3rd Young Mathematicians in Model Order Reduction Conference

4 – 8 March 2024

University of Stuttgart, Germany

YMMOR
2024

Organisers
Tobias Ehring | Robin Herkert
Sanath Keshav | Jonas Kneifl
Mattia Manucci | Jonas Nicodemus

Contact
ymmor.info@simtech.uni-stuttgart.de

Book of Abstracts

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Contents

1   Practical information

1.1   Location

The conference will take place at Pfaffenwaldring 5a on the campus in 70569 Vaihingen. It can be reached by **S1, S2, S3** from either Stuttgart central station as well as the airport (use exit "Universität"). From the S-Bahn stop, please follow the provided sketch to get to the SimTech building (Pfaffenwaldring 5a). The conference takes place on the ground floor in **room 0.009**.

Conference venue (Pfaffenwaldring 5a)

1.2   Talks

Each talk will last 30 minutes, 20 minutes for the presentation and 10 minutes for the subsequent discussion. You can use your own laptop or one that we provide.

1.3   Conference dinner

The conference dinner will take place on Thursday March 7, 2024 at Brauhaus Schönbuch, Bolzstraße 10, 70173 Stuttgart.

1.4   Excursion

A short hike is planned for the excursion. Please remember to wear appropriate clothing.

1.5   Local organizers

- Tobias Ehring (IANS), University of Stuttgart, tobias.ehring@ians.uni-stuttgart.de
- Robin Herkert (IANS), University of Stuttgart, robin.herkert@ians.uni-stuttgart.de
- Sanath Keshav (DAE), University of Stuttgart, keshav@mib.uni-stuttgart.de
- Jonas Kneifl (ITM), University of Stuttgart, jonas.kneifl@itm.uni-stuttgart.de
- Dr. Mattia Manucci (SimTech), University of Stuttgart, mattia.manucci@simtech.uni-stuttgart.de
- Jonas Nicodemus (SimTech), University of Stuttgart, jonas.nicodemus@simtech.uni-stuttgart.de

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2 Scientific Program

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	Introduction to data-driven model order reduction and surrogate modeling
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14:30–15:00	**Lukas Renelt**
	Efficient linear model order reduction for Friedrichs'systems
15:00–15:30	**Nina Beranek**
	A hybrid mixed variational formulation and discretization for the linear transport equation
15:30–16:00	**Coffee Break**
16:00–16:30	**Hongliang Mu**
	Piece-wise symplectic model reduction on quadratically embedded manifolds
16:30–17:00	**Alexander Reinhold**
	Semi-smooth Newton method for parabolic PDE-constrained optimization
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09:30–10:00	**Michael Kartmann**
	Adaptive reduced basis trust region methods for parameter identification problems
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	A parallel batch greedy algorithm in reduced basis methods: Convergence rates and numerical results
10:30–11:00	**Coffee Break**
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	Tensor Krylov subspace methods via the T-product for large Sylvester tensor equations
11:30–12:00	**Julian Roth**
	Adaptive space-time model order reduction with dual-weighted residual (MORe DWR) error control for poroelasticity
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	A nonlinear reduced basis approximation of discrete contact problems in crowd motion
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	Extending balanced truncation to general domains
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	$\mathcal{H}_2$-optimal model reduction of linear systems with quadratic outputs
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	The Kolmogorov N-width for linear transport: Exact representation and the influence of the data
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	Model order reduction techniques for multiscale systems
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	Enhancing non-intrusive reduced order methods with space-dependent aggregation models
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	Combining a priori model order reduction and Lagrangian fluid solvers with moving meshes
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	Be greedy and learn: Efficient and certified algorithms for parameterized optimal control problems
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	Optimizing groundwater heat pump placement: Extending heat plumes with CNNs and PINNs
12:30–14:00	**Lunch Break**
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3   Participants

- **Ackermann**, Michael , Virginia Tech, USA, amike98@vt.edu
- **Beckmann**, Max , Université Paris-Saclay, France, max.beckermann@centralesupelec.fr
- **Beranek**, Nina , Ulm University, Germany, nina.beranek@uni-ulm.de
- **Borghi**, Alessandro , TU Berlin, Germany, borghi@tu-berlin.de
- **Bouyghf**, Fatima , University of Caen Normandy, France, fatima.bouyghf@unicaen.fr
- **Carlucci**, Antonio , Politecnico di Torino, Italy, antonio.carlucci@polito.it
- **Fischer**, Hendrik , Leibniz University Hannover, Germany, fischer@ifam.uni-hannover.de
- **Frie**, Lennart , University of Stuttgart, Germany, lennart.frie@itm.uni-stuttgart.de
- **Gkimisis**, Leonidas , Max Planck Institute for Dynamics of Complex Techincal Systems, Germany, leogk96@gmail.com
- **Greif**, Constantin , Ulm University, Germany, constantin.greif@uni-ulm.de
- **Hornischer**, Niklas , University of Stuttgart, Germany, niklas.hornischer@outlook.com
- **Ivagnes**, Anna , SISSA, Italy, anna.ivagnes@sissa.it
- **Kartmann**, Michael , University of Konstanz, Germany, michael.kartmann@uni-konstanz.de
- **Kleikamp**, Hendrik , University of Münster, Germany, hendrik.kleikamp@uni-muenster.de
- **Marquardt**, Jannis , TU Braunschweig, Germany, j.marquardt@tu-braunschweig.de
- **Mohsin Hassan Abdalla**, Amna , University of Padua, Italy, amna.mohsin@math.unipd.it
- **Mu**, Hongliang , University of Twente, The Netherlands, h.l.mu@utwente.nl
- **Ortegón-Villacorte**, Andrés , University of Trier, Germany, ortegon@uni-trier.de
- **Padhi**, Reetish , Indian Institute of Science Education and Research Pune, India, reetish.padhi@students.iiserpune.ac.in
- **Pasco**, Alexandre , Ecole Centrale de Nantes, France, alexandre.pasco@ec-nantes.fr
- **Pashov**, Amar , KU Leuven, The Netherlands, amar.pashov@kuleuven.be
- **Pelling**, Art , TU Berlin, Germany, a.pelling@tu-berlin.de
- **Pelzer**, Julia , University of Stuttgart, Germany, julia.pelzer@ipvs.uni-stuttgart.de
- **Piller**, Lukas , University of Stuttgart, Germany, lukas.piller@ipvs.uni-stuttgart.de
- **Prusak**, Ivan , SISSA, Italy, iprusak@sissa.it
- **Reich**, Niklas , Ulm University / HRW University of Applied Sciences, Germany, niklas.reich@hs-ruhrwest.de
- **Reinhold**, Alexander , Ulm University, Germany, martin.reinhold@uni-ulm.de
- **Reiter**, Sean , Virginia Tech, USA, seanr7@vt.edu
- **Renelt**, Lukas , University of Münster, Germany, lukas.renelt@uni-muenster.de
- **Rettberg**, Johannes , University of Stuttgart, Germany, johannes.rettberg@itm.uni-stuttgart.de
- **Rohleff**, Jan , University of Konstanz, Germany, jan.rohleff@uni-konstanz.de
- **Roth**, Julian , Leibniz Universität Hannover, Germany, roth@ifam.uni-hannover.de
- **Sambataro** , Giulia , Ecole des Ponts ParisTech, France, giulia.sambataro@enpc.fr
- **Siena**, Pierfrancesco , SISSA, Italy, psiena@sissa.it
- **Trigo Trinidade**, Thomas , EPFL, Switzerland, thomas.trigotrindade@epfl.ch
- **Ullmann**, Sven , University of Stuttgart, Germany, ullmannsven@gmx.de
- **Wang**, Fan , Max Planck Institute for Dynamics of Complex Technical Systems, Germany, fwang@mpi-magdeburg.mpg.de

4 Scientific Program - Day 1

4.1 Data-driven structure preserving model order reduction for high-dimensional nonlinear optimal control problems

T. Ehring[1], P. Buchfink[1], and B. Haasdonk[1]

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

Model Predictive Control (MPC) [5] is a model-based feedback control method for both, linear and nonlinear control systems, with the goal of closed-loop stability. The feedback law of an MPC control system is based on the iterative evaluation of finite-horizon optimal control problems (OCPs) for regularly updated initial values x. In the scope of the current study, the OCP is of the form

$$\min_{\mathbf{u}\in\mathcal{U}_T} J_T(\mathbf{u}) = \min_{\mathbf{u}\in\mathcal{U}_T} \int_0^T r(\mathbf{x}(s)) + \mathbf{u}(s)^\top R\mathbf{u}(s)\,\mathrm{d}s + V(\mathbf{x}(T)) \tag{1}$$

$$\text{subject to } \dot{\mathbf{x}}(s) = f(\mathbf{x}(s)) + g(\mathbf{x}(s))\mathbf{u}(s) \text{ and } \mathbf{x}(0) = x \in \mathbb{R}^N. \tag{2}$$

Using the first-order optimal conditions of this system, called the Pontryagin Maximum Principle (PMP) [4], the optimal open-loop trajectory $\mathbf{x}_T^*(\,\cdot\,)$ is guaranteed to be the solution of a Hamiltonian two-point boundary value problem of the form

$$\dot{\mathbf{z}}_T^*(s) = J_{2N}\nabla_z H\left(\mathbf{z}_T^*\right) \ \text{ with } \ b(\mathbf{z}_T^*(0), \mathbf{z}_T^*(T); x) = 0. \tag{3}$$

Here $\mathbf{z}_T^*(s) := \begin{bmatrix} \mathbf{x}_T^*(s)^\top & \mathbf{p}_T^*(s)^\top \end{bmatrix}^\top \in \mathbb{R}^{2N}$ with $\mathbf{p}_T^*(\,\cdot\,)$ being the co-state. Solving (1)–(2) via the PMP conditions leads to an MPC procedure where (3) must be solved multiple times with x being the current initial state. The solution generation of (3) should therefore be fast, especially for nonlinear high-dimensional systems, which is one of the major challenges of real-time capable MPC. This is where model order reduction can be used to find a quickly computable approximate solution of (3). Since the latter is a Hamiltonian system, symplectic model reduction [3, 1] can be applied, which preserves the Hamiltonian structure throughout the reduction, resulting in a reduced Hamiltonian that guarantees again preservation of the energy. We compare four symplectic and non-symplectic data-based bases, including a new type of base we call biorthoSymp, in terms of their ability to generate near-optimal controls by using them to solve a reduced version of (3). Numerical tests are performed on a nonlinear heat equation of the Zeldovich type describing a combustion process, where the optimal control steers the system towards the constant zero solution. A more detailed description can be found in [2].

