro Alla)**
	· *Tommaso Bradde – A novel approach for characterizing and enforcing stability of barycentric rational models in the AAA algorithm*
	· *Linus Balicki – Parametric reduced-order modeling via low-rank barycentric forms and the p-AAA algorithm*
	· *Michael Ackermann – Optimal H_2 approximation from time-domain data*
	· *Masayuki Yano – Model reduction for parametrized aerodynamics problems : Error estimation, adaptivity, and nonlinear approximations*

Thursday, September 12

Time	Event
8 : 30 - 9 : 20	**Plenary 5 (Chair : Benjamin Peherstorfer)**
	· *Kevin Carlberg – Nonlinear model reduction for high- and low-consequence applications*
9 : 20 - 10 : 40	**Session 12 : ML (Chair : Benjamin Peherstorfer)**
	· *Jules Berman – CoLoRA : Continuous low-rank adaptation for reduced implicit neural modeling of parameterized partial differential equations*
	· *Mariella Kast – Time-evolving neural network representations for the reduced order modelling of parametrised PDEs*
	· *Daniel Alford-Lago – A generative probabilistic transformer model for ionospheric prediction*
	· *Chris Curtis – Time stepping in DMD via machine learning*
10 : 40 - 11 : 10	**Coffee**
11 : 10 - 12 : 30	**Session 13 : ML (Chair : Gianluigi Rozza)**
	· *Christophe Bonneville – Accelerating phase field simulations through time extrapolation with adaptive Fourier neural operators and U-Nets*
	· *Lukas Renelt – Efficient linear model order reduction for Friedrichs' systems*
	· *Weichao Li, Shaowu Pan – Implicit neural representation meets interpretable parameterized reduced-order modeling*
	· *Peter Benner – Transformer networks accurately predict outputs of parametric dynamical systems with time-varying external inputs*
12 : 30 - 14 : 00	**Lunch**
14 : 00 - 15 : 20	**Session 14 : ML (Chair : Serkan Gugercin)**
	· *Gianluigi Rozza – Enhancing ROM with DL for the efficient solution of parametric PDEs : applications and perspectives*
	· *Lewin Ernst – Certification of physics-informed neural networks for the solution of parameterized PDEs*
	· *Bernard Haasdonk – Kernel-based greedy collocation schemes for approximation of high-dimensional PDE boundary value problems*
	· *Marco Tezzele – Predictive digital twins of civil engineering structures*
15 : 20 - 16 : 20	**Posters & Coffee**
	· *Xuping Xie – ML based surrogate modeling for collisional radiative model in plasma disruption mitigation*
	· *Shuwen Sun – Predicting dynamics in time and parameter space with deep learning and data augmentation*
	· *Ramzi Dakhmouche – Wasserstein-robust modeling of multi-scale systems : a graph-neural-network coreset approach*
	· *Otto Lamminpää – Forward model emulator for atmospheric radiative transfer using Gaussian processes and cross validation*
	· *Birgit Hillebrecht – An application of a posteriori error quantification for physics-informed neural networks*
	· *Stefania Fresca – Neural latent dynamics models*
	· *Sandeep Reddy Bukka – Physics-informed machine learning for surrogate modeling of ultrasonic guided wave propagation in pipeline health monitoring*
	· *Caterina Millevoi – SurMoDeL : A deep learning based surrogate model for modeling fault activation*
	· *Jonas Kneifl – VENI, VINDy, VICI : A variational method to build ROMs with embedded uncertainty quantification*
	· *Teeratorn Kadeethum – Integrating improved neural operators and graph convolutional networks for scalable geological carbon storage modeling*
	· *Satoru Iwasaki – Surrogate model for partial differential equations in thin domains*
	· *Gabrielle Hobson – Physics-based uncertainty quantification for geophysical problems using data-driven reduced order modeling*
	· *Aniket Jivani – Propagation of uncertainties in data-driven learning of ODEs*
	· *Amir Sagiv – Measure transport and density estimation via surrogate models*
16 : 20 - 18 : 00	**Session 15 : Stochastic ROMs and Randomized Methods (Chair : Bernard Haasdonk)**
	· *Oliver Schmidt – A stochastic convolutional SPOD-Koopman reduced order model for turbulent flow data*
	· *Peter Frame – Model reduction for linear systems using SPOD modes*
	· *Kevin Lin – Mori-Zwanzig formalism, Wiener projections, and random dynamics*
	· *Hossein Gorji – Schrodinger bridge model-data adaptation for network dynamics*

Friday, September 13

Time	Event
8 : 30 - 9 : 20	**Plenary 6 (Chair : Peter Benner)**
	· *Francesca Bonizzoni – A greedy MOR method for the tracking of eigensolutions to parametric elliptic PDEs*
9 : 20 - 10 : 40	**Session 16 : Optimization, Control and Inverse Problems (Chair : Peter Benner)**
	· *Dane Grundvig – Line-search based optimization with online model reduction*
	· *Steffen W. R. Werner – An adaptive data sampling scheme for low-dimensional controller inference*
	· *Tea Vojkovic – Forced Stuart-Landau models for closed-loop flow control*
	· *Michael Kartmann – Adaptive reduced basis trust region methods for parameter identification problems*
10 : 40 - 11 : 10	**Coffee**
11 : 10 - 12 : 30	**Session 17 : Optimization, Control and Inverse Problems (Chair : Matthias Morzfeld)**
	· *Tia Chung, Jack Michael Solomon – Paired autoencoders for inversion and regularization with sparsity*
	· *Abed Hammoud – Data assimilation in chaotic systems using deep reinforcement learning*
	· *Pavlos Stavrinides – Faster solution of linear Bayesian smoothing problems using model reduction for ensemble Kalman inversion*
	· *Lianghao Cao – Efficient geometric MCMC for nonlinear Bayesian inversion enabled by derivative-informed neural operator*
12 : 30 - 14 : 00	**Lunch**
14 : 00 - 15 : 20	**Session 18 : UQ and Tensor Methods (Chair : Elizabeth Qian)**
	· *Thomas Coons – Adaptive covariance estimation via surrogate modeling for multi-fidelity estimation*
	· *Ruben Aylwin – Reduced basis methods for domain uncertainty quantification of periodic gratings*
	· *Patrick Blonigan, Eric Parish – A streamlined workflow for model reduction with application to aerodynamic and thermal analyses*
	· *Ye Lu – Extended tensor decomposition model reduction method : application to real-time additive manufacturing residual stress predictions and inverse problems*
15 : 20 - 15 : 25	**Closing Remarks**

3 Talk Abstracts

3.1 Monday, September 9

Exploiting Structure via Nested Operator Inference in Physics-Based Learning

Nicole Aretz[1] **and Karen Willcox**[1]

[1] *Oden Institute for Computational Engineering & Sciences, University of Texas at Austin*

We introduce the data-driven nested Operator Inference method [1] for learning projection-based reduced-order models (ROMs) from snapshot data of high-dimensional dynamical systems. Projection-based ROMs exploit the intrinsic low-dimensionality of a full-order solution manifold. They typically 1) achieve significant computational savings, 2) guarantee approximation accuracy through established error theory, and 3) remain interpretable through the governing equations. However, constructing ROMs via projection requires access to the full-order operators – a significant shortcoming for applications with legacy codes or commercial solvers. Operator Inference (OpInf) [3] circumvents this requirement by learning the intrusive ROM from available full-order data and the structure of the governing equations. Under certain conditions [2, 3], OpInf guarantees the exact reconstruction of the intrusive ROM, though meeting its data requirements in practice can be challenging, especially for highly non-linear operators: The degrees of freedom in the classic OpInf regression problem scale in $\mathcal{O}(r^p)$, where r is the dimension of the reduced space, and p is the highest polynomial degree in the governing equations. Consequently, classic OpInf requires precise regularization, balancing the numerical stability of its learning problem and the structural stability of its inferred ROM [4]. In contrast, our nested OpInf approach [1] partitions the learning problem into multiple regression problems, each with only $\mathcal{O}(p)$ degrees of freedom. Each regression problem is provably better conditioned than when all reduced-order operators are learned together, thus alleviating the need for additional regularization. The partition is based upon a nested structure in the projection-based reduced-order matrices. It exploits a hierarchy in the reduced space's basis vectors to guarantee that the ROM's dominant dynamics are learned accurately. Since only $\mathcal{O}(p)$ unknowns are learned at a time, nested OpInf is particularly applicable to higher-order polynomial systems. We demonstrate our method for the shallow ice equations with eighth-order polynomial operators.

References

[1] N. Aretz and K. Willcox. Enforcing structure in data-driven reduced modeling through nested operator inference. *submitted*, 2024.

[2] B. Peherstorfer. Sampling low-dimensional markovian dynamics for preasymptotically recovering reduced models from data with operator inference. *SIAM Journal on Scientific Computing*, 42(5):A3489–A3515, 2020.

[3] B. Peherstorfer and K. Willcox. Data-driven operator inference for nonintrusive projection-based model reduction. *Computer Methods in Applied Mechanics and Engineering*, 306:196–215, 2016.

[4] N. Sawant, B. Kramer, and B. Peherstorfer. Physics-informed regularization and structure preservation for learning stable reduced models from data with operator inference. *Computer Methods in Applied Mechanics and Engineering*, 404:115836, 2023.

Greedy construction of quadratic manifolds for nonlinear dimensionality reduction and nonlinear model reduction

Paul Schwerdtner[1] **and Benjamin Peherstorfer**[1]

[1] *Courant Institute of Mathematical Sciences, New York University*

Dimensionality reduction with quadratic manifolds augments linear approximations in subspaces with quadratic correction terms. While previous works [1, 2] rely on linear approximations given by projections onto the first few leading principal components of the training data, we instead construct subspaces so that the corresponding linear approximations can be corrected most efficiently with quadratic terms.

We propose in [3] a greedy method for the subspace construction that selects basis vectors from leading as well as later principal components. The greedy selection allows us to determine a basis that can leverage the quadratic corrections most efficiently. This is in contrast to choosing as basis the leading principle components, which results in the best linear approximation but is not necessarily most informative for the quadratic correction terms.

Properties of the greedily constructed manifold allow applying linear algebra reformulations so that the greedy method scales to data points with millions of dimensions. Numerical experiments demonstrate that an orders of magnitude higher accuracy is achieved with the greedily constructed quadratic manifolds compared to manifolds that are based on the leading principal components.

References

[1] J. Barnett and C. Farhat. Quadratic approximation manifold for mitigating the Kolmogorov barrier in nonlinear projection-based model order reduction. *J. Comput. Phys.*, 464:111348, 2022.

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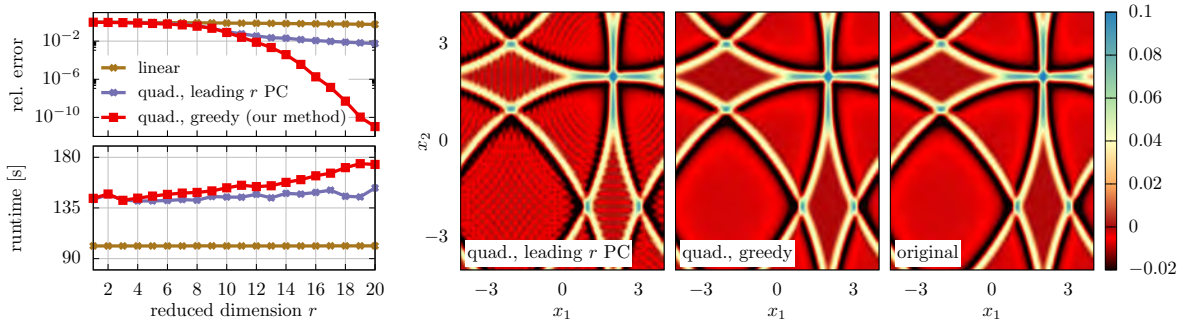

(a) relative errors and runtime

(b) reconstructions of test data point with $r = 15$

Figure 1: The proposed greedy approach leads to eight orders of magnitude more accurate approximations than using the leading principal components (PC) for the quadratic manifold construction in this 2D wave propagation problem.

Model Reduction for the Wave Equation beyond the limitations of the Kolmogorov N-width

M. Feuerle[1], **R. Löscher**[2], **O. Steinbach**[2], **and K. Urban**[1]

[1] *Institute for Numerical Mathematics, Ulm University, Germany*
[2] *Institute of Applied Mathematics, Graz University of Technology, Austria*

The Reduced Basis Method (RBM) is a well-established model reduction technique to realize multi-query and/or realtime applications of Parameterized partial differential equations (PPDEs). The RBM relies on a well-posed variational formulation of the PPDE under consideration. Since the RBM is a linear approximation method, the best possible rate of convergence is given by the Kolmogorov N-width

$$d_N(\mathcal{P}) := \inf_{\substack{X_N \subseteq X, \\ \dim(X_N)=N}} \sup_{\mu\in\mathcal{P}} \inf_{v_N\in X_N} \|u_\mu - v_N\|_X, \qquad N \in \mathbb{N}, \tag{1}$$

where X is the function space in which the solution $u_\mu \in X$ is sought, $\mathcal{P} \subset \mathbb{R}^P$ is the set of parameters and N denotes the dimension of the reduced ansatz space X_N. It is well-known that the decay of $d_N(\mathcal{P})$ is exponentially fast for suitable elliptic and parabolic problems [1, 2], but is poor for transport- or wave-type problems [4, 6]. This motivates our goal of developing a well-posed variational formulation for the wave equation, which also allows for a *nonlinear* model reduction in order to overcome the limitations of a possibly poor Kolmogorov N-width.
To this end, we consider an abstract formulation of the parameterized wave equation of the form

$$B_\mu : X \to Y',\ f_\mu \in Y', \quad \text{seek } u_\mu \in X \text{ s.t.} \quad B_\mu u_\mu = f_\mu. \tag{2}$$

In order to avoid a linear approximation process, we consider a parameter-dependent norm on X defined by $\|\cdot\|_\mu := \|B_\mu \cdot\|_{Y'}$. As this norm might not be meaningful from an application point of view, we show, that $\|\cdot\|_{L_2} \lesssim \|\cdot\|_\mu$. Using a parameter dependent norm on X (and not on Y) is a key difference of our approach compared to existing ones in the literature (see e.g. [3] for the transport problem) and leads to a nonlinear approximation scheme.
We start by showing well-posedness for the wave equation by constructing appropriate spaces X and Y. Moreover, we introduce an unconditionally stable space-time Petrov-Galerkin discretization based upon a modified Hilbert type transformation as in [5]. This discretization is then used as a "truth" solver for an RBM. Numerical experiments will be presented.

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On the Role and Computation of the Fiber in Model Reduction

Samuel E. Otto[1], **Steven L. Brunton**[1], **and J. Nathan Kutz**[1]

[1] *AI Institute in Dynamic Systems, University of Washington, Seattle, WA*

Recent advances enable accurate forecasting of nonlinear dynamical systems on low-dimensional curved manifolds learned from data [1, 3, 2]. The use of curved manifolds has proven critical in applications to high Reynolds number fluid flows where advecting flow structures are poorly approximated in low-dimensional (flat) subspaces [4, 3]. We show that choices of low-dimensional modeling variables that faithfully embed the underlying manifold can still lead to poor forecasting performance when states are condensed along fibers that fail to properly account for fast dynamics and transient amplification mechanisms associated with non-normality [6, 5]. To illustrate, we consider a non-parallel complex Ginzburg-Landau equation in a regime following a supercritical Hopf bifurcation. We project onto the unstable manifold and compare various choices for the projection fiber. We show that accurate models can be obtained by removing the most quickly decaying eigenmodes, which are orthogonal to the most slowly decaying left eigenvectors. For systems in regimes far away from relevant equilibria, low-dimensional variables with guaranteed forecasting ability can be extracted using the recently introduced Covariance Balancing Reduction using Adjoint Snapshots (CoBRAS) method and its nonlinear kernel-based variant [6]. We demonstrate this approach on a nonlinear axisymmetric jet flow discretized with $100,000$ state variables. This flow exhibits selective sensitivity to disturbances entering upstream in the shear layer, while the resulting instabilities grow large downstream. Standard data-driven methods such as those based on Proper Orthogonal Decomposition (POD) fail to capture the upstream flow features needed to forecast the system's response, while methods based on linearized analysis or low-order Volterra series expansions fail due to the rapid departure of trajectories from the neighborhood of the equilibrium where these approximations are valid. A common feature of successful methods based on left eigenvectors or CoBRAS is the reliance on adjoint-based sensitivity analysis. In the absence of additional physics-based knowledge providing implicit or explicit information about sensitivity, we explain why the adjoint is required to overcome the curse of dimensionality when selecting modeling variables.

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Randomized Local Model Order Reduction for p-Laplacian Problems

C. Beall[1] **and K. Smetana**[1]

[1]*Stevens Institute of Technology*

We seek to develop a randomized local model order reduction (MOR) method to numerically solve boundary value problems involving the p-Laplace equation

$$-\mathrm{div}(|\nabla u|^{p-2}\nabla u) = f,$$

with $2 < p < \infty$, a model nonlinear elliptic PDE. We build on previous works [1], [2] which have developed local, and randomized local, MOR in the linear elliptic setting. On a global bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$, $n = \{1, 2, 3\}$, we obtain local p-harmonic solutions on oversampling domains $\omega^* \subset \Omega$ with boundary denoted $\partial\omega^*$, and introduce a so-called transfer operator restricting solutions on ω^* to a target subdomain $\omega \subset \omega^*$ on which we construct local ansatz basis functions for the MOR scheme. However, care must be taken when considering the optimality of the space spanned by such basis functions. Here, our transfer operator corresponds to a nonlinear PDE, so the linear theory, which states that the space spanned by the leading left singular vectors of a linear transfer operator is optimal in the sense of Kolmogorov [3], no longer applies. Caccioppoli's inequality was crucial in proving compactness of linear transfer operators in [1], [2], and this inequality also applies to the p-Laplacian (proven in e.g., [4]). If we can prove compactness in this setting, it then follows that the range of our transfer operator acting on a bounded set of functions on $\partial\omega^*$ is a compact set. An optimal subspace can thus be defined as the subspace that optimally approximates this compact set, and a standard POD or Greedy algorithm can be employed to obtain reduced solutions. Since such algorithms suffer from the curse of dimensionality, we will rely on randomization and seek to exploit the concentration of measure phenomenon.

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Domain decomposition least-squares Petrov-Galerkin model reduction for time-dependent problems

Alejandro N. Diaz[1]

[1]*Rice University*

This presentation extends domain decomposition (DD) least-squares Petrov-Galerkin (LSPG) model reduction to time-dependent problems using linear subspace reduced order models (LS-ROMs) or neural network-based nonlinear-manifold ROMs (NM-ROMs). The DD LSPG approach algebraically decomposes a fully discretized full order model (FOM) into algebraic subdomains, computes a ROM for each subdomain, and minimizes the least-squares residual for each subdomain ROM at each time step while coupling the ROMs via compatibility constraints. For both LS-ROMs and NM-ROMs, applying DD has several advantages over computing a global ROM: subdomain ROMs can be trained in parallel, require smaller subdomain FOM-dimensional training data, and can be tailored to subdomain-specific features of the FOM. However, in the time-dependent setting, the compatibility constraints and reduced order representations must be carefully constructed to ensure compatibility throughout the time domain. To accomplish this, we compute so-called port ROMs and strongly enforce subdomain compatibility of the reconstructed ROM solution. The effectiveness of the time-dependent DD LSPG ROM approach using LS-ROMs and NM-ROMs is demonstrated using the 2D Burgers' equation in the advection-dominated regime.

Accelerated Simulation of Advection-dominated Flows with Automated Multifidelity Modeling and Domain Decomposition

Christopher R. Wentland[1], **Francesco Rizzi**[2], **and Irina K. Tezaur**[1]

[1]*Sandia National Laboratories*
[2]*NexGen Analytics*

Surrogate modeling is a crucial component of the modern engineer's toolbox for designing and analyzing physical systems of practical interest, shortening delivery times and decreasing life cycle costs. In the past decade, a host of data-driven surrogate models have proposed low-cost solutions rooted in experimental or high-fidelity simulation datasets, offering enticing alternatives to more traditional heuristic surrogates. Each has unique benefits and drawbacks, attempting to balance accuracy, generalizability, flexibility, training time, and inference cost. Choosing an appropriate model for a specific system is often the result of domain expert experience and trial-and-error. This is a particular issue for systems which are characterized by non-linear governing physics, a complex parameter space, and spatially-distributed and/or transient dynamics. Unsteady advection-dominated fluid flows experiencing propagating waves are prime examples of such systems for which effective data-driven surrogate modeling remains an open problem.

To overcome these issues, we propose a multifidelity modeling framework which automates the model selection process and tailors the solution to a problem's spatial dynamics. This is achieved by a novel combination of the Schwarz alternating method and automated learning algorithms. The Schwarz method allows for the decomposition of a spatial domain into arbitrary component subdomains and the communication of information between subdomains, each potentially described by vastly different mesh topologies and time integrators. The solution in each subdomain may be characterized by much simpler, localized dynamics, and hence more easily modeled and solved. An automated learning algorithm is leveraged to select both an optimal decomposition of the spatial domain and what model to apply in each region, choosing among a high-fidelity model, intrusive reduced-order models, and non-intrusive surrogates to achieve an accurate and inexpensive solution. This procedure is demonstrated for advection-dominated fluid flow problems for which monolithic approaches are prohibitively expensive or grossly inaccurate.

Latent Space Dynamics Identification

Y. Choi[1]

[1] *Lawrence Livermore National Laboratory*

This talk introduces a framework called Latent Space Dynamics Identification (LaSDI), which has significant potential for extension to other innovative data-driven algorithms. LaSDI is an interpretable, data-driven framework that operates through three key steps: compression, dynamics identification, and prediction [3, 4, 7, 6]. In the **compression** phase, high-dimensional data is reduced, allowing it to be more easily integrated into an interpretable model. The dynamics **identification** phase then derives this model, typically in the form of parameterized differential equations that accurately represent the reduced latent space data . During the **prediction** phase, these identified differential equations are solved in the reduced space for new parameter points, with the solutions subsequently projected back into the full space. A key advantage of the LaSDI framework is its efficiency, as the prediction phase operates without involving the full-order model size. The LaSDI framework supports various identification methods, including fixed forms such as dynamic mode decomposition [1] and thermodynamics-based LaSDI [6], regression forms like sparse identification of nonlinear dynamics (SINDy) and weak SINDy, and physics-driven forms such as projection-based reduced order models [5, 2]. The LaSDI family has been successfully applied to accelerate various physics problems, achieving up to 1000x speed-ups in areas such as kinetic plasma simulations, pore collapse, and computational fluid dynamics.

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Tensor-based adaptive sampling strategies for the reduced basis method with application to full-state approximation

S. Chellappa[1], L. Feng[1], and P. Benner[1]

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*

Reconstructing the entire state variable of a dynamical system is often necessary in applications such as fluid dynamics, acoustics, geomechanics, etc. Model order reduction (MOR) methods such as the reduced basis method (RBM) are preferred to achieve the real-time approximation of the state, under different parameters or initial conditions. For systems with many parameters, the offline computational cost of the RBM is often significant. To address this, our previous work [1] proposed several variants of an adaptive parameter subsampling strategy. While the approach yielded considerable speed up, it was restricted to the case of approximating a target output quantity. In this work, we propose a subsampling technique for the RBM to achieve approximation of the entire state variable, via the tensor structure of the snapshot data. Our approach is able to account for the entire space-time variation (with respect to the parameter) of the snapshot matrix, thus yielding highly relevant sampling points for the offline greedy process of the RBM. Numerical results on different problems illustrate the viability of the approach in speeding up the offline cost of RBM, while also providing reduced-order models that yield good full-state approximation for unseen parameter samples.

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Adaptive reduced-order models for high-speed flow via optimally transported meshes

R. Loek Van Heyningen[1], **Ngoc Cuong Nguyen**[1], **and Jaime Peraire**[1]

[1] *Center for Computational Science and Engineering, Department of Aeronautics and Astronautics, Massachusetts Institute of Technology*

The simulation of high-speed flow problems with parametrically varying shocks poses challenges for high-fidelity discretization methods and surrogate model construction. We use an r-adaptive mesh adaptation method introduced in [3] to aid in the accurate resolution of flows with strong shocks and the development of reduced-order models of these same flows. Using the method of [2] to construct high-order solutions of the Monge-Ampère equation for optimal transport, grid nodes of a fixed reference mesh are redistributed towards features that require more resolution. When applied to parametrized PDEs, each solution snapshot consists of a solution field and a corresponding grid deformation. The mapping defining the grid movement can be used to pull the solution back onto the reference mesh. Here, sharp and local features will be smoothed out and made more globally distributed over the domain, making them more suitable for linear basis model reduction methods like the proper orthogonal decomposition. Reduced order models can then efficiently be built on the reference mesh for the solution field and grid mappings. The effectiveness of this approach is shown for supersonic and hypersonic flows with parametrized free-stream Mach number in [4].

This presentation will detail previous results and explore extensions to viscous flows and problems with more than one parameter. For some problems, nonintrusive interpolation ROMs are sufficient for both the mesh deformation and solution fields. To reach greater accuracy levels for sparse training sets, we use an intrusive projection-based ROM for the solution fields. This requires the development of novel projection strategies for hybridized discontinuous Galerkin discretizations. Finally, this approach is coupled with the open-source uncertainty quantification framework Dakota [1] and used to perform forward propagation of uncertain boundary conditions.

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An Adaptive Surrogate Model Refinement Framework for Trajectory Simulation and Optimization

Jonathan Cangelosi[1] **and Matthias Heinkenschloss**[2]

[1] *Ph.D. Candidate, Department of Computational Applied Mathematics and Operations Research, Rice University, Houston, TX*
[2] *Noah Harding Chair and Professor, Department of Computational Applied Mathematics and Operations Research, Rice University, Houston, TX*

Determining the trajectory of an aircraft often requires the repeated computation of aerodynamic coefficients (e.g., lift, drag) which may be obtained from expensive high-fidelity CFD or wind tunnel experiments. While CFD libraries grow ever faster at running these computations, there yet remains a need to employ surrogate models to perform the tasks of trajectory simulation and optimization at a modest computational cost, and this must be done without significantly compromising solution quality. To improve the accuracy of the trajectory obtained from a surrogate, the surrogate may be refined by obtaining additional high-fidelity samples of aerodynamic coefficients at various flight configurations and fitting the surrogate to the new data. Because obtaining this data is expensive, we must select new data points in an intelligent way. In this talk, I propose a sensitivity-driven model refinement procedure that aims to select new samples that minimize the error in the trajectory resulting from model refinement at those samples. Numerical results are presented for a trajectory simulation problem and a trajectory optimization problem where aerodynamic surrogates are constructed for a nominal hypersonic vehicle. The results demonstrate that the model refinement method is effective when surrogates are slightly under-resolved, reducing the need for a priori knowledge of the physical behavior of the aerodynamic coefficients and achieving accurate trajectories with a small number of additional samples.

Transformed Model Reduction for Partial Differential Equations with Sharp Inner Layers

Tianyou Tang[1] **and Xianmin Xu**[1]

[1] *Insitute of Computational Mathematics, Chinese Academy of Sciences*

Small parameters in partial differential equations can give rise to solutions with sharp inner layers that evolve over time. However, the standard model reduction method becomes inefficient when applied to these problems due to the slowly decaying Kolmogorov N-width of the solution manifold. To address this issue, a natural approach is to transform the equation in such a way that the transformed solution manifold exhibits a fast decaying Kolmogorov N-width. In this talk, we will present a new method to deal with the difficulties. We employ asymptotic analysis to identify slow variables and perform a transformation of the partial differential equations accordingly. Subsequently, we apply the Proper Orthogonal Decomposition (POD) method and a qDEIM technique to the transformed equation with the slow variables. Numerical experiments demonstrate that the new model reduction method yield significantly improved results compared to direct model reduction applied to the original equation. Furthermore, this approach can be applied to some well-known equations, such as the Allen-Cahn equation, the convection equation and the Burgers equation, etc.

3.2 Tuesday, September 10

Tensor Decomposition meets Reproducing Kernel Hilbert Spaces (RKHS)

Tamara G. Kolda[1], **Brett Larsen**[2], **Alex Williams**[3], **and Anru Zhang**[4]

[1] *MathSci.ai*
[2] *Mosaic Research, Databricks*
[3] *NYU/Flatiron*
[4] *Duke University*

Tensor decompositions require that data live on a regular d-way grid, but many real-world datasets do not have this property. For example, time-evolving data may be measured at different intervals for different subjects and adaptive meshes in simulations are irregular by design. We can handle irregular grids by treating some modes as infinite-dimension rather than finite-dimensional; we refer to such tensors as quasi-tensors. For their decompositions, this means that we want the factors in the tensor decomposition to be smooth functions rather than vectors. This basic idea has appeared in myriad forms over the years, often using different terminology and with different applications. I will recall and build on these efforts. The result is a generic framework for incorporating continuous modes into the CP tensor decomposition. We focus on learning the infinite-dimensional modes from a reproducing kernel Hilbert space (RKHS) and present an alternating least squares algorithm that is computationally efficient. Including infinite-dimensional modes (1) enables practitioners to enforce common structural assumptions about data such as smoothness, (2) extends to situations in where the measurement times do not align by utilizing the framework of missing data, and (3) provides a more principled way to interpolate between observed points.

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The Loewner framework for parametric systems and the curse of dimensionality. Part I: Theory

A.C. Antoulas, joint work with I.V. Gosea and C. Poussot-Vassal

We propose a new approach to data-driven model reduction of linear parametrized systems. The associated transfer function $\mathbf{H}$ depends on n variables $\mathbf{H}({}^1s, {}^2s, \cdots, {}^ns)$, where ${}^1s$ is the frequency and the rest are $n-1$ parameters. Given measurements of this transfer function, first, a method is described which determines the degree $d_i = \nu_i - 1$, $i = 1, \cdots, n$, of each one of the variables ${}^is$, of the transfer function $\mathbf{H}$ of the approximate system.

Splitting of the variables into left ${}^1s, \cdots, {}^ks$ and right ${}^{k+1}s, \cdots, {}^ns$, leads to an n-D Loewner matrix $\mathbb{L}_n$, whose nullspace determines the coefficients of the n-D barycentric representation of $\mathbf{H}$. An important property of $\mathbb{L}_n$ is that it satisfies a sequence of coupled Sylvester equations. The *first* main result provides a *realization* of the approximant in the n-D case.

As a by-product we obtain a multi-linearization of the underlying nonlinear eigenvalue problem. Furthermore, by appropriately defining the left and right variables, the nonlinear eigenvalue problem becomes linear in the frequency and multi-linear in the $n-1$ parameters.

It turns out that the complexity of determining the n-D barycentric coefficients is of the order of $\left(\Pi_{i=1}^n \nu_i^3\right)$, which results in the *curse of dimensionality*.

The *second* main result shows how elements in the nullspace of $\mathbb{L}_n$ can be computed using an appropriately determined sequence of 1-D Loewner matrices. The ensuing computational complexity reduces to:

$$\nu_1^3 + (\nu_1)\nu_2^3 + (\nu_1\nu_2)\nu_3^3 + \cdots + (\nu_1\nu_2\cdots\nu_{n-1})\nu_n^3,$$

thus *breaking the curse of dimensionality*. Connections to tensor approximation will be discussed together with several examples which illustrate the theoretical results.

Reference

A.C. Antoulas, I.V. Gosea and C. Poussot-Vassal, *The Loewner framework for parametric systems: Breaking the curse of dimensionality*, Preprint, 48 pages (shortly available on arxiv).

