CSC-DMP Retreat

Sunday 16 February 2025 - Wednesday 19 February 2025

Ringberg castle

Book of Abstracts

Contents

Plenary talk / **29**

The linear algebra of Gaussian processes

Author: Martin Stoll[1]

[1] *TU Chemnitz*

Corresponding Author: martin.stoll80@gmail.com

Gaussian processes are a versatile tool in statistics and machine learning. They are suitable candidates to generate surrogate models that come with integrated uncertainty quantification of the reduced model. The quality of the model heavily depends on the choice of the hyperparameters and to train these on the given data many linear algebra challenges arise. In this talk we will briefly recall the basics of Gaussian processes and then explain the NLA challenges. We will discuss several strategies to handle these and will show how in the case of multi-output GPs we obtain a Stein equation that we then solve using low-rank techniques. We will also discuss the possibility of using mixed precision methods to speed up the training process.

Plenary talk / 36

Petrov-Galerkin Krylov methods for algebraic Riccati equations

Author: Heike Faßbender[1]

Co-author: Christian Bertram [2]

[1] *TU Braunschweig*

[2] *TU Braunschweig, Institut für Numerische Mathematik*

Corresponding Author: h.fassbender@tu-braunschweig.de

Finding the unique stabilizing solution $X = X^H$ of a large-scale continuous-time algebraic Riccati equation (CARE) $0 = R(X) := A^H X + XA + C^H C - XBB^H X$ with a large, sparse n-x-n matrix A, an $n \times m$ matrix B and a $p \times n$ matrix C is of interest in a number of applications. It is assumed, that B and C^H have full column and row rank, respectively, with $m, p << n$. The unique stabilizing solution $X = X^H$ which exists under certain assumptions is positive semidefinite and makes the closed-loop matrix $A - BB^H X$ stable. Even so A is large and sparse, the solution X will still be a dense matrix in general. However, the above assumptions on B and C often imply that the sought-after solution X will have a low numerical rank (that is, its rank is $<< n$). This allows for the construction of iterative methods that approximate X with a series of low-rank matrices X_j stored in low-rank factored form. That is, the Hermitian low-rank approximations X_j to X are of the form $X_j = Z_j Y_j Z_j^H$, where Z_j is an $n \times kj$ matrix with only few columns and Y_j is a small square $kj \times kj$ Hermitian matrix.
We will first give an overview of methods that produce such a low-rank approximation. Afterward, we will delve into projection-type methods, which reduce the large-scale Riccati equation to a smaller one by projecting it onto specific block rational Krylov subspaces. These subspaces are spanned by blocks of the form $(A^H + \sigma_j I)C^H$, where σ_j are chosen shifts. The smaller, projected Riccati equation is then solved for the matrix Y_j which contributes to constructing the low-rank approximation X_j. We propose a new algorithm that, unlike traditional approaches, does not necessarily use an orthogonal projection. Our approach constructs projections directly from the matrices generated in the block rational Arnoldi decomposition of the block rational Krylov subspace. With this algorithm, the low-rank approximations X_j and the residual norm $||R(X_j)||_F$ can be computed quickly and efficiently. Finally, we will demonstrate the effectiveness of this method through numerical examples.

Contibuted Talk / 42

Solving Dense Sylvester-like Matrix Equations - Recent Advances

Author: Martin Köhler[1]

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

Corresponding Author: koehlerm@mpi-magdeburg.mpg.de

The solution of Sylvester-like matrix equations still constitutes a core task in systems and control theory, with their solution also being required in the extensive field of eigenvalue analysis. In addition to numerous iterative algorithms, Bartels and Stewart presented an algorithm for dense matrices in the 1970s. This algorithm has been improved over the last two decades by the introduction of techniques such as recursive blocking, level-3 block partitioning, and task-based scheduling.

In the 2010s, studies demonstrated that the utilisation of GPUs yielded only a marginal enhancement in execution speed. However, contemporary computing infrastructures, characterised by the transition from multi-core to many-core systems and the integration of accelerators, have emerged as a potential solution. These advancements offer a substantial boost in floating-point operations, thereby enhancing the overall performance of these systems. These include higher floating-point performance, increased memory bandwidth, and enhanced interconnection.
The landscape has undergone a fundamental shift in terms of the relative performance of CPUs and GPUs. In addition to these hardware advancements, the author proposes two distinct methodologies for enhancing the efficiency of the Bartels-Stewart algorithm. In the first instance, an approach is adopted that considers the differing styles of parallelism developed over the last decade. On the one hand, the available parallelism on the CPU side requires hundreds of (small) tasks, as in task-based scheduling algorithms, to ensure the Bartels-Stewart algorithm runs as fast as possible. On the other hand, accelerator devices such as GPUs require a critical problem size to become efficient. The necessity to address this discrepancy has led to the extension of existing algorithms to incorporate the ideas of recursive blocking, level-3 partitioning, and
task-based scheduling using the StarPU library as a hybrid scheduling
library. The utilisation of multiple levels of block partitioning enables the effective management of the algorithm's parallel execution, ensuring its efficient operation on both CPU and GPU platforms. This approach allows us to simultaneously satisfy the block size requirements for both CPUs and GPUs. The StarPU library then schedules the individual tasks to the computing devices that are most likely to result in the minimum execution time. Secondly, the 'macroscopic' aspect of the solvers is optimised. Given that current CPUs only achieve optimal performance once a substantial amount of work is performed on top of the vector registers, techniques employed in the optimization of the GEMM operation are integrated into the level-2 BLAS inner solvers. These optimisations are expected to reduce the critical path in a parallel execution environment, thereby enhancing the overall performance.

Contibuted Talk / 43

Generalizing Reduced Rank Extrapolation to Low-Rank Matrix Sequences

Authors: Pascal den Boef[1]; Patrick Kürschner[2]; Xiaobo Liu[3]; Jos Maubach[1]; Jens Saak[3]; Wil Schilders[1]; Jonas Schulze[4]; Nathan van de Wouw[1]

[1] *TU Eindhoven*

[2] *HTWK Leipzig*

[3] *Max Planck Institute for Dynamics of Complex Technical Systems*

[4] *MPI DCTS*

Corresponding Author: jschulze@mpi-magdeburg.mpg.de

Reduced rank extrapolation (RRE) is an acceleration method typically used to accelerate the iterative solution of nonlinear systems of equations using a fixed-point process. In this context, the iterates are vectors generated from a fixed-point mapping function. However, when considering the iterative solution of large-scale matrix equations, the iterates are low-rank matrices generated from a fixed-point process for which, generally, the mapping function changes in each iteration. To enable acceleration of the iterative solution for these problems, we propose two novel generalizations of RRE. First, we show how to effectively compute RRE for sequences of low-rank matrices. Second, we derive a formulation of RRE that is suitable for fixed-point processes for which the mapping function changes each iteration. We demonstrate the potential of the methods on several numerical examples involving the iterative solution of large-scale Lyapunov and Riccati matrix equations.