References

[1] P. Buchfink, A. Bhatt, and B. Haasdonk. "Symplectic Model Order Reduction with Non-Orthonormal Bases". In: *Mathematical and Computational Applications* 24.2 (2019), p. 43.

[2] T. Ehring and B. Haasdonk. "Greedy Sampling and Approximation for Realizing Feedback Control for High Dimensional Nonlinear Systems". In: *IFAC-PapersOnLine* 55.20 (2022), pp. 325–330.

[3] L. Peng and K. Mohseni. "Symplectic Model Reduction of Hamiltonian Systems". In: *SIAM Journal on Scientific Computing* 38.1 (2016), A1–A27.

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[5] J. B. Rawlings. "Tutorial Overview of Model Predictive Control". In: *IEEE Control Systems Magazine* 20.3 (2000), pp. 38–52.

4.2 Efficient linear Model Order Reduction for Friedrichs' systems

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

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

We will discuss the class of linear Friedrichs' systems [1], defined as

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

and the corresponding PDE-problem $\mathcal{A}u = f$. Many classic partial differential equations (PDEs) can be rewritten in this form, for example diffusion problems, linear advection, linear elasticity, stationary Maxwell etc. We are interested in *parametrized* Friedrichs' systems and in particular 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 transport fields [**OhlbergerRave**]. We do not aim to tackle the latter problem (here, one should consider nonlinear approaches, see e.g. [3]) but instead aim to identify the subclass of *linearly approximable* Friedrichs' systems.

Using the theory of optimal test functions, we derive conditions under which solutions to Friedrichs' systems can be exponentially approximated [2]. We apply our result to an application-driven model problem which is based on an advection-reaction equation with parametrized reaction coefficient. The advection field is obtained as the solution to i.e. the Darcy equation (porous media), the Navier-Stokes-equation (turbulent flow) or even given as real-life data. Numerical experiments where we construct reduced spaces with a greedy-type algorithm confirm the exponential decrease of the approximation error.

References

[1] Kurt Otto Friedrichs. "Symmetric positive linear differential equations". In: *Communications on Pure and Applied Mathematics* 11.3 (1958), pp. 333–418.

[2] Lukas Renelt, Christian Engwer, and Mario Ohlberger. "Model order reduction of an ultraweak and optimally stable variational problem with application to parametrized reactive transport". In: *arXiv preprint arXiv:2310.19674* (2023).

[3] Francesco Romor, Davide Torlo, and Gianluigi Rozza. "Friedrichs' systems discretized with the Discontinuous Galerkin method: domain decomposable model order reduction and Graph Neural Networks approximating vanishing viscosity solutions". In: *arXiv preprint arXiv:2308.03378* (2023).

4.3   A hybrid mixed variational formulation and discretization for the linear transport equation

Nina Beranek [1]

[1]: Ulm University, Institute of Numerical Mathematics, Germany

This work is concerned with the theoretical study of a hybrid mixed variational formulation of the linear transport equation. A stable finite element discretization for the hybridized mixed problem is developed.

Firstly, we derive the mixed variational formulation based on the ideas of [2]. Based on the inf-sup stability of the involved bilinear forms, we show the formulation to be well-posed.

Secondly, we analyse the problem and the involved function spaces in case of a domain decomposition. It turns out that the interelement jumps of the normal components of the solution need to be controlled in order to guarantee the required regularity of the solution. Following hybridization techniques, see e.g. [1], we weaken the interelement continuity constraints by introducing a Lagrange multiplier.

Thirdly, we come up with a suitable finite element discretization for the hybridized mixed problem. Following the approach of [2], a slightly modified version of Raviart-Thomas elements of zeroth order are used for one of the unknowns. The proof of well-posedness of the problem in the chosen discrete spaces is part of our ongoing work.

References

[1]   Franco Brezzi and Michel Fortin. *Mixed and hybrid finite element methods*. Springer New York, 1991. DOI: 10.1007/978-1-4612-3172-1.

[2]   Julien Cartier and Mathieu Peybernes. "Mixed variational formulation and mixed-hybrid discretization of the transport equation". In: *Transport Theory and Statistical Physics* 39.1 (Jan. 2010), pp. 1–46.

4.4 Piece-wise Symplectic Model Reduction on Quadratically Embedded Manifolds

H. Mu[1], S. Glas[1]

[1]: University of Twente

In this work, we present a piece-wise symplectic model order reduction (MOR) method for Hamiltonian systems on quadratically embedded manifolds. For Hamiltonian systems, which suffer from slowly decaying Kolmogorov N-widths, linear-subspace reduced order models (ROMs) of low dimension can have insufficient accuracy. The recently proposed symplectic manifold Galerkin projection combined with the quadratic manifold cotangent lift approximation (SMG-QMCL)[1] is a symplectic MOR method that achieves higher accuracy than linear-subspace symplectic MOR methods. In this paper, we improve the efficiency of the SMG-QMCL by proposing a piece-wise symplectic MOR approach. First, the QMCL map is approximated piece-wisely by a linear symplectic map on each discrete time-interval. Then the symplectic Galerkin projection is applied to obtain a series of reduced-order Hamiltonian systems. In case that the Hamiltonian of the full-order model is a polynomial, the series of the Hamiltonians of the ROMs can be preserved up to a multiple of a pre-given tolerance used in the Newton iteration. In the numerical example, we demonstrate the approximation quality and the energy-preservation of the proposed algorithm.

References

[1] Harsh Sharma et al. "Symplectic model reduction of Hamiltonian systems using data-driven quadratic manifolds". In: *Computer Methods in Applied Mechanics and Engineering* 417 (2023), p. 116402. ISSN: 0045-7825. DOI: https://doi.org/10.1016/j.cma.2023.116402.

4.5   Semi-smooth Newton Method for parabolic PDE-constraint Optimization

M. A. Reinhold[1], K. Urban[1]

[1]: Institute of Numerical Mathematics, Ulm University

The solution of optimization problems constrained by parabolic PDEs is highly relevant for a wide range of applications and an interesting ongoing research subject. The usual approach to numerically solve these problems is to apply time stepping schemes to the PDE and the arising adjoint equation. In our approach we utilize a space-time variational formulation, using Lebesgue-Bochner spaces. We formulate the PDE-constraint optimization problem within this framework and use a tensor type discretizations with finite elements in time and space.

Since we consider additional constraints to the control term, we will use a semi-smooth Newton method to solve the problem. In this talk we want to discuss the derivation of the arising Newton systems in our setting. Here we want to discuss the differences between a discretize-before-optimize (DBO) and the optimize-before-discretize (OBD) approach. A comparison of the Newton like method in our Petrov-Galerkin setting with the Galerkin setting of an elliptic problem is discussed as well.

An implementation of both approaches will be presented, this implementation is supposed to be the truth solver for a parameterized version of our problem. In an outlook we will discuss a parameterized problem, where we will discuss the case with and without control constraints. We will present chances and challenges for the possibilities for Model Order Reduction (MOR) techniques for these problem as well as preliminary results of ongoing work.

5 Scientific Program - Day 2

5.1 MORe DWR applied to Manifold Learning

Hendrik Fischer [1,2], Thomas Wick[1,2],

[1]: Leibniz Universität Hannover, Institute of Applied Mathematics, Germany
[2]: Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay LMPS - Laboratoire de Mecanique Paris-Saclay, France

This presentation extends the MORe DWR method [3, 2] to parametrized problems. The MORe DWR method is an incremental, adaptive, goal-oriented reduced order modeling approach for time-dependent problems utilizing a posteriori dual-weighted residual (DWR) based error estimates [1]. The method has been successfully applied to various problems, such as the heat and elastodynamics equations [3] and lately to multiphysics problems, e.g. poroelasticity [2]. Here, the reduced bases have been altered adaptively based on the measured changes in solution behavior. This presented work innovates by introducing a parametrization to the MORe DWR method, expanding its applicability in reduced order modeling. Since the MORe DWR method tailors the bases to new solution behavior in a time-trajectory, we extend this property to solution changes caused by an underlying parametrization. For this parameter- and time-dependent problems, we are using the POD Greedy Sampling algorithm [4] as a foundation and combining it with the MORe DWR basis enrichment. The aim is to obtain a framework that can be used to explore the solution manifold in the offline phase of reduced order modeling, while also keeping the computational costs to a minimum. We introduce two strategies for the decision-making in the greedy enrichment. Further, we test the methods on the heat equation with parametrized heat coefficients and compare both approaches to the classical POD Greedy Sampling algorithm. The performance indicators used are the wall clock time, the accuracy of the estimator, and the quality of the resulting reduced basis.

References

[1] Roland Becker and Rolf Rannacher. "A feed-back approach to error control in finite element methods: basic analysis and examples". In: *East-West J. Numer. Math.* 4 (1996), pp. 237–264.

[2] Hendrik Fischer et al. *Adaptive space-time model order reduction with dual-weighted residual (MORe DWR) error control for poroelasticity*. 2023, https://doi.org/10.48550/ARXIV.2311.08907. arXiv: 2311.08907 [math.NA].

[3] Hendrik Fischer et al. *MORe DWR: Space-time goal-oriented error control for incremental POD-based ROM*. 2023, https://doi.org/10.48550/ARXIV.2304.01140. arXiv: 2304.01140 [math.NA].