The Loewner framework for parametric systems and the curse of dimensionality. Part II: Applications

Athanasios C. Antoulas[1], Ion Victor Gosea[2], and Charles Poussot-Vassal[3]

[1]*Rice University, Houston, Texas, USA, email: aca@rice.edu*
[2]*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, email: gosea@mpi-magdeburg.mpg.de*
[3]*DTIS, ONERA, Université de Toulouse, France, email: charles.poussot-vassal@onera.fr*

This contribution is a continuation of [1], which introduces the theoretical tools for multivariate realization and null-space computation in the parametric Loewner framework [3], both addressing the curse of dimensionality (CoD). For more specific details and in-depth theoretical considerations, in particular, we refer to the original full paper [2].

The current work introduces algorithms and numerical procedures for constructing parameterized realizations directly from data. Special emphasis is given to the numerical robustness and applicability of the proposed procedures to real-life examples. In this direction, several practical considerations will be investigated, such as selecting interpolation points (e.g., ad-hoc vs. via greedy approach, similar to that in the p-AAA algorithm [4]), connection to tensorization and higher-dimensional decompositions, sampling strategies (e.g., sparse vs tensorized grids), and last but not least, the efficient and accurate Loewner matrix numerical null-space (kernel) computation.

As covered in [2], we propose an exhaustive numerical study, including a fair amount of experiments. We aim to compare different implementations for a large database of test cases, data sets, and benchmarks from model reduction, control and aerospace engineering, signal processing, data science, and tensor computation communities. We report on intricate details such as tuning the input parameters of the proposed algorithms, selecting interpolation points, ways of computing the null space, etc. The compiled statistics may be proven relevant for practitioners in various fields of engineering.

From this extensive database of experiments, several numerical examples and tests will be chosen to illustrate the theoretical results. Namely, we cover a purely data-driven example (no existing model available) and also established parametric benchmarks from the MorWiki collection[1], as below:

- Flutter example (purely data-driven) in 2-D and 3-D [6].
- Modified Gyroscope model in 3-D, `https://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Modified_Gyroscope`.
- Anemometer model in 4-D, `https://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Anemometer`.

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Riemannian Optimization over the Manifold of Rational Functions

C. A. Beattie[1], **Z. Drmač**[2], **S. Güğercin**[1], **and P. Mlinarić**[1]

[1] *Virginia Tech*
[2] *University of Zagreb*

The Hardy space $\mathcal{H}_2$ is a space of matrix-valued functions defined over the open right half-plane $\mathbb{C}_+$:

$$\mathcal{H}_2 = \left\{ F\colon \mathbb{C}_+ \to \mathbb{C}^{p\times m} \;\middle|\; F \text{ is analytic and } \sup_{\xi>0} \int_{-\infty}^{\infty} \|F(\xi+\imath\omega)\|_{\mathrm{F}}^2 \,\mathrm{d}\omega \right\}.$$

The $\mathcal{H}_2$ space is a Hilbert space with inner product and norm given by, respectively,

$$\langle F, G\rangle_{\mathcal{H}_2} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle F(\imath\omega), G(\imath\omega)\rangle_{\mathrm{F}} \,\mathrm{d}\omega \quad \text{and} \quad \|F\|_{\mathcal{H}_2} = \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \|F(\imath\omega)\|_{\mathrm{F}}^2 \,\mathrm{d}\omega\right)^{1/2}.$$

Given a full-order model with transfer function $H \in \mathcal{H}_2$, which may or may not be rational, the $\mathcal{H}_2$-optimal reduced-order modeling problem is

$$\min_{\widehat{H}\in\Sigma_r} \quad \frac{1}{2}\left\|H - \widehat{H}\right\|_{\mathcal{H}_2}^2, \tag{1}$$

where Σ_r is the set of stable rational functions of order r

$$\Sigma_r = \left\{ \widehat{C}\Big(sI - \widehat{A}\Big)^{-1}\widehat{B} \;\middle|\; \widehat{A}\in\mathbb{R}^{r\times r},\ \widehat{B}\in\mathbb{R}^{r\times m},\ \widehat{C}\in\mathbb{R}^{p\times r},\ \sigma(\widehat{A})\subset\mathbb{C}_-,\ \left(\widehat{A},\widehat{B},\widehat{C}\right) \text{ is minimal} \right\},$$

where $\sigma(\widehat{A})$ is the spectrum of $\widehat{A}$ and minimality means that there are no zero-pole cancellations in $\widehat{C}(sI-\widehat{A})^{-1}\widehat{B}$. The iterative rational Krylov algorithm (IRKA) and transfer function IRKA (TF-IRKA) [1] are two well-known methods for solving (1); the former being projection-based (intrusive) while the latter data-driven (non-intrusive) only needing to evaluate H and H'. We first show that Σ_r is a Riemannian submanifold of $\mathcal{H}_2$, and thus (1) is a Riemannian optimization problem. Next we prove that both IRKA and TF-IRKA can be interpreted as Riemannian gradient descent methods with a fixed step size applied to (1). Then we develop Riemannian gradient descent with variable step size for (1), enabling to preserve stability and ensure a reduction in the $\mathcal{H}_2$ error in every step.
Both IRKA and TF-IRKA theoretically amount to re-evaluating H at iteratively corrected frequencies. However, in some instances, we might not have access to H to do re-evaluation, instead might have access only to a pre-determined (potentially experimental/noisy) data $H_i = H(\sigma_i) \in \mathbb{C}^{p\times m}$ at frequencies $\sigma_i \in \mathbb{C}$ for $i = 1, 2, \ldots, N$. In this case, we consider the discretized $\mathcal{H}_2$-optimal reduced-order modeling problem, namely

$$\min_{\widehat{H}\in\Sigma_r} \quad \sum_{i=1}^{N} \frac{\rho_i}{2}\left\|H_i - \widehat{H}(\sigma_i)\right\|_{\mathrm{F}}^2, \tag{2}$$

for weights $\rho_i > 0$. We interpret (2) as a Riemannian optimization problem and then develop a Riemannian gradient descent method for (2), and show its effectiveness by comparing its performance to existing methods on various numerical examples.

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Certified model order reduction for large-scale switched differential-algebraic equations

M. Manucci[1] **and B. Unger**[1]

[1] *Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Universitätsstr. 32, 70569 Stuttgart, Germany*

We discuss a projection-based model order reduction (MOR) for large-scale systems of switched differential-algebraic equations (sDAEs), i.e.,

$$\Sigma_q \quad \begin{cases} \mathbf{E}_{q(t)}\dot{\mathbf{x}}(t) = \mathbf{A}_{q(t)}\mathbf{x}(t) + \mathbf{B}_{q(t)}\mathbf{u}(t), \quad \mathbf{x}(t_0) = \mathbf{0}, \\ \mathbf{y}(t) = \mathbf{C}_{q(t)}\mathbf{x}(t), \end{cases} \tag{1}$$

where $q\colon \mathbb{R} \to \mathcal{J} := \{1, \dots, M\}$ is the switching signal, i.e., a piecewise constant function taking values in the index set $\mathcal{J}$, $\mathbf{x}(t) \in \mathbb{R}^n$, $\mathbf{u}(t) \in \mathbb{R}^m$, and $\mathbf{y}(t) \in \mathbb{R}^p$ denote respectively, the *state*, the controlled *input*, and the measured *output*. We emphasize that the matrices $\mathbf{E}_j \in \mathbb{R}^{n\times n}$ for $j \in \mathcal{J}$ may be singular. Control systems of sDAEs may arise in modelling physical systems with algebraic constraints and piecewise time-dependent parameters, like Stokes control system with piecewise time-dependent diffusion. If (1) has to be evaluated repeatedly, one can rely on MOR and replace (1) by the *reduced-order model*

$$\tilde{\Sigma}_q \quad \begin{cases} \tilde{\mathbf{E}}_{q(t)}\dot{\tilde{\mathbf{x}}}(t) = \tilde{\mathbf{A}}_{q(t)}\tilde{\mathbf{x}}(t) + \tilde{\mathbf{B}}_{q(t)}\mathbf{u}(t), \quad \tilde{\mathbf{x}}(t_0) = \mathbf{0}, \\ \tilde{\mathbf{y}}(t) = \tilde{\mathbf{C}}_{q(t)}\tilde{\mathbf{x}}(t), \end{cases} \tag{2}$$

with $r \ll n$, $\tilde{\mathbf{E}}_j, \tilde{\mathbf{A}}_j \in \mathbb{R}^{r\times r}$, $\tilde{\mathbf{B}}_j \in \mathbb{R}^{r\times m}$, and $\tilde{\mathbf{C}}_j \in \mathbf{R}^{p\times r}$ for $j \in \mathcal{J}$. Model reduction for systems of switched ordinary differential equations (sODEs) has been addressed in many works, see for instance [1, 3, 4] and reference therein, while, to the best of our knowledge, MOR of sDAEs only appears in [2] for a known switching signal and with several limitations to the large-scale setting, see [2, Sec. 5]. For our MOR scheme, we rely on a reformulation of (1) as a system of sODEs with state jumps at the switching times [2] and successively show that the method proposed in [3] can be successfully applied, in this generalized settings, to derive a reduced-order model for the set of generic admissible switching signals. Since the derivation of the reduced-order model is related to the solution of generalized lyapunov equations (GLEs), we show how to efficiently compute an approximate solution of these matrix equations by providing suitable stopping criteria based on derived error certificates. Then, we provide a novel computable error bound for the output error which includes the estimated error in the solution of the GLEs. To conclude, we show numerical experiments, which validate the performance of the proposed reduction method.

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Progress Towards Scalable Nonlinear Balancing Algorithms

N. A. Corbin[1] **and B. Kramer**[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California San Diego, La Jolla, CA 92093-0411 USA*

In this talk, we will discuss recent advancements in the area of computation for nonlinear balanced truncation. The first challenge we address is the computation of nonlinear balancing controllability and observability energy functions. These require solving Hamilton-Jacobi-Bellman equations [4], which are notoriously difficult to solve; we leverage the Taylor-series based approach of Al'brekht [1] as the foundation of our algorithms to compute polynomial energy functions degree-by-degree in a recursive fashion. With special attention to algorithmic implementation details, we formulate an approach based on tensor computations that enables computing energy function approximations for moderately sized problems [2].

The second major challenge in nonlinear balancing involves the computation of a nonlinear transformation that simultaneously diagonalizes the energy functions so that states that contribute little to the input-output behavior of the system can be truncated [3]. Given the polynomial approximations to the controllability and observability energy functions that we compute, we again a tensor-based algorithms for computing the input-normal/output-diagonal transformation required for balancing. The transformation is computed degree-by-degree, similar to how the energy functions are computed. Unlike previous works though, we derive the explicit form for the equations based on a Kronecker product representation for the energy functions in the interest of scalable computations. Examples are provided to demonstrate the performance and scalability of the approach.

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Nonlinear balanced truncation via infinite-dimensional Koopman lifting

T. Breiten[1], B. Höveler[1], and S. Mildenberger[1]

[1] *Technische Universität Berlin, Straße des 17. Juni 136, 10623 Berlin*

Balanced truncation is a well-known, powerful method for system theoretic model reduction [5]. Initially been proposed for linear control systems, nonlinear generalizations exist but require solutions to two nonlinear PDEs of Hamilton-Jacobi type, see [6]. On the other hand, by employing a Koopman (or composition) lifting, the evolution of a nonlinear ODE can be connected to a linear system acting on an infinite-dimensional function space [3]. In [2], a specific output energy functional for the nonlinear system

$$\dot{x}(t) = f(x(t)), \quad x(0) = z \tag{1}$$

has been related to a quadratic energy functional for the infinite-dimensional linear system

$$\dot{\psi}(t) = \mathcal{A}\psi(t), \quad \psi(0) = \delta_z \tag{2}$$

where the distributional initial condition is understood formally as the limit of a sequence of appropriate mollifiers. If considered on a suitably chosen weighted Lebesgue space, the resulting Koopman system can be shown to be exponentially stable. In [2], this has been used to discuss the solution $\mathcal{Q}$ of the following operator Lyapunov equation

$$\langle \mathcal{A}\varphi, \psi \rangle_{\mathcal{Q}} + \langle \varphi, \mathcal{A}\psi \rangle_{\mathcal{Q}} + \langle \mathcal{C}\varphi, \mathcal{C}\psi \rangle_{\ell^2} = 0 \quad \forall \varphi, \psi \in \mathcal{D}(A) \tag{3}$$

for a class of output operators $\mathcal{C}$. In this talk, equation (3) serves as the starting point for an infinite-dimensional balanced truncation strategy similar to [4]. Our interest however is to approximate the nonlinear mapping $z \mapsto x(t)$ characterized by (1). For this, a second operator Lyapunov equation is introduced and by means of an output-normalized realization of (2) and an SVD of the underlying Hankel operator, a truncated reduced-order model is obtained. This model is shown to satisfy an $\mathcal{H}_2$-type error bound as in [1] which, due to the smoothing properties of the Hankel operator, can even be obtained a priori. The result is a linear finite-dimensional system which approximates (1) not only for a single initial condition z but also if z is drawn from a known probability distribution. Numerical examples based on tensor calculus will illustrate benefits and current limitations of the method.

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Balanced truncation for bilinear systems with quadratic outputs

Reetish Padhi[1,3], **Ion Victor Gosea**[2], **Igor Pontes Duff**[2], **and Peter Benner**[2]

[1] *Indian Institute of Science Education and Research, Pune, India*
[2] *Max Planck Institute of Dynamics of Complex Technical Systems, Magdeburg, Germany*
[3] *Virginia Polytechnic Institute and State University, Blacksburg*

Bilinear systems with quadratic outputs (BQOs) are a special class of bilinear systems for which the output expression contains a quadratic form of the state variable. Such dynamical systems are characterized by the following set of differential and standard equations

$$\begin{aligned}\dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{N}\mathbf{x}(t)\mathbf{u}(t) + \mathbf{B}\mathbf{u}(t),\\ \mathbf{y}(t) &= \mathbf{C}\mathbf{x}(t) + \mathbf{x}(t)^\top\mathbf{M}\mathbf{x}(t),\end{aligned} \tag{1}$$

where $\mathbf{M} = \mathbf{M}^\top \in \mathbb{R}^{n\times n}$, $\mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{B} \in \mathbb{R}^{n\times 1}, \mathbf{C} \in \mathbb{R}^{1\times n}, \mathbf{N} \in \mathbb{R}^{n\times n}, \mathbf{x}(t) \in \mathbb{R}^n$, and $\mathbf{u}(t), \mathbf{y}(t) \in \mathbb{R}$. Such systems are of use when one is interested in observing energies or other quadratic quantities of a bilinear system as an extension from the case of linear systems [1]. However, as far as the authors are aware, model order reduction (MOR) techniques for such systems have not been studied so far.

In this contribution, we propose a balanced truncation (BT) approach for the MOR of BQO systems. We use the Volterra series representation of a BQO system and the state-space representation of its dual system [4] to derive the time-domain generalized kernels of these systems and define infinite Gramians ($\mathbf{P}$ and $\mathbf{Q}$) for such systems. We prove various relations between the newly-defined Gramians and the energy functionals of BQO systems and show that the Gramians satisfy the following generalized Lyapunov matrix equations (which are linear in both $\mathbf{P}$ and $\mathbf{Q}$ variables),

$$\mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^\top + \mathbf{B}\mathbf{B}^\top + \mathbf{N}\mathbf{P}\mathbf{N}^\top = \mathbf{0}, \tag{2}$$

$$\mathbf{A}^\top\mathbf{Q} + \mathbf{Q}\mathbf{A} + \mathbf{C}^\top\mathbf{C} + \mathbf{N}^\top\mathbf{Q}\mathbf{N} + \mathbf{M}\mathbf{P}\mathbf{M} = \mathbf{0}. \tag{3}$$

We note that the reachability Gramian $\mathbf{P}$ satisfies the same equation as that for bilinear systems with linear outputs, while if $\mathbf{M} = \mathbf{0}$, the equation of the observability Gramian $\mathbf{Q}$ becomes the standard one. Using (2) and (3), we put together the proposed BT algorithm for BQO systems. We also show that the reduced-order model is balanced in the generalized sense. It is to be noted that solving (2) and (3) can be performed employing iterative numerical methods such as in [3]. Instead of solving these generalized Lyapunov equations, we also propose using truncated Gramians similar to the approach in [2]. We then present an efficient BT algorithm based on such Gramians and also investigate the possibility of deriving error bounds to quantify the approximation quality. Finally, various numerical experiments are reported, such as a semi-discretized heat transfer model with Robin boundary conditions, for which the observed output is given by the energy of the temperature values instead of the average thereof.

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Interpolatory $\mathcal{H}_2$ model order reduction of linear systems with quadratic output functions

S. Reiter[1], I. V. Gosea[2], S. Gugercin[1], and I. Pontes Duff[2]

[1]*Department of Mathematics, Virginia Tech, Blacksburg, VA 24061, USA,*
[2]*Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany.*

In this work, we consider linear systems with quadratic output functions

$$\Sigma: \quad \mathbf{x}'(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \qquad \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{M}\left(\mathbf{x}(t) \otimes \mathbf{x}(t)\right), \tag{1}$$

where $\mathbf{A} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{n\times m}$, $\mathbf{C} \in \mathbb{R}^{p\times n}$ and $\mathbf{M} \in \mathbb{R}^{p\times n^2}$. We assume that the system in (1) is asymptotically stable. Systems that consider quadratic observables as quantities of interest arise in a variety of applications, and particularly whenever one is interested in observing quantities computed as the product of time of frequency-domain components of the state [1]. The frequency-domain response of such a system is fully specified by two rational transfer functions

$$\mathbf{H}_1(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} \quad \text{and} \quad \mathbf{H}_2(s_1, s_2) = \mathbf{M}\left((s_1\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} \otimes (s_2\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}\right). \tag{2}$$

The $\mathcal{H}_2$ norm for systems of the form (1) can be defined via these transfer functions as

$$\|\Sigma\|_{\mathcal{H}_2}^2 := \frac{1}{2\pi}\int_{-\infty}^{\infty} \|\mathbf{H}_1(\imath\omega)\|_{\mathsf{F}}^2 d\omega + \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \|\mathbf{H}_2(\imath\omega_1, \imath\omega_2)\|_{\mathsf{F}}^2 d\omega_1 d\omega_2. \tag{3}$$

In practical applications, the state dimension can be rather large (e.g., $n \geq 10^6$) and any repeated action involving the full-order model (1) becomes prohibitively expensive. Model-order reduction seeks to remedy this problem with the construction of cheap-to-evaluate surrogate models of the form

$$\widehat{\Sigma}: \quad \widehat{\mathbf{x}}'(t) = \widehat{\mathbf{A}}\widehat{\mathbf{x}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t) \qquad \widehat{\mathbf{y}}(t) = \widehat{\mathbf{C}}\widehat{\mathbf{x}}(t) + \widehat{\mathbf{M}}\left(\widehat{\mathbf{x}}(t) \otimes \widehat{\mathbf{x}}(t)\right), \tag{4}$$

where $\widehat{\mathbf{A}} \in \mathbb{R}^{r\times r}$, $\widehat{\mathbf{B}} \in \mathbb{R}^{r\times m}$, $\widehat{\mathbf{C}} \in \mathbb{R}^{p\times r}$, $\widehat{\mathbf{M}} \in \mathbb{R}^{p\times r^2}$ for $1 \leq r \ll n$, and the reduced model (4) is such that $\|\mathbf{y} - \widehat{\mathbf{y}}\|$ is small in an appropriate norm for a range of inputs. Significantly, one can show [1]

$$\|\mathbf{y} - \widehat{\mathbf{y}}\|_{\mathcal{L}_\infty^p} \leq \|\Sigma - \widehat{\Sigma}\|_{\mathcal{H}_2}\left(\|\mathbf{u}\|_{\mathcal{L}_2^m}^2 + \|\mathbf{u}\otimes\mathbf{u}\|_{\mathcal{L}_2^{m^2}}^2\right)^{1/2}.$$

Based on this bound, we consider the $\mathcal{H}_2$ optimal model reduction problem for the systems in (1). Our main contributions to this problem are threefold: First, we derive interpolation-based first-order necessary conditions for $\mathcal{H}_2$ optimal model reduction. These amount to tangential interpolation of a weighted sum of the transfer functions in (2), and generalize the analogous optimality conditions for linear $\mathcal{H}_2$ model reduction. We show how to enforce these conditions in the construction of the reduced model using projection. Secondly, we prove these conditions are equivalent to Gramian-based $\mathcal{H}_2$ optimality conditions for the systems in (1). Finally, we propose an extension of the iterative rational Krylov algorithm [2] to systems of the form (1). The algorithm enforces the necessary $\mathcal{H}_2$ optimality conditions at every step, and produces locally $\mathcal{H}_2$ optimal approximants upon convergence.

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Entropy-Stable Non-Linear Manifold ROMs for Hyperbolic Conservation Laws

R.B. Klein[1,2], B. Sanderse[1], R.A.W.M. Henkes[2], R. Pecnik[2], and P. Costa[2]

[1] *Centrum Wiskunde & Informatica, Science Park 123, Amsterdam, The Netherlands*
[2] *Delft University of Technology, Leeghwaterstraat 39, Delft, The Netherlands*

Hyperbolic conservation laws are vital in modelling the physics of fluid flow. However, due to their transport-dominated nature, solutions of these systems are inherently not contained in low-dimensional linear subspaces. This precludes the use of well-established linear model reduction methods. A popular new approach, as pioneered in [2], is to construct reduced order models (ROMs) on non-linear manifolds. The accuracy of so-called non-linear manifold ROMs is not limited by the Kolmogorov N-width of the system's solution manifold. Consequently, non-linear manifold ROMs can capture the solution manifold of transport-dominated systems.

However, for the reliability and generalizability it is crucial that non-linear manifold ROMs are stable. For non-linear hyperbolic conservation laws the natural notion of stability is entropy stability. An entropy-stable full-order model (FOM) conserves or dissipates a specific convex functional referred to as entropy depending on the solution's regularity [3]. Apart from stability, this property also assures physically correct behaviour near discontinuities. Upon constructing ROMs from entropy-stable FOMs this property is often lost though. In the linear setting results have been obtained in preserving the entropy stability property for ROMs [1]. Prohibitively large subspaces are required to accurately model the physics in this setting.

Our key contribution lies in generalizing these results to non-linear manifold ROMs which are of far lower dimensionality. Furthermore, we propose a novel rational polynomial manifold method to assure accuracy of the entropy-stable non-linear manifold ROM.

Our method works by generalizing the entropy projection method proposed in [1] to nonlinear manifolds. In this approach the ROM is evaluated at a corrected state which follows from performing an entropy projection. Evaluating the ROM at the entropy-projected state assures proper conservation or dissipation of the entropy functional. For nonlinear manifolds the entropy projection involves projecting the so-called entropy variables on the manifold's tangent space at the original state. To assure the entropy projection method remains accurate for non-linear manifolds, we propose a novel tangent space enrichment (TSE) method. With TSE we lift the manifold in such a way so that the entropy variables are well-resolved by the appropriate tangent spaces of the lifted manifold. At the cost of introducing an extra reduced variable we can then assure the ROM remains accurate and entropy-stable.

We test our proposed method on several well-known one-dimensional hyperbolic conservation laws with moving discontinuities like the Burgers equation, shallow-water equations and compressible Euler equations. Our experiments validate the theoretical framework and show that our method significantly outperforms linear and quadratic manifold ROMs while also possessing stability guarantees.

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Flexible and variationally consistent Hamiltonian model reduction

A. Gruber[1] **and I. Tezaur**[2]

[1] *Center for computing research, Sandia National Laboratories, Albuquerque, NM*
[2] *Quantitative modeling and software engineering, Sandia National Laboratories, Livermore, CA*

Hamiltonian systems offer a simple description of conservative dynamics which presents many challenges for model reduction, particularly when canonical position and momentum variables are separated in scale by orders of magnitude. This talk presents a novel and variationally consistent method for the model reduction of canonical Hamiltonian systems. Its distinguishing factors are (1) its ability to accommodate nearly arbitrary reduced bases, (2) its applicability in both intrusive and nonintrusive settings, and (3) its interpretable error estimate involving a projection term and a deviation-from-canonicity term, both of which must balance for accurate state approximation. Results are presented using examples from 3D solid mechanics, showing that the proposed method offers several advantages when compared to the existing state of the art.

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Lagrangian operator inference enhanced with structure-preserving machine learning for nonintrusive model reduction of mechanical systems

Harsh Sharma[1], **David A. Najera-Flores**[2,3], **Michael D. Todd**[2], **and Boris Kramer**[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California San Diego*
[2]*Department of Structural Engineering, University of California San Diego*
[3]*ATA Engineering, Inc., San Diego*

Complex mechanical systems often exhibit strongly nonlinear behavior due to the presence of nonlinearities in the energy dissipation mechanisms, material constitutive relationships, or geometric/connectivity mechanics. Numerical modeling of these systems leads to nonlinear full-order models that possess an underlying Lagrangian structure. This work proposes a Lagrangian operator inference method enhanced with structure-preserving machine learning to learn nonlinear reduced-order models (ROMs) of nonlinear mechanical systems. This two-step approach first learns the best-fit linear Lagrangian ROM via Lagrangian operator inference and then presents a structure-preserving machine learning method to learn nonlinearities in the reduced space. The proposed approach can learn a structure-preserving nonlinear ROM purely from data, unlike the existing operator inference approaches that require knowledge about the mathematical form of nonlinear terms. From a machine learning perspective, it accelerates the training of the structure-preserving neural network by providing an informed prior (i.e., the linear Lagrangian ROM structure), and it reduces the computational cost of the network training by operating on the reduced space. The method is first demonstrated on two simulated examples: a conservative nonlinear rod model and a two-dimensional nonlinear membrane with nonlinear internal damping. Finally, the method is demonstrated on an experimental dataset consisting of digital image correlation measurements taken from a lap-joint beam structure from which a predictive model is learned that captures amplitude-dependent frequency and damping characteristics accurately. The numerical results demonstrate that the proposed approach yields generalizable nonlinear ROMs that exhibit bounded energy error, capture the nonlinear characteristics reliably, and provide accurate long-time predictions outside the training data regime.

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Learning passive dynamical systems via spectral factorization

J. Nicodemus[1], S. Gugercin[2], and B. Unger[1]

[1]*Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart*
[2]*Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech*

Inferring mathematical models of physical systems from data is a fundamental task in engineering and science. In previous work [2], we have developed a method for the identification of passive dynamical systems from time domain data. Now we extend this framework to the frequency domain. We are interested in the identification of passive dynamical systems of the form

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

with matrices $A \in \mathbb{R}^{n\times n}$, $B, C \in \mathbb{R}^{n\times m}$, and $D \in \mathbb{R}^{m\times m}$. One well-known condition to ensure passivity is the Kalman-Yakubovich-Popov lemma, i.e., the existence of matrix $X \in \mathbb{R}^{n\times n}$ such that

$$\mathcal{W}_\Sigma(X) := \begin{bmatrix} -A^\mathsf{T}X - XA & C^\mathsf{T} - XB \\ C - B^\mathsf{T}X & D + D^\mathsf{T} \end{bmatrix} \succeq 0.$$

Our method is based on the spectral factorization of the Popov function

$$\Phi(s) = \begin{bmatrix} (-sI_n - A)^{-1}B \\ I_m \end{bmatrix}^\mathsf{T} \mathcal{W}_\Sigma(X) \begin{bmatrix} (sI_n - A)^{-1}B \\ I_m \end{bmatrix},$$

which motivates a two-step approach. First, we obtain A and B from traditional identification methods such as the Loewner framework or Vector fitting. Then, observing that samples of the transfer function on the imaginary axis can be used to infer the Popov function on the imaginary axis, we fit $\mathcal{W}$ to this data. With $\mathcal{W}$ at hand, we obtain C and D in a computationally efficient way that at the same time guarantees passivity of the realization. To overcome the course of dimensionality, we reduce the number of decision variables and get rid of the semi-definite constraint by fitting Cholesky-like factors of $\mathcal{W}$ to the data instead of $\mathcal{W}$ itself

$$\mathcal{W}_\Sigma(X) = \begin{bmatrix} L & M \end{bmatrix}^\mathsf{T} \begin{bmatrix} L & M \end{bmatrix} \succeq 0.$$

Combining this approach with the result of [3], which states that there exists always X such that $\operatorname{rank}(\mathcal{W}_\Sigma(X)) = m$, we can restrict the dimensions of L and M to $n \times m$ and $m \times m$ respectively. Now, instead of solving a constrained convex optimization problem, we solve an unconstrained non-convex optimization problem with (potentially) a much smaller number of decision variables. We have already applied a similar strategy with great success in [1]. Secondly, we observe that with the framework outlined above, we can also tackle the $\mathcal{H}_2$-optimal passivation problem in a large-scale setting. We illustrate the effectiveness of our methods on several numerical examples.

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Data-driven identification of reduced port-Hamiltonian systems

J. Rettberg[1], J. Kneifl[1], J. Herb[1], P. Buchfink[2,3], J. Fehr[1], and B. Haasdonk[2]

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

Conventional modeling techniques involve high effort and expert knowledge, while data-driven methods often lack interpretability, structure and sometimes reliability. To mitigate this, we present a data-driven system identification framework that derives models in the port-Hamiltonian (pH) formulation, which is suitable for multi-physics modeling. At the same time, these systems incorporate the useful system theoretical properties of passivity and stability [2]. Our framework combines linear and nonlinear reduction with structured, physics-motivated system identification, see Fig. 1. In this process, high-dimensional and possibly nonlinear state data serves as the input for the autoencoder, which then performs two tasks: (i) nonlinearly transforming and (ii) reducing this data onto a low-dimensional manifold following the approach of [1]. In the resulting latent space, a pH system is identified by using the weights of a neural network as entries of triangular matrices that strongly satisfy the pH properties. In a joint optimization process over the loss term, the pH matrices are adjusted to match the dynamics of the data, and the latent coordinates automatically become pH variables. The identified (parameter-dependent) pH system can be solved in the reduced space to obtain solutions for varying initial conditions, parameters and inputs. Furthermore, it can be shown that the decoded pH system on the state space fulfills pH properties under certain assumptions. The learned, linear low-dimensional pH system can describe even nonlinear systems and is rapidly computable due to its small size [3]. An academic nonlinear example of a pendulum and the high-dimensional model of a disc brake with linear thermoelastic behavior exemplify the approach.

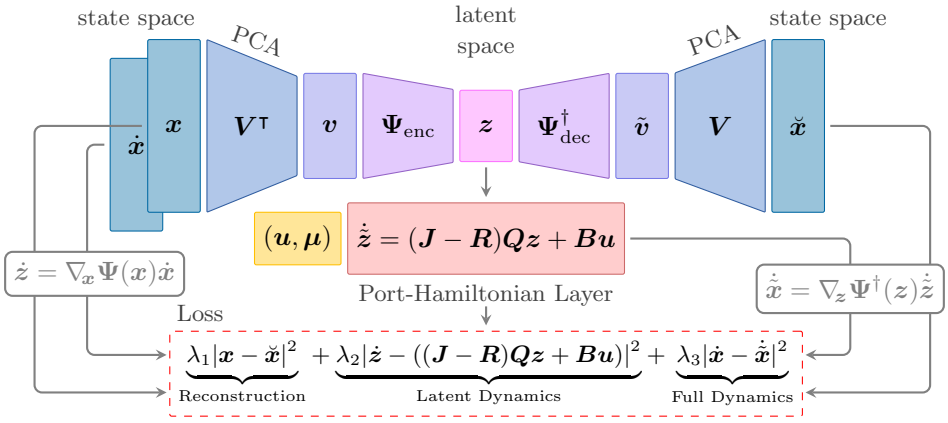

Figure 1: Port-Hamiltonian deep learning framework [3].