Contibuted Talk / 39

Low-synchronization variants of reorthogonalized block classical Gram-Schmidt

Author: Eda Oktay[1]

Co-authors: Erin Carson [2]; Yuxin Ma [2]; Kathryn Lund [3]

[1] *MPI DCTS*

[2] *Charles University*

[3] *STFC RAL*

Corresponding Author: oktay@mpi-magdeburg.mpg.de

Interest in communication-avoiding orthogonalization schemes for high-performance computing has been growing recently. In this talk, we discuss some open questions about the numerical stability of various block classical Gram-Schmidt variants that have been proposed in the past few years. We introduce an abstract framework, the flexibility of which allows for new rigorous bounds on the loss of orthogonality in these variants. With this framework, we first analyze a generalization of (reorthogonalized) block classical Gram-Schmidt, and then, using this variant, which has four synchronization points per block column, we remove the synchronization points one at a time and analyze how each alteration affects the stability of the resulting method. Our analysis shows that the variant requiring only one synchronization per block column cannot be guaranteed to be stable in practice, as stability begins to degrade with the first reduction of synchronization points.

Contibuted Talk / 49

Optimizing Rayleigh quotient with Hermitian and symmetric constraints

Author: Anshul Prajapati[1]

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

Corresponding Author: prajapati@mpi-magdeburg.mpg.de

Let $G, H \in \mathbb{C}^{n,n}$ be Hermitian and $S \in \mathbb{C}^{n,n}$ be a symmetric matrix. We consider the problem of maximizing the Rayleigh quotient of G with respect to constraints involving symmetric matrix S and Hermitian matrix H. More precisely, we compute

$$m(G,H,S) := \sup\left\{ \frac{v^*Gv}{v^*v} : \ v \in \mathbb{C}^n \setminus \{0\},\ v^TSv = 0,\ v^*Hv = 0 \right\}, \tag{1}$$

$$tag\mathrm{P} \tag{2}$$

where T and $*$ denote respectively the transpose and the conjugate transpose of a matrix or a vector.

Such problems occur in stability analysis of uncertain systems and in the eigenvalue perturbation theory of matrices and matrix polynomials [1, 2, 3]. A particular case of problem $(\mathcal{P})$ with only symmetric constraint (i.e., when $H = 0$) is used to characterize the μ-value of the matrix under skew-symmetric perturbations [3].

An explicit computable formula was obtained for $m(G,S)$ in [3, Theorem 6.3] and given by

$$\mathrm{m(G,S)}=\inf_{t\in[0,\infty)} \lambda_2 \left(\begin{bmatrix} G & t\overline{S} \\ tS & \overline{G} \end{bmatrix} \right),$$

where $\lambda_2(A)$ stands for the second largest eigenvalue of a Hermitian matrix A. The case where only Hermitian constraint (i.e., when $S = 0$) was also considered and an explicit computable formula was obtained for $m(G,H)$ in [3, Theorem 6.2] and given by

$$\mathrm{m(G,H)}=\inf_{t\in\mathbb{R}} \lambda_{max}(G + tH),$$

where λ_{max} stands for the largest eigenvalue. However, the solution to the problem $(\mathcal{P})$ is still not known.

———-

[1] S. Bora, M. Karow, C. Mehl, P. Sharma. Structured eigenvalue backward errors of matrix pencils and polynomials with Hermitian and related structures. SIAM J. Matrix Anal. Appl., 35: 453–475 (2014).

[2] J. Doyle. Analysis of feedback systems with structured uncertainties. IEE Proc. Part D, Control Theory Appl., 129: 242–250 (1982).

[3] M. Karow. μ-values and spectral value sets for linear perturbation classes defined by a scalar product. SIAM J. Matrix Anal. Appl., 32: 845–865 (2011).

Contibuted Talk / 65

On empirical interpolation under the tensor t-product algebra

Author: Harshit Kapadia[1]

Co-authors: Lihong Feng [1]; Peter Benner [1]

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

Corresponding Author: kapadia@mpi-magdeburg.mpg.de

We present a novel tensor empirical interpolation method operating within the tensor t-product framework. Compared to traditional empirical interpolation, our approach significantly enhances the reconstruction accuracy of tensor-valued datasets by using optimally placed sparse sensor measurements along the dimension of interest. This improvement is achieved by preserving the native tensor structure of the dataset rather than matricizing it, which allows us to leverage the inherent relationships within the data. Moreover, our formulation naturally supports an augmentation that permits us to gather more sensor measurements than the size of the generated tensorial bases set, thereby expanding its applicability to data-scarce scenarios. Numerical results from various large-scale complex systems demonstrate the robustness of our method, which we will illustrate with selected examples.

Contibuted Talk / 34

A hybrid Chebyshev-Tucker tensor format with applications to multi-particle modelling

Authors: Peter Benner[None]; Venera Khoromskaia[1]; Boris Khoromskij[2]; Bonan Sun[3]

[1] *Max-Planck-Institute for mathematics in the Sciences*

[2] *Max-Planck Institute for Mathematics in the Sciences, Leipzig*

[3] *Max Planck Institute Dynamics of Complex Technical System*

Corresponding Author: bsun@mpi-magdeburg.mpg.de

In this talk, we introduce a mesh-free two-level hybrid Tucker tensor format for the approximation of multivariate functions. This new format combines the product Chebyshev interpolation with the ALS-based Tucker decomposition of the coefficients tensor. The benefits of this tensor approximation are two-fold. On the one hand, it allows to avoid the rank-structured approximation of functional tensors defined on large spatial grids, while on the other side, this leads to the Tucker decomposition of the core coefficient tensor with nearly optimal ε-rank parameters, which are shown to be much smaller than both the polynomial degree of the Chebyshev interpolant and the potential number of spatial grid points in the commonly used grid-based discretizations. We discuss the error and complexity estimates of the presented method and demonstrate its efficiency on the demanding example of multi-particle interaction potentials generated by the 3D Newton kernel.