[4] Jan S. Hesthaven, Gianluigi Rozza, and Benjamin Stamm. "Parametrized Differential Equations". In: *Certified Reduced Basis Methods for Parametrized Partial Differential Equations*. Ed. by Jan S Hesthaven, Gianluigi Rozza, and Benjamin Stamm. SpringerBriefs in Mathematics. Springer International Publishing, 2016, pp. 15–25. ISBN: 978-3-319-22470-1.

5.2 Adaptive Reduced Basis Trust Region Methods for Parameter Identification Problems

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

[1]: Universität Konstanz, Germany
[2]: Universität 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. More details can be found in the corresponding preprint [1].

References

[1] M. Kartmann et al. "Adaptive Reduced Basis Trust Region Methods for Inverse Parameter Identification Problems". In: (2023). DOI: https://doi.org/10.48550/arXiv.2309.07627.

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

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

[1]: Institute for Numerical Mathematics, Ulm Universtiy
[2]: Institute of Natural Sciences, University of Applied Sciences Ruhr West

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.

References

[1]   Peter Binev et al. "Convergence rates for greedy algorithms in reduced basis methods". In: *SIAM journal on mathematical analysis* 43.3 (2011), pp. 1457–1472.

[2]   Ronald DeVore, Guergana Petrova, and Przemyslaw Wojtaszczyk. "Greedy algorithms for reduced bases in Banach spaces". In: *Constructive Approximation* 37.3 (2013), pp. 455–466.

5.4 Tensor Krylov subspace methods via the T-product for large Sylvester tensor equations

Fatima Bouyghf[1], Alaa El Ichi[2], Mohamed El Guide[3]

[1]: LMNO, University of Caen Normandie, France
[2]: ULCO, France
[3]: UMIVP, Morocco

The aim of this talk is to present numerical Tensor Krylov subspace methods for solving the Sylvester tensor equation

$$\mathcal{M}(\mathcal{X}) = \mathcal{C}, \tag{4}$$

where $\mathcal{M}$ is a linear operator that could be described as

$$\mathcal{M}(\mathcal{X}) = \mathcal{A} \star \mathcal{X} - \mathcal{X} \star \mathcal{B} \tag{5}$$

where $\mathcal{A}$, $\mathcal{X}$, $\mathcal{B}$ and $\mathcal{C}$ are three-way tensors leaving the specific dimensions to be defined later, and $\star$ is the T-product introduced by Kilmer and Martin [2].

Consider the following Sylvester matrix equation

$$AX + XB = C. \tag{6}$$

In the literature, several methods to solve equation (6) have been established. When matrices are of small sizes, the well-know direct methods are recommended. These methods are based on Schur decomposition to transform the original equation into a form that is easily solved by a forward substitution. For large Sylvester matrix equations, iterative projection methods have been developed, see for example [3,4]. These methods use Galerkin projection methods, such the classical and the block Arnoldi techniques, to produce low-dimensional Sylvester matrix equations that are solved by using direct methods.

In the current talk, we are interested in developing robust and fast iterative Krylov subspace methods via T-product to solve the Sylvester tensor equation *STE* (17). In fact, when the tensors in equations (17) are of small sizes, the purpose is to extend matrix version of direct methods to third order tensors using the T-product formalism. This give us the *t-Bartels-Stewart* algorithm. For large size tensors, we describe first a new methods that will be defined as orthogonal and oblique projection onto a tensor Krylov subspace. In particular, the tensor Full orthogonalization method (tFOM) and tensor generalized minimal residual method (tGMRES) will be examined. We will also introduce the well-Know tensor Tubal block Krylov methods via T-product for transforming the original large Sylvester equation to a low-dimensional *STE* . In particular, we will describe the Tubal Block Arnoldi (TBA) as a generalization of the block Arnoldi matrix [5].

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5.5 Adaptive space-time model order reduction with dual-weighted residual (MORe DWR) error control for poroelasticity

Hendrik Fischer [1,2], Julian Roth [1,2], Ludovic Chamoin [2], Amelie Fau [2], Mary Wheeler [3], Thomas Wick [1,2]

[1]: Leibniz Universitat Hannover, Institut fur Angewandte Mathematik, Hannover, Germany
[2]: Universite Paris-Saclay, CentraleSupelec, ENS Paris-Saclay, CNRS, LMPS - Laboratoire de Mecanique Paris-Saclay, France
[3]: The University of Texas at Austin, Oden Institute, Austin, USA

In this presentation, the space-time MORe DWR (Model Order Reduction with Dual-Weighted Residual error estimates) [4] framework is extended and further developed for single-phase flow problems in porous media [3]. Specifically, our problem statement is the Biot system [5] which consists of vector-valued displacements (geomechanics) coupled to a Darcy flow pressure equation. The MORe DWR method introduces a goal-oriented adaptive [2, 1] incremental proper orthogonal decomposition (POD) based-reduced-order model (ROM). The error in the reduced goal functional is estimated during the simulation, and the POD basis is enriched on-the-fly if the estimate exceeds a given threshold. This results in a reduction of the total number of full-order-model solves for the simulation of the porous medium, a robust estimation of the quantity of interest and well-suited reduced bases for the problem at hand. We apply a space-time Galerkin discretization with Taylor-Hood elements in space and a discontinuous Galerkin method with piecewise constant functions in time. The latter is well-known to be similar to the backward Euler scheme. We demonstrate the efficiency of our method on the well-known two-dimensional Mandel benchmark and a three-dimensional footing problem.

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5.6 A nonlinear reduced basis approximation of discrete contact problems in crowd motion

V. Ehrlacher [1,2], G. Sambataro [1,2]

[1]: Cermics, École des Ponts ParisTech, Marne la Vallée Cedex 2, France
[2]: Inria, MATHERIALS team, Paris, France

In this work we develop new model reduction approaches to predict the solutions of time-dependent parametrized problems describing crowd motion in the presence of obstacles. The problem of interest is described by a discrete contact model (DCM) (Ref.[2]): we consider N_{P} agents identified to rigid disks of radius r and we define the feasibility region for the positions $\mathcal{Q} = \{\mathbf{q} \in \mathbb{R}^{2N_{\mathrm{P}}} \text{ s.t. } D_{ij}(\mathbf{q}) = |q_i - q_j| - 2r \geq 0, \forall i < j\}$, where D_{ij} is the signed distance between disks i and j.

The DCM problem is formulated as a constrained least-squares optimization statement: the velocity field is seeked as the projection of the spontaneous velocities of each particle $\mathbf{U}_i = \mathbf{U}_i(\mathbf{q})$ into a closed convex cone of admissible velocities:

$$\begin{cases} \frac{d\mathbf{q}}{dt} = \mathrm{P}_{\mathcal{C}_{\mathbf{q}}}(\mathbf{U}(\mathbf{q})), \\ \mathbf{q}(0) = \mathbf{q}_0 \in \mathcal{Q}, \end{cases} \tag{7}$$

where

$$\mathcal{C}_{\mathbf{q}} = \{\mathbf{v} \in \mathbb{R}^{2N_{\mathrm{P}}}, \forall i < j \text{ s.t. } D_{ij}(\mathbf{q}) = 0 \implies \nabla D_{ij}(\mathbf{q}) \cdot \mathbf{v} \geq 0\}.$$

The parametric variations in the problem are associated to the geometric configuration of the system (for example, the exit width) and to the initial positions of the particles. Parametric variations have a dramatic impact in the solution, both in terms of the particles positions and in the contact forces, which are represented by the Lagrange multipliers of the underling saddle-point problem.

We investigate new developments of the reduced-basis method and supervised machine-learning techniques to effectively find, in a decorrelated manner, primal and dual reduced spaces. Indeed, for the DCM of interest, linear approximation methods become ineffective, as outlined by the slow decay of the Kolmogorov n-width: the combination of a reduced basis technique with nonlinear methods is promising to achieve a more satisfactory level of accuracy. The reduced basis for the primal variables is found by a Proper Orthogonal Decomposition (POD), and the basis for the dual variables is constructed by a cone-projected greedy algorithm that preserves the non-negativity of the dual basis vectors. As in [1], we perform a non-linear reconstruction (e.g. by Random Forest regression) of reduced coordinates from a small number of first coordinates of a linear reduced basis approximation, in order to achieve a better performance than the linear reconstruction.

To assess the validity of the method, the nonlinear compressive strategy is then compared to more standard linear and nonlinear approximations.

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5.7 Extending balanced truncation to general domains

A. Borghi [1], T. Breiten[1], S. Gugercin[2]

[1]: Technical University of Berlin, Mathematics department,10623 Berlin, Germany
[2]: Virginia Tech, Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Blacksburg, VA 24061, USA

Model order reduction aims to alleviate the computational burden of large-scale systems by computing a lower order surrogate model with approximately the same input-output behaviour. While many established techniques exist in this field, a substantial amount assumes the underlying model to be asymptotically stable.

The objective of this work is to extend existing methodologies to linear time invariant systems with transfer functions having poles in more general domains in the complex plane. In particular, we generalize the concept of balanced truncation through conformal maps. To this aim, we reformulate the Gramians of the full order system. We demonstrate that, for particular conformal maps, these Gramians are the solution to Lyapunov equations. Lastly, we show that there exists a bound for a newly defined $\mathcal{H}_2$ norm (see [1]). We propose a balanced-truncation-based algorithm and assess its performance against the Schrödinger equation and the wave equation with spectra on the imaginary axis .