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Structure-preserving model order reduction of linear time-varying port-Hamiltonian systems

K. Cherifi[1] **and R. Morandin**[1]

[1] *Technische Universität Berlin, Insitut für Mathematik*

Many physical processes can be naturally modeled using port-Hamiltonian (pH) systems [4], which are inherently passive and stable, and allow for structure-preserving interconnection, making them particularly suitable for the modeling of complex networks. Furthermore, many dedicated numerical methods have been developed to exploit and preserve the structure of pH systems, e.g. for space- and time-discretization, and model order reduction (MOR).

In our work, we focus on the structure-preserving MOR of linear time-varying (LTV) pH systems [1], which have the form

$$\begin{aligned} \dot{x}(t) &= ((J(t) - R(t))Q(t) - K(t))x(t) + (G(t) - P(t))u(t), \\ y(t) &= (G(t) + P(t))^\top Q(t)x(t) + (S(t) - N(t))u(t), \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^n$, and $u, y \in \mathbb{R}^m$ denote the state, input and output variables, respectively, and the coefficients J, R, Q, K, G, P, S, N are matrix functions depending on the time variable, satisfying $J(t) = -J(t)^\top$, $N(t) = -N(t)^\top$, $Q(t) = Q(t)^\top \geq 0$, $\dot{Q}(t) = Q(t)K(t) + K(t)^\top Q(t)$, and

$$W(t) := \begin{bmatrix} R(t) & P(t) \\ P(t)^\top & S(t) \end{bmatrix} = W(t)^\top \geq 0 \tag{2}$$

for all times t. The Hamiltonian $\mathcal{H}(x,t) := \frac{1}{2}x^\top Q(t)x$ is then a storage function for (1).

LTV systems appear quite naturally in many applications, e.g. in the linearization of nonlinear systems around non-stationary reference solutions, or when some of the system parameters are time-dependent. In the literature there are few works on the MOR of general LTV systems [3], but even fewer on the MOR of LTV-pH systems. In this talk, we introduce a general approach based on (Petrov)-Galerkin projection for the structure-preserving MOR of LTV-pH systems. In particular, we show that the effort constraint method extended to the case of LTV-pH systems falls into this category. Then, we present a variant of the usual balanced truncation method that combines balancing with effort constraint to obtain a reduced pH model, similarly to what was done in [2] for linear time-invariant systems. Numerical experiments to validate our methods are exhibited.

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Beyond linear – a differential geometric framework for nonlinear projections

P. Buchfink[1,2], **S. Glas**[1], **B. Haasdonk**[2], **and B. Unger**[3]

[1]*Faculty of Electrical Engineering, Mathematics and Computer Science, University of Twente*
[2]*Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*
[3]*Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart*

While classical linear-subspace MOR is well-established, it cannot approximate a dynamical system with a low-dimensional surrogate with high fidelity if the Kolmogorov n-widths (respectively the Hankel singular values; see [4]) decay slowly, which is the prevalent scenario in transport-dominated applications. To remedy this issue, several nonlinear approximation schemes have been proposed over the last decade in the literature, and the use of nonlinear projections, including deep learning architectures in model order reduction (MOR), is still a very active research field. In this talk, we provide a first attempt towards a unifying framework for (many of) these methods by acknowledging that general nonlinear projections can benefit from a differential geometric viewpoint [1]. In more detail, we provide a novel framework for model reduction on smooth manifolds, emphasizing the objects' geometric nature. The crucial ingredient is the construction of an embedding for the low-dimensional submanifold and a compatible reduction map that maps a subset of the tangent bundle of the manifolds onto the tangent bundle of the reduced manifold. In this talk, we demonstrate how the classical (Petrov-)Galerkin framework using linear projections can be generalized to the manifold setting, thus generalizing results from [2, 3], and prove a general exact reproduction result. To connect our framework to existing work in the field, we demonstrate that various nonlinear MOR techniques presented in the literature can be included.

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Structure-preserving model reduction: From the formulation on manifolds to data-driven realizations

P. Buchfink[1,2], **S. Glas**[1], **B. Haasdonk**[2], **H. Mu**[1], **and B. Unger**[3]

[1]*Faculty of Electrical Engineering, Mathematics and Computer Science, University of Twente*
[2]*Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*
[3]*Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart*

Capturing and preserving physical properties, e.g., system energy, stability and passivity, using data-driven methods is currently a highly-researched topic in surrogate modeling. To ensure that the desired physical properties are retained, structure-preserving projection techniques are used in the field in model reduction (MOR), see e.g., [3].

In this talk, we present structure-preserving MOR with nonlinear projections, which are needed for problems with slowly decaying Kolmogorov-n-widths. To precisely define and highlight the quantities that we would like to retain, we start with a formulation of initial value problems on manifolds, which we consider as the full-order model (FOM). Already at this level, we define what we mean by adding structure to the FOM and how this can be detailed geometrically. This formalism allows to introduce a novel projection technique, the *generalized manifold Galerkin* (GMG) [2]. By adapting the underlying non-degenerate tensor field, this GMG projection can be used for a structure-preserving reduction of various initial value problems that give rise to interesting physical properties, which include, but are not restricted to, Lagrangian and Hamiltonian systems.

Once that we have derived the geometric formulation, we focus on data-driven ansatzes to realize the presented reduction methods. In this part of the talk, we will connect several existing techniques for data-driven realizations with GMG projections [1, 4].

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3.3 Wednesday, September 11

Registration in bounded domains for model reduction of parametric conservation laws

Tommaso Taddei[1,2]

[1] *IMB, UMR 5251, Univ. Bordeaux, 33400 Talence, France*
[2] *Inria Bordeaux Sud-Ouest, Team MEMPHIS, Univ. Bordeaux, 33400 Talence, France*

In this talk, I review recent efforts on the development of registration methods [2] for parametric model order reduction (MOR), with emphasis on advection-dominated flows. In computer vision and pattern recognition, registration refers to the process of finding a parametric transformation that aligns two datasets; in model order reduction, registration methods seek a parametric bijection Φ that tracks coherent structures (e.g., shocks, shear layers) of the solution field. Formally, given the computational domain $\Omega \subset \mathbb{R}^d$, the vector of parameters μ in the parameter region $\mathcal{P} \subset \mathbb{R}^P$, and the solution set $\mathcal{M} = \{u_\mu : \mu \in \mathcal{P}\}$, the bijection Φ is designed to make the mapped manifold $\widetilde{\mathcal{M}} = \{u_\mu \circ \Phi_\mu : \mu \in \mathcal{P}\}$ (more) suitable for linear compression methods (e.g., POD).

We integrate registration in the offline/online model reduction framework to tackle problems with parameter-dependent discontinuities [1]. Our approach combines registration with three additional building blocks: (i) an hyper-reduced least-squares Petrov-Galerkin (LSPG) reduced-order model, to estimate the mapped solution; (ii) a parametric mesh adaptation procedure to build a parsimonious yet accurate representation of the solution field; and (iii) a multi-fidelity strategy to reduce offline training costs. We present numerical results for several two-dimensional inviscid compressible flows, to show the potential of the method.

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Greedy frequency domain model reduction for parametric systems: New theory and algorithms

Filip Belik[1], **Yanlai Chen**[2], **and Akil Narayan**[1]

[1]*Department of Mathematics and Scientific Computing and Imaging (SCI) Institute, University of Utah, USA*
[2]*Department of Mathematics, University of Massachusetts Dartmouth, USA*

We propose and investigate weak greedy snapshot-based model reduction for linear differential equations posed in the frequency domain with parametric dependence. The full order model is,

$$\boldsymbol{x}'(t) = \boldsymbol{A}(\boldsymbol{p})\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t), \qquad \boldsymbol{y}(t) = \boldsymbol{C}(\boldsymbol{p})\boldsymbol{x}(t),$$

where $\boldsymbol{u} \in \mathbb{R}^{n_{\text{in}}}$ is a given input signal, $\boldsymbol{y} \in \mathbb{R}^{n_{\text{out}}}$ is an output, and the matrices $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$ are dependent on a parameter $\boldsymbol{p} \in \mathbb{R}^d$. The frequency domain representation of this system is a stationary linear problem that defines the frequency response of the output $\boldsymbol{y}$. Our main strategy is to deploy a certain type of reduced basis method-type solver for the frequency domain problem. Similar approaches for this problem include interpolatory methods [1] and moment matching-type procedures [2, 3].

Our contributions are as follows. Our particular reduced basis method representation uses frequency domain parametric snapshots to build low-dimensional approximation spaces. The algorithmic ingredients employ techniques from reduced basis methods such as empirical interpolation, successive constraint methods, and *a posteriori* error estimators. The procedure is an algorithmic realization of recent theory that connects Kolmogorov n-width decay to rational approximability of the transfer function of the full order model. We discuss how this procedure is backed by corresponding *a priori* theoretical guarantees on approximation of the full order parametric system transfer function. We also demonstrate how this theory translates into practical performance of the algorithm, including certification of error. Our examples reveal the efficacy of this procedure and in particular how the *a priori* theory informs expected performance of the reduced order model.

We will showcase deployment of this new method through our newly developed Julia package, `ModelOrderReductionToolkit.jl`. This package achieves several goals. It provides replicable, implementable, and extendable numerical examples that illustrate the efficacy of the method, including rates of error decay. To promote the numerical computing of reduced order models, the package contributes new functionality to the Julia reduced order modeling community by providing a set of open source tools that could be applied to several model order reduction problems. While the current focus is on linear parametric reduced order modeling techniques, the long-term goal of the package is to provide a starting point for learning about and implementing more general reduced order models used in various applications.

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Snapshot-based modeling of parametric linear systems

Art J. R. Pelling[1], **Karim Cherifi**[1], **and Ion Victor Gosea**[2]

[1] *Technical University Berlin, Germany.*
[2] *Max Planck Institute for Dynamics of Complex Technical Systems, Germany.*

Parametric data-driven modeling is relevant for many applications where the model depends on some varying parameter. Consider parametric linear time-invariant systems of the form

$$\begin{aligned} \tfrac{d}{dt}x(t,p) &= A(p)x(t,p) + B(p)u(t), \\ y(t,p) &= C(p)x(t,p) + D(p)u(t), \end{aligned} \tag{1}$$

with *transfer function*

$$H(s,p) = C(p)(sI - A(p))^{-1}B(p) + D(p). \tag{2}$$

This work falls in the category of data-driven modeling and reduction of parametric systems[1]. In particular, we focus on modeling parametric linear systems based on a sampling of the parameter space into snapshots of system matrices. Each snapshot is given by

$$\boldsymbol{\Sigma}_i = \big(A(p_i), B(p_i), C(p_i), D(p_i)\big), \tag{3}$$

where $i \in \{1, \ldots, n_p\}$ at $n_p \in \mathbb{N}$ fixed parameter samples $p_i \in P$, the aim is to construct an approximate bivariate transfer function $\hat{H}(s,p)$ of the form (2) that interpolates the data, i.e. $\hat{H}(s,p_i) = H(s,p_i)$, for any given value of $p_i \in P$ and $s \in \mathbb{C}$ and matches the original transfer function $H(s,p)$ as closely as possible at intermediate parameter values $p_i \neq p \in P$. In order to obtain the matrices that constitute the transfer function, each global parametric matrix is obtained by interpolation of individual snapshot matrices in (3). This type of parametric systems interpolation is called matrix interpolation. The main constraint of this method is that all snapshots have to lie in the same subspace. This problem is dealt with by the projection of all the snapshots in a common subspace as discussed in [2]. We assume in our case that the snapshots are already given in a common subspace. If not, one can follow the framework of [2]. Then, the parameter snapshots are interpolated using the classical univariate Loewner framework. This avoids the computational burden of multivariate Loewner matrices and their truncation. Then, the global bivariate transfer function of the form (2) is extracted using a linear fractional transformation (LFT) where the LFT is defined for LTI systems as

$$G(s) = C(sI_n - A)^{-1}B + D = \mathcal{F}_u\left(\begin{bmatrix} A & B \\ C & D \end{bmatrix}, s^{-1}I_n\right). \tag{4}$$

With this method we are also able to derive a priori rank bounds for the Loewner matrices based on the parametric structure of the transfer function. These bounds are derived for an affine dependence of the parametric transfer function on p and a higher-order polynomial dependence on p. Finally, the implementation details are discussed where we propose a switching strategy to speed up computations and support our results by multiple numerical examples.

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A parallel batch greedy algorithm in reduced basis methods: Convergence rates and numerical results

N. Reich[1,2]**, K. Urban**[1]**, and J. Vorloeper**[2]

[1] *Ulm University, Institute for Numerical Mathematics, Ulm, Germany*
[2] *University of Applied Sciences Ruhr West, Institute of Natural Sciences, Mülheim, Germany*

The classical (weak) greedy algorithm is used within the reduced basis method in order to compute a reduced basis in the offline training phase. To this end, either the actual error or an a posteriori error estimator is maximized and the snapshot corresponding to the maximizer is added to the current basis.
We aim at exploring the potential of parallel computations in the offline phase to obtain some speed-up in particular in those cases where the snapshot computation is extremely costly. In order to do so, we introduce a batch size b and add b snapshots to the current basis in every greedy iteration. These snapshots are computed in parallel.
First, we prove convergence rates for this new batch greedy algorithm for polynomial and exponential decay of the Kolmogorov width and compare them to those of the classical (weak) greedy algorithm, [1, 2]. Then, we present numerical results where we apply a (parallel) implementation of the proposed algorithm to some benchmark problems. We analyze the quality of the final reduced basis, as well as the offline and online wall-clock times for different batch sizes and show that the proposed variant can, in fact, be used to speed-up the offline phase.

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An Iterative Active Subspace Approach for Model Order Reduction of Parametric Systems with High-Dimensional Parameter Spaces

Chenzi Wang[1], Page Yu[1], Lihong Feng[2], Peter Benner[2], Wenshuai Lu[1], and Zheng You[1]

[1] *Department of Precision Instrument, Tsinghua University*
[2] *Max Planck Institute for Dynamics of Complex Technical Systems*

The active subspace approach [1] has been successfully applied to parametric model order reduction (PMOR) for systems with many parameters (1). This work considers a linear parametric system with a large dimensional parameter space $\mathcal{P}$, represented by its transfer function

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

where $p \in \mathcal{P} \subset \mathbb{R}^{n_p}$ is the vector of parameters; s is the Laplace variable; $E(p), A(p) \in \mathbb{R}^{n\times n}$, $B(p) \in \mathbb{R}^{n\times n_I}$, $C(p) \in \mathbb{R}^{n_O\times n}$ are the system matrices. Using the active subspace method, a matrix $U \in \mathbb{R}^{n_p\times r_p}, r_p < n_p$, is computed so that its columns span the active subspace $\mathcal{U}$ of the parameter domain $\mathcal{P}$. Based on the active subspace, the parameter sampling can be done in $\mathcal{U}$, the reduced transfer function

$$H_r(p,s) = C(UU^Tp)V(sV^TE(UU^Tp)V - V^TA(UU^Tp)V)^{-1}V^TB(UU^Tp)$$

is computed by using U and a projection matrix $V \in \mathbb{R}^{n\times r},\ r \ll n$ via, e.g., the PMOR method in [2].

While the active subspace approach is able to achieve decent accuracy with a relatively small Reduced Order Model (ROM), its accuracy often fails to scale with the size of the ROM. In this paper, we propose an iterative approach that aims to improve the accuracy of the active subspace approach, while keeping the ROM size as small as possible. The reduced transfer function $H_r(p,s)$ is iteratively updated by applying PMOR with the active subspace method [1] to the error system at the current iteration.

Our proposed method is applied to analyze a structural mechanical system of a micro-electro-mechanical system (MEMS) accelerator, which consists of $n_p = 416$ parameters and $n = 15652$ state variables generated by the finite element method with a parametric mesh [3]. To obtain an acceptable ROM with an average accuracy of around 80% over the entire parameter space, we need at least a ROM with $r = 500$ (by Latin hypercube sampling in parameter space). In comparison, the original active subspace method is able to achieve 50% accuracy with a single ROM $r = 20$. However, we do not observe significant accuracy improvements when the ROM size is further increased. In contrast, the ROM constructed by our iterative active subspace method, is updated by several small ROMs with $r = 20$ at each iteration. The final ROM, in the form of the sum of 7 small ROMs, achieves 78.8% accuracy after 3 iterations. In summary, the proposed method improves the efficiency of the standard PMOR method and the accuracy of the original active subspace method [1] for systems with large-dimensional parameter spaces.

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Multi-fidelity Learning of Reduced Order Models

M. Ohlberger[1]

[1] *Institute for Analysis and Numerics, University of Münster, , Einsteinstraße 62, D-48149 Münster*

Classically, model order reduction it is based on a so-called offline phase, where reduced approximation spaces are constructed and the reduced parameterized system is built, followed by an online phase, where the reduced system can be cheaply evaluated in a multi-query context. In this contribution, instead, we follow an active learning or enrichment approach where a multi-fidelity hierarchy of reduced order models is constructed on-the-fly while exploring a parameterized system.

To this end we focus on learning based reduction methods in the context of PDE constrained optimization [1, 2, 4] and inverse problems [3] and evaluate their overall efficiency. We discuss learning strategies, such as adaptive enrichment within a trust region optimization framework as well as a combination of reduced order models with machine learning approaches.

We propose a hierarchical framework of full order, reduced order, and machine learning models [5] for parameterized parabolic equations that can be queried in any context with a prescribed accuracy. The resulting hierarchical model adaptively updates its hierarchy if it is queried for parameters where either the machine learning model or the reduced order model is not accurate enough. The accuracy is thereby measured by a rigorous a posteriori error estimator that can be used by both the reduced order and machine learning model. As machine learning approaches, we studied deep neural networks as well as kernel and deep kernel methods. Following the multi-fidelity approach, the hierarchy may also only consists of a full order model and a deep neural network based machine learning model built from snapshots of the full order model [6]. Concepts of rigorous certification and convergence will be presented, as well as numerical experiments that demonstrate the efficiency of the proposed approaches.

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Multi-fidelity reduced-order surrogate modelling

P. Conti[1], M. Guo[2], A. Frangi[1], A. Manzoni[3], S. Brunton[4], and J. N. Kutz[4]

[1]*Department of Civil Engineering, Politecnico di Milano, Milano, Italy*
[2]*Department of Applied Mathematics, University of Twente, Enschede, the Netherlands*
[3]*MOX – Department of Mathematics, Politecnico di Milano, Milano, Italy*
[4]*Department of Mechanical Engineering, and* [5]*Department of Applied Mathematics, University of Washington, Seattle, United States*

High-fidelity numerical simulations of partial differential equations (PDEs) given a restricted computational budget can significantly limit the number of parameter configurations considered and/or time window evaluated. Multi-fidelity surrogate modeling aims to leverage less accurate, lower-fidelity models that are computationally inexpensive in order to enhance predictive accuracy when high-fidelity data are scarce [4]. However, low-fidelity models, while often displaying the qualitative solution behavior, fail to accurately capture fine spatio-temporal and dynamic features of high-fidelity models.

To address this shortcoming, we present a data-driven strategy that combines dimensionality reduction with multi- fidelity neural network surrogates [1]. The key idea is to generate a spatial basis by applying proper orthogonal decomposition (POD) to high-fidelity solution snapshots, and approximate the dynamics of the reduced states – time-parameter-dependent expansion coefficients of the POD basis – using a multi-fidelity long short-term memory network [2, 3]. By mapping low-fidelity reduced states to their high-fidelity counterpart, the proposed reduced-order surrogate model enables the efficient recovery of full solution fields over time and parameter variations in a non-intrusive manner. A further extension to the case of multiple data sources, with low-fidelity models of different type, is also considered, in the spirit of progressive learning from multiple sources.

The generality of the proposed approach is demonstrated by a collection of PDE problems where the low-fidelity model can be defined by coarser meshes and/or time stepping, as well as by misspecified physical features.

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Learning Bayesian reduced-order operators with Gaussian processes

Shane A. McQuarrie[1], **Mengwu Guo**[2], **and Anirban Chaudhuri**[3]

[1] *Sandia National Laboratories*
[2] *University of Twente*
[3] *The University of Texas at Austin*

This work presents a non-intrusive Bayesian inference method for learning reduced-order models whose predictions are endowed with uncertainty estimates. The strategy is based on operator inference (OpInf), which poses the problem of learning reduced operators as a regression of state space data and corresponding time derivatives. When time derivative data are not natively available, as is often the case in applications, they must be estimated from the state data, usually via finite differences. An inaccurate estimation adversely affects the quality of the learned reduced-order model, hence OpInf is challenging when state data are sparse or noisy. Our approach builds on our previous work [1] by combining OpInf with Gaussian process surrogate modeling to probabilistically describe uncertainties in the state data and procure analytical time derivative estimates with uncertainty. A Bayesian formulation is used to define a posterior distribution for the reduced-order operators, hence predictions subsequently issued by the reduced-order model are endowed with uncertainty, with statistical moments that can be estimated efficiently via Monte Carlo sampling. The Bayesian inference problem is equivalent to a weighted, Tikhonov-regularized least-squares regression. We select the regularization term, which relates statistically to the Bayesian prior, using an optimization-based strategy that ensures operators sampled from the posterior distribution result in numerically stable models. We demonstrate the approach for a quadratic system describing the compressible flow of an ideal gas (see Figure 1) and a nonlinear diffusion model with a parameterized forcing term. The numerical results show that sparse, noisy data can be handled effectively to non-intrusively construct probabilistic reduced-order models that can issue accurate predictions in time and for parametrically varying input terms.
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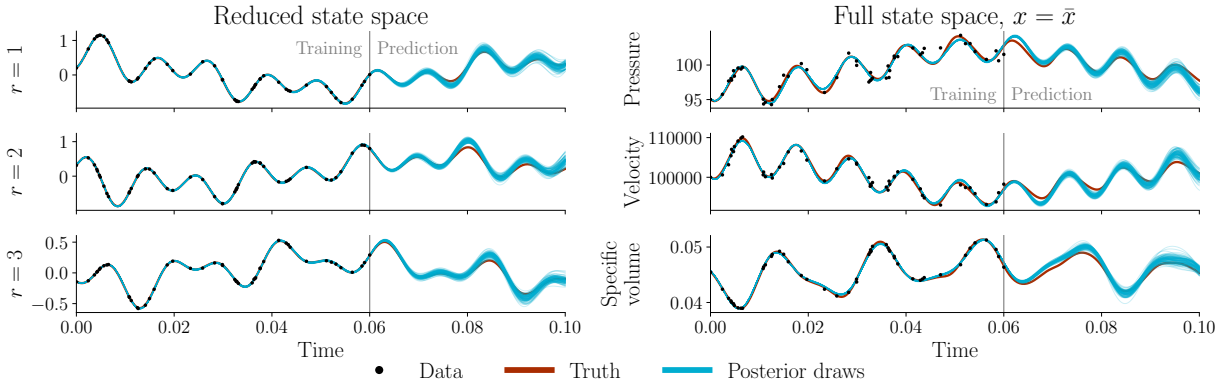

Figure 1: GP-Bayesian operator inference for the compressible Euler equations of an ideal gas. A set of 50 state observations with 5% relative noise is used to construct a quadratic probabilistic reduced-order model. Results are shown for the first three modes and for the full state space at one point in space.

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Building dynamical stability into data-driven quadratic ROMs

M. Peng[1], A. Kaptanoglu[2], C. Hansen[3], K. Manohar[1], and S. Brunton[1]

[1]*Dept. of Mechanical Engineering, University of Washington, Seattle, WA, 98195, USA*
[2]*Courant Institute of Mathematical Sciences, NYU, New York, NY, 10012, USA*
[3]*Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, 10027, USA*

Quadratically nonlinear reduced-order models (ROMs) are commonly used for approximating the dynamics of fluids, plasmas, and many other physical systems. However, it is challenging to a-priori guarantee the local or global dynamical stability of reduced-order models built from data. For instance, a minimal requirement for physically-motivated ROMs is long-time boundedness for any initial condition, yet many ROMs in the literature still fail this basic requirement. For quadratically nonlinear systems with energy-preserving nonlinearities, the Schlegel and Noack trapping theorem [5] provides necessary and sufficient conditions for long-time boundedness to hold. This analytic theorem was subsequently incorporated into system identification and machine learning techniques in order to produce a-priori bounded models directly from data [2, 3, 1]. However, many dynamical systems exhibit weak breaking of the quadratically energy-preserving nonlinear structure required for the trapping theorem. To address this important case, we present recent work that relaxes the quadratically energy-preserving constraint and derives local stability guarantees for data-driven models. The analytic results are subsequently used with system identification techniques to build models with a-priori local stability properties [4]. Lastly, we comment on alternative methods and future work for promoting dynamical stability in data-driven models.

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Data-driven Approximation of Linear Switched Systems

Antonio Carlucci[1], **Tommaso Bradde**[1], **and Stefano Grivet-Talocia**[1]

[1] *Dept. of Electronics and Telecommunications, Politecnico di Torino, Italy*

This contribution addresses the problem of learning dynamical Linear Switched System (LSS) models from input/output observations [1]. The method is illustrated on systems switching between two modes, according to the value of an exogenous signal $p(t) : \mathbb{R}_+ \to \{0, 1\}$. The LSS G maps its input $u(t)$ to the output $y(t)$, i.e. $y(t) = G[u(t), p(t)]$, see [1] for a rigorous definition.

First, we observe that G can be viewed as a family of linear time-varying (LTV) systems, each corresponding to a fixed switching trajectory. In particular, restricting $p(t)$ to the set of square-wave signals $p_{\omega_0}(t)$ of frequency ω_0, the collection of periodic LTV systems G_{ω_0} (indexed by ω_0) is defined by $y_{\omega_0}(t) = G_{\omega_0}[u(t)] \triangleq G[u(t), p_{\omega_0}(t)]$. According to Zadeh's theory [3], G_{ω_0} is represented by an ω_0-periodic transfer function $H_{\omega_0}(\mathrm{j}\omega, t)$, that admits a complex Fourier expansion with coefficients $H^{(n)}_{\omega_0}(\mathrm{j}\omega)$, $n \in \mathbb{Z}$. Isolating $n = 1$, we define the bivariate function $F(\mathrm{j}\omega, \mathrm{j}\omega_0) \triangleq H^{(1)}_{\omega_0}(\mathrm{j}\omega)$, that is a purely I/O representation, measurable by experiment or simulation in periodic steady-state conditions. Hence, the training dataset is a collection of evaluations $F(\mathrm{j}\omega^{(k)}, \mathrm{j}\omega_0^{(h)})$.

With this premise, we look for a model $\tilde{G}$ whose associated bi-variate function $\tilde{F}(\mathrm{j}\omega, \mathrm{j}\omega_0)$ approximates F in a least-squares sense. To this aim, we adopt a Wiener-like model structure [2] for $\tilde{G}$, whose output is $\tilde{y}(t) = \tilde{G}[u(t), p(t)] = \sum_{i=1}^{\bar{\imath}} \phi_i[p](t) \cdot \psi_i[u](t)$, where $\phi_i[\cdot]$ and $\psi_i[\cdot]$ are LTI systems. Its $\tilde{F}$-function can be written in pole-residue form as

$$\tilde{F}(\mathrm{j}\omega, \mathrm{j}\omega_0) = (\mathrm{j}\pi)^{-1} \sum_{i,j} r_{ij} (\mathrm{j}\omega - \alpha_i)^{-1} (\mathrm{j}\omega_0 - \beta_j)^{-1}. \tag{1}$$

We highlight that in the selected model structure, the components $\phi_i[p](t), \psi_i[u](t)$ are the outputs of scalar LTI systems. Model fitting, i.e. optimization of poles α_i, β_j and residues r_{ij}, can be performed using a suitable adaptation of a multivariate rational fitting algorithm. In our experiments, we used the Vector Fitting (VF) algorithm in two steps. First, we view ω_0 as a parameter and run VF to find a set of basis poles α_i to approximate the frequency dependence w.r.t. ω for all sampled values $\omega_0^{(h)}$ collectively. Then, a second run of VF, with fixed α_i, gives poles β_j and residues r_{ij}. Finally, $\tilde{G}$ results from assigning $\phi_i(s) = (s - \alpha_i)^{-1}$, $\psi_i(s) = \sum_j r_{ij}(s - \beta_j)^{-1}$. The input/output stability of the proposed model structure is guaranteed by enforcing strictly negative real part of the estimated poles α_i, β_i using standard techniques. The proposed approach is demonstrated using several benchmark examples of practical interest, including a Buck voltage regulator commonly used to stabilize the microprocessor power supply in electronic systems.

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Distributed computing for physics-based data-driven reduced modeling at scale

Ionut Farcas[1], **Rayomand P. Gundevia**[2], **Ramakanth Munipalli**[3], **and Karen E. Willcox**[1]

[1]*Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712*
[2]*Jacobs Engineering Group, Inc., Edwards Air Force Base, Edwards, CA 93524*
[3]*Air Force Research Laboratory, Edwards Air Force Base, Edwards, CA 93524*

High-performance computing (HPC) and data-driven reduced modeling offer two complementary perspectives on numerical simulations of complex systems. HPC focuses on parallel architectures, algorithms, and software implementations to conduct high-fidelity simulations on supercomputers. On the other hand, data-driven reduced modeling aims to construct computationally inexpensive yet sufficiently accurate approximations to enable tasks that are computationally too expensive in terms of high-fidelity models. The work discussed in this presentation enables a fast and scalable construction of predictive physics-based reduced models from data in problems at a scale and complexity the exceed what standard approaches used in the model reduction community can afford. Such a capability is essential for enabling many-query engineering tasks, real-time control and decision making, as well as digital twins in large-scale, real-world applications. This is achieved by a distributed algorithm that integrates high-performance computing into the data-driven reduced modeling procedure. Our algorithm enables the efficient and scalable processing of extremely large-scale datasets, and the learning of structured physics-based reduced models that approximate the dynamical systems underlying those datasets. We demonstrate its effectiveness using up to 1 024 processing units on the Frontera supercomputer at the Texas Advanced Computing Center. We focus on a real-world three-dimensional rotating detonation rocket engine simulation with more than 75 million degrees of freedom for which two milliseconds of simulated physical time necessitate six million core hours on more than 16 000 processing units on a supercomputer. We first demonstrate the strong and weak scalability of our distributed algorithm, as depicted in Figure 1. We then show that our method enables the preprocessing of the large training data set as well as the construction of a predictive physics-based data-driven reduced model in a mere four seconds on 1 024 processing units.

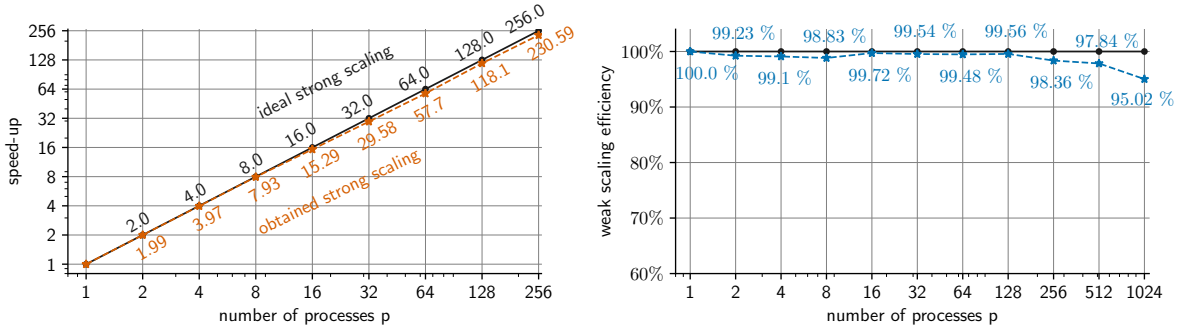

Figure 1: Scaling results performed on the Frontera supercomputer. The left figure plots the strong scaling speed up whereas the right figure plots the weak scaling efficiency of our distributed algorithm.