Plenary talk / 73

What to Interpolate for L2 Optimal Approximation: Reflections on the Past, Present, and Future

Author: Serkan Gugercin[1]

[1] *Virginia Tech*

Corresponding Author: gugercin@vt.edu

In this talk, we revisit the L2 optimal approximation problem through various formulations and applications, exploring its rich mathematical structure and diverse implications. We begin with the classical case where the optimal approximant is a rational function, highlighting how Hermite interpolation at specific reflected points emerges as the necessary condition for optimality. Building on this foundation, we consider extensions that introduce additional structure to rational approximations and relax certain restrictions, revealing new dimensions of the problem. Throughout, we demonstrate how Hermite interpolation at reflected points serves as a unifying theme across different domains and applications.

Plenary talk / 32

Fluid-structure interactions with elastic contact - Numerical Modeling and Benchmarking

Author: Thomas Richter[1]

[1] *Otto-von-Guericke Universität Magdeburg*

Corresponding Author: thomas.richter@ovgu.de

We consider an elastic solid, e.g. a ball, which sinks towards the ground in a container filled with a liquid. The ball bounces off the bottom.

From a mathematical point of view, it is not clear what exactly happens. Assuming that the Navier-Stokes equations describe the situation, contact should not occur. The common hypothesis is that if the surface of the sphere is assumed to be perfectly smooth, a thin film of liquid always remains, the forces are transferred into the solid body via this film and are released again due to the elasticity. This results in a rebound without any contact.

In the lecture, the numerical difficulties of simulating such a problem are discussed. The various common approaches, e.g. ALE coordinates or purely Eulerian formulations, all have their own challenges to overcome.

We show that a simulation is possible without adding parameterized additional models to describe the rebound. However, this requires an immense effort. In addition, we present experimental and numerical benchmark problems as well as computational results.

Plenary talk / **46**

Modeling and numerical analysis of sea ice

Author: Carolin Mehlmann[None]

Corresponding Author: carolin.mehlmann@ovgu.de

Sea ice is one of the important components in global circulation models used for weather forecasting and especially for climate prediction. Sea ice is modeled as a 2D layer between the atmosphere and the ocean. While sea ice covers only the polar regions of the Earth, the sea ice component usually takes on the role of a coupler between the ocean and the atmosphere and is responsible for all energy transfer between these two phases.

We focus on the dynamics of sea ice and provide an introduction to modeling it as a 2D fluid. Different rheologies are considered. The most established are approximations to a viscous plastic model.

Finally, we describe the special requirements in terms of numerical discretization and implementation of such a sea ice model, which should fit well into the general framework of global climate models.

Contibuted Talk / 52

Non-intrusive reduced-order modeling for dynamical systems with spatially localized features

Author: Leonidas Gkimisis[1]

Co-authors: Karen E. Willcox [2]; Marco Tezzele [3]; Nicole Aretz [2]; Peter Benner ; Thomas Richter [4]

[1] *MPI Magdeburg*

[2] *The University of Texas at Austin*

[3] *Emory University*

[4] *Otto-von-Guericke Universität Magdeburg*

Corresponding Author: gkimisis@mpi-magdeburg.mpg.de

spatially localized features characterized by slow singular value decay. The proposed approach builds upon two existing methodologies for reduced and full-order non-intrusive modeling, namely Operator Inference (OpInf) and sparse Full-Order Model (sFOM) inference. We decompose the domain into two complementary subdomains which exhibit fast and slow singular value decay, accordingly. The dynamics on the subdomain exhibiting slow singular value decay are learned using sFOM while the
dynamics with intrinsically low dimensionality on the complementary subdomain are learned using OpInf. The resulting, coupled OpInf-sFOM formulation leverages the computational efficiency of OpInf and the high spatial resolution of sFOM and thus enables fast non-intrusive predictions for localized features with slow singular value decay, such as transport-dominated dynamics. Furthermore, we propose a novel, stability-promoting regularization technique with a closed-form solution based on the Gershgorin disk theorem for both sFOM and OpInf models and evaluate the efficiency of the coupled approach in terms of offline and online speedup. Finally, we demonstrate the capabilities of the coupled OpInf-sFOM formulation for testcases such as the one-dimensional, viscous Burgers'equation and a two-dimensional parametric model for the Pine Island Glacier ice thickness dynamics.

Contibuted Talk / 45

Approximating Metastable Dynamics with Koopman Operators

Author: Feliks Nüske[1]

[1] *MPI for Dynamics of Complex Technical Systems*

Corresponding Author: nueske@mpi-magdeburg.mpg.de

Metastablility is a phenomenon which often inhibits the efficient simulation of dynamical systems, or the generation of samples from high-dimensional probability measures. In particular, metastability is frequently encountered in computer simulations of biological macromolecules using molecular dynamics. It is well-known that metastable transitions and their time scales are encoded in the dominant spectrum of certain transition operators, also called Koopman operators. The study of Koopman operators, and their data-driven approximation by algorithms like the Extended Dynamic Mode Decomposition (EDMD), have gained significant traction in the study of dynamical systems, and have led to widespread application.
In this talk, we will report on recent progress in this field for large-scale systems. First, we will present a study showing that a fairly basic linear dimensionality reduction, combined with a clever design of the basis set, can lead to very accurate Koopman models. The second study we will present is on using equilibrium samples produced by a generative model to feed a model for the Koopman generator. This method allows to extrapolate dynamical properties across different thermodynamic parameters, such as temperature.

Contibuted Talk / 67

Generator-extended DMD method for control-affine SDEs

Authors: Lei Guo[1]; Jan Heiland[None]

Co-author: Feliks Nüske [2]

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

[2] *MPI for Dynamics of Complex Technical Systems*

Corresponding Author: lguo@mpi-magdeburg.mpg.de

Stochastic dynamics with metastability are a recurring theme in many scientific disciplines, for instance, in simulations of macro-molecules, in climate systems, and in applications of uncertainty quantification. Metastability describes the existence of long-lived macro-states in a dynamical system's state space, such that transitions between these macro-states are rare events. It is thus also closely related to control systems. There is a wide range of biased sampling algorithms, which seek to overcome the rare event nature of the dynamics using a time-dependent input.