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5.8 $\mathcal{H}_2$-optimal model reduction of linear systems with quadratic outputs

Sean Reiter [1], Serkan Gugercin [1], Igor Pontes Duff[2], Ion Victor Gosea[2]

[1]: Department of Mathematics and Computational Modeling and Data Analytics, Virginia Tech, USA
[2]: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

We consider dynamical systems that are linear in the state equation with a quadratic output term:

$$\Sigma : \left\{ \dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{b}u(t), \quad y(t) = \mathbf{c}^T\mathbf{x}(t) + \mathbf{x}(t)^T\mathbf{M}\mathbf{x}(t), \right. \tag{8}$$

where $\mathbf{A}, \mathbf{M} \in \mathbb{R}^{n \times n}$, and $\mathbf{b}, \mathbf{c} \in \mathbb{R}^n$. We assume that $\mathbf{M} = \mathbf{M}^T$, and that Σ is asymptotically stable, i.e. $\lambda(\mathbf{A}) \subset \mathbb{C}_-$. The frequency response of Σ is fully characterized by two rational transfer functions:

$$H_1(s) = \mathbf{c}^T(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}, \qquad H_2(s_1, s_2) = \mathbf{b}^T(s_1\mathbf{I} - \mathbf{A}^T)^{-1}\mathbf{M}(s_2\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}. \tag{9}$$

The $\mathcal{H}_2$-norm of such a system (8) is defined as

$$\|\Sigma\|_{\mathcal{H}_2}^2 := \frac{1}{2\pi}\int_{-\infty}^{\infty}|H_1(i\omega)|^2 d\omega + \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|H_2(i\omega_1, i\omega_2)|^2 d\omega_1 d\omega_2 \tag{10}$$

Such systems arise when observing, e.g., the product of time or frequency domain components of the state [3]. In a large-scale setting (e.g., $n \sim \mathcal{O}(10^6)$), repeated simulation of the model (8) poses a significant computational burden. This motivates the computation of reduced-order models (RoMs):

$$\Sigma_r : \left\{ \dot{\mathbf{x}}_r(t) = \mathbf{A}_r\mathbf{x}_r(t) + \mathbf{b}_r u(t), \quad y_r(t) = \mathbf{c}_r^T\mathbf{x}_r(t) + \mathbf{x}_r(t)^T\mathbf{M}_r\mathbf{x}_r(t), \right. \tag{11}$$

where $\mathbf{A}_r, \mathbf{M}_r \in \mathbb{R}^{r \times r}$, and $\mathbf{b}_r, \mathbf{c}_r \in \mathbb{R}^r$, $r \ll n$, and Σ_r accurately reproduces the response characteristics of (8) in the sense that $y_r(t) \approx y(t)$ for admissible inputs $u(t)$. The error bound [1]

$$\|y - y_r\|_{\mathcal{L}_\infty} \leq \|\Sigma - \Sigma_r\|_{\mathcal{H}_2}\left(\|u\|_{\mathcal{L}_2} + \|u \cdot u\|_{\mathcal{L}_2}\right),$$

motivates the construction of a RoM Σ_r as in (11) that approximates Σ well in the $\mathcal{H}_2$-norm (10). To this end, we study the $\mathcal{H}_2$-optimal model reduction problem for linear systems with quadratic outputs. Our significant contributions are twofold: First, we derive first-order necessary conditions for $\mathcal{H}_2$ optimality. These conditions amount to rational interpolation of H_1 and H_2 in (9) by the transfer functions of Σ_r at the mirror images of the poles of Σ_r, i.e. $\lambda(\mathbf{A}_r)$.

Secondly, we adapt the iterative rational Krylov algorithm [2] as an efficacious approach for computing locally $\mathcal{H}_2$-optimal reduced-order models as in (11). Numerical experiments validate the effectiveness of the proposed framework.

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5.9 Finite-Dimensional RHC Control of linear time-varying parabolic Parabolic PDEs: Stability Analysis and Model-Order Reduction

Behtad Azmi [1], Jan Rohleff [1], Stefan Volkweini[1]

[1]: Universität Konstanz

This chapter deals with the stabilization of a class of linear time-varying parabolic partial differential equations employing reduced receding horizon control (RHC). Here, RHC is finite-dimensional, i.e., it enters as a time-depending linear combination of finitely many indicator functions whose total supports cover only a small part of the spatial domain. In detail, we are concerned with the stabilization of the control system of the form

$$\begin{cases} \dot{y}(t) - \nu \Delta y(t) + a(t)y(t) + \nabla \cdot (b(t)y(t)) = \sum_{i=1}^{N} u_i(t)\mathbf{1}_{R_i} & \text{in } (0, \infty) \times \Omega, \\ y = 0 & \text{on } (0, \infty) \times \partial\Omega, \\ y(0) = y_0 & \text{on } \Omega \end{cases} \qquad (12)$$

with a time depending control vector $u(t) = [u_1(t), \ldots, u_N(t)]^\top \in L^2((0, \infty); \mathbb{R}^N)$, where $\Omega \subset \mathbb{R}^n$ is a bounded domain with the smooth boundary $\partial\Omega$ and $\nu > 0$. The functions $\mathbf{1}_{R_i}$ represent the actuators. They are modeled as the characteristic functions related to open sets $R_i \subset \Omega$ for $i = 1, \ldots, N$, and the support of these actuators are contained in a *small* open subset of the domain Ω. Moreover, the reaction term $a(t) = a(t, x)$ and convection term $b(t) = b(t, x)$ are, respectively, real- and $\mathbb{R}^n$-valued functions of real variables t and x. Further, we consider the squared ℓ_1-norm as the control cost. This leads to a nonsmooth infinite-horizon problem which allows a stabilizing optimal control with a low number of active actuators over time. First, the stabilizability of RHC is investigated. Then, to speed up numerical computation, the data-driven model order reduction (MOR) approaches are adequately incorporated within the RHC framework. Numerical experiments are also reported which illustrate the advantages of MOR approaches.

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5.10 Generalized transfer function approximation for nonlinear MOR

Antonio Carlucci[1]

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

This work is concerned with data-driven, non-intrusive reduced modeling of nonlinear systems, using only input-output (I/O) data that can be easily obtained from evaluation of system responses, i.e. without accessing a first-principles description (see [2] for relevant previous work). The adopted I/O representation for the time-invariant system $G : u(t) \to y(t)$ is the Volterra series [3], whereby $y(t)$ is expanded as a sum of repeated convolutions between the input $u(t)$ and the degree-n multidimensional kernels $h_n(\tau_1, \ldots, \tau_n)$, so that $y(t) = \sum_{n=1}^{\infty} \int_0^t h_n(\tau_1, \ldots, \tau_n) u(t - \tau_1) \cdots u(t - \tau_n) \, d\tau_1 \cdots d\tau_n$.

The multidimensional Laplace transform of the degree-n symmetric Volterra kernel $h_n(\tau_1, \ldots, \tau_n)$ is denoted with $H_n(s_1, \ldots, s_n)$ and it generalizes the transfer function concept that is central to linear systems theory. Samples of these transfer functions can be directly inferred from I/O experiments.

We start from transfer function values $\breve{H}_n(\mathbf{s}_n^{(k)})$, where $\mathbf{s}_n^{(k)} = (s_1^{(k)}, \ldots, s_n^{(k)})$ and the superscript k refers to the k-th sample. We look for the best-fitting model with the following bilinear structure

$$\dot{x}_1 = A_1 x_1 + B_1 u, \quad \dot{x}_n = A_n x_n + D_n x_{n-1} u, \quad 2 \leq n \leq N \tag{13}$$

and output $y(t) = \sum_{n=1}^{N} C_n x_n(t)$. The n-th state equation in (13) corresponds to the degree-n *homogeneous subsystem*. In order to write the symmetric transfer functions of (13) following [3], let us introduce $\mathbf{s}_n \backslash s_i \triangleq (s_1, \ldots, s_{i-1}, s_{i+1}, \ldots, s_n)$, and

$$X_1(s_1) = (s_1 I - A_1)^{-1} B_1, \qquad Q_n(\mathbf{s}_n) = \sum_{i=1}^{N} X_{n-1}(\mathbf{s}_n \backslash s_i), \tag{14a}$$

$$X_n(\mathbf{s}_n) = [(s_1 + \cdots + s_n)I - A_n]^{-1} D_n Q_n(\mathbf{s}_n), \qquad \text{for } n \geq 2. \tag{14b}$$

With this notation, $H_n(\mathbf{s}_n) = C_n X_n(\mathbf{s}_n)$. The recursion in (14) suggests a greedy approach where N independent systems are fitted sequentially, starting from (A_1, B_1, C_1), followed by (A_n, D_n, C_n) for $n = 2$ up to $n = N$. As for $n = 1$, *rational approximation* of the samples $\breve{H}_1(s_1)$ (e.g. via Vector Fitting [4]) yields A_1, B_1, C_1. For $n \geq 2$, the key observation is that Q_n in (14a) only depends on lower-degree subsystems, and the model H_n can be written as

$$H_n(\mathbf{s}_n) = F_n(s_1 + \cdots + s_n) Q_n(\mathbf{s}_n), \quad \text{where } F_n(s) = C_n(sI - A_n)^{-1} D_n. \tag{15}$$

This implies that the approximation problem $H_n \approx \breve{H}_n$ can again be tackled through rational fitting to find a uni-variate rational function $F_n(s)$ that minimizes the error of the approximation

$$F_n\left(s_1^{(k)} + \cdots + s_n^{(k)}\right) Q_n\left(\mathbf{s}_n^{(k)}\right) \approx \breve{H}\left(\mathbf{s}_n^{(k)}\right) \tag{16}$$

An extended description including numerical results is in preparation [1].

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5.11 Quadrature-based balanced truncation for quadratic-bilinear systems

Reetish Padhi [1], Ion Victor Gosea [2]

[1]: Indian Institute of Science Education and Research, IISER Pune, India
[2]: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

Quadratic-bilinear (QB) systems are an important class of dynamical systems since many systems are characterized by such nonlinearities. They are given by the following set of equations

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{N}\mathbf{x}(t)\mathbf{u}(t) + \mathbf{H}(\mathbf{x}(t) \otimes \mathbf{x}(t)),$$
$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t).$$

Balanced truncation (BT) is a classical, established model reduction method that computes balanced reduced-order models. The authors in [1] extend the definition of Gramian from the linear to the QB case and use truncated Gramians for QB systems to provide a BT algorithm for such systems. By writing the Volterra series representation of the system, the time-domain generalized kernels of the QB system can be derived.