Stability Guarantees of Non-Intrusive Data-Driven Model Reduction for Nonlinear Systems

Tomok Koike[1] **and Elizabeth Qian**[1]

[1] *Georgia Institute of Technology*

In many-query computations, particularly those involving large-scale or highly complex models, the development of an efficient surrogate model is essential. This is especially true for real-time applications, such as control systems, which require high-efficiency computations across many queries. To address this requirement, we focus on constructing surrogate models using projection-based model reduction methods. These methods project the original system onto a reduced subspace, yielding reduced surrogate models. Through projection, the reduced models can inherit the stability properties of the original system, which are essential for system control. This inheritance, however, primarily applies to *intrusive* projection methods, where the model operators and underlying code are accessible. In contrast, many practical scenarios are *non-intrusive*, meaning the original model is unavailable. In these scenarios, non-intrusive methods have been developed to construct reduced surrogate models from empirical data. Unlike intrusive methods, non-intrusive ones do not directly project the original model onto the reduced subspace, thereby leaving the preservation of stability guarantees within the reduced models as an open question.

The *Lyapunov function* V is central to analyzing stability guarantees and synthesizing controllers for nonlinear systems. It provides a sufficient condition for stability if it satisfies the conditions: $V > 0$ and $\dot{V} < 0$. It also defines the domain of attraction, indicating the region under which the system states asymptotically converge to equilibrium. Although constructing Lyapunov functions analytically is feasible for low-dimensional ordinary differential equations, this task becomes considerably more challenging for large-scale systems governed by partial differential equations since identifying a function that fulfills stability conditions in these high-dimensional settings is difficult. While various methods for constructing Lyapunov functions for lower-dimensional systems exist, they are yet nontrivial to solve. For instance, Krasovskii's method requires solving a linear matrix inequality and approaches such as linear programming and sum-of-squares methods involve optimizations that are computationally intensive [1, 2]. Moreover, extending these methods to high-dimensional systems becomes impractical due to the curse of dimensionality.

In this presentation, we will introduce new work in developing Lyapunov functions for data-driven reduced models learned using the Operator Inference method [3]. The approach aims to provide stability guarantees for data-driven nonlinear reduced models. Additionally, we will demonstrate the method through various numerical examples.

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Data-driven Models of Nonautonomous Systems

Hannah Lu[1] **and Daniel M. Tartakovsky**[2]

[1]*Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[1]*Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[2]*Department of Energy Science and Engineering, Stanford University, Stanford, CA 94305, USA*

Nonautonomous dynamical systems are characterized by time-dependent inputs, which complicates the discovery of predictive models describing the spatiotemporal evolution of the state variables of quantities of interest from their temporal snapshots. When dynamic mode decomposition (DMD) is used to infer a linear model, this difficulty manifests itself in the need to approximate the time-dependent Koopman operators. Our approach is to approximate the original nonautonomous system with a modified system derived via a local parameterization of the time-dependent inputs. The modified system comprises a sequence of local parametric systems, which are subsequently approximated by a parametric surrogate model using the DRIPS (dimension reduction and interpolation in parameter space) framework[1]. The offline step of DRIPS relies on DMD to build a linear surrogate model, endowed with reduced-order bases for the observables mapped from training data. The online step interpolates on suitable manifolds to construct a sequence of iterative parametric surrogate models; the target/test parameter points on these manifolds are specified by a local parameterization of the test time-dependent inputs. We use numerical experimentation to demonstrate the robustness of our method[2] and compare its performance with that of deep neural networks.

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A novel approach for characterizing and enforcing stability of barycentric rational models in the AAA algorithm

Tommaso Bradde[1], **Ion Victor Gosea**[2], **and Stefano Grivet-Talocia**[1]

[1]*Dept. of Electronics and Telecommunications, Politecnico di Torino, Italy*
[2]*Max Planck Institute for Dynamics of Complex Technical Systems*

Rational approximation algorithms based on barycentric model structures are some of the methods of choice for learning Reduced-Order Models (ROMs) of large-scale Linear Time-Invariant (LTI) systems in non-intrusive, data-driven settings. In this work, we address the problem of characterizing and enforcing the asymptotic stability of a ROM with transfer function $\hat{H}(s)$ in barycentric form

$$\hat{H}(s) = \frac{N(s)}{D(s)} \in \mathbb{C}, \quad N(s) = \sum_{i=1}^{k} \frac{h_i w_i}{s - q_i}, \quad D(s) = \sum_{i=1}^{k} \frac{w_i}{s - q_i}, \quad D^*(s) = D(s^*), \quad w_i \neq 0 \; \forall i. \tag{1}$$

In the above, q_i, h_i are assumed to be fixed quantities, while the coefficients w_i (the so-called barycentric weights) are model unknowns, to be optimized so that $\hat{H}(s)$ matches samples of the underlying full-order system transfer function, according to a prescribed accuracy criterion, i.e., as in [3]. Our first result is deriving a set of novel algebraic conditions on the barycentric weights w_i's that characterize the stability of $\hat{H}(s)$. This characterization is obtained by proving that, under mild conditions, a ROM with transfer function $\hat{H}(s)$ is asymptotically stable if and only if the denominator $D(s)$ is an *Almost Strictly Positive-Real* (ASPR) transfer function [1], i.e., a transfer function that fulfills the requirement

$$\exists g \in \mathbb{R} : G(s) = \frac{D(s)}{1 + gD(s)} \quad \text{is Strictly Positive Real,} \tag{2}$$

see [2] for further details and proofs. Exploiting this fact, and defining a suitable state-space realization for $D(s)$, requirement (2) is translated into a set of non-convex algebraic constraints involving the unknowns w_i by means of the Positive Real Lemma [1], which provides the proposed characterization.

Our second contribution illustrates how to proficiently exploit the above results for performing reduced-order modeling with guaranteed stable ROMs. We present a constrained version of the AAA (Adaptive Antoulas-Anderson) algorithm [3], in which the unknowns optimization is forced to return solutions that allow the verification of (2), and thus generate stable ROMs. Applying an ad-hoc relaxation strategy, we show that the involved constrained optimization problem can be solved via semidefinite programming, by suitably weighting the linearized error function minimized by the standard AAA iteration. Furthermore, we propose an efficient extension of the resulting algorithm to the Multi-Input-Multi-Output (MIMO) case, and we test experimentally the efficiency and the reliability of the approach, by tackling model order reduction problems arising from different physical domains. Finally, we compare its performance with those of other state-of-the-art methods that use different types of strategies to enforce the stability of rational barycentric models.

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Parametric Reduced-Order Modeling via Low-Rank Barycentric Forms and the p-AAA Algorithm

L. Balicki[1] **and S. Gugercin**[1]

[1] *Department of Mathematics, Virginia Tech, Blacksburg, USA*

Rational approximation is a widely used tool for data-driven reduced-order modeling of linear dynamical systems. In recent years the adaptive Antoulas-Anderson (AAA) algorithm [1] has established itself as a successful method for computing rational approximations from a set of sampled data. Our recent work [2] introduced the p-AAA algorithm, extending the original AAA framework to multivariate rational functions, which allows for effectively capturing the dynamics of parameter-dependent systems. In p-AAA, rational approximations are represented via baryentric forms of the type

$$\widehat{\mathbf{H}}(s,p) = \left(\sum_{i=1}^{k}\sum_{j=1}^{q} \frac{\alpha_{ij}\mathbf{H}(\sigma_i,\pi_j)}{(s-\sigma_i)(p-\pi_j)}\right) \Bigg/ \left(\sum_{i=1}^{k}\sum_{j=1}^{q} \frac{\alpha_{ij}}{(s-\sigma_i)(p-\pi_j)}\right), \tag{1}$$

where $\mathbf{H}(\sigma_i,\pi_j)$ corresponds to transfer function data sampled from a high-fidelity model or real-world measurements. Aside from choosing suitable interpolation points (σ_i,π_j) via a greedy selection, the p-AAA algorithm determines the matrix of barycentric coefficients $\alpha \in \mathbb{C}^{k\times q}$ via a linear least-squares (LS) problem of the form

$$\min_{\|\alpha\|_{\mathrm{F}}=1} \|\mathbb{L}_2 \operatorname{vec}(\alpha)\|_2^2. \tag{2}$$

Solving the LS problem (2) is the dominant cost of p-AAA and is done via a singular value decomposition of the 2D Loewner matrix $\mathbb{L}_2 \in \mathbb{C}^{(d-kq)\times kq}$ where d corresponds to the number of available samples. This problem becomes computationally demanding when the underlying system depend on many more parameters. In this case the barycentric coefficients form a tensor in $\mathbb{C}^{k\times q\times z\times\cdots}$ and solving the corresponding LS problem often becomes impractical. To overcome these shortcomings, we introduce a new barycentric form which uses low-rank matrix and tensor decompositions to implicitly store the barycentric coefficients. For $\widehat{\mathbf{H}}$ in (1) we use the factorization $\alpha = \beta\gamma^\top$ where $\beta \in \mathbb{C}^{k\times r}$, $\gamma \in \mathbb{C}^{q\times r}$ and $r \ll \min(k,q)$. We show that in this case the p-AAA objective function can be written as

$$\|\mathbb{L}_2 \operatorname{vec}(\alpha)\|_2^2 = \|\mathbb{L}_\gamma \operatorname{vec}(\beta)\|_2^2 = \|\mathbb{L}_\beta \operatorname{vec}(\gamma)\|_2^2,$$

where $\mathbb{L}_\gamma \in \mathbb{C}^{(d-kq)\times kr}$ and $\mathbb{L}_\beta \in \mathbb{C}^{(d-kq)\times qr}$. This connection allows for leveraging an alternating LS (ALS) procedure to compute α in an iterative manner. Our ALS approach is particularly appealing when moving to systems with many parameters. In this case the complexity of computing α reduces to $\mathcal{O}(dr^2(k^2+q^2+z^2+\cdots))$ as opposed to $\mathcal{O}(dk^2q^2z^2\cdots)$ for the original p-AAA LS problem. We demonstrate the effectiveness of our proposed approach via various numerical experiments. Aside from discussing practical aspects of our method, we establish theoretical connections to separable function approximation. In particular, we establish conditions for the underlying dynamical system under which our proposed method is particularly effective.

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Optimal H_2 Approximation from Time-Domain Data

M. S. Ackermann[1] **and S. Gugercin**[1]

[1] *Department of Mathematics, Virginia Tech, Blacksburg, 24061, VA, United States*

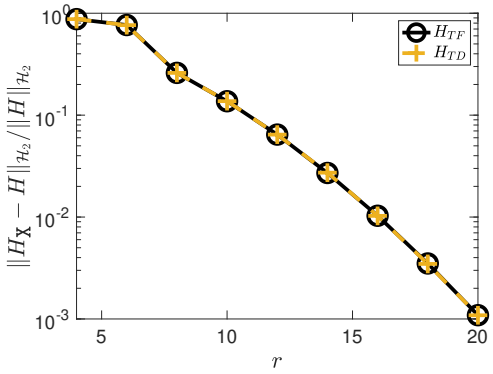
We consider the optimal $\mathcal{H}_2$ approximation of a discrete-time, single-input single-output system

$$\mathbf{x}[k+1] = \mathbf{A}\mathbf{x}[k] + \mathbf{b}u[k]; \quad y[k+1] = \mathbf{c}^\top \mathbf{x}[k] \quad \text{with transfer function} \quad H(z) = \mathbf{c}^\top (z\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}, \quad (1)$$

where $\mathbf{x}[k] \in \mathbb{R}^n$, $u[k] \in \mathbb{R}$, and $y[k] \in \mathbb{R}$ are, respectively, the states, input, and output at time k; $\mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{b} \in \mathbb{R}^n$, and $\mathbf{c} \in \mathbb{R}^n$. Even though we explicitly write the state-space matrices in (1), in this work, we will *never* assume access to the model, but only to *time-domain input-output data*

$$\mathbb{U} = [u[0] \ \dots \ u[T]] \in \mathbb{R}^{T+1} \quad \text{and} \quad \mathbb{Y} = [y[0] \ \dots \ y[T]] \in \mathbb{R}^{T+1}. \quad (2)$$

Given the input/output data (2), our goal is to construct a data-driven reduced-order model (DDROM) with form as in (1) but with the reduced quantities $\mathbf{A}_r \in \mathbb{R}^{r\times r}, \mathbf{b}_r \in \mathbb{R}^r$, and $\mathbf{c}_r \in \mathbb{R}^r$ with $r \ll n$, to minimize the $\mathcal{H}_2$ distance $\|H - H_r\|^2_{\mathcal{H}_2} = \frac{1}{2\pi}\int_{-\pi}^{\pi} |H(e^{\mathbf{i}\omega}) - H_r(e^{\mathbf{i}\omega})|^2 d\omega$.
The Realization independent Iterative Rational Krylov Algorithm (TF-IRKA) [2] constructs $\mathcal{H}_2$ optimal DDROMs from transfer function data $H(\sigma)$ and $H'(\sigma)$. However, it requires repeated evaluations of $H(z)$ and $H'(z)$ at a priori unknown points. Such information may not be feasible to obtain during the iteration or we may only have time-domain data (2).



In our recent work [1] based on [3], we developed a robust framework, complete with an error indicator, for recovering $H(\sigma)$ and $H'(\sigma)$ from purely time-domain data (2). This approach requires solving two linear systems with Hankel-like structure that also involve powers of σ, i.e., σ^k for $k = 1, \dots, N$ where N is usually large. The work [1] only considered σ on the unit disc, which prevented the powers of σ from causing further ill-conditioning. However, the $\mathcal{H}_2$ optimal modeling problem requires evaluating H and H' outside the disk, leading to extremely ill-conditioned linear systems to solve in the framework of [1].
In this work, we first develop the theory on how to optimally scale these linear systems so that recovery of $H(\sigma)$ for $|\sigma| > 1$ is computationally feasible. We directly connect conditioning of these linear systems to the properties of the underlying dynamics. These considerations then lead to a time-domain variant of TF-IRKA which produces (nearly) $\mathcal{H}_2$ optimal DDROMs from a single time-domain simulation. We illustrate the effectiveness of TD-IRKA on several numerical examples. One such result for a linear advection model is depicted in the figure above showing the relative $\mathcal{H}_2$ error vs reduced order, due to TF-IRKA (using exact evaluations of $H(\sigma)$ and $H'(\sigma)$) and TD-IRKA (using only single time-domain simulation). The figure shows that TD-IRKA almost exactly replicates the performance of TF-IRKA.

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Model reduction for parametrized aerodynamics problems: error estimation, adaptivity, and nonlinear approximations

Masayuki Yano[1]

[1] *University of Toronto*

We consider projection-based model reduction of parametrized nonlinear partial differential equations (PDEs) with applications to large-scale aerodynamics problems. Our emphasis is on transonic flows with parameter-dependent shocks, which induce a parametric solution manifold with slowly decaying Kolmogorov n-width and hence is not amenable to linear model reduction. The key ingredients of our nonlinear model reduction formulation are as follows: an adaptive high-order discontinuous Galerkin (DG) method, which provides stable solution of convection-dominated problems while efficiently controlling the full-order model (FOM) discretization error; nonlinear reduced approximation spaces, which incorporate geometrically transformed solution snapshots to effect rapid approximation of parametric solution manifolds with slowly decaying Kolmogorov n-width; the dual-weighted residual (DWR) method, which provides effective error estimates for quantities of interest in both the FOM and reduced-order model approximations; the empirical quadrature procedure (EQP), which identifies point-wise reduced quadrature rules to enable efficient hyperreduction of high-order DG discretizations; and a spatio-parameter adaptive greedy algorithm, which simultaneously trains the DG spaces, nonlinear reduced approximation spaces, and reduced quadrature rules to meet the user-specified output error tolerance in a fully automated manner.

We demonstrate the efficacy and versatility of the framework using parametrized aerodynamics problems governed by the Euler and Reynolds-averaged Navier-Stokes (RANS) equations in two and three dimensions. We consider the following applications: flight parameter sweep, where we demonstrate that the formulation provides efficient offline training and online speedup of several of orders of magnitude; uncertainty quantification (UQ) of RANS turbulence model, where we employ greedy algorithm with adaptively enriched training set to address UQ problems with many parameters; aerodynamic shape optimization, where we incorporate a trust-region method informed by DWR error estimate to accelerate optimization on the fly; and data assimilation, where we accelerate ensemble-based state estimation on the fly.

3.4 Thursday, September 12

Nonlinear model reduction for high- and low-consequence applications

Kevin Carlberg[1,2]

[1] *University of Washington*
[2] *AI at Meta*

Model reduction has become a widely used tool for reducing the dimensionality and complexity of simulating large-scale nonlinear dynamical systems across a wide range of problems. However, the requirements of the application of interest have a profound implication on the proper way to approach model reduction.

This talk will cover nonlinear model reduction for two vastly different application areas:

1. *High-consequence* many-query engineering applications characterized by extreme-scale parameterized initial value problems; and

2. *Low-consequence* real-time virtual-interaction applications characterized by free-form hand interactions with geometrically complex deformable objects.

The first application imposes the following demands on reduced-order models: (1) *accuracy* as measured in quantities of interest over the parameter domain, (2) *low cost* to enable simulation at many parameter instances using large-scale computing resources, (3) *certification* in the form of error/uncertainty quantification, and (4) *reliability* in the form of error/uncertainty control. The talk will briefly cover several methodological approaches to deliver these capabilities with a focus on finite-volume simulations, including nonlinear-manifold kinematic approximation [5], structure preservating projection [6], error modeling [7], and *a posteriori* adaptivity [1, 4].

The second application imposes the following demands: (1) *accuracy* as measured by human perception and enjoyment of the interaction, and (2) *low cost* to enable real-time simulation on virtual reality headsets. Certification and reliability are not important in such cases. The talk will introduce a new software package for enabling real-time virtual interactions with deformable objects as well as nonlinear model-reduction techniques that leverage implicit neural representations [2, 3] and contact awareness [8] that are tailored to this problem.

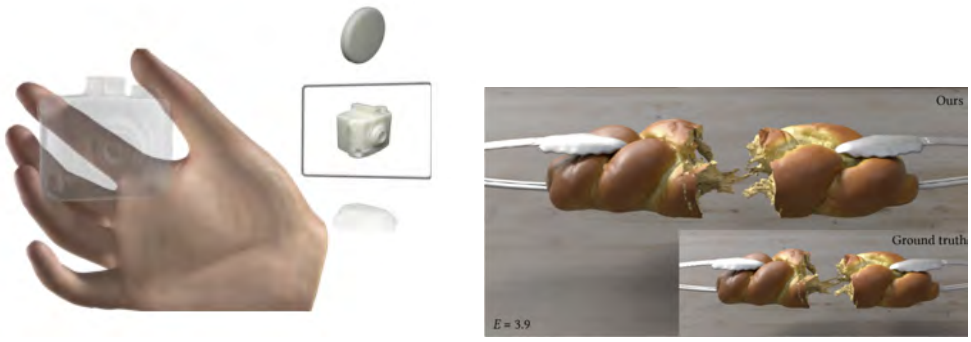

Figure 1: Model reduction applied to low-consequence virtual interactions

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CoLoRA: Continuous low-rank adaptation for reduced implicit neural modeling of parameterized partial differential equations

Jules Berman[1] **and Benjamin Peherstorfer**[1]

[1] *Courant Institute of Mathematical Sciences, New York University, New York, NY 10012*

This work introduces reduced models based on Continuous Low Rank Adaptation (CoLoRA) [1] that pre-train neural networks for a given partial differential equation and then continuously adapt low-rank weights in time to rapidly predict the evolution of solution fields at new physics parameters and new initial conditions. CoLoRA provides nonlinear parameterizations that circumvent the Kolmogorov barrier of transport-dominated problems and provide orders of magnitude speedups compared to full models.

CoLoRA is a sequential-in-time (online adaptive) method that adapts nonlinear representations in time. In contrast to dynamic low-rank methods, CoLoRA applies low-rank updates to the weight matrices of multi-layer neural networks. The multi-layer structure greatly reduces the number of online parameters that have to be updated while maintaining high expressiveness, which is key to achieving online speedups. In addition, having network weights that depend on time allows one to combine CoLoRA with variational approaches [2] to obtain reduced solutions that are Galerkin-optimal. This opens the door to analyses, error bounds, and goes far beyond purely data-driven forecasting. In particular, we show that variational approaches with CoLoRA can be formulated so that they preserve physical quantities such as mass, momentum, and energy.

Numerical experiments show that CoLoRA requires a low number of training trajectories, which makes it well suited for scarce data applications. CoLoRA achieves orders of magnitude speedups compared to classical full models and outperforms existing state-of-the-art neural-network-based model reduction methods such as operator learning in parameter count and accuracy in our experiments.

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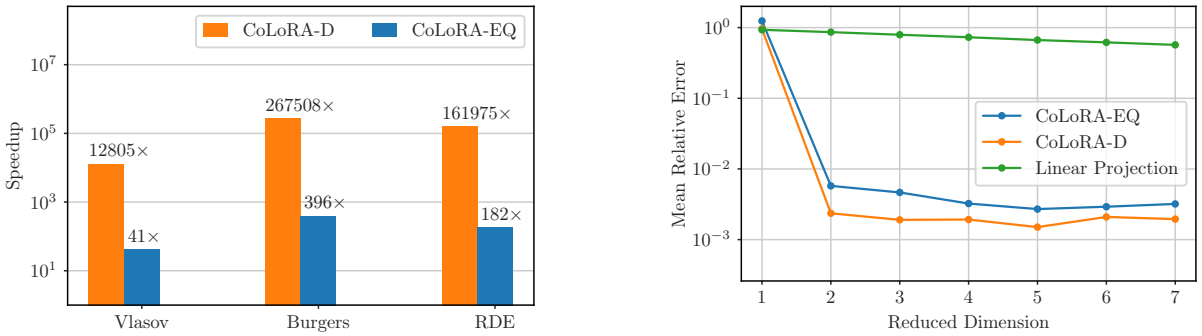

Figure 1: **Left**: Purely data-driven CoLoRA (CoLoRA-D) is more than four orders of magnitude faster than full models. If the governing equation is solved in a Galerkin-optimal variational sense (CoLoRA-EQ), we obtain about two orders of magnitude speedups. **Right**: CoLoRA models achieve orders of magnitude lower errors than linear model reduction methods. Details in [1].

Time-evolving neural network representations for the reduced order modelling of parametrised PDEs

Mariella Kast[1] **and Jan S. Hesthaven**[1]

[1] *EPFL - Ecole Polytechnique Federale de Lausanne, Switzerland*

Neural networks have emerged as usefool tools for reduced order modelling of parametrized partial differential equations (PDEs) since they offer universal function approximation and efficient treatment of high-dimensional inputs. Evolutional deep neural networks (EDNNs) [1] represent the PDE solution as the output of a neural network and and use a time-stepping scheme based on the PDE residual to evolve the network parameters. Based on the paradigm of EDNNs, we develop a novel method to efficiently solve parametric time-dependent PDEs, which obtains the solution for all parameter instances from a single time-integration and does not require training data from a high fidelity solver. This creates a promising surrogate model for use in many-query applications such as uncertainty quantification, inverse problems and optimisation, especially in cases where reduced bases methods fail to obtain efficient surrogates.

We particularly focus on extending EDNNs for problems of realistic complexity, by using positional embeddings that can encode domains with geometrical features and automatically enforce Dirchlet, Neumann and periodic boundary conditions on the predicted PDE solution fields [2]. Connections between the eigenfunctions of the Laplace Beltrami operator and Fourier Features are drawn to explain the success of the positional embedding layer.

As EDNNs are nonlinear models, the PDE dynamics are projected onto the tangent space of the neural network at each time step, which requires the solution of a dense, and possibly ill-conditioned, linear system. We argue that the Krylov solver LSMR is especially suited for this task as it avoids explicit assembly of Jaccobians and enables scaling to larger neural networks and thus more complex problems. We further propose a modified linearly implicit Rosenbrock method, which significantly alleviates the time step requirements of stiff PDEs. We also showcase how automatically encoding invariants into the neural network can simplify the loss terms and therefore speed up the learning process, which can also be exploited in the training of physics informed neural networks (PINNs).

We showcase our method on the Korteweg-de Vries equation, and several parametrized PDEs, including a nonlinear heat equation, advection-diffusion problems on domains with holes and 2D Navier Stokes flow. We particularly highlight the challenges in balancing accuracy and computational time and why EDNNs are promising surrogate models for parametrized PDEs with slow decaying Kolmogorov n-width.

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A Generative Probabilistic Transformer Model for Ionospheric Prediction

D. Alford-Lago[1,2,3], C. Curtis[2], A. Ihler[3], and D. Drob[4]

[1] *Naval Information Warfare Center Pacific, Atmospheric Propagation Branch*
[2] *San Diego State University, Department of Mathematics and Statistics*
[3] *University of California Irvine, Department of Computer Science*
[4] *Naval Research Laboratory, Space Science Division*

The Earth's ionosphere provides a medium for reliably transmitting radio waves far beyond the horizon. However, it is a highly variable environment, so the development and operation of many radio communications and radar systems that utilize the ionospheric channel require accurate forecasting of the prevailing space weather conditions. We propose a new model for forecasting key ionospheric parameters based on a modern deep learning architecture, the transformer [2]. Although transformers were initially motivated by natural language processing (NLP), their flexibility and efficiency in processing sequential data make them prime candidates for time series prediction.

Current state-of-the-art ionospheric forecast models are categorized roughly as physics-based or empirical. Many physics models, such as SAMI3 [1], solve the ion and electron continuity and momentum equations and allow for highly accurate nowcast and hindcast when parameterized with good initial and boundary conditions. However, the ionosphere is a damped, driven system, so without knowledge of the geomagnetic and solar drivers, the forecast skill often drops precipitously over relatively short time windows. Additionally, the simulations themselves come with a high computational cost. On the other hand, empirical ionospheric models are usually much cheaper to run, and the forecast horizon may be much longer, since many conventional models like IRI combine mode decompositions and Fourier analysis to generate stable, time-evolving models of the ionosphere. Nevertheless, the predictions are limited to merely point forecasts of the statistical average.

To address these limitations, we developed a transformer-based model that generates forecasts in a single step rather than sequentially. Moreover, instead of predicting a discrete time series, it predicts distributions for the parameter of interest at each forecast time step. These learned probability densities are generated from prior observations of the data and relevant geomagnetic and solar indices. The attention mechanism of the transformer enables the model to dynamically weigh these inputs when generating a forecast. Additionally, the model embedding layers learn predictive latent features from the data that may not be captured in the canonical physical equations or are lost in the statistical averaging of the empirical climatological models. We demonstrate these results with a model trained on twenty-three years of ionospheric observations from around the globe, establishing its ability to generalize to different geographic locations as a surrogate for larger computational models.

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Time Stepping in DMD via Machine Learning

Christopher W. Curtis[1], Daniel Jay Alford-Lago[1,2], Alexander Ihler[3], and Erik Bollt[4]

[1]Dept. of Mathematics and Statistics, SDSU
[2]Naval Information Warfare Center
[3]Dept. of Computer Science, UC Irvine
[4]Dept. of Electrical and Computer Engineering, Clarkson University

Dynamic Mode Decomposition (DMD) plays a significant role in reduced order modeling (ROM), where it provides a non-intrusive means of identifying fundamental modes and time scales which can facillitate parametric exploration and uncertainty quantification. However, the problem of using DMD based approaches for time stepping time-series from initial data is challenging due to the dilemma of proper observable choices. Adressing this issue should be of use across problems domains where DMD is used in ROM or surrogate modeling contexts. We thus present a neural-network based autoencoding method, [1, 2], which when coupled to an adaptive Hankel DMD approach allows for learning models which are able to accurately forecast chaotic time series. The method relies on three key innovations. The first is a choice of loss-function in our machine learning algorithm which ensures both the one-step convergence and global stability of our DMD based forecasts. The second is a global approximation to the Koopman operator. The third is an epoch by epoch adaptation of the window size in a Hankel DMD method which allows the machine to learn optimal numbers of encoded observables. We explore our method over the Lorenz-63, Rossler, and Kuramoto–Sivashinksy equations, where we see excellent performance at reconstruction and even the potential for generating ARIMA like forecasts. We also explore using a transfer-entropy like measurement to characterize the encoding process over different strange attractors.

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Accelerating phase field simulations through time extrapolation with Adaptive Fourier Neural Operators and U-Nets

Christophe Bonneville[1], **Arun Hegde**[1], **Cosmin Safta**[1], **and Habib Najm**[1]

[1]*Sandia National Laboratories, Livermore CA*

Computational simulation of phase field dynamics can be prohibitively expensive when using standard numerical solvers. For example, high-fidelity simulations often use very small time steps due to stability considerations, which can become a bottleneck when the target quantities of interest require predictions far out in time. To address this challenge, we employ machine learning-based surrogate models to help predict key dynamics forward in time, enabling predictions at time horizons far beyond what is achievable through traditional methods alone. Specifically, we investigate a combination of two popular deep learning architectures: a special kind of vision transformers, namely Adaptive Fourier Neural Operators (AFNO) [2], and U-Nets [3]. We train them to predict future states with much coarser time steps − thus encapsulating multiple high-fidelity steps within a single surrogate evaluation. While this approach enables more rapid predictions through autoregressive evaluation of the surrogate, the incurred error is essentially uncontrolled. To alleviate this, we adopt a hybrid prediction strategy which alternates between surrogate evaluations − which leap forward in time − and high fidelity simulation steps − which reduce errors and bring the system state back to the solution manifold. Moreover, we show that including periodic retraining or online fine-tuning can provide further control on the error growth. We illustrate these methods on two examples, a Cahn-Hilliard toy-problem and a chaotic liquid-metal dealloying problem [1].

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Efficient linear Model Order Reduction for Friedrichs' systems

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

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

In this contribution we discuss the class of parametrized linear Friedrichs' systems [1] i.e. operators of the form

$$\mathcal{A}_\mu u := \sum_{i=1}^{d} A_\mu^i \frac{\partial u}{\partial x_i} + C_\mu u, \qquad A_\mu^i \in [L^\infty(\Omega)]^{m\times m}_{sym},$$

and the corresponding problems $\mathcal{A}_\mu u = f$. Many classic partial differential equations (PDEs) can be rewritten in this form, for example diffusion problems, linear advection, linear elasticity, the curl-curl problem etc. In particular, we are interested in the approximability (in the sense of Kolmogorov) of their solution set. While under certain conditions an exponential decrease of the Kolomogorov N-width (i.e. good approximability) is known for diffusion problems, slowly decreasing lower bounds have been shown for e.g. parametrized advection fields [2]. We do not aim to tackle the latter problem (here, one should consider nonlinear approaches, see e.g. [4]) but instead aim to identify the subclass of *linearly approximable* Friedrichs' systems.

Using the theory of optimal test functions, we derive conditions on $\mathcal{A}_\mu$ under which solutions to Friedrichs' systems can be exponentially approximated [3]. In addition to the known results for diffusion problems we obtain theoretical justification to apply linear reduction techniques to e.g. advection-reaction problems with prescribed velocity field $\vec{b} \neq \vec{b}_\mu$ and parametrized reaction or the curl-curl problem with parametrized premeability and permittivity. Numerical experiments using a greedy-type algorithm confirm an exponential decay of the approximation error. For problems with spatially strongly varying data functions a localized model order reduction approach based on solving local problems with randomized boundary information (localized training) will also be discussed.