In this study, we join the ideas of Koopman-based modeling and biased sampling. The key ingredient is the generator extended dynamic mode decomposition algorithm (gEDMD), a variant of EDMD to approximate the Koopman generator. For control-affine stochastic differential equations (SDEs), application of gEDMD reduces the Kolmogorov backward equation into an ODE that is bi-linear in expectation and input. This simplified structure can be utilized for designing controllers which are geared towards accelerated sampling of rare events.

In this talk, we will report on recent progress concerning the data-driven analysis of metastable systems using Koopman generators. First, we will introduce Koopman operators for (controlled) stochastic systems, the gEDMD method, and its application to optimal control problem. Second, we will present the numerical results showing that the gEDMD method for control-affine SDEs can be used to a) accurately predict the expectation of observable functions of interest for fixed control input; b) solve optimal control problems (OCPs) with integrated running cost and terminal cost; c) design OCPs which enforce accelerated transitions between metastable states.

Contibuted Talk / 64

Sensor selection using an end-to-end differentiable network with application to nonlinear function approximation

Authors: Sridhar Chellappa[1]; Pawan Goyal[2]; Peter Benner[None]

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

[2] *appliedAI Initiative GmbH*

Corresponding Author: chellappa@mpi-magdeburg.mpg.de

Reconstructing nonlinear parametric functions based on sparse measurements or partially observed sensor data is an important problem arising in a number of practical applications such as climate science, fluid dynamics, and biology. To achieve accurate approximation, two crucial aspects need to be considered: (a) choosing the optimal location for data sampling and (b) identifying a suitable model to map the measured data to the corresponding high-dimensional state. Existing approaches to address this challenge either adopt a linear model for reconstruction [1], leading to poor approximations or follow an ad-hoc (random) choice of sensor locations that fail to efficiently recover the true underlying field [2, 3]. Our solution to address this problem uses a neural network architecture that combines the functionalities of data sampling and reconstruction in the form of a pseudo-autoencoder setup. Importantly, it is differentiable and can be trained end-to-end. Once trained, our setup requires only the sparsely sensed data as input, which is then lifted to the true dimension via the decoder. To perform differentiable sampling, we use stochastic optimization, taking advantage of recent developments in statistical techniques to sample from categorical distributions. We illustrate the benefits of the new approach on numerical examples arising in fluid dynamics and climate science.

There is a close similarity between the above framework and hyperreduction methods [4]. We discuss this connection and explore how our method can be put in the same mathematical setting as hyperreduction. This similarity will also illustrate how the new approach is a natural extension of hyperreduction using neural networks.

[1] K. Manohar, B. W. Brunton, J. N. Kutz and S. L. Brunton, Data-Driven Sparse Sensor Placement for Reconstruction: Demonstrating the Benefits of Exploiting Known Patterns, IEEE Control Systems Magazine, vol. 38, no. 3 (2018), pp. 63-86.

[2] N. B. Erichson , L. Mathelin, Z. Yao, S. L. Brunton, M. W. Mahoney, J. N. Kutz, Shallow neural networks for fluid flow
reconstruction with limited sensors, Proceeding of the Royal Society A, 476: 20200097, 2020.

[3] K. Fukami, R. Maulik, N. Ramachandra, K. Fukagata, and K. Taira, Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, Nature Machine Intelligence 3, no. 11 (2021): 945-951.

[4] C. Farhat, S. Grimberg, A. Manzoni, and A. Quarteroni, Computational bottlenecks for PROMs: precomputation and hyperreduction. In P. Benner, S. Grivet-Talocia, A. Quarteroni, G. Rozza, W. Schilders & L. Silveira (Ed.), Volume 2 Snapshot-Based Methods and Algorithms, pp. 181-244, De Gruyter, 2021.

Contibuted Talk / 57

An Adaptive Procedure to Solve Stochastic Shape Optimization Problems

Author: Hamdullah Yücel[None]

Corresponding Author: yuecel@mpi-magdeburg.mpg.de

In this talk, we present an adaptive based algorithm to solve a robust shape structural optimization problem governed by a linear elasticity model that accounts for uncertainties in the loading and material inputs. A posteriori error estimators are developed to adjust both the sample size and the spatial domain. Within the dual-weighted residual framework, a weighted goal functional is established to consider the errors arising from the approximation of the underlying PDE as well as the approximation of the domain geometry. Finally, the proposed estimation-based adaptive stochastic optimization procedure is tested on the well-known compliance minimization problem of cantilever beams under the load and material uncertainties.

Contibuted Talk / 50

Predicting multiple outputs of parametric dynamical systems using multiple-output temporal fusion transformer

Author: Shuwen Sun[1]

Co-authors: Lihong Feng ; Peter Benner

[1] *MPI Magdeburg*

Corresponding Author: ssun@mpi-magdeburg.mpg.de

With the capability of modern computers for processing large amounts of data, machine learning (ML) is being more and more applied in computational science. Many of the ML learning methods aim to accurately predict the whole solution vector of dynamical systems via data compression, such as convolutional autoencoder. These works focus on predicting only the quantities of interests (QoIs) or outputs using ML without data compression.

Transformer models have been proposed to overcome the difficulties of recurrent neural networks, such as LSTM, for long-term prediction. Many transformer models have been suggested for time series forecast. Most of the transformer models are applied to predict daily life activities, such as customer electricity usage, traffic road occupancy rate, etc. In this work, we explore the promising performance of a transformer model: temporal fusion transformer (TFT) on predicting outputs of parametric dynamical systems. The outputs of such systems vary not only with physical parameters but also with external time-varying input signals. Accurately catching the dynamics of such systems is challenging. We have adapted and extended the original TFT for single output prediction to a multiple-output TFT that is able to predict multiple outputs. The multiple-output transformer generalizes the interpretability of the original TFT model. The generalized interpretable attention weight matrix explores not only the temporal correlations in the sequence, but also the interactions between the multiple outputs.