In [2], the authors introduce a non-intrusive data-based balanced truncation method to obtain lower-order models for linear systems (named QuadBT). They do so by approximating the system Gramians using quadrature weights and writing all associated quantities as samples of the system kernels. For the extension of QuadBT to QB systems, we use the definitions given in [1] and follow the original method in [2] and the recent extension for bilinear systems in [3]. We approximate the reachability Gramians using quadrature nodes. For example, the components of the reachability Gramian can be approximated as

$$\tilde{\mathcal{P}}_1 = \sum_{i=1}^{N_p} \rho_i^2 e^{\mathbf{A}\mu_i} \mathbf{B}\mathbf{B}^\top e^{\mathbf{A}^\top \mu_i} = \tilde{\mathbf{U}}_1 \tilde{\mathbf{U}}_1^\top, \quad \tilde{\mathcal{P}}_2 = \sum_{i=1}^{N_p} \rho_i^2 e^{\mathbf{A}\mu_i} \mathbf{N}\tilde{\mathbf{U}}_1 \tilde{\mathbf{U}}_1^\top \mathbf{N}^\top e^{\mathbf{A}^\top \mu_i} = \tilde{\mathbf{U}}_2 \tilde{\mathbf{U}}_2^\top,$$

$$\tilde{\mathcal{P}}_3 = \sum_{i=1}^{N_p} \rho_i^2 e^{\mathbf{A}\mu_i} \mathbf{H} \left(\tilde{\mathbf{U}}_1 \otimes \tilde{\mathbf{U}}_1 \right) \left(\tilde{\mathbf{U}}_1^\top \otimes \tilde{\mathbf{U}}_1^\top \right) \mathbf{H}^\top e^{\mathbf{A}^\top \mu_i} = \tilde{\mathbf{U}}_3 \tilde{\mathbf{U}}_3^\top.$$

We then construct the projection matrices $\mathcal{V}, \mathcal{W}$ using the SVD of the matrix $\tilde{\mathbf{L}}^\top \tilde{\mathbf{U}}$. Finally, we replace the expression for the reduced order model terms $\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}}, \hat{\mathbf{H}}$ and $\hat{\mathbf{N}}$ in terms of samples of the time-domain kernels and their derivatives. Extending QuadBT to such systems also allows one to construct data-driven reduced-order models for a more general class of systems by employing lifting transforms.

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6 Scientific Program - Day 3

6.1 Model order reduction techniques for the prediction of railway induced vibration

A. Pashov [1], S. François [1], G. Degrande[1]

[1]: KU Leuven, Department of Civil Engineering, Kasteelpark Arenberg 40,3001 Leuven, Belgium

When designing new railway tracks or new buildings in the vicinity of existing railway lines, it is essential to conduct parametric studies to quantify the impact of design changes. Existing computational models demand substantial computational effort when predicting the full propagation path from track to building. Although computational complexity has been reduced by exploiting the geometrical invariance of the railway track, studies involving many design parameters are still hindered by the curse of dimensionality. By applying model order reduction techniques to predict railway induced vibration in buildings, a computational vademecum of the response is constructed, integrating soil and track parameters and facilitating fast parametric studies on vibration mitigation.

The objective is to develop a model order reduction method addressing the high-fidelity complex dynamic soil-structure interaction problem across a wide frequency range. To tackle this, Proper Generalized Decomposition (PGD) has been employed [1]. The PGD formulation is based on the assumption of a separable form of the multi-dimensional field. Each contribution therefore consists of a rank-one tensor that is computed iteratively in a greedy manner. To this end, the PGD formalism is introduced into the weak form and the resulting non-linear problem is solved using fixed point iterations. Damping terms result in non-Hermitian properties of the operator, hindering convergence of the standard Galerkin PGD approach. Therefore, alternative solution strategies, like Petrov-Galerkin based solvers, are considered [3]. We compare the classical greedy rank one update with a greedy Tucker approximation method [2].

We elaborate the PGD formulation for three problems with different complexity: a simplified source model of an Euler-Bernoulli beam on a Winkler foundation; a 2.5D model of a ballast track on a heterogenous soil medium, modelled with finite elements in combination with complex frequency-shifted perfectly matched layers; and Green's functions for in-plan (P-SV) and out-of-plane (SH) wave propagation in a layered halfspace. Apart from the frequency and wavenumber, we take along the foundation stiffness, ballast and soil properties, or source and receiver positions as coordinates in the PGD formulation. The considered algorithms are compared in terms of convergence, memory requirements, and CPU time.

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6.2 Proper Orthogonal Decomposition for port-Hamiltonian energy networks

A. Ortegón-Villacorte [1], S.-A. Hauschild [1], N. Marheineke [1]

[1]: Universität Trier

Proper network simulation of flows in gas or water pipes is important when we want to improve the efficiency of an energy distribution system, for example to save energy or resources. The port-Hamiltonian framework is applied to the non-isothermal Euler equations in pipe networks. Thanks to the pH modeling, mass and energy conservation are encoded in the system and appropriate coupling conditions are used in the ports and pipe connections. The structure of the system must be preserved when new network components are added, such as consumers, producers or compressor stations. The system is discretized in space preserving the structure of the original pH system. These systems often require a fine discretization in space to converge to proper results and for this reason a strategy of model order reduction is useful to significantly reduce the computational cost of the simulation. Building on previous work [1, 2], we present numerical results for large energy networks where proper orthogonal decomposition is used for model order reduction.

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6.3 Kernel Trust-Region algorithm for solving optimization problems

Sven Ullmann [1]

[1]: Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Pfaffenwaldring 57, Stuttgart 70569, Germany

Solving optimization tasks for problems with computationally expensive objective functions often results in impractical methods. One approach to enhance computational efficiency are so-called Trust-Region methods. These methods aim to approximate the objective function by a surrogate model in a region around the current iterate of the algorithm. The surrogate model is intentionally designed to be more manageable and less intricate than the original objective function that we aim to optimize.

In this work, kernel functions, which have found widespread use in high-dimensional interpolation problems [3], are utilized to construct the surrogate model of the objective function [2]. The algorithmic approach for our kernel Trust-Region algorithm is inspired by Algorithm 1 in [1], which uses gradually enriched Reduced Basis surrogate models instead of kernel functions to approximate the objective function. To establish convergence under reasonable assumptions for the kernel Trust-Region algorithm, we extend the convergence analysis provided in [4], aligning it with the conditions of the kernel surrogate model. We discuss how to thoughtfully select the interpolation points to construct the kernel surrogate model, ensuring its capability to adequately approximate both the objective function and its gradient. Moreover, we conduct a comparative analysis of the optimization outcomes achieved by the kernel Trust-Region algorithm against state-of-the-art optimization methods, using various numerical examples.

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6.4 Approximating the smallest eigenvalue of large Hermitian matrices that depend on parameters

N. Guglielmi [1], M. Manucci[2] , E. Mengi [3]

[1]: Gran Sasso Science Institute, Italy
[2]: University of Stuttgart, Germany
[3]: Koç University, Turkey

We investigate the efficient and certified approximation of smallest singular value

$$\lambda_{\min}(\boldsymbol{\mu}) \; := \; \min_{\boldsymbol{v} \in \mathbb{C}^N, \, |\boldsymbol{v}|=1} \boldsymbol{v}^* \boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{v}, \quad \boldsymbol{\mu} \in \mathcal{D}; \tag{17}$$

where $\mathcal{D}$ is a compact subset of $\mathbb{R}^p$ and $\boldsymbol{A}(\boldsymbol{\mu})$ is such that

$$\boldsymbol{A}(\boldsymbol{\mu}) := \sum_{l=1}^{\kappa} f_l(\boldsymbol{\mu})\boldsymbol{A}_l \tag{18}$$

with $\boldsymbol{A}_l \in \mathbb{C}^{n \times n}$ Hermitian matrix and $f_l : \mathcal{D} \to \mathbb{R}$ is a real-analytic functions, for $l = 1, ..., \kappa$. Being able to approximate in a fast and reliable way (17) is crucial in *projection Model Order Reduction*, in particular for the construction of reduced spaces through *greedy algorithms* [1].

To deal with this problem we relay to the *subspace* framework, see [2], and following what proposed in [4], we approximate the smallest eigenvalues using a greedy strategy based on efficiently computable upper and lower bounds of the smallest eigenvalues, i.e.

$$\lambda_{\mathsf{LB}}(\boldsymbol{\mu}) \leq \lambda_{\min}(\boldsymbol{\mu}) \leq \lambda_{\mathsf{UB}}(\boldsymbol{\mu}).$$

Our main contributions consists in $i)$ approximating (17) over the uniform parametric domain, by means of the software EigOpt [3] and $ii)$ showing rigorous global convergence of the method under suitable assumptions. We also propose an heuristic strategy to deal with non-Hermitian matrices in (18). Finally, we show through several numerical test examples that the proposed method is efficient and reliable in approximating (17).

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6.5   The Kolmogorov N-width for linear transport: Exact representation and the influence of the data

Florian Arbes [1], Constantin Greif [2], Karsten Urban[2]

[1]: IFE, Institute for Energy Technology, Instituttveien 18, 2007 Kjeller (Norway)

[2]: Ulm University, Institute of Numerical Mathematics, Helmholtzstr. 20, 89081 Ulm (Germany)

The Kolmogorov N-width describes the best possible error one can achieve by elements of an N-dimensional linear space. Its decay has extensively been studied in Approximation Theory and for the solution of Partial Differential Equations (PDEs). Particular interest has occurred within Model Order Reduction (MOR) of parameterized PDEs e.g. by the Reduced Basis Method (RBM).

While it is known that the N-width decays exponentially fast (and thus admits efficient MOR) for certain problems, there are examples of the linear transport and the wave equation, where the decay rate deteriorates to $N^{-1/2}$. On the other hand, it is widely accepted that a smooth parameter dependence admits a fast decay of the N-width. However, a detailed analysis of the influence of properties of the data (such as regularity or slope) on the rate of the N-width seems to lack.

In this paper, we use techniques from Fourier Analysis to derive exact representations of the N-width in terms of initial and boundary conditions of the linear transport equation modeled by some function g for half-wave symmetric data. For arbitrary functions g, we derive bounds and prove that these bounds are sharp. In particular, we prove that the N-width decays as $c_r N^{-r}$ for functions with Sobolev regularity $g \in H^{r-\varepsilon}$ for all $\varepsilon > 0$ even if $g \notin H^r$. Our theoretical investigations are complemented by numerical experiments which confirm the sharpness of our bounds and give additional quantitative insight.