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Implicit Neural Representation Meets Interpretable Parameterized Reduced-Order Modeling

Weichao Li[1] **and Shaowu Pan**[1]

[1]*Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180*

Learning interpretable reduced-order models of nonlinear PDE dynamics has been a long-standing problem in data-driven modeling of dynamical systems. Early works can be traced back to Operator Inference, Sparse Identification of Nonlinear Dynamics (SINDy), and SINDy-Autoencoder, among others. However, these approaches still suffer from scalability issues in scalable nonlinear dimensionality reduction. On the other hand, novel dimensionality reduction frameworks that leverage implicit neural representation, such as Neural Implicit Flow, show great promise for scalable 3D PDE data, even on dynamic meshes. Here, we propose a novel framework combining the idea of implicit neural representation with learning interpretable nonlinear dynamics from data. We compare our framework against state-of-the-art operator learning techniques (e.g., FNO) and a recent related work called DINo that leverages a vanilla feedforward neural network to learn the nonlinear latent dynamics. Furthermore, we extend our interpretable reduced-order learning framework to a parametric setting. Our testing cases range from forced 2D Navier-Stokes equations to incompressible flow over a 2D cylinder.

Transformer accurately predicts outputs of parametric dynamical systems with time-varying external inputs

L. Feng[1] **and P. Benner**[1,2]

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
[2] *Fakultät für Mathematik, Otto-von-Guericke-Universität Magdeburg, Germany*

With the capability of modern computers for processing large amounts of data, machine learning (ML) is being more and more applied in computational science. Dynamics of large-scale systems are being learned by neural networks as a new kind of surrogate models. Many of the ML learning methods aim to accurately predict the whole solution vector, for which autoencoders are often used to first compress the data of the solution trajectories into a latent space with much lower dimension. Different data-driven methods are then used to learn the dynamics in the latent space [1]. Most of these works consider dynamical systems without external time-varying input signal. There are a few works on predicting only the quantities of interests (QoIs) or outputs using ML [3] without data compression. There, long-short-term-memory (LSTM) is used to predict the parametric outputs changing with external input signals. However, LSTM is known to suffer from long-term predictions.
Transformer models have been proposed to overcome the difficulties of recurrent neural networks, such as LSTM, for long-term prediction. Many transformer models have been suggested for time series forecast [4]. Most of the transformer models are applied to predict daily life activities, such as customer electricity usage, traffic road occupancy rate, etc. In this work, we explore the promising performance of a transformer model: temporal fusion transformer (TFT) [2] on predicting outputs of parametric dynamical systems with external time-varying input signals. It is shown in [2] that TFT is accurate in long-term (multi-horizon) prediction of time series dependent on a complex mix of inputs, including time-invariant (static) covariates, known future inputs, and time series that are only observed in the past. The TFT model was used to predict the electricity usage, the traffic flow, etc., in a future time period [2]. Translating these terminologies into those in system theory, we expect that the TFT model should be able to do prediction of the outputs in both parameter and time domain. Based on this understanding of TFT, we have successfully applied it to three parametric dynamical systems, including systems with both physical/geometrical parameters and external input signals.

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Enhancing ROM with DL for the efficient solution of parametric PDEs: applications and perspectives

Gianluigi Rozza[1]

[1] *SISSA, International School for Advanced Studies, Mathematics Area, mathLab, Trieste, Italy*

Parametric Partial Differential Equations (PDEs) serve as indispensable tools in modeling physical phenomena, finding applications across academic research and industrial sectors. However, the analytical solutions for these equations are limited in scope, leaving the majority necessitating computationally intensive numerical approximations. These approximations, while effective, often prove impractical for scenarios requiring rapid computations, as in industry. Consequently, Reduced Order Models (ROMs) have emerged as a promising avenue within computational sciences, offering streamlined computational frameworks for real-time simulations. Deep Learning algorithms have played a pivotal role in advancing efficient ROM methods, characterized by their exceptional generalization capabilities and reduced computational overhead. In this talk, we delve into the synergies between classical ROM techniques and deep learning methodologies, exploring how the integration of the latter can elevate the former. Our discussion spans innovative approaches aimed at addressing longstanding challenges associated with ROMs, such as the curse of dimensionality, linearity constraints, and the abundance of data required for constructing robust ROMs. By leveraging the power of deep learning, we aim to not only enhance the performance of existing ROM frameworks but also pave the way for novel applications and advancements in computational modeling and simulation. Work in collaboration with Dario Coscia, Nicola Demo, Guglielmo Padula, Niccoló Tonicello, Federico Pichi, Moaad Khamlich at SISSA mathLab group

Certification of physics-informed neural networks for the solution of parameterized partial differential equations

L. Ernst[1] **and K. Urban**[1]

[1]*Institute for Numerical Mathematics, Ulm University, Germany*

Parameterized partial differential equations (PPDEs)

$$u \in \mathcal{X}: \quad F_\mu(u_\mu) = 0 \quad \text{in } \mathcal{Y}',\ \mu \in \mathcal{P} \subset \mathbb{R}^p \tag{1}$$

arise to describe linear and nonlinear physical phenomena. Here, $(\mathcal{X}, \|\cdot\|_\mathcal{X}), (\mathcal{Y}, \|\cdot\|_\mathcal{Y})$ are Banach spaces, $(\mathcal{Y}', \|\cdot\|_{\mathcal{Y}'})$ is the dual space of $\mathcal{Y}$ and $F_\mu \in C(\mathcal{X}, \mathcal{Y}')$ is a continuous function. 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.
The recent success in solving various PPDEs with neural networks, particularly with physics-informed NNs (PINNs) (see e.g. [3], [1], [4]) suggests that they are a natural candidate for nonlinear model order reduction techniques. Even though the range of PDEs that can be approximated seemingly well by PINNs is quite impressive, a rigorous a posteriori error control is at least not straightforward.
Classical PINNs are usually trained with loss functions based upon the pointwise residual. The advantage of this is, that the method is meshfree, although it makes the error control difficult due to the fact that a error-residual relation of the form

$$c\|F_\mu(u_\mu^\delta)\|_{\mathcal{Y}'} \leq \|u_\mu - u_\mu^\delta\|_\mathcal{X} \leq C\|F_\mu(u_\mu^\delta)\|_{\mathcal{Y}'}$$

is only available if the problem (1) is well-posed. Therefore, the goal of our work is to certify PINN approximations for linear and nonlinear PPDEs while preserving their broad applicability and keeping the additional cost of discretizing the underlying physical domain $\Omega \subset \mathbb{R}^d$ low. Given a trained PINN Φ_μ approximating the solution $u : \mathcal{P} \times \Omega \to \mathbb{R}$ of a PPDE, we imbed the domain Ω into a simple shaped domain $\square$ and construct a computable upper bound $\eta(F_\mu(\Phi_\mu))$ such that

$$\|u_\mu - \Phi_\mu\|_\mathcal{X} \leq C \cdot \eta(F_\mu(\Phi_\mu)).$$

The advantage of this ansatz is, that discretizing $\square$ is straightforward. Further, to evaluate η we use Riesz-representations if $\mathcal{Y}$ is a Hilbert space and wavelet-methods as proposed in [2] in the case of a Banach space. The evaluation is efficient due to the simple shape of the domain.

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Kernel-based Greedy Collocation Schemes for Approximation of High-Dimensional PDE Boundary Value Problems

B. Haasdonk[1], T. Wenzel[2], G. Santin[3], and D. Winkle[4]

[1]*Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*
[2]*Department of Mathematics, University of Hamburg*
[3]*Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice*
[4]*Institute of Stochastics and Applications, University of Stuttgart*

We consider general linear PDE boundary value problems in the strong form on arbitrary bounded Lipschitz-domains. For such problems, we recently presented a scale of meshless greedy kernel-based collocation techniques [5]. The approximation spaces are incrementally constructed by carefully collecting Riesz-representers of (derivative operator) point-evaluation functionals. The approximants are obtained by generalized interpolation [3, Chap. 16]. The scale of methods naturally generalizes existing approaches of PDE approximation [2] as well as function approximation techniques [1, 4]. Assuming well-posedness and a stability estimate of the given PDE-problem, we can rigorously prove convergence rates of the resulting approximation schemes [5]. Interestingly, those rates show that it is possible to break the curse of dimensionality and potentially reach high input dimensions. For cases with polygonal domains in small input space dimensions the schemes allow experimental comparison with, e.g., standard finite element methods. The strength of the procedure, however, is the ease of treating high-dimensional input space dimensions due to the mesh-independence and ommitting spatial integrals. We present numerical experiments demonstrating these aspects. When considering additional parametric inputs, the overall procedure can be interpreted as an a-priori model reduction approach.

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Predictive digital twins of civil engineering structures

M. Tezzele[1], M. Torzoni[2], S. Mariani[2], A. Manzoni[2], and K. E. Willcox[1]

[1] *University of Texas at Austin*
[2] *Politecnico di Milano*

In this talk, I will present a digital twin (DT) formulation for the structural health monitoring of civil engineering structures [1], with a focus on railway bridges. A DT is a virtualization of a physical asset built upon a set of computational models that dynamically update to persistently mirror a unique asset of interest throughout its operational lifespan, enabling informed decisions that realize value.

The talk covers the health monitoring, predictive maintenance, and management planning of civil structures. The asset-twin coupled dynamical system is encoded using a probabilistic graphical model (PGM) [2] which provides a general framework for data assimilation, state estimation, prediction, planning, and learning while accounting for the associated uncertainty. The assimilation of high-dimensional multivariate time series describing the vibration response is carried out by exploiting physics-based reduced order methods and deep learning models. The numerical models allow automated selection and extraction of optimized damage-sensitive features and real-time assessment of the structural state of a bridge.

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A stochastic convolutional SPOD-Koopman reduced order model for turbulent flow data

T. Chu[1] **and O. T. Schmidt**[1]

[1] *Dept. of MAE, University of California San Diego, La Jolla, CA, USA*

We introduce a stochastic reduced-order model for modeling turbulent flows, leveraging Koopman theory and Spectral Proper Orthogonal Decomposition (SPOD). This data-driven approach, not reliant on governing equations, utilizes Koopman analysis on time-delay observables, specifically SPOD coefficients, for linear dynamics, and models nonlinear interactions as time-invariant forcing. The model is validated through Monte Carlo simulations and applied to various turbulent experimental and numerical fluid dynamics data, demonstrating its ability to accurately reproduce the dynamics and statistics of turbulent flows.

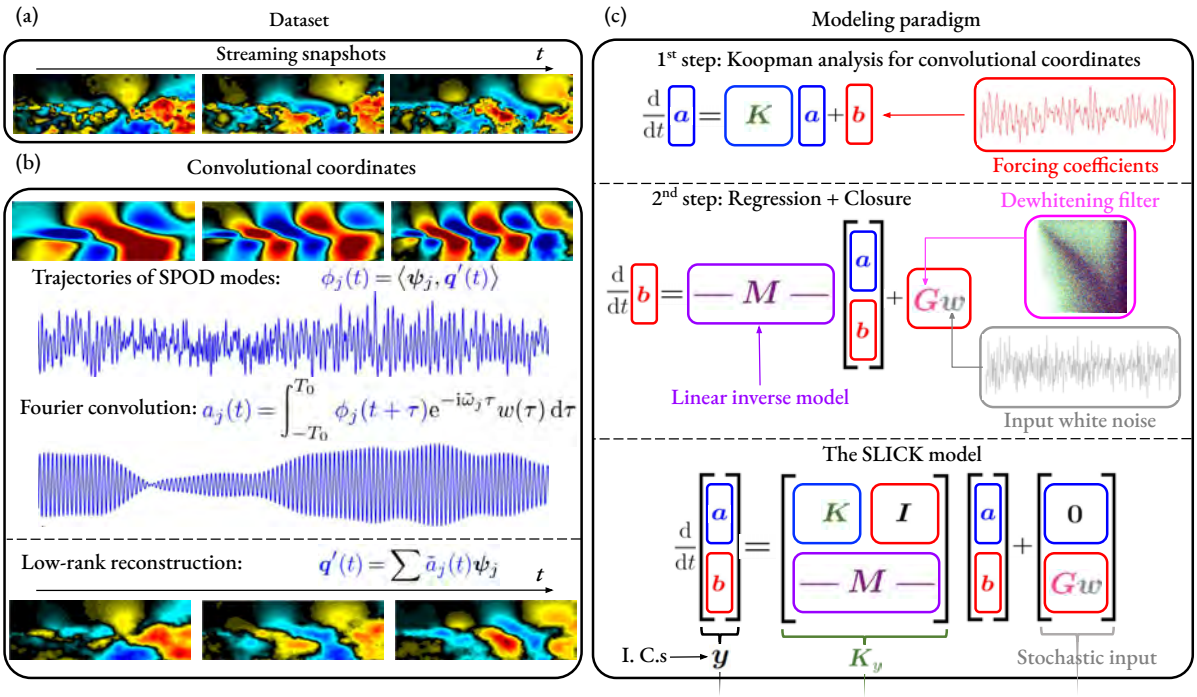

Figure 1: Schematic of the stochastic ROM: (a) snapshot data; (b) model-order reduction and Fourier convolution; (c) training phase. The example is experimental particle image velocimetry data of an open cavity flow.

The SPOD basis decomposes the flow into energy-ranked structures that evolve coherently in both space and time, optimally capturing the flow's second-order statistics and dynamically significant features. A significant aspect of the model is its stochastic closure, which addresses the residual error inherent in the finite-dimensional approximation of turbulent dynamics. This closure models the residue as a stochastic source, incorporating a dewhitening filter informed by the data to maintain second-order flow statistics. The model employs the two-step process illustrated in Fig. 1: Koopman analysis for linear dynamics and a regression-based method with a closure model for nonlinear interactions, effectively capturing the essential features of turbulence for forecasting.

Model reduction for linear systems using SPOD modes

Peter Frame[1], **Cong Lin**[2], **Oliver Schmidt**[2], **and Aaron Towne**[1]

[1] *University of Michigan, Department of Mechanical Engineering*
[2] *University of California, San Diego, Department of Mechanical and Aerospace Egineering*

Most model reduction methods employ the following two-step strategy: first, they find a compressed representation of the state of the system at a particular time, then they obtain equations that evolve the reduced set of variables that encode the state in this representation in time. Examples of the first step include representing the state using proper orthogonal decomposition (POD) modes, balanced truncation modes [2], or an autoencoder, and examples of the second step include Galerkin and Petrov-Galerkin projection of the governing equations, and machine learning techniques to learn the dynamics in the reduced set of variables.

In this work, we explore a different strategy and apply it to forced linear dynamical systems. Instead of using a compact representation of the state, we use a compact representation of the entire trajectory of the state over some time interval $[0, T]$ using a basis of modes that are functions of both space and time. In particular, we use spectral POD (SPOD) modes, which both have analytic properties that make them suitable for model reduction, and are known to provide an accurate representation of trajectores using relatively few coefficients [1]. In fact, with the SPOD basis, the trajectory of a system can be represented substantially more accurately with the same total number of coefficients than it can if the coefficients pertain to a space-only basis, e.g., POD modes. Thus, if the coefficients that encode the trajectory in the SPOD basis can be obtained accurately, the trajectory they represent will be more accurate than any trajectory representable by the same number of POD coefficients. The goal of the proposed method is therefore to solve accurately, and in a reduced manner, for the SPOD coefficients given the forcing and initial condition.

The method works as follows. The SPOD coefficients at a particular frequency are given by the Fourier transform of the state at that frequency multiplied on the left but the transpose of the SPOD modes. We derive an analytic expression for Fourier transform of the state as a linear function of the initial condition and forcing. By multiplying this expression of the left by the transpose of the modes, we obtain an expression for the SPOD mode coefficients. Crucially, the linear operators involved can be precomputed, leaving only small matrix-vector multiplications to be done online.

We demonstrate the method's accuracy and CPU time on two examples: a linearized Ginzburg-Landau system, and an advection-diffusion problem. In both cases, the proposed method achieves roughly two orders of magnitude lower error than both POD-Galerkin and balanced truncation applied to the same problem. In fact, the proposed method achieves substantially lower error than the projection of the solution onto the POD modes, which itself is a lower bound on the error for any Petrov-Galerkin method with the same number of modes. The method is also comparable to POD-Galerkin and balanced truncation in terms of CPU time, as we show it should be from scaling analysis. We hope that the orders-of-magnitude accuracy improvement over balanced truncation, the standard method for linear model reduction, will both prove useful in applications and increase interest in space-time model reduction methods.

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Mori-Zwanzig formalism, Wiener projections, and random dynamics

Kevin K. Lin[1] **and Fei Lu**[2]

[1]*Department of Mathematics, University of Arizona*
[2]*Department of Mathematics, Johns Hopkins University*

In the absence of sharp timescale separation, reduced models of many-degree-of-freedom dynamical systems can exhibit both memory and noise effects. The Mori-Zwanzig projection operator formalism, originally developed by statistical physicists, has been found useful for capturing the effect of memory and noise on steady-state statistics, including a variety of deterministic chaotic dynamical systems [7, 1, 2] as well as certain classes of stochastic systems [3, 6].
In this talk, I will review a data driven approach to model reduction motivated by a discrete-time version of the Mori-Zwanzig formalism that makes use of Koopman operators (rather than the Liouville operator used in continuous-time approaches) [5, 4]. Through a construction which we call *Wiener projection*, we can relate the resulting models to classical Wiener filtering and derive a version of the NARMAX representation of stochastic processes. The formalism can be naturally extended to general dynamical systems with random forcing. Time permitting, I will discuss the relationship between the discrete-time Mori-Zwanzig and other formalisms commonly used for data-driven modeling of nonlinear dynamical systems, as well as some open issues with this approach to model reduction.

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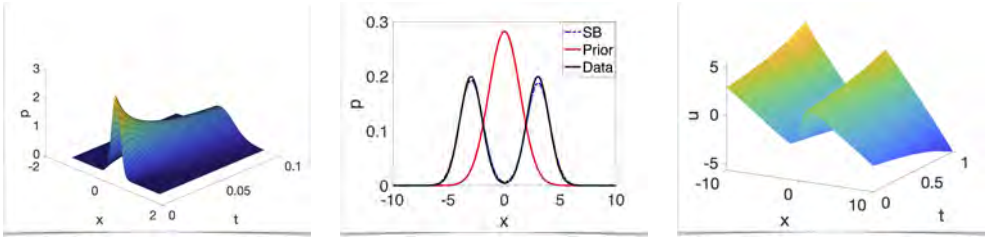
Schrödinger bridge model-data adaptation for network dynamics

H. Gorji[1], **R. Dakhmouche**[1,2], **N. Stauffer**[1,2], **and I. Lunati**[1]

[1] *Laboratory for Computational Engineering, Empa, Dübendorf, Switzerland*
[2] *Chair of Computational Mathematics and Simulation Science, EPFL, Switzerland*

Recent advances in data-driven techniques and digital-twin concepts have refreshed the interest in integrating data with mechanistic and stochastic models [2]. Beyond the conventional Bayesian inference approach, which calibrates model parameters with input data, there is a widespread interest in *dynamic* model adaptation, which focuses on learning and adjusting the described dynamic. The main challenge behind this class of problems is to find optimal adjustments of the high-dimensional *prior* models, given the state variables that are often only partially observed.



(a) (b) (c)

Figure 1: Adaptation with random walk prior. (a) Density $p(x|t)$ produced by the prior model. (b) Density at $t = 0.1$, with and without correction in blue and red, respectively. (c) Correction $u(x, t)$.

To address this challenge, we study the model-data adaptation problem in the context of stochastic dynamics, where the Schrödinger bridge (SB) setting naturally arises [1]. To illustrate the problem setup, consider a random variable X_t with values in $\mathbb{R}$ following the random walk as the prior dynamical model. Our objective is to find the optimal correction force

$$u \quad = \quad \underset{u^* \in \mathcal{U}}{\arg\min} \frac{1}{2} \mathbb{E}\left[\int_0^T \|u^*(X_t, t)\|_2^2 dt\right] \tag{1}$$

over a feasible set $\mathcal{U}$, subject to the constraint that the dynamic has the measure μ at some finite time $t = T$ (see Fig 1). Besides this classical SB problem, we investigate more elaborated scenarios where the prior is enriched by network models, such as Port-Hamiltonian and Kuramoto dynamics. Furthermore, we present results on two interesting extensions of the SB, where instead of the full distribution μ, the input data are limited to (a) noisy observables of the form $h(X) + \epsilon$, where ϵ is the noise and $h(.)$ the map; and (b) moments $\mathbb{E}[Q_i(X)]$, where $Q_i(.)$ are polynomials. By providing novel solution algorithms tailored to these realistic variations, we demonstrate accessible and robust model-data adaptations for complex dynamical systems.

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3.5 Friday, September 13

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

M. Alghamdi[1], **D. Boffi**[1,2], **and F. Bonizzoni**[3]

[1] *KAUST, Kingdom of Saudi Arabia*
[2] *Università di Pavia, Italy*
[3] *Politecnico di Milano, Italy*

The present talk concerns with the following parametric eigenvalue problem discretized by means of the finite element (FE) method: for all $\mu \in \mathcal{M}$, find real eigenvalues $\lambda_h(\mu)$ and non-vanishing eigenfunctions $u_h(\mu) \in V_h$ such that

$$a(u_h, v_h; \mu) = \lambda_h(\mu)(u_h, v_h)_{L^2} \quad \forall v_h \in V_h,$$

where $\mathcal{M} \subset \mathbb{R}^p$ is the parameter space, V_h is the FE subspace of the Hilbert space V and $a(\cdot, \cdot, \mu)$ is elliptic in V for all $\mu \in \mathcal{M}$. In particular, we are interested in detecting the behavior of the hypersurfaces defined by $\{\lambda_{h,j}(\mu)\}_{j\geq 1}$ as the parameter μ varies in $\mathcal{M}$. These hypersurfaces may intersect, leading in general to multiple eigenvalues at one point of intersection. When a crossing occurs, clearly the eigenvalues involved in the crossing are not smooth functions of the parameters and the corresponding eigenspaces are not even continuous if the eigenvalues are sorted by their magnitude. The question addressed in [1] concerns the matching of the eigenvalues across their intersections so that a new sorting of the eigenmodes can be introduced that restores the smoothness of eigenvalues and eigenspaces with respect to the parameters.

To better define our problem, we restrict the range of eigenvalues we are interested in to an interval $I_\lambda = [\lambda_{\min}, \lambda_{\max}]$. Consequently, we only examine the hypersurfaces in the region $\mathcal{M} \times I_\lambda$. This implies in particular that hypersurfaces can enter or exit this region of interest when the corresponding eigenvalues cross the values of $\lambda_{\min}$ or $\lambda_{\max}$.

We design an adaptive algorithm which minimizes the number of FE solves to guarantee the correct tracking 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 based on how close the eigenvalues and the eigenfunctions at each pair neighboring parameter $\mu_i,\ \mu_k$ are to each other. The a-priori phase is followed by the application of a suitable a-posteriori strategy, based on the orthogonality of the eigenfunctions. If the a-posteriori error indicator detects a mistake in the output of the a-priori phase, we mark the subinterval $[\mu_i,\ \mu_k]$ for refinement. To tackle the curse of dimensionality, at a given refinement level, a sparse grid approach is adopted for the construction of the grid of the next level.

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Line-Search Based Optimization With Online Model Reduction

Dane Grundvig[1]

[1] *Rice University*

When applying model reduction to optimization, an online only approach can help to alleviate the expense of model construction by leveraging locally accurate models. We propose a line-search algorithm that uses objective function models with tunable accuracy to solve smooth optimization problems with general nonlinear equality constraints. This algorithm specifies how objective function models can be used to generate new iterates in the context of line-search methods, and specifies approximation properties these models have to satisfy. Moreover, the algorithm assumes that a bound for the model error is available and uses this bound to explore regions where the model is sufficiently accurate. The algorithm has the same first-order global convergence properties as standard line-search methods. However, this algorithm uses only the models and the model error bounds, but never directly accesses the original objective function. Examples include problems where the evaluation of the objective requires the solution of a large-scale system of nonlinear equations. The models are constructed from reduced order models of this system. Numerical results for partial differential equation constrained optimization problems show the benefits of the proposed algorithm. Extensions to constraint optimization are presented.

An adaptive data sampling scheme for low-dimensional controller inference

Steffen W. R. Werner[1] **and Benjamin Peherstorfer**[2]

[1] *Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech, Blacksburg, VA 24061, USA, (steffen.werner@vt.edu).*
[2] *Courant Institute of Mathematical Sciences, New York University, New York, USA, (pehersto@cims.nyu.edu).*

Stabilizing dynamical systems in science and engineering is a challenging task, in particular when only limited amounts of data are available. In this work, we propose an adaptive data sampling scheme for generating small yet informative data sets for the task of stabilizing dynamical systems via the controller inference approach [1]. The key is to generate suitable input signals for the data generation via intermediate low-dimensional controllers that stabilize the system dynamics over limited subspaces.

As we have shown in our previous work [1], the sample complexity of constructing stabilizing state-feedback controllers directly from data scales with the intrinsic dimension of the system rather than its state or input dimensions. However, to use a data set of that minimal or any size for the task of stabilization, the data must contain the right information about the task. In particular in the case of unstable systems, the collection of large numbers of informative data samples is typically prevented by the instabilities that yield redundant or destructive system behavior. This leads to the question of how to generate data that is informative for system stabilization. In this presentation, we provide an approach that is based on our previous theoretical findings and related to the idea of iterative controller design, which allows us to adapt the input signal online for appropriate data generation and which avoids catastrophic unstable system behavior in the process. Numerical experiments including fluid dynamics (Figure 1), chemical reactors, power networks and particle models demonstrate that this adaptive approach further improves on the low-dimension controller inference method.

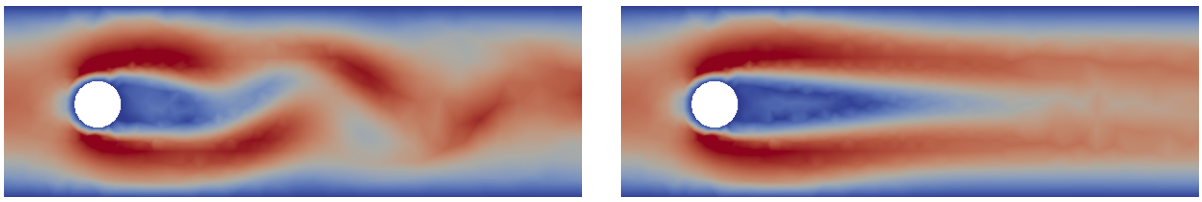

Figure 1: The behavior of laminar flows behind obstacles tends to unstable oscillations after perturbation (left) in contrast to the desired steady state behavior (right). Using the data from our proposed adaptive sampling approach only 10 system queries are needed to stabilize the system, while classical low-dimensional controller inference needs one order of magnitude more evaluations.

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Forced Stuart-Landau models for closed-loop flow control

Tea Vojkovic[1,2], Dimitris Boskos[2], and Abel-John Buchner[1]

[1] *Laboratory for Aero and Hydrodynamics, Delft University of Technology, The Netherlands*
[2] *Delft Center for Systems and Control, Delft University of Technology, The Netherlands*

We present a methodology for the extraction of parametric reduced order models (pROMs) for systems governed by the Navier-Stokes equations when they undergo a supercritical Hopf bifurcation. The purpose of the constructed models is to enable the design of closed-loop control laws that robustly stabilize the system.

The incompressible Navier-Stokes equations are the system of partial differential equations

$$\mathscr{E}\frac{\partial \mathbf{U}}{\partial t} = \mathscr{N}(\mathbf{U}, \mathbf{f}, \epsilon), \tag{1}$$

where the state $\mathbf{U}$ is comprised of the velocity and pressure fields, $\mathscr{E}$ denotes projection onto the velocity space, $\mathscr{N}$ is the nonlinear Navier-Stokes operator, and $\mathbf{f}(t)$ is an external forcing term. Here the model parameter ϵ is considered in a neighborhood of a critical point $\epsilon = 0$ where the bifurcation occurs. The starting point of our approach is the weakly nonlinear analysis from [1, 2] where the state $\mathbf{U}$ of (1) is asymptotically expanded as $\mathbf{U} = \mathbf{U}_0 + \sqrt{\epsilon}\mathbf{U}_1(t,\epsilon) + \epsilon\mathbf{U}_2(t,\epsilon) + \sqrt{\epsilon}^3\mathbf{U}_3(t,\epsilon) + ...$ around the equilibrium point at the critical value $\epsilon = 0$. Our key contribution is to consider a forcing of the form $\mathbf{f}(t) = E(t,\epsilon)\mathbf{f}_E + c.c.$, which generalizes existing approaches that consider $E(t,\epsilon)$ to be harmonic with a constant frequency, and enables the design of closed-loop controllers. Substituting the asymptotic expansions of the state and the forcing into the governing equation (1) leads to a series of linear equations at various orders $\sqrt{\epsilon}^i$, which are successively solved. At the order $\sqrt{\epsilon}^3$ we obtain the forced Stuart-Landau equation

$$\frac{dA}{dt} = \epsilon a_0 A - a_1 A|A|^2 + a_2 E(t,\epsilon), \tag{2}$$

for the evolution of the global mode associated with the Hopf bifurcation, which together with the expansion of the state serves as a surrogate model of (1). The Stuart-Landau model provides a reliable approximation of the nonlinear system (1) for a broad range of initial conditions and a reasonable set of parameter values. At the same time, our formulation accounts for time-varying forcing, enabling the design of closed-loop control laws that can be implemented in real time.

We exploit this methodology to model and control the flow around both a single cylinder and two cylinders in tandem configurations. Furthermore, we present an alternative data-driven approach where the Stuart-Landau coefficients are fitted from data in the least-squares sense. This is also convenient for other important classes of forced systems which exhibit supercritical Hopf bifurcation.

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Adaptive Reduced Basis Trust Region Methods for Parameter Identification Problems

M. Kartmann[1], T. Keil[2], M. Ohlberger[2], S. Volkwein[1], and B. Kaltenbacher[3]

[1] *University of Konstanz, Germany*
[2] *University of Münster, Germany*
[3] *Alpen-Adria-Universität Klagenfurt, Austria*

In this talk, we are concerned with model order reduction in the context of iterative regularization methods for the solution of inverse problems arising from parameter identification in elliptic partial differential equations. Such methods typically require a large number of forward solutions, which makes the use of the reduced basis method attractive to reduce computational complexity. However, the considered inverse problems are typically ill-posed due to their infinite-dimensional parameter space. Moreover, the infinite-dimensional parameter space makes it impossible to build and certify classical reduced-order models efficiently in a so-called offline phase. We thus propose a new algorithm that adaptively builds a reduced parameter space in the online phase. The enrichment of the reduced parameter space is naturally inherited from the Tikhonov regularization within an iteratively regularized Gauss-Newton method. Finally, the adaptive parameter space reduction is combined with a certified reduced basis state space reduction within an adaptive error-aware trust region framework. Numerical experiments are presented to show the efficiency of the combined parameter and state space reduction for inverse parameter identification problems with distributed reaction or diffusion coefficients. The talk is based on [1].

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Paired Autoencoders for Inversion and Regularization with Sparsity

Matthias Chung[1] **and Jack Michael Solomon**[1]

[1] *Department of Mathematics, Emory University,*
{matthias.chung,jack.michael.solomon}@emory.edu

Surrogate models utilize compression and embedding techniques to reduce computational cost and improve efficiency of simulating physical systems or forward processes while maintaining interpretability and accuracy of subsequent tasks such as solving an inverse problem. We consider a novel approach based on data-driven scientific machine learning tools for large-scale inverse problem with the aim to reconstruct a quantity of interest $\mathbf{x} \in \mathbb{R}^n$ given observations $\mathbf{b} \in \mathbb{R}^m$ perturbed by additive noise and a computationally challenging and ill-conditioned forward process $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^m$.