Contibuted Talk / 63

Parametric interpolation for nonlinear dynamical systems using barycentric rational approximation of matrix-valued functions

Author: Ion Victor Gosea[1]

Co-authors: Karim Cherifi ; Sridhar Chellappa [2]

[1] *MPI Magdeburg*

[2] *Max Planck Institute for Dynamics of Complex Technical Systems*

Corresponding Author: gosea@mpi-magdeburg.mpg.de

Parametrized nonlinear dynamical systems often arise upon discretizing parametrized partial differential equations (PDEs). Typically, the former tends to be of a large scale, i.e., the number of state variables could be significantly high (the state vector is denoted with x(t, p), p is the vector of parameters, the nonlinearity is f(x(t, p), p), while the matrices corresponding to the linear part are E(p), A(p), and B(p)). Solving it repeatedly at different parameter samples p (e.g., in the context of optimization and/or uncertainty quantification) tends to be an expensive pursuit. To address this, a reduced-order model (ROM) of the same structure can be obtained using well-known approaches such as proper orthogonal decomposition (POD), reduced basis method (RBM), and balanced truncation (BT). The number of equations in this formulation is usually far lesser compared to the full-order model, which makes it amenable to rapid, real-time evaluations, thereby circumventing expensive simulations associated with large-scale system evaluation.

In the context of the POD or RBM, snapshots of the solution vectors x(t, p), obtained at different time instances and different parameter samples are used to obtain a suitable projection matrix V which can be used to obtain the ROM via Galerkin projection.
A key implicit assumption in defining the reduced quantities thus obtained is that the matrices E(p), A(p), B(p), f(x(t, p), p) have an affine parameter dependence. While the affine parametric dependence assumption indeed holds in several applications, there are many cases where it does not hold. That is, it is impossible to know, a priori, the parameter affine form. In such scenarios, there is a need for a cheap and effective approximation technique to learn a function mapping the parameter p to the reduced matrices.

Pre-existing works that tackle the issue of non-affine parametrized matrices and/or vectors are only a few; in [Negri et al. '15] the authors introduced the matrix discrete empirical interpolation method (MDEIM) which leverages DEIM [Chaturantabut/Sorensen '10] to learn the mapping from the parameter to the reduced system matrix. However, this method needs data/entries of E(p) evaluated at a sparse set of locations. In the work [Degroote et al. '10], the authors propose an entry-wise interpolation of E(p) using splines. The same work also introduces a different technique of interpolating the reduced matrices over a Riemannian manifold for better approximation.

Recently, [Pelling et al. '24] exposed an interesting application of the classic Loewner approach for rational approximation in the context of parametric linear time-invariant (pLTI) systems. The authors utilize the snapshots of parametrized system matrices and the linear fractional transform to obtain ROMs of pLTIs. An intermediate step involved in the approach proposed in [Pelling et al. '24] is the use of the univariate Loewner approximation method in [Mayo/Antoulas '07] to interpolate large-scale system matrices E(p), A(p), and B(p). In our work, we rely on the observation of [Pelling et al. '24], but instead use it to learn a map from the parameter p to the reduced system matrices obtained via Galerkin projection. We do this by utilizing extensions of the Loewner framework for multiple parameters [Ionita/Antoulas '14], that rely on multivariate barycentric forms. Challenges that occur in this process come from dealing with a higher number of parameters (in the vector p) and with the non-scalar format of the data. We deal with these by accommodating the generalized barycentric forms to the matrix format (using barycentric formulas with matrix-valued weights as in [G./Guettel '21]), as well as allowing an adaptive choice of interpolation points (parameter values). Several numerical examples attest to the practical applicability of the proposed method.

Poster Presentations / 69

A mixed-precision algorithm for the Sylvester matrix equation

Author: Xiaobo Liu[1]

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

Corresponding Author: xliu@mpi-magdeburg.mpg.de

In the usual one-precision environment the Bartels–Stewart algorithm is the standard algorithm for solving small dense Sylvester matrix equations AX+XB=C. their algorithm consists of three steps, including the computation of the Schur decompositions, the substitution for solving the Sylvester equation with quasi-triangular coefficients, and the final recovering transformation.

In the new mixed-precision algorithm we propose, the computation of the Schur decompositions, which are the most expensive part of the algorithm, is performed in a low precision. Then the algorithm *refines* via a stationary iteration the approximate solution obtained by solving the quasi-triangular Sylvester equation with the low-precision quasi-triangular coefficient matrices; and this is in fact an iterative refinement scheme for the quasi-triangular Sylvester equation with the coefficient matrices in a perturbed form. Finally, in order to recover the solution from the Schur decompositions we need the unitary factors to be unitary to the working precision. In order to do so, we propose two efficient approaches to orthonormalize to the working precision the low-precision unitary factors, one based on orthonormalization and the other on inversion of the unitary factors.

We test the new mixed-precision methods on various problems from the literature containing both Sylvester and Lyapunov matrix equations. Numerical experiments show that the new methods are comparable with the classical Bartels–Stewart method in terms of accuracy, and they can be faster if the employed low-precision arithmetic is sufficiently cheaper than the working-precision arithmetic.

Poster Presentations / 71

Linear $\mathcal{L}$-structured matrix equations

Authors: Peter Benner[None]; Sergii Chuiko[1]; Mykhailo Chuiko[2]

[1] *Donbass State Pedagogical University, Donetsk region, Slavyansk, Ukraine*

[2] *Taras Shevchenko National University of Kyiv, Ukraine*

Corresponding Author: chuiko@mpi-magdeburg.mpg.de

We study the problem of constructing solutions [1, 2] $X \in \mathbb{R}^{\alpha\times\beta}$ of a linear matrix equation
$LX = F, F \in \mathbb{R}^{\gamma\times\delta}$, (1)
where $L : \mathbb{R}^{\alpha\times\beta} \to \mathbb{R}^{\gamma\times\delta}$ is a linear bounded matrix functional. A partial case of the matrix algebraic equation (1) is the well-known Sylvester and Lyapunov equations [1, 3, 4]. In the article [5], the definition of several partial cases was introduced for a matrix algebraic equation (1) with a $\mathcal{L}$-structure
$\mathcal{L}X = F$, (2)
which determines the linear relationship between the elements of the solution of the matrix algebraic equation. In particular, the $\mathcal{L}$-structure defines symmetric, skew-symmetric, diagonal matrices, as well as quaternions. Thus, we obtain the problem of finding solutions of a linear matrix equation (1) with a $\mathcal{L}$-structure defined by a linear bounded matrix functional
$\mathcal{L} : \mathbb{R}^{\alpha\times\beta} \to \mathbb{R}^{\lambda\times\mu}$;
here $\mathcal{F} \in \mathbb{R}^{\lambda\times\mu}$ is a known matrix. In partial case, the $\mathcal{L}$-structure defines magic squares [6], Hilbert, Hankel and Toeplitz matrices [7], Hermitian [8], symmetric and skew-symmetric matrices, as well as quaternions and biquaternions [9, 10].