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6.6 Active Subspace Methods for Parametrized Partial Differential Equations

N. Hornischer [1,2], N. Shah [2], G. Wells [2], D. Göddeke[1,3]

[1]: Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Germany
[2]: Department of Engineering, University of Cambridge, United Kingdom
[3]: Institute for Applied Analysis and Numerical Simulation (IANS), University of Stuttgart, Germany

Conducting parameter studies in science and engineering often necessitates computationally intensive simulations to model complex processes. However, classical parameter studies become infeasible when faced with high-dimensional parameter spaces due to limited computational resources and the curse of dimensionality. To reduce the complexity of these parameter studies, model order reduction techniques provide a promising workaround. These techniques often require multiple snapshots representing the full parameter space, in order to construct the reduced basis. However, selecting useful snapshots from the parameter space is a non-trivial task since the number of snapshots should be kept as low as possible to reduce the computational costs, while still capturing the relevant information in the parameter space.

Active subspace methods offer a relatively new approach to dimension reduction, aiming to identify significant directions within the parameter space [3]. These key directions of the parameter space can be used directly in the parameter study to only explore the most relevant directions, or to select the most informative snapshots for the construction of the reduced basis.

However, applying active subspace methods directly to complex simulation models, especially within active simulation platforms, presents challenges. We present an easy-to-use framework tailored for models involving parametric partial differential equations on the FEniCSx computing platform [2, 4, 1]. In that way, we aim to provide tools to analyze the usability of the active subspace methods for given problems and basic functionality to construct the active subspace. This talk provides an overview of active subspace methods, providing the mathematical background and the necessary details to use the framework. We demonstrate the capabilities of the framework by applying the method to a multivariate quadratic model and a parametrized Stokes equation.

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7 Scientific Program - Day 4

7.1 Frequency-Domain Based Learning of Dynamical Systems from Purely Time-Domain Data

M. S. Ackermann[1], S. Gugercin[1,2]

[1]: Department of Mathematics, Virginia Tech, Blacksburg, 24061, VA, United States
[2]: Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech, Blacksburg, 24061, VA, United States

Frequency-based reduced order modeling techniques have been very successful in creating high-fidelity reduced order models (ROMs). Here, we consider the discrete-time, single-input single-output system

$$\mathcal{S} : \begin{cases} \mathbf{x}[k+1] = \mathbf{A}\mathbf{x}[k] + \mathbf{b}u[k] \\ y[k+1] = \mathbf{c}^\top \mathbf{x}[k], \end{cases} \tag{19}$$

with transfer function

$$H(z) = \mathbf{c}^\top (z\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}, \tag{20}$$

where $\mathbf{A} \in^{(\beta)} R^{n \times n}, \mathbf{b} \in^{(\beta)} R^n$, and $\mathbf{c} \in^{(\beta)} R^n$. The goal of frequency-based reduced order modeling is to well-approximate the transfer function (20) in some sense (such as the $\mathcal{H}_2$ norm). Classically, frequency-based ROMs are obtained *intrusively* by projecting the system matrices in (19) to smaller system matrices: $\mathbf{A}_r \in^{(\beta)} R^{r \times r}, \mathbf{b}_r \in^{(\beta)} R^r$, and $\mathbf{c}_r \in^{(\beta)} R^r$. An example of such a technique is the Iterative Rational Krylov Algorithm (IRKA) [3], which computes locally $\mathcal{H}_2$ optimal ROMs. Recently, many of these classical techniques have been formulated in a *data-driven* framework, where one assumes access to $\{H(\sigma_i)\}_{i=1}^m$, the values of (20) at $\{\sigma_i\}_{i=1}^m \subset^{(\beta)} C$ (and sometimes its derivative) and produces reduced system matrices directly from data. IRKA is one such method; the realization independent iterative rational Krylov algorithm (TF-IRKA) [1] only requires values and derivatives of (20). However, in practical settings it can be difficult to obtain frequency data $H(\sigma)$; one may only have time-domain data from (19)

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

In [2], the authors present a method to calculate frequency data $H(\sigma)$ from time-domain data $^{(\beta)}U, ^{(\beta)}Y$. However, due to numerical ill-conditioning and an assumption that the system order n is known, the method faces challenges when applied to large-scale dynamical systems. First, we provide the necessary analysis to increase the robustness of the framework in [2] for large-scale dynamical systems, while assuming access to only a single time-domain input-output trajectory. This analysis also leads to an error indicator that accurately predicts the relative error in recovered frequency data. We illustrate that the frequency information we recover can be used in established frequency domain data-driven techniques by demonstrating a time-domain variant of TF-IRKA which constructs locally $\mathcal{H}_2$ optimal ROMs of large-scale dynamical systems from only a single time-domain simulation of (19).

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7.2 Reformulation of the data assimilation problem as a new foundation for model order reduction methods

J. Marquardt [1], C. Gräßle [1]

[1]: Institut für Partielle Differentialgleichungen, TU Braunschweig

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 $0 \le i \le N$ 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 $x_{i+1} = \mathcal{M}_i(x_i)$. A connection between the states and observations may be realised by 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

$$\operatorname*{argmin}_{x_0 \in \mathbb{R}^d} \left\{ J(x_0) := \frac{1}{2} \sum_{i=0}^{N} \|\mathcal{H}_i(x_i) - y_i\|_{\mathbb{R}^{d_{\text{obs}}}}^2 + \frac{\alpha}{2} \left\|x_0 - x_0^{(b)}\right\|_{\mathbb{R}^d}^2 \right\}, \tag{21a}$$

subject to

$$x_{i+1} = \mathcal{M}_i(x_i) \quad \forall i \in \{0, ..., N-1\} \tag{21b}$$

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 usual solution techniques such as variants of the Gauss-Newton method and different versions of Kalman filters all require the numerical treatment of large systems. Therefore, it is not surprising that the search for reduced order models is a focus of various researches (for an overview of data assimilation and model order reduction techniques see [2]).

In this talk, a reformulation of data assimilation problems governed by a parabolic partial differential equation (pde) will be presented. This reformulation allows to find the solution of the optimisation problem (21) by solving a fourth order elliptic pde with i.e. finite elements. The idea which motivated the transition between these problems has already been successfully used by other authors in different contexts (i.e. [1, 3]). It involves the interpretation of (21) as an optimal control problem and the utilisation of the arising optimality conditions in order to establish the fourth order system.

Switching from an optimisation problem to the discretisation of a pde now allows to investigate the possibilities of model order reduction from a new angle. While the author will present the outcome of some first model order reduction attempts such as the proper orthogonal decomposition for the system matrices, he also seeks the discussion and exchange of ideas coming from different directions with other participants of the YMMOR conference.

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7.3 Model Order Reduction Techniques for Multiscale Systems

Fan Wang [1,2]

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

The problem of model reduction in multiscale systems arises, e.g., in climate dynamics. Climate dynamics blend multiscale data, including multilayers of atmosphere and hydrosphere. Although in a high-fidelity model, it is difficult to track all data but large-scale data. Thus a model of unresolved/unmeasured parts of the dynamical system is important to forecast the weather accurately. Moreover, subgrid modeling plays an important role in turbulence modeling in the fluid dynamics community.

Recent approaches call on Neural Ordinary Differential Equations (NODE) [1] as a continuous case of well-known ResNet, to fit the dynamical systems together with ODE solvers. Inspired by NODE, the Universal Differential Equations (UDE) [5] framework successfully integrates unresolved scales / subgrid scales with the solved scales. Apart from UDE, Empirical Model Reduction (EMR) [3, 4] is a numerical algorithm to model multiscale problems.

In this work, we try to find the similarity between EMR and DMD/Koopman [2], then use DMD/Koopman together with Neural Networks (NN) to guide the modeling of the multiscale problems. The challenge is that "traditional" MOR methods like DMD/Koopman assume fully observed data and then reduce the full dimension n to reduced dimension r by some optimization algorithms. On the contrary, EMR is a method to deal with partially observed/measured systems with solved dimension r' which is generally not optimized for a full model with dimension n.

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7.4   An Optimisation–Based Fully Segregated Reduced Order Model for Fluid Structure Interaction Problems

I. Prusak[1], D. Torlo[1], M. Nonino[2], G. Rozza[1]

[1]: SISSA, Mathematics Area, mathLab
[2]: University of Vienna, Department of Mathematics

Even though there has been extensive research in computational methods for solving Fluid–Structure interaction (FSI) problems in the last decades, a comprehensive presentation from a mathematical point of view is still missing nowadays: one of the reasons for this is the fact that the two subproblems, namely the Navier–Stokes equation and the elastic solid equation, are two big mathematical challenges on their own. FSI problems describe the dynamic interplay between a fluid and a solid. This interplay takes place because of the coupling of the two different physics at the FSI interface, namely the part of the physical domain that is common to the fluid subdomain and the solid subdomain. The FSI interface profile is unknown *a priori* and depends on the dynamics of the fluid and the structure problem.

Classically, there are two different approaches to solving an FSI problem: a partitioned (or segregated) procedure and a monolithic procedure. The idea behind partitioned algorithms is to try to combine available well–developed computational tools for fluid dynamics and structural dynamics and couple them with some iterative procedure. On the other hand, in monolithic algorithms, the fluid and the solid problem are solved simultaneously.

Our work aims to introduce a framework where Domain Decomposition (DD) algorithms and Reduced–Order Models (ROMs) are combined to achieve better performance of numerical simulations. We choose to model the DD using an optimisation approach (see, for instance, [2]) to ensure the coupling of the interface conditions between fluid and structure subdomains and it leads to a complete separation of the solvers on the subdomains. The snapshots for the high–fidelity model are obtained with the Finite Element (FE) discretisation, and the model order reduction is then proposed both in terms of time and physical parameters with a standard Proper Orthogonal Decomposition (POD)–Galerkin projection.