Our goal is to learn autoencoder mappings for dimensionality reduction of the inverse process. Let $a = d \circ e \approx \mathbf{A}$ be an *autoencoder*, where $e : \mathbb{R}^n \to \mathbb{R}^r$ denotes an *encoder* and $d : \mathbb{R}^r \to \mathbb{R}^n$ denotes the corresponding decoder, see Figure 1. Instead of utilizing a single autoencoder to learn a mapping $\mathbf{x} \mapsto \mathbf{b}$, we propose a decoupled approach for surrogate modeling, where unsupervised learning approaches are used to efficiently represent the input $\mathbf{x}$ and target spaces $\mathbf{b}$ separately, and a supervised learning approach is used to represent the mapping from one latent space to another. We refer to this approach as *paired autoencoders for inversion and regularization (pair)*. Standard autoencoders reduce dimensionality of the latent space. In our approach, we instead embed the latent variable in a *large* dimensional space while enforcing a sparse representation in the latent space. One may formulate the encoder $e(\,\cdot\,;\theta_e)$ decoder $d(\,\cdot\,;\theta_d)$ learning by

$$\min_{\theta_e,\theta_d} \; \mathbb{E}\, \|d(e(\mathbf{x};\theta_e);\theta_d) - \mathbf{x}\|_2^2 + \mu \, \|e(x;\theta_e)\|_1$$

where θ_e, θ_d denote the network parameters and $\mathbb{E}$ the expectation over the input.

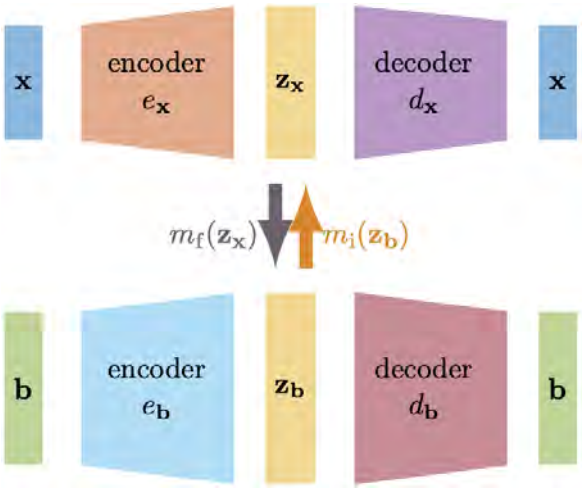

Figure 1: Paired autoencoders for inversion and regularization with sparsity features in the latent spaces. Inversion and forward propagation can be efficiently performed with sparse mappings m_{f} (forward) and m_{i} (inverse) between the latent space $\mathbf{z_x}$ and $\mathbf{z_b}$.

This approach confers several advantages compared to, for instance, full mapping approaches. First, the reduced approach decouples the model and the dimension reduction processes. Thus, unsupervised learning techniques can be used for autoencoders. Different sizes of datasets can be used in the input and target spaces. For example, in medical imaging, datasets corresponding to observed sinograms may be significantly larger than datasets of true images/phantoms. Furthermore, the training of the autoencoders is independent and can be run in parallel. Utilizing the sparsity constraints allows for efficient representation of forward models such as in medical imaging.

Data Assimilation in Chaotic Systems Using Deep Reinforcement Learning

Mohamad Abed El Rahman Hammoud[1], Naila Raboudi[1], Edriss S. Titi[2,3], Omar Knio[1], and Ibrahim Hoteit[1]

[1]*King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia*
[2]*Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, UK*
[3]*Department of Mathematics, Texas A & M University, College Station, TX 77843, USA*

Data assimilation (DA) plays a pivotal role in diverse applications, ranging from climate predictions and weather forecasts to trajectory planning for autonomous vehicles. A prime example is the widely used ensemble Kalman filter (EnKF), which relies on linear updates to minimize variance among the ensemble of forecast states. Recent advancements have seen the emergence of deep learning approaches in this domain, primarily within a supervised learning framework. However, the adaptability of such models to untrained scenarios remains a challenge. In this study, we introduce a novel DA strategy that utilizes reinforcement learning (RL) to apply state corrections using full or partial observations of the state variables. Our investigation focuses on demonstrating this approach to the chaotic Lorenz '63 system, where the agent's objective is to minimize the root-mean-squared error between the observations and corresponding forecast states. Consequently, the agent develops a correction strategy, enhancing model forecasts based on available system state observations. Our strategy employs a stochastic action policy, enabling a Monte Carlo-based DA framework that relies on randomly sampling the policy to generate an ensemble of assimilated realizations. Results demonstrate that the developed RL algorithm performs favorably when compared to the EnKF. Additionally, we illustrate the agent's capability to assimilate non-Gaussian data, addressing a significant limitation of the EnKF.

Faster solution of linear Bayesian smoothing problems using model reduction for ensemble Kalman inversion

P. Stavrinides[1] **and E. Qian**[1]

[1] *Georgia Institute of Technology*

We consider the Bayesian smoothing problem of inferring the initial state of a linear dynamical system, given noisy linear output measurements after the initial time. The ensemble Kalman inversion (EKI) method is an adjoint-free iterative method for estimating the posterior distribution of this inference problem. However, accuracy of EKI depends on having a large ensemble of particles, where each particle requires evolving the dynamical system. When the system is high-dimensional, the cost per particle is high, leading to EKI either having prohibitive cost or high sampling error. In this work, we use Balanced truncation for Bayesian smoothing (BTBS) to accelerate solution of the smoothing problem via EKI. BTBS is a model reduction method that adapts balanced truncation, a system-theoretic projection-based model reduction method, to the Bayesian smoothing problem. Numerical results show that reduced EKI models achieve the same accuracy as the full EKI algorithm with multiple-orders-of-magnitude reduction in computational cost.

Efficient Geometric MCMC for Nonlinear Bayesian Inversion Enabled by Derivative-Informed Neural Operator

Lianghao Cao[1], **Thomas O'Leary-Roseberry**[2], **and Omar Ghattas**[2]

[1] *California Institute of Technology*
[2] *The University of Texas at Austin*

We propose an accelerated geometric Markov chain Monte Carlo (MCMC) method for fast and consistent solutions to infinite-dimensional nonlinear Bayesian inverse problems. Such problems are relevant for inferring uncertain parameters of continuum physical systems based on sparse, noisy, and indirect observations. Geometric MCMC methods [1] employ proposals that adapt to posterior local geometry and thus can generate high-quality Markov chains for posterior sampling. However, these methods require computing a Hessian approximation of the likelihood at each chain position, which can be costly when the parameter-to-observable (PtO) map is defined through large-scale partial differential equations (PDEs).

To address this challenge, we consider a delayed-acceptance geometric MCMC method that utilizes a neural operator surrogate of the PtO map to alleviate cost while retaining posterior consistency. To achieve a superior quality-cost trade-off, the surrogate must make fast and accurate predictions on both the observable and its parametric derivative. In this work, we leverage an infinite-dimensional formulation of derivative-informed operator learning [2] utilizes input-output-derivative samples. Such an operator learning scheme leads to derivative-informed neural operators (DINOs) that accurately predict both the observable and its parametric derivative at a significantly lower training cost than conventional training based on input-output samples. Our numerical examples on challenging problems, such as coefficient inversion for nonlinear diffusion–reaction and hyperelastic material properties discovery, show that (i) DINO-accelerated geometric MCMC can reliably generate effective posterior samples around 3–9 times faster than geometric MCMC and 60–97 times faster than MCMC based on prior geometry (e.g., preconditioned Crank–Nicolson), and (ii) DINO-accelerated geometric MCMC is more cost-effective than geometric MCMC if one aims to collect more than merely 10–25 effective posterior samples.

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Adaptive Covariance Estimation via Surrogate Modeling for Multi-fidelity Estimation

T. Coons[1], A. Jivani[1], T. Dixon[2], A. Gorodetsky[2], and X. Huan[1]

[1] *University of Michigan, Department of Mechanical Engineering*
[2] *University of Michigan, Department of Aerospace Engineering*

Multi-fidelity variance-reduction techniques (e.g., multi-fidelity Monte Carlo [3], approximate control variates [2, 1], and multilevel BLUEs [4]) have seen considerable attention in recent years, in many cases providing orders-of-magnitude computational savings in estimating statistics of a high-fidelity model. Given the exact covariance matrix between model fidelities and the computational costs of each model, these methods solve the multi-fidelity sample allocation strategy and produce an optimal estimator by minimizing variance while remaining unbiased with respect to the highest fidelity model available. However, the covariance matrix across model fidelities is usually not known *a priori* and is instead often estimated via pilot sampling or reinforcement-learning techniques [5] in conjunction with the sample covariance formula. Depending on the model ensemble available, this covariance estimation can be costly or inaccurate, leading to suboptimal estimators or prohibitive offline costs. Furthermore, most multi-fidelity estimators are not designed with an outer design optimization loop in mind, where covariance information and thus estimator properties may vary substantially from design to design. In this work, we explore probabilistic surrogate methods to model the covariance information across the domain, adaptively taking additional pilot samples only when the uncertainty in the covariance at a given location in the domain is too high for accurate multi-fidelity estimation. As the overall stochastic optimization process converges and the covariance uncertainty is reduced, far fewer pilot samples are needed and the overall optimization cost is greatly reduced.

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Reduced Basis Methods for Domain Uncertainty Quantification of Periodic Gratings

R. Aylwin[1], J. Pinto[2], and G. Silva-Oelker[3]

[1] *Universität Ulm*
[2] *Universidad Adolfo Ibañez*
[3] *Universidad Mayor*

March 1, 2024

We present a reduced basis method and accompanying implementation for the computation of statistical information of scattered electromagnetic fields by two-dimensional periodic gratings and its resolution through the boundary element method. In particular we build a surrogate model that allows for the fast and precise computation of first and second order moments of the scattered field (and smooth quantities of interes, e.g., the diffraction efficiency) in the setting of uncertain geometry, simulating manufacturing errors and wear and tear of the optical devices. The approach allows us to avoid the small perturbation assumption required by, e.g., the Fist-Order-Second-Moment (FOSM) approach considered in [5] and treat perturbations of arbitrary size. Moreover, we consider the efficient estimation of failure probabilities in the context of reliability analysis of optimal structures for the applications considered in [4, 2]. Furthermore, we solve the periodic problem through the Boundary Element Method and the approach developed in [1, 3]. Applications in the shape optimization of periodic gratings and the consideration of statistical information in optimization algorithms.

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A streamlined workflow for model reduction with application to aerodynamic and thermal analyses

Patrick Blonigan[1], Eric Parish[1], Elizabeth Krath[1], John Tencer[1], Andrew Kurzawski[1], and Francesco Rizzi[2]

[1]*Sandia National Laboratories*
[2]*NexGen Analytics*

Projection-based reduced-order models (ROMs) of high-fidelity computational physics simulations have shown great potential to accelerate outer-loop analyses such as uncertainty quantification and optimization [1, 2, 3]. Translating these algorithms into methods that are usable by non-experts requires easy-to-use tools and workflows for sampling the full-order model (FOM) at desired locations, constructing the ROM to a desired tolerance, and deploying the ROM in the analysis of interest. This presentation covers a Python-based library being used at Sandia, called "rom-tools-and-workflows", which facilitates both the offline construction of the ROM as well as its online deployment. The library is part of the Pressio project and provides a suite of tools for constructing reduced subspaces, hyper-reduction, and relies on simple APIs that enable pre-defined workflows such as multifidelity UQ with a coupling to Dakota and greedy sampling.

The presentation will outline these workflows with demonstrations on two example problems. The first example is ROM-accelerated forward UQ for a computational fluid dynamics problem. Specifically, we present forward uncertainty propagation of a high-speed compressible flow with respect to uncertain turbulence model parameters in the Reynolds-Averaged Navier-Stokes equations. We couple Sandia's Parallel Aerodynamics and Reentry Code (SPARC) with Pressio to implement a projection-based ROM, and we drive the outer-loop analysis with rom-tools-and-workflows and Dakota. We show that ROMs reduce the variance of mean estimators for a given computational budget and provide accurate output distributions.

The second example we consider is the solution of a thermal inverse problem. In this example, we infer material properties and boundary conditions given temperature readings at a handful of locations over time, using ROMs implemented in Sierra-Thermal/Fluid and Pressio. We show that ROMs can bring down the cost of inverse problems while finding similar optimal solutions to more expensive analyses that leverage the full-order high-fidelity model alone.

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Extended tensor decomposition model reduction method: application to real-time additive manufacturing residual stress predictions and inverse problems

Ye Lu

University of Maryland, Baltimore County

Simulation-based science and engineering, including design, uncertainty quantification, and general inverse problems, usually necessitate fast responses of numerical models. Despite the significant improvement of the computer hardware over the last decades, real-time simulations of large-scale nonlinear systems, such as additive manufacturing, are still intractable with conventional finite element analysis (FEA). The repetitive nonlinear FEA makes general inverse problems computationally prohibitive.

To address the above challenges, this work presents an eXtended Tensor Decomposition (XTD) method [1] for nonlinear model reduction. The idea of XTD is to introduce a sparse non-separated enrichment to the conventional tensor decomposition based model reduction methods, such as proper generalized decomposition [2, 3, 4], to enhance the efficiency of model reduction for dealing with localized highly nonlinear problems, such as additive manufacturing or fracture problems. The XTD method can significantly improve the approximation accuracy and the reducibility (compressibility) of such problems and makes the nonlinear model reduction much more efficient.

The method has been successfully applied to parametric elastoplastic problems for real-time additive manufacturing residual stress predictions and inverse problems, including uncertainty quantification. Significant speedups are obtained with comparison to full-order FEA. The proposed method can enable a powerful computational framework for many science and engineering problems, such as manufacturing process design under uncertainty.

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4 Poster Abstracts

4.1 Posters for Tuesday, September 10

Model reduction of large-scale sparse systems in MATLAB and Octave with the MORLAB toolbox

S. W. R. Werner[1], P. Benner[2], and J. Saak[2]

[1] *Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech, Blacksburg, VA 24061, USA, (steffen.werner@vt.edu).*

[2] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany (benner@mpi-magdeburg.mpg.de, saak@mpi-magdeburg.mpg.de).*

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] is providing such implementations in MATLAB and Octave. 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. While being originally developed for medium-scale ($n \in \mathcal{O}(10^3)$) dense systems, since its latest version, the toolbox now supports the reduction of systems with large-scale ($n \in \mathcal{O}(10^5)$ and larger) sparse coefficient matrices via balancing-related methods such as balanced truncation, as well as Krylov subspace methods such as moment matching. To this end, the Matrix Equation Sparse Solvers (M-M.E.S.S.) library [2] is used as backbone of MORLAB for the efficient implementation of solvers for matrix equations such as Lyapunov and Riccati equations as well as the correct handling of systems with structured differential-algebraic equations.

This poster describes the latest release, version 6.0, of the MORLAB toolbox. It features new implementations of balancing-related and Krylov subspace model reduction methods for large-scale sparse, linear systems.

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Reduction of periodic systems with partial Floquet transforms

S. Bender[1] **and C. Beattie**[1]

[1] *Department of Mathematics, Virginia Tech, Blacksburg, 24061, VA, United States*

We consider systems of single input, single output systems with periodic parameters:

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{b}(t)u(t), \quad y(t) = \mathbf{c}(t)^*\mathbf{x}(t), \tag{1}$$

where $\mathbf{A}(t) \in \mathbb{R}^{n\times n}$, $\mathbf{b}(t), \mathbf{c}(t) \in \mathbb{R}^n$ all have period T. Such systems arise as the result of modeling phenomena related to fluid dynamics, structural mechanics, and electronic circuits. Specifically, linearization around known periodic orbits of a nonlinear model produces a periodic system of partial differential equations, then semi-discretization in space yields large scale linear time-periodic (LTP) dynamical systems. The need to simulate responses to a variety of inputs motivates the development of effective model reduction tools for these systems.

While the research on model reduction for LTP systems is limited, there is a sizeable amount of literature devoted to control, spectral analysis, and harmonic response of LTP systems [1, 2, 3]. Essential to the advances developed in these settings is the *Floquet transform*: If $\mathbf{A}(t)$ is locally integrable for $t \in \mathbb{R}$, then there exists an absolutely continuous, T-periodic, invertible matrix-valued function $\mathbf{P}(t) \in \mathbb{C}^{n\times n}$ such that the time-varying change of basis determined by $\mathbf{z}(t) = \mathbf{P}(t)^{-1}\mathbf{x}(t)$ (the Floquet transform) transforms solutions, $\mathbf{x}(t)$, satisfying the equation $\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t)$ to solutions, $\mathbf{z}(t)$, satisfying the constant coefficient differential equation $\dot{\mathbf{z}}(t) = \mathbf{R}_0\mathbf{z}(t)$, where $\mathbf{R}_0 \in \mathbb{C}^{n\times n}$ [4]. Applying this Floquet transform to (1) results in a dynamical system whose time dependency is isolated to the input and output ports:

$$\dot{\mathbf{z}}(t) = \mathbf{R}_0\mathbf{z}(t) + \mathbf{P}(t)^{-1}\mathbf{b}(t)u(t), \quad y(t) = \mathbf{c}(t)^*\mathbf{P}(t)\mathbf{z}(t). \tag{2}$$

Computation of the Floquet transform is expensive, making it intractable for large scale systems. Our research explores ways constructing a *partial* Floquet transform. Beyond being computationally feasible, our approach simultaneously isolates the time dependency to the input and output ports and produces an effective reduced order model.

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Randomized Symplectic MOR for Hamiltonian Systems

R. Herkert[1], P. Buchfink[1,3], B. Haasdonk[1], J. Rettberg[2], and J. Fehr[2]

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

Symplectic model order reduction (MOR) [6, 7] is used to reduce the computational complexity of high-dimensional Hamiltonian systems in a structure-preserving way. The mathematical structure of such systems ensures conservation of the Hamiltonian (i.e., the energy of the system) and under certain assumptions stability properties. In contrast to classical basis generation techniques such as the Proper Orthogonal Decomposition (POD), which do not ensure that the reduced order model (ROM) is a Hamiltonian system, symplectic MOR transfers the Hamiltonian structure to the ROM. Additionally, numerical experiments often show advantages of symplectic MOR compared to a classical, non-structure-preserving MOR [7]. To compute a symplectic basis, techniques like the complex SVD (cSVD) [7] or the SVD-like decomposition (SVD-like) [2] can be used. However, for large-scale Hamiltonian systems, computing the low-rank matrix approximations required by these techniques can lead to prohibitively high computational costs during the offline-phase.
We present the randomized cSVD (rcSVD) and the randomized SVD-like to reduce this computational costs. We provide numerical experiments that highlight their computational efficiency while preserving the approximation quality compared to their classical versions [4]. We further derive error bounds which show that the rcSVD is quasi-optimal in the set of ortho-symplectic matrices. This means that with a proper choice of hyperparameters, the projection error of the rcSVD is at most a constant worse than that of the cSVD [3]. As alternative approach, we accelerate the computation of the reduced Hamiltonian system in the offline-phase by random sketching techniques where inner products of high-dimensional matrices are approximated using randomized subspace embeddings. We follow ideas from [1] where linear, time-independent systems are approximated by their random sketch. These techniques significantly reduce computational complexity and memory requirements by avoiding operations with and storing of the full basis vectors. We merge these ideas with the concepts of symplectic MOR [5].

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Entropy stable reduced order modeling of nonlinear conservation laws using discontinuous Galerkin methods

Ray Qu[1] **and Jesse Chan**[1]

[1] *Department of Computational Applied Mathematics and Operations Research, Rice University*

We generalize the construction of entropy stable reduced order models (ROMs) for nonlinear conservation laws from finite volume methods (FVM) [1] to high order discontinuous Galerkin (DG) methods. This generalization preserves entropy stability while simplifying the hyper-reduction step by utilizing the Caratheodory pruning for the hyper-reduction of boundary conditions.

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Discovering Quadratic Representations of PDEs: Algorithms and Software

A. Olivieri[1], G. Pogudin[2], and B. Kramer[1]

[1] *Department of Mechanical and Aerospace Engineering, University of California San Diego*
[2] *LIX, CNRS, École Polytechnique, Institute Polytechnique de Paris*

Nonpolynomial and nonquadratic PDEs are used to describe complex dynamical processes in science and engineering. Some examples are the cubic FitzHugh-Nagumo model, which describes the activation and deactivation dynamics of a spiking neuron; the also cubic Brusselator model, used to predict oscillations in chemical reactions; and the quartic model of the nonadiabatic tubular reactor, which describes the evolution of the species concentration and temperature. Transforming, or lifting, such systems into quadratic form (as introduced for MOR in [1]) has been used to obtain better variables for model learning [2], for system-theoretic MOR [3] and data-driven MOR [4]. In all of these, the lifting transformation to quadratic form was done by hand on either the ODE or PDE. This is tedious, error-prone, and often results in suboptimal lifted transformations.

Quadratization of PDEs is the process of finding a lifting transformation that turns a PDE system with nonpolynomial or higher-degree polynomial drift into systems with quadratic drift. To obtain a quadratic form, it is often required to add new variables to the system. The set of variables introduced is called a quadratization. For illustration, consider the PDE describing the evolution of the space and time-varying function $u(t, x)$ as

$$u_t = u_x u^2 \tag{1}$$

To quadratize (1) we introduce the variable $y := u^2$ and calculate its first derivative in x: $y_x = 2u_x u$, which allows us to write

$$y_t = 2u_x u^3 = 2u_x uy = y_x y \quad \textit{and} \quad u_t = u_x y. \tag{2}$$

This is a quadratic equation in $u(t, x)$ and $y(t, x)$, so that the set $\{u^2\}$ is a quadratization for (1).

There exist quadratization algorithms and software for ODE models, e.g., [5], yet they cannot directly handle the PDE case. We present an algorithm and accompanying software that finds optimal quadratizations of complex PDE systems, where optimality is defined in terms of the number of the dimension of the quadratization. The presented algorithm searches a combinatorial tree of possible transformations, uses branch-and-bound techniques to curb its computational complexity, and outputs a minimal set of variables that effectively quadratize a PDE system. To the best of our knowledge, these are the first results of automated quadratization for PDEs.

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Conservative Reduced Order Modeling of the Plasma Kinetic Equations

Opal Issan[1] **and Boris Kramer**[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California San Diego, La Jolla, CA, USA*

We propose a data-driven projection-based reduced-order model (ROM) to reduce the computational cost of the spectral plasma solver (SPS) of the Vlasov-Poisson equations, which describe the equations of motions of collisionless electrostatic plasma. The SPS solver is based on a Fourier spectral expansion in space, asymmetrically-weighted Hermite expansion in velocity, and an implicit temporal integrator [1, 2]. The main advantages of the SPS solver are its conservation and fluid-kinetic coupling property, where the first three expansion coefficients correspond to the macroscopic description of the plasma, while higher-order expansion coefficients correspond to higher-order fluid moments capturing the kinetic effects of the plasma. A core contribution of this work is to introduce a ROM for the kinetic effects into SPS while keeping the macroscopic description intact. We show that this preserves its fluid-kinetic property, and conserves mass, momentum, and energy. Moreover, the suggested strategy overcomes the nonlinear bottleneck by efficiently handling convolutions. The numerical results show that our method can adequately emulate the SPS simulations at a fraction of the cost, which we test on the following benchmark problems: 1D-1V weak Landau damping, 1D-1V bump-on-tail instability, 1D-1V two-stream instability, and 2D-2V current-driven ion acoustic instability.

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Robust Implicit Adaptive Low Rank Time-Stepping Methods for Matrix Differential Equations

Daniel Appelö[1] **and Yingda Cheng**[1]

[1] *Department of Mathematics, Virginia Tech*

In this work, we develop implicit rank-adaptive schemes for time-dependent matrix differential equations. The dynamic low rank approximation (DLRA) is a well-known technique to capture the dynamic low rank structure based on Dirac-Frenkel time-dependent variational principle. In recent years, it has attracted a lot of attention due to its wide applicability. Our schemes are inspired by the three-step procedure used in the rank adaptive version of the unconventional robust integrator (the so called BUG integrator) [1] for DLRA. First, a prediction (basis update) step is made computing the approximate column and row spaces at the next time level. Second, a Galerkin evolution step is invoked using a base implicit solve for the small core matrix. Finally, a truncation is made according to a prescribed error threshold. Since the DLRA is evolving the differential equation projected on to the tangent space of the low rank manifold, the error estimate of the BUG integrator contains the tangent projection (modeling) error which cannot be easily controlled by mesh refinement. This can cause convergence issue for equations with cross terms.

To address this issue, we propose a simple modification, consisting of merging the row and column spaces from the explicit step truncation method together with the BUG spaces in the prediction step. In addition, we propose an adaptive strategy where the BUG spaces are only computed if the residual for the solution obtained from the prediction space by explicit step truncation method, is too large. We prove stability and estimate the local truncation error of the schemes under assumptions. We benchmark the schemes in several tests, such as anisotropic diffusion, solid body rotation and the combination of the two, to show robust convergence properties.

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An online algorithm to identify and control unknown PDEs

Alessandro Alla[1] **and Agnese Pacifico**[2]

[1] *Università Ca' Foscari Venezia (Italy)*
[2] *Sapienza Università di Roma (Italy)*

We address the control of Partial Differential equations (PDEs) with unknown parameters. Our objective is to devise an efficient algorithm capable of both identifying and controlling the unknown system. We assume that the desired PDE is observable provided a control input and an initial condition. The method works as follows, given an estimated parameter configuration, we compute the corresponding control using the State-Dependent Riccati Equation (SDRE) approach. Subsequently, after computing the control, we observe the trajectory and estimate a new parameter configuration using Bayesian Linear Regression method. This process iterates until reaching the final time, incorporating a defined stopping criterion for updating the parameter configuration. We also focus on the computational cost of the algorithm, since we deal with high dimensional systems. To enhance the efficiency of the method, indeed, we employ model order reduction through the Proper Orthogonal Decomposition (POD) method. The considered problem's dimension is notably large, and POD provides impressive speedups. Further, a detailed description on the coupling between POD and SDRE is also provided. Finally, numerical examples will show the accurateness of our method across.

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Model order reduction for parabolic PDE constrained optimization in a space time variational setting

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

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

In this talk we want to present research regarding parameterized time-dependent optimization problems. Using a tracking type objective function, this problem reads as:

$$\min_{(y\times u)\in\mathcal{Y}\times\mathcal{U}} J(y,u;\mu) = \frac{1}{2}(y-y_{d,\mu}, y-y_{d,\mu})_{L_2(I;L_2(\Omega)} + \frac{\lambda}{2}(u,u)_{L_2(I;L_2(\Omega)} \tag{1}$$

$$\text{s.t.} \qquad A_\mu y - F_\mu u - c_\mu = 0 \quad \in \mathcal{Z}', \tag{2}$$

where the state equation (2) is a parametric linear parabolic PDE formulated in the space-time variational setting, as e.g. in [3]. We know that using this formulation as well as a simultaneous space-time discretization has favorable properties regarding stability [4] and model order reduction [2]. This motivates the application of this setting to the field of PDE-constrained optimization. We have already shown results regarding the well-posedness and stability of this approach for a non parameterized version in [1].

Now we want to extend this approach to a parameterized setting. The parameter $\mu \in \mathcal{P}$ can appear in the constraining parabolic PDE (2) or the objective function (1). The control u is in our setting *not* parameter dependent and not regarded as a parameter. Therefore we consider our problem in a multi-query context, i.e. we want to solve a large number of optimization problems for varying parameters and therefore have a need for MOR.

In her master's thesis (2021), Nina Beranek has shown some preliminary results regarding the decay of the Kolmogorov n-width. Currently Linus Heinzelmann, within his master's thesis, is working on an implementation of the MOR to confirm these preliminary results numerically.

Additionally we are currently investigating optimization problems with additional constraints for the control. The optimal control $\bar{u}$ has to fulfill e.g. box constraints of the form $u_a(t,x) \leq \bar{u}(x,t) \leq u_b(t,x)$. Regarding the full order optimization problem, we can then solve this high dimensional problem quite efficiently using a semi-smooth Newton method. However the application of MOR to these systems is an open problem that we are currently investigating.

In this talk we want to present the results of this ongoing research of applying MOR to the parameterized PDE-constrained optimization problem in a space-time variational setting with and without additional control constraints.

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Parametric Proper Orthogonal Decomposition approaches for high-dimensional design optimization problems

Sebastiaan P. C. van Schie[1] **and John T. Hwang**[1]

[1]*Department of Mechanical and Aerospace Engineering, UC San Diego*

Proper Orthogonal Decomposition (POD) is one of the most widely-used reduced basis methods for model reduction. It uses the Singular Value Decomposition (SVD) to find a low-dimensional subspace which is optimally close to the span of a data matrix generated by a high-dimensional model. Despite its attractive approximation properties POD is not inherently suitable for parametric models, as it does not explicitly take into account the parametric model structure.

Let X denote a data matrix that contains data snapshots X_i from multiple parameter vectors $\boldsymbol{\mu}_i$ in parameter space $P \subset \mathbb{R}^p$, such that $X = \begin{bmatrix} X_1(\boldsymbol{\mu}_1) & \dots & X_s(\boldsymbol{\mu}_s) \end{bmatrix}$. Standard POD constructs a single reduced basis for all of P by using all of X. This results in inaccurate and unstable reduced bases when the model behavior changes significantly over P. Various approaches have been proposed to make POD more robust and accurate under parameter changes. These include Grassmann manifold interpolation [1] and clustering data to construct local POD bases on disjoint subspaces that cover P [2]. While these methods rely only on state information, other approaches use the state sensitivities as well. Example approaches include adding the sensitivities to a weighted snapshot matrix [3] and computing the sensitivity of the POD modes under parameter changes [4].

These and other parametric POD approaches in literature perform best for low-dimensional P and sometimes require an offline data acquisition phase that covers P with data snapshots. This limits their usefulness for design optimization problems, where high-dimensional P are often of interest. In this talk we instead focus on parametric POD approaches for high-dimensional optimization problems without offline phase. We propose a new approach for efficient online weighted POD that avoids having to recompute the entire SVD when new weights are assigned. Furthermore, we present ways to incorporate state sensitivities into the parametric POD computation process. We show results for static and dynamic optimization problems and compare the performance of various parametric POD models in terms of accuracy and speed.

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Optimal control based reformulation of a data assimilation problem as a new approach for applying model order reduction methods

J. Marquardt[1] **and C. Gräßle**[1]

[1]*Institute for Partial Differential Equations, TU Braunschweig, Germany.*

The goal of data assimilation is to update a mathematical model with observations from the real world. In 4D-var data assimilation, the observations $y_i \in \mathbb{R}^{d_{\text{obs}}}$ for $0 \leq i \leq N$ are taken at multiple time instances $0 = t_0 < ... < t_N = T < \infty$. The current state of the model at time t_i is given by $x_i \in \mathbb{R}^d$. The forward evolution of the model is governed by some dynamics $\mathcal{M}_i : \mathbb{R}^d \to \mathbb{R}^d$ such that $x_{i+1} = \mathcal{M}_i(x_i)$. Further, we introduce the observation operators $\mathcal{H}_i : \mathbb{R}^d \to \mathbb{R}^{d_{\text{obs}}}$. In order to match the model prediction with the observation, the initial state x_0 can be chosen as a solution of

$$\underset{x_0 \in \mathbb{R}^d}{\operatorname{argmin}} \Big\{ J(x_0) := \frac{1}{2} \sum_{i=0}^{N} \|\mathcal{H}_i(x_i) - y_i\|^2_{\mathbb{R}^{d_{\text{obs}}}} + \frac{\alpha}{2} \left\| x_0 - x_0^{(b)} \right\|^2_{\mathbb{R}^d} \Big\}, \tag{1}$$

subject to

$$x_{i+1} = \mathcal{M}_i(x_i) \quad \forall i \in \{0, ..., N-1\} \tag{2}$$

with initial guess $x_0^{(b)}$ and trust coefficient $\alpha > 0$, which describes how much confidence can be put into $x_0^{(b)}$ compared to the measurements y_i. The common solution techniques in data assimilation usually require the numerical treatment of large systems. Therefore, it is not surprising that the search for reduced order models is a focus of various contributions (see e.g. [2] for an overview).