References

[1] Benner P., Bollhofer M., Kressner D., Mehl C., Stykel T. Numerical Algebra, Matrix Theory, Differential-Algebraic Equations and Co Numerical Algebra, Matrix Theory, Differential-Algebraic Equations and Control Theory. —2015 .—Springer International Publishing. —608 p.
[2] Chuiko S.M. The solution of the linear matrix equations // Visnyk of
V.N. Karazin Kharkiv National University. Ser. mathematics, applied mathematics and mechanics. —2015. —29. —P. 27 —33.
[3] Boichuk A.A., Krivosheya S.A. Criterion of the solvability of matrix equations of the Lyapunov type // Ukrainian Mathematical Journal. –1998.–50 (8). –pp. 1162 –1169.
[4] Boichuk A.A., Krivosheya S.A. A Critical Periodic Boundary Value Problem for a Matrix Riccati Equation // Differential Equations. —2001.—37 (4). —pp. 464 —471.
[5] Magnus J.R. L-structured matrices and linear matrix equations //Linear and multilinear algebra. —1983. —14. —P. 67 —88.
[6] Pinn K., Wieczerkowski C. Number of magic squares from parallel temperingMonte Carlo // arxiv.org, April 9, 1998.
[7] Fiedler M. Hankel and Loewner Matrices // Linear algebra and its application.—1984. —58. —P. 75 —95.
[8] Khatri C.G., Mitra K. Hermitian and nonnegative definite solutions of linear matrix equations // SIAM Journal on Applied Mathematics. —1976. —31(4). —P. 579 —585.
[9] Ahmad S.S., Bhadala N. L-structure least squares solutions of reduced biquaternion matrix equations with applications //ArXiv.2311.06461 DOI:10.48550.
[10] Long-Sheng Liu, Shuo Zhang A coupled quaternion matrix equations with applications // Journal of Applied Mathematics and Computing. —2023. —69.—P. 4069 —4089.

Poster Presentations / 66

Molecular Kinetics with Koopman Operators: Application to large-scale Systems

Author: Hauke Sprink[1]

[1] *MPI Magdeburg*

Corresponding Author: sprink@mpi-magdeburg.mpg.de

Biomolecular processes often involve transitions between metastable states governing molecular function. Extracting this information is challenging due to the high dimensionality of simulation data. Kernel methods are a powerful tool for automated analysis of complex systems, yet their need for pairwise kernel evaluations leads to scalability issues, particularly in large datasets.
To address this, we integrate Random Fourier Features (RFF) into Kernel-based Extended Dynamic Mode Decomposition (EDMD), providing a scalable method for studying long-time kinetics in biomolecular systems. By comparing and combining this approach with other dimensionality reduction techniques, we demonstrate its robustness and potential for enabling efficient analysis of molecular data.

Poster Presentations / 47

Diffusion Monte Carlo as a Stochastic Optimal Control Problem

Authors: Feliks Nüske[1]; Lei Guo[1]; Luís Tadeu Nascimento Pires[1]

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

Corresponding Author: pires@mpi-magdeburg.mpg.de

Solving the Schrödinger equation is a central task in quantum chemistry. Diffusion Monte Carlo (DMC) is a stochastic method that utilizes the connection between this equation and those governing diffusion phenomena to obtain accurate estimates of the eigenvalues and eigenfunctions involved. This is made possible by the well-known Feynman-Kac formula, which allows the Schrödinger equation to be expressed in terms of the expectation of the solution to a stochastic differential equation. However, efficient evaluation of the required quantities remains an open problem. In this work, we show that bypassing the sampling from an unknown distribution with a variational principle leads to a recasting of the problem as a stochastic optimal control task. In this setting, the linearity of observables permits us to employ Koopman operator methods to approximate the desired solutions in a computationally tractable manner.

Poster Presentations / 61

Prescribed-Time Asynchronous Boundary Control for Uncertain Delay Reaction-Diffusion Systems

Author: Xuelian Wang[1]

[1] *MPI*

Corresponding Author: xwang@mpi-magdeburg.mpg.de

There have been a number of works in the literature dealing with the stabilization of processes with input delays for a reaction-diffusion partial differential equation, mainly by using finite-time control strategies, where their settling time depends on the initial conditions. However, in many practical applications, it is difficult or even impossible to obtain system initial values in advance, which makes it impossible to control the settling time. Recently, the prescibed-time control method has aroused extensively research interests, because for the upper bound of settling time, it can be arbitrarily selected by suitably tuning control parameters, and the true convergence time in prescribed-time stabilization results is independent of initial conditions. Thus far, the research on prescribed–time stabilization of reaction-diffusion systems is interesting and meaningful. In this talk, the prescribed-time stabilization is considered for uncertain delay reaction–diffusion systems via asynchronous boundary control.

Poster Presentations / 37

DEIM-spirited hypred reduction for nonlinear constraint projectiond

Authors: Peter Benner[None]; Shaimaa Monem[None]

Corresponding Author: monem@mpi-magdeburg.mpg.de

We introduce a novel reduction bases to accelerate the nonlinear term evaluation of constraints projections on different mesh elements. Our method determines an approximate reduced subspace that is computed on the constrained elements (vertices, triangles, tetrahedrons) which show the largest deformation on the provided set training snapshots. We achieve low error bounds by incorporating the differential operator that maps constrained projections to position space and use a discrete empirical interpolation to determine a small set of interpolation elements which then can be used instead of full elements dimension in order to internal forces computation. Our method works with any mesh. We compare to the state of are using linear-blend skinning for the same purpose and show lower ranges of relative norm errors and rotations, our results show high computational efficiency, stability using much smaller subspace dimension as well as constrained elements.