Although the partitioned approach is more attractive because of its computational efficiency, it might lead to unstable algorithms, under some physical and geometrical conditions, while the monolithic approach does not suffer from this issue. This happens, for example, if the physical domain has a slender shape, or, as in our numerical test, if the fluid density is close to the solid density, and this is usually the case in haemodynamics applications, where the density of the blood is quite close to the density of the walls of the vessel. This phenomenon is the so–called "added mass" effect; see, for instance, [1] for a detailed derivation of the "added mass" effect and related consequences. The approach undertaken in our work leads to a fully–segregated algorithm which is nevertheless stable under the "added mass" effect. It is evidenced by the numerical experiments of the model presented for a two–dimensional haemodynamics benchmark FSI problem.

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7.5   Reduced order models for cardiovascular flows

P. Siena [1], C. Balzotti [1], M. Girfoglio [1], A. Quaini [2], G. Rozza [1]

[1]: SISSA, International School for Advanced Studies, Mathematics Area, mathLab, via Bonomea 265, I-34136 Trieste, Italy
[2]: University of Houston, Department of Mathematics, 3551 Cullen Blvd, 77204, Houston TX, USA

Heart disease represents one of the leading causes of death worldwide, thus several research areas pay particular attention to cardiovascular disorders. The formulation of mathematical models dedicated to patient-specific cases [4] or appropriate benchmarks [2] can be useful to analyse the blood perfusion in critical areas. In this work, features commonly encountered in the vascular system and medical devices, such as flow contraction, expansion, recirculation zones are studied through a Reduced Order Model (ROM) in the Food and Drug Administration (FDA) nozzle benchmark.

The incompressible Navier-Stokes equations represent the mathematical model employed at the full order level, where space-dependent boundary conditions are imposed for the inlet velocity. High Reynolds numbers are taken into account and the finite volume method is adopted to find the full order solutions in a large eddies simulation approach. The features of the mesh, the discretization parameters and the numerical schemes to obtain proper results are taken from [2].

A Proper Orthogonal Decomposition (POD) with Galerkin projection is implemented in the ROM framework. The lifting function method is adopted to introduce non-homogeneous Dirichlet boundary conditions at reduced level [1]. For a turbulent flow treated with a large eddies simulation approach, one of the main sources of errors is the truncation of the modes. Therefore, stabilization methods to properly recover neglected data are introduced. The first consists of an additional global constant viscosity (constant kernel) in the reduced model formulation. A comparison is performed with a linear kernel approach where the amount of added viscosity is modified for each mode [3].

Several analyses are performed as the number of modes and the added viscosity change. Qualitative and quantitative comparisons are carried out for mean pressure and velocity by reaching good agreements between FOM and ROM solutions.

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7.6 Model Order Reduction for Partitioned Linear FSI Systems

L. Frie [1], P. Eberhard [1]

[1]: Institute of Engineering and Computational Mechanics, University of Stuttgart, Germany

For the simulative analysis of many systems, different physical domains have to be considered. One example is the frequently occurring fluid-structure interaction (FSI). Systems, where FSI is very important are various. Two examples that are considered in this talk are a classical guitar and the very complex system of a helicopter in flight. In both systems, the different physical domains, i.e. structure and air, influence each other significantly and, thus, both have to be simulated in an interacting coupling framework. These coupling frameworks are divided into monolithic coupling and its counterpart, the partitioned methods or non-monolithic coupling. The non-monolithic coupling has the advantage that specially adapted solvers can be used for each subsystem and that different working groups can work on each different subsystem separately [2, 3].

For the modeling of mechanical systems, the finite element method is frequently used. To achieve an adequate description of complex systems, however, a fine discretization in space is necessary leading to very high-dimensional systems of differential equations. In order to still enable efficient and effective simulations, model order reduction (MOR) is essential. By coupling the different domains, the individual subsystems often have numerous inputs and outputs through which forces are exchanged over the common interaction surface. This is a special challenge for many MOR approaches, though. Furthermore, not only a good approximation of the full-system states is important, but also the approximation of their derivatives. This is because the derivatives are used to compute the forces that act on the complement subsystem.

In this talk, projection-based MOR using Krylov subspaces is used to reduce the structural part of the FSI system. It is shown that a good approximation of states does not necessarily lead to good approximations of the interaction forces. Different advancements in moment matching, e.g. ESVDMOR [1], are reviewed for use with systems that have numerous inputs, and are enhanced for the present use case. Their functionality is shown with the two above-mentioned examples. The classical guitar has the advantage that also the used full-order model has a moderate size and can be evaluated to receive a reference solution. The application to the helicopter model demonstrates the suitability for very large and very complex systems.

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7.7 Structure-preserving model order reduction and error analysis of port-Hamiltonian systems

J. Rettberg[1], D. Wittwar[2], P. Buchfink[2], R. Herkert[2], J. Fehr[1], B. Haasdonk[2]

[1]: University of Stuttgart, Institute of Engineering and Computational Mechanics
[2]: University of Stuttgart, Institute of Applied Analysis and Numerical Simulation

The modeling of modern technical systems typically includes the consideration of different physical domains to represent a realistic behavior. The method of port-Hamiltonian (pH) systems manages to describe such systems in a unified framework by defining the energy as the *lingua franca* between the involved subsystems [3]. High-dimensional systems result from the spatial discretization of these models, leading to computationally demanding simulations and making model order reduction (MOR) techniques indispensable to allow for real-time scenarios or multi-query simulations.

Port-Hamiltonian systems fulfill the useful properties of passivity, stability and modularity, which are worth maintaining through structure-preserving reduction even in reduced space. Usually, the reduction introduces an approximation error. Error estimation approaches help to build confidence in the reduced model and can be used to work on adaptive basis generation, e.g. greedy algorithms, to improve the projection basis iteratively.

The authors present a sensitivity analysis of different structure-preserving projection and basis generation methods for the reduction of linear port-Hamiltonian systems [2]. Based on this, residual-based error estimators are adapted to the pH systems and the error overestimation is reduced by using linear auxiliary problems [1]. The methods are illustrated using a coupled fluid-structure interaction model of a classical guitar.

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7.8 Wasserstein-VAEs in Monte Carlo Simulations

A. Mohsin [1], M. Putti [2], G. Santin[3]

[1]: Department of Mathematics, University of Padova
[2]: Department of Agronomy, Food, Natural Resources and Environment, University of Padova
[3]: Department of Environmental Sciences, Informatics and Statistics, University of Venice

Uncertainty Qualification in Partial Differential Equations (PDEs) tries to approximate the probability distribution of the PDE solution given the uncertainty on the data. This is typically addressed by the method that requires a large number of simulations, called the Monte Carlo (MC) ensemble. MC method is a common quadrature strategy and can be used effectively to approximate the moments (e.g., mean and variance) of the PDE solution. The computational cost of building the MC ensemble can be prohibitively large for real-world application and tools for reducing this effort must be developed.

In this talk we will discuss several aspects of a promising approach in this direction, which is the use of Deep Learning - based methods to generate data that resemble the unknown distribution, such as Generative Adversarial Networks (GANs) [2] and Variational Auto Encoders (VAEs) [3], and use them to approximate the MC estimations cheaply and without requiring any full model solution after the training of the model.

Nevertheless, these techniques are usually based on the estimation of appropriate distances between distributions. Typically, the Kullback-Leibler and Jensen-Shannon divergences [1] are used. Unfortunately, often these distances are unable to detect important differences between distributions, leading to loss of accuracy in the final approximation. To address this issue, we investigate the use in this setting of VAEs based on the Wasserstein distance (Wasserstein-VAE), which has the potential to overcome the limitations of the existing approaches. We expect the uses of this distance to be especially important when dealing with PDEs whose solutions display peculiar features, such as shocks or discontinuities.

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7.9   Data-driven and Low-rank Implementations of the Generalized Singular Perturbation Algorithm

Art J. R. Pelling [1], Sean J. Reiter [2], Bjön Liljegren-Sailer[3], Ion Victor Gosea[4]

[1]: Technische Universität Berlin, Berlin
[2]: Virginia Tech, Blacksburg
[3]: Johann Radon Institute for Computational and Applied Mathematics, Linz
[4]: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

The Balanced Generalized Singular Perturbation Algorithm (GSPA) [6] is a classic model order reduction method for linear time-invariant systems with an a priori error bound. The connection between GSPA and Balanced Truncation (BT) in the form of a Möbius transformation [1] is long known and has been employed to derive theoretical properties of GSPA-reduced models and to prove aforementioned error bounds [1, 4]. Recently, the relationship of the Singular Perturbation Algorithm (SPA) [2] and BT via a reciprocal transformation was exploited to enable new algorithmic strategies for low-rank and data-driven approaches for the method [5].

BT is a staple of the model order reduction community and can be conceived of as a special case of GSPA; a connection that is seldomly mentioned the literature, e.g. in review papers. We will show that the new algorithmic results for SPA extend naturally to GSPA and present numerical examples of low-rank and data-driven implementations. The low-rank version is realized by following the algorithmic counterparts of BT with the additional expense of solving a least-squares problem of reduced order. The data-driven implementation uses the QuadBT framework [3] which bases on an approximation of the system gramians via numerical quadrature. Furhtermore, we will look briefly at possible connections that arise to frequency-weighted model order reduction and discretization schemes.

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7.10 Stabilised Dynamical Low Rank Methods for random Advection-Dominated Problems

Fabio Nobile [1], Thomas Trigo Trindade [1]

[1]: CSQI, Department of Mathematics, EPFL

The efficient and accurate simulation of random unsteady advection-dominated problems in a multi-query context is challenging.

On the one hand, those problems are not amenable to the POD paradigm. While the solution may at all times exhibit a low-rank structure, the subspaces capturing that structure can vary significantly over time. The Dynamical Low Rank framework can be an interesting alternative, in which we approximate

$$u(t,x,\xi) \approx \sum_{i=1}^{R} U_i(t,x)Y_i(t,\xi).$$

This method can be understood as a Reduced Basis method with the peculiarity that both bases (called *physical* modes $\{U_i\}_{i=1}^{R}$ and *stochastic* modes $\{Y_i\}_{i=1}^{R}$ in this context) are time-dependent. The aim is consequently to track a (quasi-)optimal approximation of the best rank-R approximation over time.