In this presentation, we consider data assimilation problems governed by parabolic partial differential equations and apply a reformulation technique, which allows us to assimilate the data by solving an elliptic differential equation with e.g. finite elements. The transition between these problems is based on the interpretation of the data assimilation task as an optimal control problem and the further utilisation of the arising optimality conditions in order to establish the elliptic system. The presented reformulation technique is not only limited to data assimilation and and has already been successfully implemented by other authors for distributed control problems in the past (cf. [1, 3]).

Switching from (1) - (2) to the task of discretising a partial differential equation allows to exploit new ideas for the reduction of the model's complexity. Both our results from first approaches of applying model order reduction to the reformulated system and our investigations for the identification of good time instances for the incorporation of data to the model will be presented.

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Real-time aerodynamic load estimation for hypersonics via strain-based inverse maps

Julie Pham[1], **Omar Ghattas**[1], **and Karen Willcox**[1]

[1] *The University of Texas at Austin*

We present an efficient inverse formulation for estimating aerodynamic pressure loads on a hypersonic vehicle using a strain-based sensing strategy and dimension reduction for aerodynamic pressure fields. Real-time characterization of aerodynamic loads is critical for guidance, navigation, and control applications. In hypersonic flight environments, direct measurement of these quantities of interest is often intractable due to the harsh aerothermal conditions. Our work targets the hypersonic environment by employing strain-based sensing to infer the aerodynamic surface loads from sparse measurements of the structural strain field. The strain response induced by the aerodynamic loads is governed by the partial differential equations (PDE) of linear elasticity, leading to a PDE-constrained inference problem, for which model reduction is often critical for computational tractability [1]. In this work, we embed the physics in a compressed inverse map, which is a surrogate for enabling real-time estimation.

To construct the inverse map, we pose the inference task as a least-squares problem with a high-dimensional linear constraint arising from a finite element discretization of the governing PDE [2]. Due to the linearity of the constraint, a closed-form solution is available via the normal equations, which provides an inverse map from strain measurements to the aerodynamic pressure quantities of interest. Pre-computation of the least-squares solution (estimator), which comprises the high-dimensional system matrices, enables a compression of the high-fidelity physics into a reduced inverse map. This estimator reduces the inverse map via either (1) a low-dimensional parameterization of the surface pressure field via the proper orthogonal decomposition, or (2) a prior regularization term that eliminates higher spatial-frequency modes of the surface pressure field [2]. We employ a data-driven prior for regularization, constructed using computational fluid dynamics solutions of the surface pressure field over a range of flight conditions. Additionally, the analytical covariance of the estimator provides explicit uncertainty quantification in the presence of sensor noise. Numerical studies are conducted using the Initial Concept 3.X (IC3X) conceptual hypersonic vehicle. The results demonstrate the estimator performance for surface pressure reconstruction, as well as the corresponding force and moment coefficients, for a given noise level. We provide a discussion of accuracy, uncertainty, regularization, and optimal sensor placement for the IC3X testbed problem.

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Surrogate Model Generation in CFD with Machine Learning-Aided Design Optimization Method (MLADO)

F.-J. Granados-Ortiz[1] **and J. Ortega-Casanova**[2]

[1]*Department of Engineering, University of Almeria (Spain)*
[2]*Department of Mechanical, Thermal and Fluid Engineering, University of Malaga (Spain)*

In engineering applications it is often complicated to find optimal designs, especially in simulation-based design, due to each computational simulation may take long time to converge. This situation worsens when the planned design life cycle involves many design parameters, which dramatically increases the number of simulations to achieve an optimal design.

A widely accepted approach in the literature to obtain optimal designs in CFD (Computational Fluid Dynamics) is to construct surrogate models, which can be later sampled. However, the construction of these surrogates must be smart enough, since brute force leads to inefficient procedures, especially when the number of design parameters in the optimisation approach is large and thus hundreds or thousands of simulations must be converged to obtain reliable and useful surrogates. In unsteady engineering problems, each simulation may take from several days to weeks to converge, thus an efficient and data-driven construction of surrogates is an important advantage.

In this presentation, a proposed solution to this problem is to embed a classification algorithm (predictor) in the making of the surrogates (may exist more than one for a specific problem), as shown in Figure 1. This process is supported by the namely Machine Learning-Aided Design Optimization (MLADO) [1]. The classifier predicts whether the objective feature yields $VS = 1$ (desired feature) or $VS = 0$ (undesired feature). The classifier can be trained with lower-quality data from many possible sources (ROMs such as SINDy models, low-fidelity simulations on coarse grids, data-bases, etc.) and then be used to make a surrogate that incorporates the most relevant features and efficiently. The use of the predictor allows to also explore the design space to reduce its dimension, since the classification is monitored to see whether the number of $VS = 1$ is increasing or not by following a parameter exploration. In addition, if desired, uncertainty estimates can be obtained from these surrogates. During the talk, we will show successful cases of application of this method to unsteady CFD problems and discuss what has been done to date, future plans and other potential improvements of the method, as well as its extension to other scientific problems.

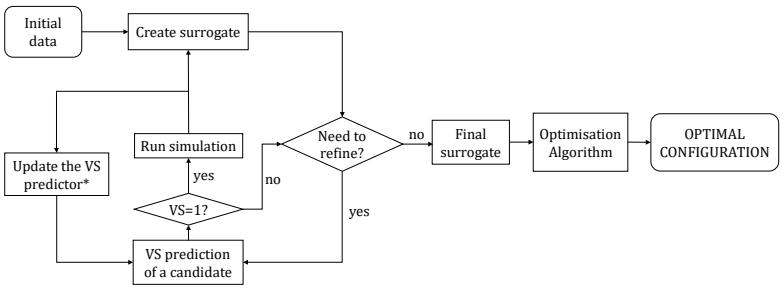

Figure 1: Framework to improve surrogate models by relying on a classification algorithm (predictor).

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Score-based diffusion models for PDE-based inverse problems

Yilin Zhuang[1], **Christian Jacobsen**[1], **and Karthik Duraisamy**[1,2]

[1]*Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI, United States of America*
[2]*Michigan Institute for Computational Discovery, University of Michigan, Ann Arbor, MI, United States of America*

Despite recent advancement in reduced order and surrogate models, applications in field inversion [1] - i.e. the task of solving inverse problems for fields rather than parameters - presents a substantial challenge, especially due to the difficulties in optimizing data matching to accurately represent the physical phenomena of interest.

This study aims to explore the potential of employing diffusion models, specifically score-based models [2] for field inversion tasks. In image generation, a similar technique known as inpainting has proven efficient in approximating data distributions through score matching [2, 3]. Our investigation into score-based diffusion models is motivated by their ability to model complex distributions. However, these models often lose physical consistency across simulations. We have developed a method that enforces physical constraints during the reverse sampling process by evaluating the governing equations on each cell and has been demonstrated to perform well in a range of scientific machine learning tasks [4]. Although this enforcement does not require evaluation at every sampling step, the associated evaluation costs may restrict certain applications from obtaining a posteriori field distributions from measured inputs. We introduce an efficient framework that integrates physical laws and spatial dependence into the model's training process, aiming to reduce the computational efforts required for evaluation. Additionally, we demonstrate the computation of field uncertainty through repetition samplings from the Gaussian prior. The method is demonstrated in several applications including flow in porous media.

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4.2 Posters for Wednesday, September 11

Stochastic Subspace Descent with Surrogate-adjusted Line Search

Nuojin Cheng[1], **Stephen Becker**[1], **and Alireza Doostan**[2]

[1]*Department of Applied Mathematics, University of Colorado Boulder*
[2]*Smead Aerospace Engineering Sciences Department, University of Colorado Boulder*

Gradient-free optimization (GFO) is the optimization approach when the gradient of the objective function is unavailable, commonly happen in black-box optimizations. Traditional GFO methods that estimate gradients using finite differences face significant challenges in high-dimensional spaces, as the number of required function evaluations grows with dimensionality. To address these challenges, Kozak et al. [1] introduced the Stochastic Subspace Descent (SSD) method, which enhances efficiency by estimating gradients within a randomly selected subspace. This approach has demonstrated substantial effectiveness, particularly in cases where the objective function exhibits weak dependence on most of its inputs—a situation frequently encountered in practice. However, the optimization performance of SSD, particularly regarding step size selection, remains suboptimal due to unknown variables such as the Lipschitz constant of the objective function gradient and the projected energy of the effective objective function onto the subspace.

To overcome these limitations, recent developments have utilized reduced-order or surrogate models, such as polynomial chaos and deep learning-based surrogates, which offer cost-effective approximations of the original expensive models while maintaining a consistent performance. Building on these advancements, this work proposes a novel method that leverages reduced-order surrogate models to refine the step size selection process through a surrogate-adjusted line search method. This approach aims to harmonize the efficiency of surrogate models with the robustness of SSD, thereby enhancing the overall optimization process.

This paper makes several significant contributions to the field of gradient-free optimization:

1. We introduce a novel surrogate-adjusted line search algorithm that utilizes reduced-order surrogate models to approximate the optimal step size, effectively addressing the prevalent challenge of step size tuning in gradient-free optimization.

2. We provide a comprehensive theoretical analysis of the surrogate-adjusted line search algorithm, which includes a rigorous convergence analysis and a detailed discussion on the trade-offs between the number of iterations and the accuracy of surrogate construction required for optimal step size adjustment.

3. We validate the effectiveness of our proposed method through extensive numerical experiments across various applications. The results confirm the advantages of the proposed algorithm, showcasing its potential to significantly improve the performance of gradient-free optimization methods.

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Physics-informed neural networks assisted operator inference framework for noisy data

Sandeep Bukka[1,2], **Pawan Goyal**[2], **and Peter Benner**[2]

[1]*National Energy Technology Laboratory, 626 Cochran Mill Road, Pittsburgh, PA USA*
[2]*Max Planck Institute for Dynamics of Complex Technical Systems, 39106 Magdeburg, Germany*

The framework of operator inference is used to build a reduced order model directly from data and to make use of the knowledge at the level of partial differential equations. However, the operator inference approach is sensitive to noise and poses a significant challenge, particularly in approximating the derivative information. In this work, we propose the construction of reduced-order models via operator inference for noisy data, which is two fold. First, we clean the data by constructing an implicit neural representation of data such that the output of the implicit neural network is not only in the vicinity of the noisy measurement but also enforces the known form of the partial differential equation. Consequently, we obtain denoised data, which, in the next step, is used to construct reduced-order models via operator inference. The performance of the proposed approach is investigated using two numerical examples, and a comparison with operator inference applied to low-pass filtered data is presented.

Rapid 3D Green's functions using reduced-order models of physics-based seismic wave propagation simulations

J. M. Rekoske[1], D. May[1], and A.-A. Gabriel[1]

[1]*Institute of Geophysics and Planetary Physics, Scripps Institution of Oceanography, University of California, San Diego*

Elastodynamic Green's functions are essential in seismology, and form a connection between direct observations of seismic waves and earthquake sources. They are key to enabling various seismological tasks, including physics-based ground motion prediction and kinematic or dynamic source inversions. In regions with comparably well-constrained 3D models of the Earth's elastic structure, such as Southern California, approximate 3D Green's functions can be computed using physics-based numerical simulations of seismic wave propagation. However, these simulations are computationally expensive, which presents a challenge for real-time ground motion prediction (e.g., ShakeMap and ShakeAlert), physics-based Probabilistic Seismic Hazard Assessment (PSHA, e.g., CyberShake), and uncertainty quantification in source inversions. Here, we address this challenge by using a reduced-order model (ROM) which enables rapid computation of approximate Green's functions by using the proper orthogonal decomposition combined with radial basis function interpolation. We train the ROM using three-component seismograms for six elementary moment tensors, computed with SeisSol, selecting 500 source locations to calculate 1.0 Hz elastodynamic Green's functions for approximately 10,000 sites in southern California. Using leave-one-out cross-validation, we assess the accuracy of our Green's functions for the SCEC CVM-S4.26-M01 velocity model in both the time domain and frequency domain. We show that the ROM can accurately and rapidly reproduce simulated seismograms for generalized moment tensor sources in our 3D region, as well as kinematic sources by using a finite fault model of the 1987 Mw 5.9 Whittier Narrows earthquake as an example. In these demonstrators, the accuracy is quantified using the mean absolute error of the velocity waveforms and the Fourier amplitude spectra. We envision that our rapid Green's functions would be useful for physics-based PSHA, improving the uncertainty quantification in earthquake source inversions, and constructing rapid ShakeMovies with high spatial resolution.

Construction of nonlinear models from input-output data for atmospheric pollution simulations

Dimitrios Xylogiannis[1], **Charles Poussot-Vassal**[1], **and Claire Sarrat**[1]

[1] *Onera-The French Aerospace Lab, Toulouse, France*

Atmospheric pollution models are essential for understanding and predicting episodes of high concentration that may occur in a defined area (e.g., cities, sensitive areas such as industrial sites, etc.). These models typically involve complex, heterogeneous, and multi-scale dynamics and physical phenomena, whose simulation results in significant computational time. In order to produce forecasts and estimate of local air pollution more quickly, it is relevant to develop dynamic reduced order models that can be quickly and easily used in place of complex and expensive simulators. Typical applications include observer design, parametric optimization, and potentially closed-loop control design, for which many query model-based processes are usually needed.

In this work, based on simulation outputs of limited time-domain data, the goal is to construct nonlinear structured models (e.g. bilinear, quadratic and quadratic-bilinear). The considered time-domain data consists of input-output pairs based on pollutant dispersion simulations of a real, documented with observations, event of atmospheric pollution. The proposed methodology aims to construct a nonlinear model in a non-intrusive way. First, from the input-output data we built a linear model using the Pencil method described in [2]. Due to the large complexity of the model its order is reduced by applying the Loewner Framework [3]. The states of the identified reduced linear model are combined with the original input-output data in order to enrich the model structure with nonlinear terms, by solving a least-square problem similar to [1]. Convergence conditions of the proposed sequential process are provided, thus providing a framework for this configuration setup. Finally, the conducted simulations and the constructed reduced models are validated through comparison with output observations. Last but not least, the considered setup data will be made available to the research community.

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Data-driven Model Reduction via Block-structured Operator Inference for Coupled Aeroelastic Flutter

Benjamin G. Zastrow[1], **Anirban Chaudhuri**[1], **and Karen E. Willcox**[1]

[1] *The University of Texas at Austin*

This work presents a data-driven, physics-informed reduced-order modeling (ROM) approach for computationally efficient prediction of coupled aeroelastic flutter. We develop a coupled ROM based on the operator inference method [2] with embedded physics-based knowledge. We use a full-order model for flutter simulation that couples a high-dimensional computational fluid dynamics (CFD) solver with a modal decomposition from a finite element model to generate the snapshots. We infer both the structural dynamics and the fluid dynamics reduced operators via the solution of least squares problems to learn a block-structured coupled ROM of the form

$$\begin{bmatrix} \dot{\widehat{\mathbf{q}}}_{\mathrm{s}} \\ \dot{\widehat{\mathbf{q}}}_{\mathrm{f}} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \widehat{\mathbf{c}}_{\mathrm{f}} \end{bmatrix} + \begin{bmatrix} \widetilde{\mathbf{A}}_{\mathrm{s}} & \widehat{\mathbf{E}}_{\mathrm{sf}} \\ \widehat{\mathbf{E}}_{\mathrm{fs}} & \widehat{\mathbf{A}}_{\mathrm{f}} \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{q}}_{\mathrm{s}} \\ \widehat{\mathbf{q}}_{\mathrm{f}} \end{bmatrix}, \tag{1}$$

where $\widehat{\mathbf{q}}_{\mathrm{s}}$ and $\widehat{\mathbf{q}}_{\mathrm{f}}$ are the structural and fluid reduced state vectors, $\widehat{\mathbf{c}}_{\mathrm{f}}$ is the constant fluid reduced operator, $\widetilde{\mathbf{A}}_{\mathrm{s}}$ is the linear structural dynamics operator, $\widehat{\mathbf{A}}_{\mathrm{f}}$ is the linear fluid dynamics operator, and $\widehat{\mathbf{E}}_{\mathrm{sf}}$ and $\widehat{\mathbf{E}}_{\mathrm{fs}}$ are the linear coupling operators. We incorporate intrusive knowledge of the structural dynamics operator, $\widetilde{\mathbf{A}}_{\mathrm{s}}$, from the modal decomposition, thus eliminating the need to infer it. The remaining operators ($\widehat{\mathbf{c}}_{\mathrm{f}}, \widehat{\mathbf{A}}_{\mathrm{f}}, \widehat{\mathbf{E}}_{\mathrm{sf}}, \widehat{\mathbf{E}}_{\mathrm{fs}}$) are learned non-intrusively. The block structure allows us to effectively combine intrusive and non-intrusive learning for the coupled ROM and enables improved inference of the coupling and fluid dynamics operators with limited training snapshots. We demonstrate our method on the AGARD 445.6 wing [3], a canonical large-scale aeroelastic prediction testbed problem. We use NASA's FUN3D CFD solver with its aeroelasticity capability [1] to couple the structural and fluid dynamics to generate our full-order model snapshots.

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Non-intrusive reduced order models for geophysics applications: Adaptive sampling for the small data regime

Dave A. May[1]

[1] *University of California San Diego, Scripps Institution of Oceanography, Institute of Geophysics and Planetary Physics*

Physics-based models defined by conservation laws are ubiquitous within geophysics, with the majority being parametric Partial Differential Equations (PDEs). Such PDEs are used in both forward and inverse modelling contexts. In the "forward" context, the objective is often to explore the parameter-to-observable map so as to: identify and classify dynamical regimes; scaling laws; and or to conduct a global sensitivity analysis. In the "inverse" context, the objective is typically parameter estimation, and if adjoint methods are adopted, a by-product is the capability to efficiently perform a local sensitivity analysis. Whether exploring the parameter-to-observable map, or solving an inverse problem, many evaluations of the forward model are required, a situation which can be computationally prohibitive for very large scale simulations. In this work, the many-query scenario is made computationally tractable by employing a data-driven, non-intrusive reduced order model (ROM) - specifically the interpolated Proper Orthogonal Decomposition (iPOD).

There are numerous application areas within geophysics where non-intrusive ROMs are highly beneficial. However, exploiting non-intrusive reduced order models in geophysics appears to be in its infancy. Here I will present two distinct geophysical applications where iPOD has been successfully applied. The first application concerns modeling the thermal structure within a subduction zone. Here the forward model is non-linear and consists of a coupled set of elliptic and parabolic PDEs that describe viscous flow and the conservation of energy. The second application considers the modeling of ground motion generated by seismic waves originating from an earthquake. The forward model in this application consists of the linear elastic wave equation, with a sub-surface 3D velocity model and topography consistent with Southern California. Despite the highly distinct application contexts and the PDEs defining the forward model, the iPOD ROM is both accurate and highly efficient.

The offline cost of building these non-intrusive ROMs is non-negligible as the forward models are computational expensive. In a very practical sense, the number of forward models allowed to be executed is finite due to the computational resources they require. Hence, in order to minimize the offline cost, I compare several new techniques for constructing iPOD ROMs adaptively, in which adaptivity in parameter space is driven by an error estimate of the difference between the high-fidelity model and the ROM.

Wavelet-based Dynamic Mode Decomposition in the context of Extended Dynamic Mode Decomposition and Koopman Theory

C. Tilki[1] **and S. Gugercin**[1]

[1] *Department of Mathematics, Virginia Tech, Blacksburg, 24061, VA, United States*

Dynamic mode decomposition (DMD) [3] is extensively used in data-driven modeling of dynamical systems where the data is sampled from a dynamical system of the form

$$\dot{\boldsymbol{x}} = \mathcal{T}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{M} \subseteq \mathbb{R}^n.$$

The analytical connection between DMD and the *Koopman theory* has paved the way for the Extended DMD algorithm (EDMD) [4]. In simplest terms, EDMD can be considered as constructing an approximation of the Koopman operator on a finite-dimensional subspace. This subspace is predetermined, mostly by designating the *observables* $\psi : \mathcal{M} \to \mathbb{C}^M$. In short, given the time-domain data $\{\boldsymbol{x}(t_i)\}_{i=0}^N \subseteq \mathcal{M}$, EDMD proceeds by solving the least squares problem

$$\boldsymbol{K} = \underset{\hat{\boldsymbol{K}} \in \mathbb{C}^{M \times M}}{\arg\min} \ \|\Psi_1 - \hat{\boldsymbol{K}}\Psi_0\|_F^2 \qquad \text{for } \Psi_j := \begin{bmatrix} \psi(\boldsymbol{x}(t_j)) & \psi(\boldsymbol{x}(t_{j+1})) & \dots & \psi(\boldsymbol{x}(t_{j+N-1})) \end{bmatrix},$$

where $\boldsymbol{K}$ inherits a finite-dimensional approximation to the underlying Koopman operator. In practice choosing good observables ψ is a big challenge. To overcome this problem one can employ strategies from the signal processing domain and use *wavelets* as a candidate for these observables. This idea of incorporating wavelets was proposed in [2] leading to the so-called Wavelet-based DMD (WDMD).

WDMD considers an input-output dynamical system and does not assume access to the state data $\boldsymbol{x}(t_i)$, but only to input-output data $\{\boldsymbol{u}(t_i), \boldsymbol{y}(t_i)\}$. Then by using *discrete wavelet transform* (DWT) at the samples of output trajectory $\boldsymbol{y}(t_i)$ WDMD obtains auxiliary state variables to perform DMD.

In this work, we prove that the EDMD algorithm with wavelets coincides with a specific case of WDMD, up to an error introduced by DWT, thus establishing the analytical connection to the Koopman theory. This theoretical connection clarifies how WDMD needs to be modified for approximating non-linear input-output systems. Mainly to have convergence guarantees, one needs to consider bilinear approximations [1]. One can achieve this by employing linear parameter-varying (LPV) methods. It has been shown that this framework can be used in the bilinear approximation of the *input-parametrized* Koopman operator for the continuous-time dynamical systems [1]. In that vein, we propose a bilinear generalization of WDMD for guaranteeing convergence properties when the system is control-affine.

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Surrogate modeling for data-scarce applications using projection-based multifidelity linear regression

V. Sella[1], **J. Pham**[1], **K. Willcox**[1], **and A. Chaudhuri**[1]

[1] *University of Texas at Austin, TX 78712, USA*

Tasks in science and engineering such as uncertainty quantification, risk analysis, optimization, and sensitivity analysis, that require many queries of an expensive-to-evaluate model, are often hindered by computational cost constraints. One strategy to alleviate the computational cost burden involves the development of surrogates, such as linear regression models aimed at approximating outputs from the high-fidelity model. Nevertheless, accurate surrogate modeling poses a persistent challenge, particularly in the low data regime for high-dimensional problems. This work presents projection-based multifidelity (MF) approaches for multivariate linear regression for data-scarce applications with high-dimensional outputs. We tackle the sparse data issue by projecting the outputs to a lower-dimensional subspace through proper orthogonal decomposition basis vectors and using information from multiple models of varying cost and fidelity. The proposed MF linear regression approaches leverage many training data points from multiple low-cost, lower-fidelity information sources with few training data points from the high-fidelity source.

We implement and contrast two projection-enabled MF linear regression methods. First, we show an additive approach based on the Kennedy-O'Hagan [1] framework. Second, we propose a data augmentation approach that merges both high-fidelity and low-fidelity datasets into a single training set in two ways: (i) directly using the low-fidelity data and (ii) using an explicit linear regression mapping between low-fidelity and high-fidelity data. We assign user-defined weights to each dataset corresponding to the fidelity levels of the models. Subsequently, the multifidelity linear regression model is trained utilizing weighted least squares. The multifidelty setup using data augmentation enables the fitting of higher-order polynomials by utilizing the larger sample pool available from the low-fidelity models along with the high-fidelity data in a single training phase.

We apply the projection-enabled MF linear regression methods to approximate the surface pressure field on a hypersonic vehicle in flight. The projected MF linear regression using data augmentation outperforms the single-fidelity linear regression in the low data regime of $3 - 10$ high-fidelity samples with an improvement in the range of approximately $3 - 12\%$ in median accuracy for similar computational cost with higher accuracy gains for lower number of high-fidelity samples.

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Reduced-order modeling as a catalyst and enabler for digital twinning in process and chemical engineering

Peter Benner[1] **and Ion Victor Gosea**[1]

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106, Magdeburg, Germany, email: benner,gosea@mpi-magdeburg.mpg.de*

A digital twin (DT) is a digital model of an intended or actual real-world physical product, system, or process (physical twin) that serves as the effectively indistinguishable digital counterpart of it for various practical purposes. In line with advances in many industrial sectors, the confluence of Industry 4.0 principles, digital transformation initiatives, and the accuracy of mathematical modeling techniques have collectively triggered an increase in the exploration of DTs in process engineering [1]. The application of DTs offers benefits such as enabling real-time monitoring, facilitating predictive maintenance through future state prediction, supporting process design and optimization, or improving control mechanisms. Model order reduction and reduced-order modeling (RoMod) can be viewed as enabling tools for the construction of reliable DTs. Lowering the complexity of the original system, i.e., the number of degrees of freedom, allows for increasing the speed of model execution while maintaining the required accuracy & predictability. A key feature of most RoMod approaches is the data-driven aspect, which alleviates the need to explicitly access the (complex) model. These are especially important when a large number of evaluations are needed from a complex/large simulation model, which is required to be continuously updated based on changes in parameters and operating conditions.

In this work, we address the challenge of RoMod of dynamical systems in the field of process engineering, by employing RoMod and scientific machine learning (SciML) techniques. One method of interest is operator inference (OpInf) [5], a non-intrusive data-driven method for learning dynamical systems from time-domain data. The other approach to be applied here is SINDy, which enables the discovery of governing equations from data by sparse identification of nonlinear systems. By harnessing some latest developments of these methods [4, 2], robust stable quadratic surrogate models are inferred directly from data. The test case investigated here is driven by carbon dioxide (CO_2) methanation i.e., the conversion of CO_2 to methane, which facilitates the recycling of CO_2 emissions and enables green carbon processing. However, this reaction is strongly exothermic creating a major bottleneck for dynamic operation. Based on an intricate mathematical model of a reactor, we apply the proposed methods for real-time collected data and investigate the behavior of the ROMs for different operating conditions, together with their predictive capabilities [3]. We compare results to other, classical ML methods and present a detailed conclusion towards the goal of implementing a DT infrastructure.

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Enabling Model Reduction of Meshless Nonlocal Methods via Modal Reference Spaces

Steven N. Rodriguez[1], Steven L. Brunton[2], Liam K. Magargal[3], Parisa Khodabakhshi[3], Justin W. Jaworski[4], Nicole A. Apetre[1], John C. Steuben[1], John G. Michopoulos[1], and Athanasios P. Iliopoulos[1]

[1] *U.S. Naval Research Laboratory*
[3] *University of Washington*
[3] *Lehigh University*
[4] *Virginia Tech*

Meshless nonlocal methods (MNMs) are versatile computational frameworks that enable effective modeling and simulation of complex multiphysics phenomena involving large-deforming numerical domains, e.g., magnetohydrodynamics in astrophysics, free-surface and multiphase flows in additive manufacturing, etc. However, MNM methods can be more computationally expensive than mesh-based counterparts due to their dense and unstructured numerical stencil. Recent progress has been made to reduce the computational cost of meshless numerical methods by Rodriguez et al. [1] via Projection Tree Reduced-Order Modeling (PTROM). However, their approach relies on low-dimensional manifold discovery techniques built for mesh-based methods and assumes non-mixing and structured numerical topology. Therefore, this approach cannot project dynamics onto a low-dimensional subspace that is directly discovered from unstructured and mixing numerical points, as illustrated in Figure 1.

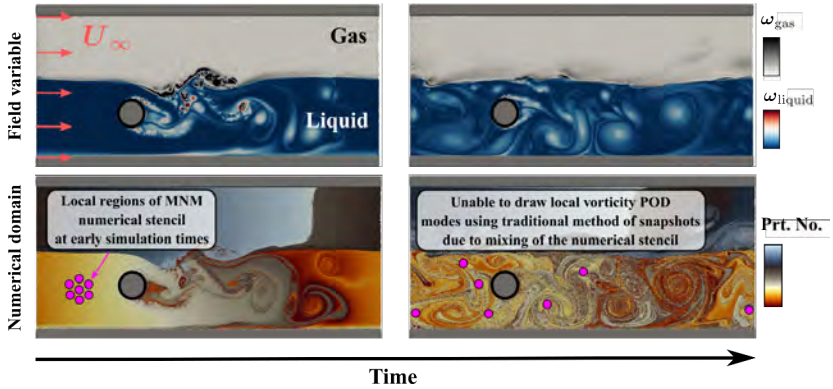

Figure 1: Snapshots of field variable time evolution (top row) and snapshots of numerical domain time evolution (bottom row).

The present work focuses on addressing the limitations of PTROM with unstructured data via reference modal spaces, akin to reference finite elements. The presented approach is designed to construct low-dimensional projection maps on reference spaces where a meshless numerical topology can dynamically evolve. The proposed projection approach is showcased on smoothed-particle hydrodynamic simulations with significant numerical point mixing such as natural convection instabilities, vortex flows, and surface tension-driven phenomena often seen in multiphase flows.

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Oblique projection for scalable rank-adaptive reduced-order modeling of nonlinear stochastic PDEs with time-dependent bases

Hossein Naderi[1] **and Hessam Babaee**[1]

[1]*Department of Mechanical Engineering and Materials Science, University of Pittsburgh, 3700 OâHara Street, Pittsburgh, PA 15213, USA*

Time-dependent basis reduced order models (TDB ROMs) have successfully been used for approximating the solution to nonlinear stochastic partial differential equations (PDEs). For many practical problems of interest, discretizing these PDEs results in massive matrix differential equations (MDEs) that are too expensive to solve using conventional methods. While TDB ROMs have the potential to significantly reduce this computational burden, they still suffer from the following challenges: (i) inefficient for general nonlinearities, (ii) intrusive implementation, (iii) ill-conditioned in the presence of small singular values, and (iv) error accumulation due to fixed rank. To this end, we present a scalable method for solving TDB ROMs that is computationally efficient, minimally intrusive, robust in the presence of small singular values, rank-adaptive, and highly parallelizable. These favorable properties are achieved via oblique projections that require evaluating the MDE at a small number of rows and columns. The columns and rows are selected using the discrete empirical interpolation method (DEIM), which yields near-optimal matrix low-rank approximations. We show that the proposed algorithm is equivalent to a CUR matrix decomposition. Numerical results demonstrate the accuracy, efficiency, and robustness of the new method for a diverse set of problems using both explicit and implicit time integration methods [1].