Poster Presentations / 51

Structure-preserving symplectic neural networks for parametric Hamiltonian systems

Author: Konrad Janik[1]

Co-author: Peter Benner

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

Corresponding Author: janik@mpi-magdeburg.mpg.de

The numerical integration of Hamiltonian systems is a central topic in computational physics and theoretical chemistry. Intrinsic structure-preserving symplectic networks (SympNets) [1] are a widely used tool when it comes to learning symplectic integrators for Hamiltonian systems from data. More often then not Hamiltonian systems of interest depend on a set of parameters. Currently, SympNets do not respect parameters. Therefore, SympNets have to be retrained for every new parameter combination. To eliminate this necessity, we propose to extend the SympNet architecture to handle parameters explicitly, making it suitable for parametric Hamiltonian systems. This approach is coined "ParSympNets". We perform different numerical experiments to investigate the approximation and generalization capabilities of ParSympNets. Furthermore, we present a new universal approximation theorem, which shows that ParSympNets can approximate arbitrary parametric symplectic maps.

References
[1] P. Jin, Z. Zhang, A.Zhu, Y. Tang, and G. E. Karniadakis., SympNets: intrinsic structure-preserving symplectic networks for identifying Hamiltonian system, Neural Networks, 132:166–179, 2020.

Poster Presentations / 55

Efficient iterative solution of nonstandard algebraic Riccati equations via indefinite factorizations

Authors: Jens Saak[1]; Steffen W.R. Werner[2]

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

[2] *Virginia Tech*

Corresponding Author: saak@mpi-magdeburg.mpg.de

For the standard algebraic generalized Riccati equation

$C^TQC + A^TXE + E^TXA - E^TXBR^{-1}B^TXE = 0$

different algorithms inspired by the low-rank alternating directions implicit (LR-ADI) iteration and Krylov subspace projection have successfully been applied, based on the ZZ^T factorization of the iterates, when Q, R are both symmetric, and $Q \geq 0$ and $R > 0$.

In this contribution, we investigate the more general equations of the type

$C^TQC + A^TXE + E^TXA - (E^TXB + S)^TR^{-1}(B^TXE + S^T) = 0$

allowing for $R > 0$, $R < 0$ or even indefinite R. While for the specific cases we investigate, the solution is always the stabilizing solution which can be shown to be semi-definite, the latter is not always true for intermediate iterates. Thus, in order to avoid complex arithmetic, and to simplify algorithmic representations, we suggest the use of indefinite factorizations of the form LDL^T for the representation of solution approximations and residuals. The main goal of this research is to bring low-rank Riccati solvers closer to the capabilities of, e.g., `icare` in MATLAB. This, in turn, enables balancing based model order reduction methods, such as positive-real or bounded-real balanced truncation, for large-scale linear time-invariant (LTI) systems.

Poster Presentations / 59

Benchmarking pyMOR QR decompositions

Author: Maximilian Bindhak[1]

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

Corresponding Author: bindhak@mpi-magdeburg.mpg.de

pyMOR, a Python toolbox for building reduced order models, supports a variety of solver backends, such as dune-gdt, FEniCS, NGSolve, NumPy and potentially MPI distributed variants. An abstract interface, the VectorArray, is used to wrap vectors and matrices from these backends on which pyMOR's algorithms work. For compatibility reasons direct access of entries has to be avoided, which restricts possible algorithms.

Projection based methods used in model order reduction rely on a numerically stable QR decomposition, i.e. $A = QR$ for $A \in \mathbb{C}^{m \times n}, r = \text{rank}(A), Q \in \mathbb{C}^{m \times r}, R \in \mathbb{C}^{r \times n}$, where A is "tall" and "skinny", i.e. $m \gg n$. The current implementation is a repeated modified Gram-Schmidt, which is numerically robust at the cost of high runtimes. In order to increase the performance promising algorithms from papers are implemented and quantified. The "classical Gram-Schmidt with normalization lag and re-orthogonalization lag" performs the best if only a few vectors have to be orthogonalized or have to be orthogonalized against an orthonormal basis. In contrast, the novel "shifted Cholesky QR" scales better for large n. Essential for this algorithm is the evaluation of the Gramian $X = A^T A$. In case the Gramian is not positive definite, a shift, based on its norm, has to be evaluated and applied onto the diagonal. The algorithm can compute good approximations even for high matrix condition numbers if the shift is recomputed in every iteration. Using symmetric eigenvalue solvers one can further decrease the runtime of the norm computation for large n.

Poster Presentations / 62

A realization-free approach for constructing surrogate bilinear reduced-order models

Author: Jan Lilienblum[1]

Co-authors: Igor Pontes Duff ; Ion Victor Gosea [2]; Peter Benner

[1] *Max-Planck-Institute for Dynamics of Complex Technical Systems*

[2] *MPI Magdeburg*

Corresponding Author: jan.lilienblum@ovgu.de

The class of bilinear dynamical systems often arises in the description and approximation of large-scale nonlinear systems with analytic nonlinearities. This bilinear structure allows the extension of various established model order reduction (MOR) approaches, from their linear counterparts. In this work, our aim is to introduce a realization-free, data-based MOR method, inspired by the TF-IRKA method in [Beattie/Gugercin ‘12] and the BIRKA method in [Benner/Breiten ‘12, Flagg/Gugercin ‘15]. The former one is applicable solely to linear systems, but is non-intrusive, while the latter one is applicable to bilinear systems, but is intrusive (requires system matrices).

We propose an approach that we call TF-truncBIRKA, which is a novel non-intrusive reduction method, based on constructing quasi-Loewner matrices (similar to those in the bilinear Loewner frameworks [Antoulas/G./Ionita ‘16] and [G./Pontes Duff ‘22]), and therefore relies solely on the evaluation of generalized transfer functions (corresponding to the original system). Starting from a cascaded form of underlying generalized Sylvester equations and based on the standard BIRKA approach, data-based Loewner matrices are computed at each step as system matrices of the surrogate reduced model. To make the presentation as clear as possible, we will stop at the second level in the Volterra series decomposition, hence the prefix “trunc” (truncated) appearing in the name of the method. However, extensions to higher-order truncation levels are indeed feasible and may be explored. The method is indeed iterative (in the fashion of all IRKA-based approaches), and will be stopped based on a termination criterion similar to that of BIRKA (when the poles of the linear subsystem do not change much, i.e., w.r.t. a tolerance value).

The proposed iterative, realization-free approach TF-truncBIRKA reaches the goal of reducing bilinear systems in a data-based manner and successfully replaces the computation of standard projection matrices. Interpolation conditions are also derived, and in order to validate the practical applicability of the method, several numerical test cases are presented.