On the other hand, the use of the standard Finite Element method is also problematic as the numerical solutions thus obtained display oscillations. These numerical artifacts are unphysical and must be removed or at least alleviated. To tackle this, we introduce a framework of stabilised Dynamical Low Rank methods. The framework naturally integrates any stabilisation technique that is expressed as a generalised Petrov-Galerkin method for a time-dependent problem. The streamline Upwind/Petrov-Galerkin and Interior Penalty methods fall into this category. A family of time-stepping algorithms is introduced and their properties analysed. Under certain assumptions, the stabilised DLR method is shown to inherit the properties of the stabilised full-order model. Numerical experiments will illustrate the effectiveness of the stabilising methods.

8 Scientific Program - Day 5

8.1 Sequential nonlinear dimension reduction using gradient evaluations

A. Pasco [1], A. Nouy [1]

[1]: Ecole Centrale de Nantes, Laboratoire de Mathematiques Jean Leray, UMR CNRS 6629

Our goal is to approximate a differentiable function $u : \mathbb{R}^d \to \mathbb{R}$, $d \gg 1$, by a composition of functions $f \circ g$ where $g : \mathbb{R}^d \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}$. The approximation error is assessed in the L^2_μ-norm where μ is some probability measure on $\mathbb{R}^d$. First the feature map g is selected among some prescribed functional class by minimizing an upper bound of the approximation error based on evaluations of ∇u. Then the function f is built using classical regression methods.

If g is taken linear, this problem has been extensively studied under the name Active Subspace, see for example [2]. This approach is easy to implement, computationally efficient, has robust theoretical guarantees for some classical probability laws μ, and showed good performances in various numerical applications. However, there are many functions u for which such an approximation with $m < d$ is known to be not efficient.

Therefore, recent works consider non-linear feature maps in order to produce better dimension reduction. More especially, we will focus on the work from [1], where for a fixed mapping $\phi : \mathbb{R}^d \to \mathbb{R}^K$, $K \geq d$, they consider g as a function of the form $g(x) = A^T \phi(x)$ with $A \in \mathbb{R}^{K \times m}$. Although theoretical guarantees require more restrictive assumptions, numerical experiments showed improved performances compared with linear featuring, even when the assumptions were not satisfied.

Our goal is to find a sequential approach to build a good mapping ϕ. While [1] also considered this approach using a greedy algorithm, we will consider an approach for constructing a more structured map ϕ.

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8.2 Enhancing Non-intrusive Reduced Order Methods with Space-dependent Aggregation Models

A. Ivagnes[1], N. Tonicello[1], P. Cinnella[2], G. Rozza[1]

[1]: International School of Advanced Studies SISSA, Trieste, 34136
[2]: Institut Jean Le Rond D'Alembert, Sorbonne University, Paris, 75252

The novelty of the present contribution is the exploitation of space-dependent aggregation techniques [3] to combine different data-driven Reduced Order Models (ROMs) [1]. The prediction of the model-mixture formulation, the *mixed-ROM*, consists in a convex linear combination of the predictions of some previously-trained non-intrusive ROMs, where we assign a space-dependent weight to each model.

The ROMs taken into account to build the mixture model exploit different reduction techniques, both linear –the Proper Orthogonal Decomposition (POD)– and non-linear –an Auto-Encoder (AE)– and/or different approximation techniques, including interpolation –Radial Basis Function Interpolation (RBF)– or regression techniques –a Gaussian Process Regression (GPR) or a feed-forward neural network [2]. The contribution of each model is retained with higher weights in the regions where the model performs best, and, vice versa, with small weights where the model has a lower accuracy with respect to the other models. Finally, a machine learning technique, namely a Random Forest, is exploited to infer the weights for unseen parameters.

The performance of the aggregated model is evaluated on the parametric test case of the 2D flow past an airfoil, considering as parameters the angle of attack and/or the Reynolds number. In this test case, the mixed-ROM provided improved accuracy with respect to the standard ROM techniques, while providing an estimate for the predictive uncertainty.

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8.3 Combining a priori model order reduction and Lagrangian fluid solvers with moving meshes

Max Beckermann [1], Andrea Barbarulo [1], Massimilano Cremonesi[2]

[1]: Laboratoire de Mécanique Paris-Saclay, 91190 Gif-Sur-Yvette, France
[2]: Politecnico di Milano, 20133 Milano, Italy

The Particle Finite Element method is a fluid solver based on Lagrangian finite elements combined with efficient re-meshing algorithms [2]. It was shown to be effective in a large amount of applications, especially in the case of free surface fluids flows or fluid-structure interactions as the different interfaces are intrinsically dealt with within the method. Up to now, this method has never been paired up with any model-order reduction technique because of the difficulties linked to the re-meshing schemes. This remains however, an important area of research to uncover as it could drastically reduce the computational cost of the method.

In this work, we focus on an *a priori* reduction method called Proper Generalized Decomposition (PGD) [1] with a space-time decomposition. Contrary to the *a posteriori* family of reduced order modelling techniques the PGD does not require any knowledge of past solutions. The reduced solution is instead built iteratively solving several problems of lower dimension. This technique has been used extensively over the years and has been given a solid mathematical framework [4]. In fluid dynamics, PGD was used in the context of Eulerian finite element fluid solvers [3] but the performance improvement was limited by the non-linear convective term. This justifies the hopes we have to be able to solve higher convective cases with a Lagrangian description of motion, in which the convective term vanishes entirely.

The PGD formulation requires a complete time integration of all points of our system. To be able to deal with moving mesh and remeshing, a new expanded formulation is introduced. This formulation extends the degrees of freedom to all particles that have existed throughout our simulation. Particular efforts have to be made to ensure both correct mesh and solution interpolation at the re-meshing instances and adequate update of the mesh after every new mode calculation. The proposed technique has been validated with simple tests showing very promising results.

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8.4 Be greedy and learn: efficient and certified algorithms for parametrized optimal control problems

H. Kleikamp [1], M. Lazar [2], C. Molinari[3]

[1]: Institute for Analysis and Numerics, Mathematics Münster, University of Münster, Germany
[2]: Department of Electrical Engineering and Computing, University of Dubrovnik, Croatia
[3]: Dipartimento di Matematica, University of Genova, Via Dodecaneso 35, 16146, Genoa, Italy

In this talk we consider parametrized linear-quadratic optimal control problems and provide their online-efficient solutions by combining greedy reduced basis methods and machine learning algorithms [2]. To this end, we first extend the greedy control algorithm [3], which builds a reduced basis for the manifold of optimal final time adjoint states, to the setting where the objective functional consists of a penalty term measuring the deviation from a desired state and a term describing the control energy. Afterwards, we apply machine learning surrogates to accelerate the online evaluation of the reduced model by approximating the map from parameter to coefficients with respect to the reduced basis [1]. The error estimates proven for the greedy procedure are further transferred to the machine learning models and thus allow for efficient a posteriori error certification. We show by means of numerical examples the potential of the proposed methodology.

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8.5   Optimizing Groundwater Heat Pump Placement: Extending Heat Plumes with CNNs and PINNs

J. Pelzer [1], L. Piller [1], M. Schulte[1], D. Pflüger[1]

[1]: Institute for Parallel and Distributed Systems, Universität Stuttgart, 70569 Stuttgart, Germany

Part 1: Unlocking the full potential of groundwater heat pump deployment in a given region presents a fascinating challenge, demanding a good understanding of the specific groundwater flow dynamics to model the formation of heat plumes and their interactions. This talk presents an extended two-stage learning strategy to model the groundwater flow with the goal of optimizing the placement of additional heat pumps at the example of the metropolitan region of Munich. For practical use in the field, this has to be orders of magnitude more efficient than classical simulations.

The first stage involves the prediction of standard-shaped heat plumes such as in Fig. 1 within realistic subsurface parameter ranges, achieved through the utilization of a Convolutional Neural Network (CNN) trained on simulations. In the second stage, another CNN adjusts the temperature field of this independent plume based on its interaction with neighboring plumes, see Fig. 2.
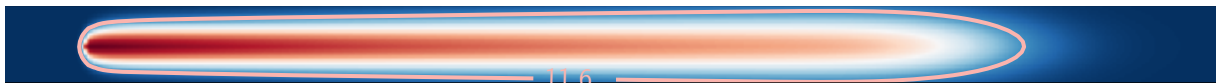

Figure 1: 1st stage: predict one heat plume.

Figure 2: 2nd stage: learn interaction with neighboring heat plumes.

Part 2. However, a novel challenge arises after the first stage. Depending on the subsurface property input-combinations, heat plumes can assume arbitrary lengths, necessitating either excessively large simulations or extending predicted plumes. Here, we introduce a physics-informed machine learning method to extend heat plumes. Our goal is to minimize the number of expensive simulations required as training data, while covering rare scenarios such as extremely long heat plumes.

Introducing a pragmatic methodology in Fig. 3, we segment datasets by cutting the label (temperature field) into rectangles. The first rectangles's temperature field (containing the origin of a heat pump) is then forecasted using CNNs (see initial first stage), based on subsurface input properties. Following this, we extend the heat plume until its ends using a Physics-Informed Neural Network (PINN) combined with a classical data loss. This streamlined approach not only enhances computational efficiency but also paves the way for extrapolating plumes with minimal data requirements.
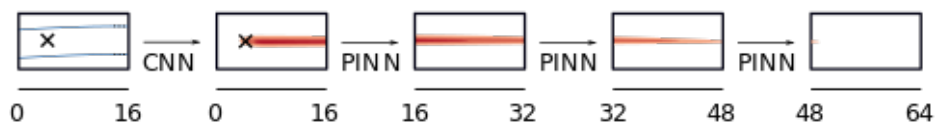

Figure 3: Approach to extend the plumes in two steps.