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Randomized Local Model Order Reduction for Nonlinear Partial Differential Equations

M. Whitby [1] **and K. Smetana**[1]

[1] *Stevens Institute of Technology*

The importance of developing accurate and efficient numerical simulations for large multiscale systems is apparent in applications such as monitoring the structural integrity of engineering systems and creating digital twins. Often, these applications require working with complex problems, which may involve the need for multiple solutions, rapidly varying strongly heterogeneous coefficients, or geometrically varying domains. In these cases, the implementation of finite elements and finite volumes can prove to be computationally infeasible or exceed the permissible time frame. Localized model order reduction (MOR), which includes combinations of domain decomposition, reduced basis, and multiscale methods, is often used to circumnavigate these issues. Central to this approach is the need for an efficient and easily implemented methodology for selecting local spaces that yield a (quasi-) optimally convergent approximation. For linear problems, optimal local approximation spaces are found by taking the leading left singular vectors of a transfer operator that maps boundary data on the boundary of the oversampling domain to the respective solution restricted to the target domain [1, 2]. As this concept of optimality does not transfer to nonlinear operators, we consider the range of the transfer operator when applied to a bounded set. We may then use a POD or the Greedy algorithm to construct a (quasi-) optimal reduced space to approximate this set. However, due to the high-dimensional parameter set (which is the same dimension as the dimension of the high-fidelity discretization space on the boundary of the oversampling domain) these algorithms suffer from the curse of dimensionality [3]. Therefore, in this talk, we present and analyze a randomized Greedy algorithm for the construction of local reduced basis spaces.

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Extracting Markovian description of high-dimensional dynamics via Mori-Zwanzig formalism

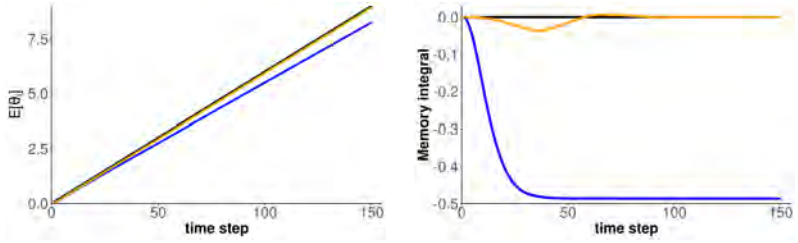
N. Stauffer[1,2], H. Gorji[1], and I. Lunati[1]

[1] *Laboratory for Computational Engineering, Empa, Dübendorf, Switzerland*
[2] *Chair of Computational Mathematics and Simulation Science, EPFL, Switzerland*

Developed in the context of statistical mechanics, the Mori-Zwanzig (MZ) formalism [1] provides a rigorous model reduction technique, where only a subset of variables is tracked in time (t). By virtue of the projection operator (P), the Liouvillian (L) of the resolved variable (θ) is split according to

$$\frac{d\theta_j}{dt} = b_j(\theta) = \overbrace{e^{Lt}Pb_j}^{\text{Markovian term}} + \overbrace{\int_0^t e^{(t-s)L}PLe^{s(1-P)L}(1-P)Lb_j ds}^{\text{Memory integral}} + \overbrace{e^{t(1-P)L}(1-P)b_j}^{\text{Noise}}, \quad (1)$$

where the Markovian term depends only on the current value, the memory depends on the whole history, and the noise term is orthogonal to the projected space. The latter requires the full knowledge of the system. Even though formally well defined, the memory integral is the main computational bottleneck of the MZ formalism. Its computational cost is similar to that of the original high-dimensional system and its explicit computation involves solving the orthogonal dynamics [1]. As a consequence, the memory integral has been approximated by different approaches [1] (see Fig.1). However, there is still lack of flexible and reliable computational treatment of the memory integral, hindering the applicability of the MZ formalism for high-dimensional systems. To tackle this challenge, in this study, we reduce



(a) (b)

Figure 1: Application of the MZ formalism to a Kuramoto model using different approximations for the memory integral and orthogonal dynamics generated by $(1-P)L$. (a) Evolution of the resolved variable θ_i, (b) Memory integral. Exact solution (blue), weak interactions limit (black), pseudo-orthogonal dynamics [1] (orange).

the corresponding computational cost by transforming the generalized Langevin system (1) into a quasi-Markovian one by exploring two paths: a) we derive a cascade of MZ equations for the successive memory kernels until the contribution of the kernel can be neglected; and b) we leverage the idea of dynamic low-rank approximation in order to contain the memory kernel arising from the conditional expectation projector P. This results in an optimization problem aiming to look for the optimal transformation, while minimizing the memory integral in the transformed space.

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Linear and Non-linear Reduced Dimensional Manifolds for Global Weather Predictions

Amirpasha Hedayat[1] **and Karthik Duraisamy**[1]

[1] *Computational Aerosciences Laboratory*
Department of Aerospace Engineering
University of Michigan
Ann Arbor, MI 48109, USA

Weather prediction poses significant challenges due to the complex and chaotic nature of atmospheric dynamics. While advanced AI models have shown promise in this area [1, 2], they often require extensive computational resources and training time. In this work, we explore alternatives to large Neural Operator/Transformer-based models by extracting reduced dimensional manifolds and inferring time-evolving operators on these manifolds. Dimensionality reduction techniques that we explored include Proper Orthogonal Decomposition, Convolutional Autoencoders, and different types of hybrid architectures. To further enhance the model's capability, we augment the state space with time-delayed states. Our approach, tested on the ERA5 benchmark data [3], shows promising results in predicting the dynamics for short-range weather forecasts (about 5 days), though challenges persist with medium-range predictions, as with existing approaches.

Particularly, our study highlights the effectiveness of a simple linear time-delayed model, as more advanced neural operator/transformer-based architectures offer only marginally better accuracy while imposing a computational burden that is several orders of magnitudes larger. We also observed that projection error is the primary contributor to the overall prediction error, indicating that the inference error is a relatively small contributor.

These findings suggest that, with further refinement, our framework could serve as an efficient base predictor for weather systems with the residuals being potentially modeled using modern, heavy-duty machine learning architectures. Our work also reinforces the notion that modern ML/AI architectures require better baselines to demonstrate accuracy and effectiveness, and can potentially greatly benefit from simple structures imposed on the architectures.

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4.3 Posters for Thursday, September 12

ML based surrogate modeling for collisional radiative model in plasma disruption mitigation

Xuping Xie[1], **Qi Tang**[1], **and Xianzhu Tang**[1]

[1]*Los Alamos National Laboratory*

Collisional-radiative (CR) models describe the atomic processes in a plasma by tracking the population density in ground and excited states for each charge state of the atom/ion. These models predict important plasma properties such as charge state distributions and radiative emissivity and opacity. Accurate descriptions of the CR balance of the plasma are essential in fusion whole device modeling, especially when significant impurities are introduced into the plasmas. In a coupled plasma and CR simulation, the CR model, which is a high-dimensional ODE, is solved on each grid point for the plasma solver, and can overwhelm the plasma simulation cost. In this work, we introduce a machine learning (ML) based method that discovers a latent space and learns its corresponding reduced order modeling (ROM) dynamics that can capture the essential physics to make accurate predictions of the quantities of interest, at much reduced online computational cost.

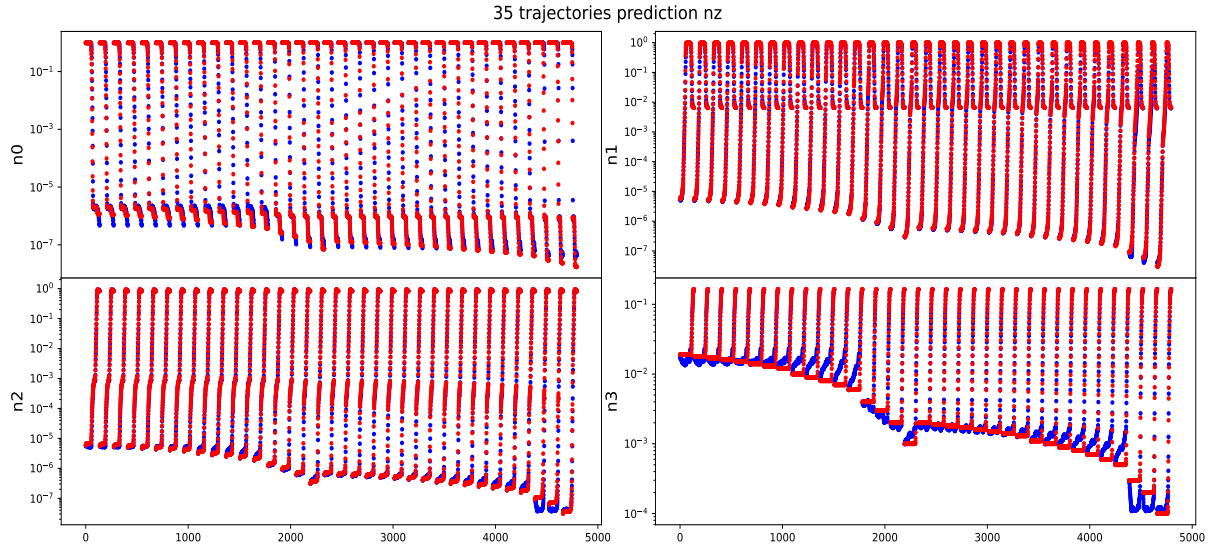

Figure 1: Trajectory prediction from the learned latent dynamics of the CR model

Predicting dynamics in time and parameter space with deep learning and data augmentation

Shuwen Sun[1], **Lihong Feng**[1], **and Peter Benner**[1,2]

[1] *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
[2] *Otto von Guericke University, Magdeburg, Germany*

Analyzing dynamics of a system by numerically solving a large parametric nonlinear dynamical system is challenging due to its high complexity and the high computational costs involved. Conventional model order reduction (MOR) based on projection relies on the full knowledge of the system and its dynamical behaviour. Non-intrusive or data-driven MOR methods extend their applicability in various situations. In recent years, machine learning-aided MOR methods are being actively researched [2, 1]. Solely based on data, a nonlinear mapping between the physical and the reduced space can be constructed via neural networks (NNs). However, many methods fail in accurate generalization in the whole time interval $[0, T]$, when the training data is available only in a training time interval $[0, T_0]$, with $T_0 < T$.

To achieve better extrapolation in time domain, we propose two new frameworks by combining kernel dynamic mode decomposition (kDMD) [3] with neural networks. In the first basic framework, the convolutional autoencoder (CAE) is responsible for compressing the data into a latent space. Meanwhile, a feed-forward neural network (FFNN) learns the latent variables from the physical parameters and time. CAE-FFNN is trained in the training time interval $[0, T_0]$. At the online stage, FFNN first learns the latent dynamics in $[0, T_0]$ at any testing parameter, then passes them to kDMD for dynamics evolution in the out-of-training time period $(T_0, T]$. The decoder then reproduces physical dynamics in the whole time interval $[0, T]$. This framework, referred to as CAE-FFNN-kDMD, can predict nonlinear parametric dynamics quickly and accurately. The second framework aims to further enhance the extrapolation capability of the first framework. During the training stage, kDMD derives the latent variables in $(T_0, T]$ based on the latent data in $[0, T_0]$ obtained from the encoder. The decoder is used to recover the physical dynamics from the latent variables in $(T_0, T]$. Those recovered physical data in $(T_0, T]$ are combined with the original training data in $[0, T_0]$ to retrain CAE-FFNN without regenerating any new data in $(T_0, T]$ from the original model. During the online prediction, this retrained FFNN is only combined with the retrained decoder for more accurate time-domain generalization. These two frameworks are tested on two examples: a FitzHugh-Nagumo model and a model of incompressible flow past a cylinder. Numerical results show their promising prediction performance in both the time and the parameter domain.

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Wasserstein-robust modeling of multi-scale systems: A Graph-Neural-Network coreset approach

R. Dakhmouche[1, 2], **I. Lunati**[2], **and H. Gorji**[2]

[1] *Chair of Computational Mathematics and Simulation Science, EPFL, Switzerland*
[2] *Laboratory for Computational Engineering, Empa, Dübendorf, Switzerland*

Learning the effective dynamics of multi-scale systems is a powerful approach to trade-off between model fidelity and computational cost, as recently demonstrated for regular geometries [2]. Yet, more complex settings with unstructured discretizations, and presence of noise, require more tailored schemes. We devise a model reduction approach leveraging time-varying Graph Neural Networks (GNNs) to address these challenges. Our scheme integrates a Bayesian coreset algorithm to down-sample the discretization graph in an adaptive probabilistic way. This leads to a multi-scale embedding of the spatial-features, which can then be efficiently evolved in time using recurrent neural networks. The model is trainable in an end-to-end fashion allowing improved feature learning. Besides, to enhance the robustness of the proposed model, we leverage a distributionally robust loss [1] given by

$$\mathcal{L}(\theta) = \sup_{\mathbb{Q}\in\hat{\mathcal{P}}_N} \mathbb{E}^{\mathbb{Q}}\left[(Y - f_\theta(X))^2\right],$$

where $\theta \in \mathbb{R}^p$ is the training parameter and $\hat{\mathcal{P}}_N$ is the 2-Wasserstein ball centered at the empirical distribution of the training data $\hat{\mu}_{(X,Y)}$. As shown in Figure 1, the robustness of the Wasserstein metric

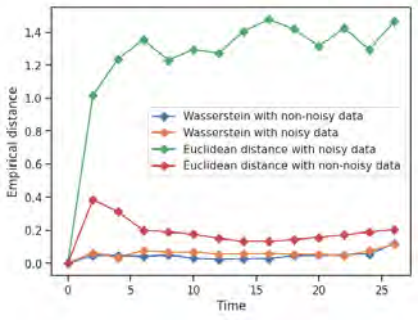

Figure 1: Distance between estimated and ground-truth data distribution in Kuramoto dynamic.

in comparison to the standard Euclidean L^2 norm motivates the training via the Wasserstein distance. We validate the performance of the approach on two canonical models: the Kuramoto system of ODEs and an advection fluid model around a circular cylinder. Additionally, we provide a comparison against a single-scale GNN baseline.

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Forward Model Emulator for Atmospheric Radiative Transfer Using Gaussian Processes And Cross Validation

Otto Lamminpää[1], Jouni Susiluoto[1], Jonathan Hobbs[1], James McDuffie[1], Amy Braverman[1], and Houman Owhadi[2]

[1] *NASA Jet Propulsion Laboratory, California Institute of Technology*
[2] *California Institute of Technology*

Remote sensing of atmospheric carbon dioxide (CO2) carried out by NASAâs Orbiting Carbon Observatory-2 (OCO-2) satellite mission and the related Uncertainty Quantification (UQ) effort involves repeated evaluations of a state-of-the-art atmospheric physics model. The retrieval, or solving an inverse problem, requires substantial computational resources. In this work, we propose and implement a statistical emulator to speed up the computations in the OCO-2 physics model. Our approach is based on Gaussian Process (GP) Regression, leveraging recent research on Kernel Flows ([1]) and Cross Validation to efficiently learn the kernel function in the GP. We demonstrate our method by replicating the behavior of OCO-2 forward model within measurement error precision, and further show that in simulated cases, our method reproduces the CO2 retrieval performance of OCO-2 setup with orders of magnitude faster computational time. The underlying emulation problem is challenging because it is high dimensional. It is related to operator learning in the sense that the function to be approximated is mapping high-dimensional vectors to high-dimensional vectors. Our proposed approach is not only fast but also highly accurate (its relative error is less than 1%). In contrast with Artificial Neural Network (ANN) based methods, it is interpretable and its efficiency is based on learning a kernel in an engineered and expressive family of kernels.

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An application of a posteriori error quantification for physics-informed neural networks

B. Hillebrecht[1] **and B. Unger**[1]

[1] *SimTech, University of Stuttgart*

Modeling a system by a physics-informed neural network (PINN) is beneficial compared to using a purely data-driven neural network because it incorporates a priori knowledge about the system dynamics. This a priori knowledge and the extended network training strategy can also be used to develop an a posteriori error estimator of the neural network prediction [1, 2]. Technical details aside, this means in particular that for a system governed by the abstract linear differential equation

$$\begin{aligned} \dot{x}(t) &= \mathcal{A}x(t), \\ x(0) &= x_0, \end{aligned}$$

with the PINN-determined solution denoted by $\hat{x}(t)$ the prediction error of the PINN can be estimated by the following formula

$$\|\hat{x}(t) - x(t)\| \leq M\|x_0 - \hat{x}(0)\|\mathrm{e}^{\omega t} + \int_0^t M\mathrm{e}^{\omega(t-s)}\|\dot{\hat{x}}(t) - \mathcal{A}\hat{x}(t)\| \,\mathrm{d}s.$$

All terms containing the norm on the right-hand side can be determined without knowledge of the solution of the original system. However, the system-dependent parameters M and ω can only be determined by understanding the original operator semigroup $\mathcal{S}(t)$ generated by $\mathcal{A}$. This information is conventionally not accessible or determined for real-world problems goverened by PDEs.

To overcome this, we extend the Trotter-Kato approximation theorem [3] to derive the parameters M, ω from finite dimensional approximations. We perform an additional extension of the theorem which incorporates control operators to compute the parameters describing the impact of errors in the boundary condition on the prediction accuracy of the neural network.

We illustrate the results using an application which is governed by a PDE on a complex geometry.

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Neural latent dynamics models

S. Fresca[1], **N. Farenga**[1], **and A. Manzoni**[1]

[1]*MOX - Department of Mathematics, Politecnico di Milano, P.zza Leonardo da Vinci 32, 20133 Milano, Italy*

Solving differential problems using full order models (FOMs), like the finite element method, incurs prohibitively computational costs in real-time simulations and multi-query routines. Reduced order modeling aims at replacing FOMs with reduced order models (ROMs), that exhibit significantly reduced complexity while retaining the ability to capture the essential physical characteristics of the system.
In this respect, the novel concept of the Latent Dynamics Problem (LDP) is introduced and the class of Latent Dynamics Models (LDMs), along with their specialized deep learning counterpart, Neural Latent Dynamics Models (NLDMs) is presented. NLDMs constitute a neural differential equations-based model architecture designed for continuous-time modeling. This architecture is embedded within a reduced order modeling framework, with the primary objective of capturing the latent, low-dimensional dynamics of high-dimensional dynamical systems.
In a series of numerical experiments, the effectiveness of NLDMs in addressing challenging problems is demonstrated, particularly in the context of large-scale high-fidelity models governed by time-dependent parameterized PDEs. The results not only underscore the remarkable performance of NLDMs but also highlight their potential as a valuable tool for understanding and modeling complex dynamic systems.

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Physics-Informed Machine Learning for Surrogate Modeling of Ultrasonic Guided Wave Propagation in Pipeline Health Monitoring

Sandeep Bukka[1,2], Nageswara Lalam[1,2], Ruishu Wright[1], Pengdi Zhang[3], and Paul Ohodnicki[3]

[1] *National Energy Technology Laboratory, 626 Cochran Mill Road, Pittsburgh, PA USA*
[2] *NETL Research Support Contractor, 626 Cochran Mill Road, Pittsburgh, PA USA*
[3] *University of Pittsburgh, 3700 OâHara street, Pittsburgh , PA, USA*

The detection and characterization of structural defects in gas pipelines, such as welding inconsistencies, pitting, and both localized and general corrosion, present significant challenges in the maintenance and operation of these critical infrastructures. Traditional methodologies for inspecting such defects often rely on ultrasonic guided wave propagation techniques, which, while effective, are hampered by the complexity of conducting comprehensive experimental studies across the myriad conditions encountered in operational pipelines. The necessity to generate extensive datasets for the training of artificial intelligence (AI) models for corrosion detection exacerbates these challenges, as creating simulations that accurately reflect the diverse and complex nature of pipeline defects demands considerable computational resources and time. Addressing these challenges necessitates an innovative approach that can circumvent the computational bottlenecks associated with conventional simulation-driven AI training methods. Physics-informed machine learning (PIML) emerges as a transformative solution, offering a framework that integrates domain-specific physical laws directly into the learning process.The implementation of a Physics-Informed Machine Learning (PIML) framework, despite its initial higher financial investment, presents a singular expenditure for the designated domain, enabling rapid inference capabilities that can encompass a broad spectrum of scenarios. These scenarios notably include various forms of corrosion across different locales. In this context, the introduction of Physics-Informed Neural Operators, as pioneered by [1], marks a significant advancement. This novel approach has been adeptly applied within the current study to emulate the propagation of ultrasonic guided waves in gas pipelines, a critical component in identifying a range of physical anomalies. Moreover, this work endeavors to build upon the previous work conducted by [2], which utilized Finite Element Modeling (FEM) to explore similar phenomena. By integrating more sophisticated physics-informed neural operators, our study not only extends but also enhances the existing framework, providing a more robust and efficient computational model. Experimental validation is also carried out for the developed surrogate model. The surrogate model is trained on a range of physical defects with varying degrees of location and type of corrosion. The generated datasets from surrogate model were compared and found to be in excellent agreement with datasets generated from standard finite element based simulation framework. The cost of surrogate model is found to be at a fraction of simulations costs.

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SurMoDeL: A Deep Learning based Surrogate Model for modeling fault activation

C. Millevoi[1], C. Zoccarato[1], and M. Ferronato[1]

[1]*Dept. of Civil, Environmental and Architectural Engineering, University of Padova, Italy*

Robust geomechanical modeling is necessary to assess the safety and environmental implications of subsurface resource exploitation and management. Predictability is, however, compromised by uncertainties arising from model assumptions, variability of the governing parameters, and inaccuracies in the data. To solve this problem, sensitivity analysis and uncertainty quantification are crucial. Inverse modeling and stochastic data assimilation techniques can provide reliable outcomes in the absence of direct measurements, but the computing cost may become unaffordable when modeling fault activation, since it involves the solution of complex and large-scale problems [1].

A proxy model based on Neural Networks (NNs) is created to approximate the geomechanical outcome in a faulted reservoir application. The aim is to simulate the beginning of fault slippage that could result in an induced seismic event, by utilizing in-situ observations of the seismic moment [2]. A deterministic forward geomechanical model is used to create a set of snapshots on which the Deep Learning based Surrogate Model (SurMoDeL) is trained. The SurMoDeL turned out to accurately simulate the outputs of interest, hence to be useful for multi-query or real-time applications where quick estimation is essential. Indeed, what makes NNs effective in this context is their ability to approximate even discontinuous functions, which are required to represent the displacement field in fault activation modeling. Moreover, SurMoDeL physical consistency can also be guaranteed by requiring predictions to follow physical rules and/or imposing physics-awareness on the model. After training and validation, the proxy model is applied in order to reduce uncertainty on input parameters by means of seismic data assimilation.

This work aims to integrate deep learning with traditional modeling approaches in order to decrease uncertainty in reservoir simulations, improve prediction reliability, and enable robust simulations for design and optimization.

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VENI, VINDy, VICI: A variational method to build ROMs with embedded uncertainty quantification

J. Kneifl[1], **P. Conti**[2], **J. Fehr**[1], **A. Manzoni**[3], **A. Frangi**[2], **S. L. Brunton**[4], **and J. N. Kutz**[5]

[1]*Institute of Engineering and Computational Mechanics, University of Stuttgart, Stuttgart, Germany*
[2]*Politecnico di Milano, Department of Civil and Environmental Engineering, Milano, Italy*
[3]*Politecnico di Milano, MOX - Department of Mathematics, Milano, Italy*
[4]*Department of Mechanical Engineering, University of Washington, Seattle, United States*
[5]*Department of Applied Mathematics, University of Washington, Seattle, United States*

Numerous complex phenomena in the realms of technology and science require the solution of expensive, high-dimensional systems of partial differential equations (PDEs). Reduced order models (ROMs) have been developed to overcome this issue and accelerate the calculations [2, 4]. In scenarios involving experimental measurements or constrained access to full-order solvers, non-intrusive reduced-order modeling techniques offer a solution. However, these methods often lack interpretability and uncertainty quantification (UQ) of the predicted solutions.
Consequently, we present a data-driven, non-intrusive reduced order modeling scheme that identifies the latent dynamics in an interpretable manner while it inherently embeds UQ. Utilizing a limited dataset with high-dimensional noisy data, our proposed framework employs variational autoencoders for dimensionality reduction and a variational adaptation of sparse identification of nonlinear dynamics (SINDy) [1, 3, 2] to proficiently construct ROMs.
In detail, the method consists of **Variational Encoding of Noisy Inputs** (VENI) to identify the distribution of reduced coordinates. At the same time, we introduce **Variational Identification of Nonlinear Dynamics** (VINDy) to learn the distribution of coefficients determining the contribution of terms from a predefined set of candidate functions. Following the offline training, the identified model can be queried for new parameter instances and/or new initial conditions in order to calculate the corresponding full-time solutions. The probabilistic framework inherently facilitates UQ, as online testing involves **Variational Inference** that naturally provides **Certainty Intervals** (VICI). The performance of the proposed method is validated on a diverse set of PDE benchmarks including structural mechanics and fluid dynamics.

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Integrating Improved Neural Operators and Graph Convolutional Networks for Scalable Geological Carbon Storage Modeling

Teeratorn Kadeethum[1], Birendra Jha[2], Stephen J. Verzi[1], John D. Jakeman[1], and Hongkyu Yoon[1]

[1]*Sandia National Laboratories, New Mexico, USA*
[2]*University of Southern California, California, USA*

Introduction: The computational intensity of Full Order Models (FOM) for field-scale parameter estimation, optimization, and real-time control in subsurface modeling necessitates an alternative approach to manage computational demands effectively. Reduced Order Models (ROM) emerge as a viable solution, providing a simplified yet efficient means to approximate complex systems. However, their utility in large-scale industrial applications is often hampered by the extensive computational resources required, especially when machine learning (ML)–based ROMs are employed. This challenge is predominantly due to the need to account for each degree of freedom (DOF), which corresponds to the discretization of the problem domain and serves as input features, thereby exponentially increasing the computational load as the computational domain expands.

Methodology: Addressing the computational bottleneck, we introduce the Improved Neural Operator (INO) [1], a neural operator framework designed to enhance the performance of ROMs in large-scale settings. The INO approach involves a strategic division of the computational region into smaller, manageable subdomains during the training process, significantly reducing the size of training sets and, consequently, the computational overhead. This method efficiently handles multiple DOFs with high accuracy, even when operating within a limited subset of the computational domain. A practical application of INO to the Illinois Basin - Decatur Project underscores its effectiveness, where it achieved an average relative error of less than 1 % in pressure predictions with a relatively small training set of 90 samples over four years of geological carbon storage operation.

Challenges and Innovations: Despite its proven efficacy, the INO model encounters limitations in capturing global phenomena due to its subsampling strategy, which might overlook the extensive connectivity and complexities within geological fields. Specifically, the reliance on localized states during the training phase restricts the model's ability to comprehensively understand and predict behaviors across an entire heterogeneous permeability field. To surmount this challenge, we propose the integration of Graph Convolutional Networks (GCNs) with the INO framework. GCNs utilize graph structures to represent intricate relationships within the data, such as those in heterogeneous permeability fields, thereby enhancing the model's capacity to incorporate global impact factors while still benefiting from localized training samples.

Contribution: The proposed integration of GCNs with the INO model marks a significant advancement in the modeling of geological storage phenomena, enabling a more nuanced, accurate, and computationally efficient representation of complex subsurface environments. This breakthrough can transform the landscape of large-scale geological storage modeling, offering a scalable, accurate, and resource-efficient solution for the industry.

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Surrogate Model for Partial Differential Equations in Thin Domains

S. Iwasaki[1]

[1] *Department of Information and Physical Sciences, Osaka University, Osaka, Japan*

Spatial domain reduction theories [1] aim to reduce partial differential equations (PDEs) in high-dimensional spatial domains to those in lower–dimensional spatial domains. Within spatial domain reduction theories, there is theoretical analysis concerning the errors present in the solutions of the original PDE and the those of the spatially reduced PDE.

In this research, we propose and analyze a surrogate model with reduced learning costs and enhanced interpretability by leveraging spatially reduced partial differential equations as the dynamics within the latent space. The learning outcomes of the proposed model exhibit a clear structure comprising the "core spatially reduced PDE approximations" and "small-error neural networks," enhancing the interpretability of the results. In the presentation, we will explain the structures of proposed surrogate model and show some learning results.

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Physics-Based Uncertainty Quantification For Geophysical Problems Using Data-Driven Reduced Order Modeling

Gabrielle Hobson[1] **and Dave A May**[1]

[1]*Institute of Geophysics and Planetary Physics, Scripps Institution of Oceanography, University of California San Diego*

Subduction zones can host large earthquakes, which are capable of causing strong ground shaking and generating tsunamis. Physical models are used to better understand subduction zones processes and potential hazards. These physical models are typically computationally intensive and simulate many parametrized physical processes. Since the parameters describing these processes are representing characteristics of the deep Earth, they are naturally uncertain. Quantifying the effects of variability in model input parameters on output quantities of interest is key to understanding subduction zones and earthquake hazard. The challenge lies in the combination of a large parameter space to explore and the computational expense of the models. To address this challenge, we build reduced-order models using the interpolated Proper Orthogonal Decomposition (iPOD) [2, 5, 3, 1, 4]. We interpolate the POD coefficients using radial basis function (RBF) interpolation [6]. This method is non-intrusive, requiring no modification of the forward model code, so our framework can be readily applied to different forward models simulating a variety of physical processes in subduction zones. iPOD is also a data-driven method, so it is suitable to apply to nonlinear problems. The ROMs are $10^4 - 10^5$ times faster to evaluate than the forward model, making robust global sensitivity analysis (SA) tractable. We apply this combined ROM and SA methodology to several geophysical problems of interest, including thermal models of subduction zones and simulations of dynamic rupture during earthquakes. Given reasonable variability in model input parameters, we quantify the variability in geophysically important quantities such as the thermally-inferred width of the seismogenic zone, the moment magnitude of earthquakes, pressure-temperature conditions along slab interfaces, and characteristics of dynamic rupture during an earthquake.

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Propagation of Uncertainties in Data-driven Learning of ODEs

Aniket Jivani[1] **and Xun Huan**[1]

[1] *Department of Mechanical Engineering, University of Michigan*

There have been a number of developments in learning surrogate models and/or reduced order models of systems described by ODEs/PDEs (e.g. [5], [4] [6]) from observed or simulated snapshots of quantities of interest (QoIs). These need to go hand in hand with techniques for uncertainty quantification (UQ), especially for expensive experiments or forward model evaluations that may arise in critical applications such as space weather forecasting. The UQ aspect is critical for evaluating and improving the predictive performance of surrogate models and enabling parameter inference among other downstream tasks. Some post-hoc techniques calibrate heuristic estimates of the uncertainty to provide model-agnostic valid prediction intervals on otherwise deterministic outputs [7]. In contrast, recent works ([8], ([2], [9]), non-exhaustive list) and extensions of these have focused on a Bayesian treatment combined with known / data-learnt dynamics. These explored variational inference (VI) and Gaussian Process (GP) based-methods to enable UQ.

However, adopting such methods of uncertainty propagation remains challenging for applications with limited high-dimensional, parametrized spatiotemporal data, where extrapolation in time is desirable and inference of the true system parameters may be of interest for designing future experiments. In this work, we focus on using neural ordinary differential equations (NODEs) [1] as a surrogate model to approximate the dynamics. Specifically, we build parametrized NODEs [3] and propagate uncertainties on an exemplar problem in this setting.

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Measure Transport and Density estimation via Surrogate Models

A. Sagiv[1]

[1] *Faculty of Mathematics, Technion - Israel Institute of Technology, Haifa 32000, Israel*

Uncertainty propagation accounts for the effect of uncertain parameters in an otherwise deterministic model. Traditionally, the analysis of surrogate models in this context is done through the lens of moment approximation, or conversely, L^2 approximation. However, in many applications, the "full statistics" are required, i.e., we wish to approximate the probability density function (PDF) of the quantity of interest. In this talk, we will identify the fundamental mathematical problem underlying this computational task: if two "similar" functions pushforward the same measure, would the new resulting measures be close, and if so, in what sense? We will show how the PDF of the quantity of interest can be approximated, using a spline-based method [2] and then using more popular spectral methods [4], both with theoretical guarantees. We will then present an alternative viewpoint: through optimal transport theory, a Wasserstein-distance formulation of our problem yields a much simpler and widely applicable theory [3]. Finally, we will see how these ideas are crucial in the analysis of another core task in UQ - sampling and generative modeling [1].

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