Poster Presentations / 54

Optimization and Stability of Chemical Reactor Models

Authors: Yevgeniia Yevgenieva[1]; Alexander Zuyev[None]; Peter Benner[None]

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

Corresponding Author: yevgenieva@mpi-magdeburg.mpg.de

We analyze two classes of mathematical models describing chemical reactions of the type "$A \to$ product," conducted in tubular reactors. The first class involves nonlinear hyperbolic partial differential equations modeling a plug flow reactor (PFR) in the presence of an inert component. For this system, an isoperimetric optimal control problem is formulated to maximize the mean product yield over a period under input constraints. The optimality of a bang-bang control strategy is rigorously proved within the class of bounded measurable inputs. Additionally, numerical case studies demonstrate the efficiency of the proposed strategies.

The second class involves a nonlinear parabolic partial differential equation that models a dispersed flow tubular reactor with a single boundary control input. The existence and uniqueness of solutions to the associated nonlinear Cauchy problem are established using the theory of strongly continuous semigroups. Furthermore, by employing Lyapunov's direct method, we design a feedback control strategy that ensures the exponential stability of the steady state and evaluates the decay rate of the solutions. Together, these results provide a comprehensive framework for the analysis and control of chemical reactor models.

Poster Presentations / 48

A Multi-Layered CSE Workflow Framework for FAIR Numerical Experiments

Author: Pavan L. Veluvali[1]

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

Corresponding Author: veluvali@mpi-magdeburg.mpg.de

Numerical algorithms and computational tools are essential for managing and analyzing complex data processing tasks. As meta-data and parameter-driven simulations have become more prevalent, the need for automated workflows to reproduce computational experiments across platforms has significantly increased. In general, a computational workflow is defined as a step-by-step description for accomplishing a scientific objective. Characterized through their input-output relation, computational workflows are designed such that the associated meta-data can be used interchangeably and redundantly. In the present work, we develop a computational framework, namely, MaRDIFlow, that focuses on the abstraction of meta-data while negating the underlying dependencies through multi-layered descriptions. Notably, by allowing the complete range between abstract descriptions and concrete numerical realizations (or even plain input-output data) of the tasks to serve equivalently and possibly redundantly in the definition of the workflows, we provide the lowest possible barrier for findable, accessible, interoperable and reusable (i.e. FAIR) workflow definitions. We showcase minimum working examples and how they are systematically incorporated into our workflow framework.

Poster Presentations / 41

Data-Driven Generalised eigenvalue problems in Tensor Train Format

Authors: Feliks Nüske[None]; Minakshi Verma[None]; Peter Benner[None]

Corresponding Author: mverma@mpi-magdeburg.mpg.de

This poster introduces an approach to solving the Generalised eigenvalue problems arising from the tensor- based Extended Dynamic Mode Decomposition (EDMD). The Extended Dynamic Mode Decomposition (EDMD) is a data-driven technique used for approximating the Koopman operator, a linear operator which is particularly useful for understanding the behavior of nonlinear dynamical systems from observational data. But solving high-dimensional eigenvalue problems is very challenging in terms of storage consumption and computational robustness. So, we are presenting EDMD as a Tensor (a multidimensional generalisation of matrices) based method. Tensors arise from a multi-linear structure; for example, when constructing a large basis set of from products of lower-dimensional functions. We are using the Tensor Train (TT) format which is one of the promising candidates for approximating high-dimensional tensors by low-rank decompositions.

Poster Presentations / 58

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

Author: Chenzi Wang[1]

[1] *MPI magdeburg*

Corresponding Author: cwang@mpi-magdeburg.mpg.de

The increasing complexity in design and manufacturing has driven the need for advanced techniques for fast modeling problems with high-dimensional parameter spaces. Avoiding high-fidelity finite element models while achieving fast and accurate simulations in such contexts is challenging. Projection-based parametric model order reduction (pMOR) has drawn significant attention in recent years. Nevertheless, the curse of dimensionality in parameter spaces has severely limited its effectiveness. The active subspace (AS) approach has been successfully applied to pMOR for systems with many parameters. However, the balance between accuracy and compactness of the reduced model remains problematic for systems with high-dimensional parameter spaces. It often results in models that are either small enough or accurate enough. We propose an iterative active subspace (IAS) approach for parametric model order reduction, which, to some extent, addresses the trade-off between accuracy and reduced model size and achieves substantial computational gains compared to the original active subspace method.

Poster Presentations / 56

Port Hamiltonian connection of pipes

Authors: Ashwin Nayak[1]; Sara Grundel[None]

[1] *CSC group*

Corresponding Author: grundel@mpi-magdeburg.mpg.de

The poster will present a comparison of different Port Hamiltonian models focusing on the interconnection of two or more PH models to generate a new PH model. Starting from a standard linear finite dimensional system a few steps will be presented how one could model the generalized framework of nonlinear and infinite dimenisonal systems. Some examples will be shown in the context of interconnections of two or more pipes to a network of pipes. The industrial application in mind being gas or liquid transportation networks.

Poster Presentations / 60

Structure-preserving learning for multi-symplectic PDEs

Author: Süleyman Yildiz[1]

Co-authors: Pawan Goyal [2]; Peter Benner

[1] *Group of Computational Methods in Systems and Control Theory (CSC), Max Planck Institute for Dynamics of Complex Technical Systems*

[2] *Max Planck Institute for Dynamics of Complex Technical Systems*

Corresponding Author: yildiz@mpi-magdeburg.mpg.de

We present a novel machine learning approach to develop energy-preserving reduced-order models (ROMs) by exploiting the multi-symplectic structure of partial differential equations (PDEs). Traditional energy-preserving ROMs often rely on the symplectic Galerkin projection, which requires fully discrete operators - often unavailable in black-box PDE solvers. Our method circumvents this limitation by inferring the PDE dynamics directly from the data, eliminating the need for fully discrete operators and maintaining a non-intrusive framework. The proposed approach is gray-box in the sense that it requires only minimal knowledge of the multi-symplectic model at the PDE level. We show that our method ensures spatially discrete local energy conservation and preserves multi-symplectic conservation laws. Validation of the method is performed on the linear wave equation, the Korteweg-de Vries equation, and the Zakharov-Kuznetsov equation, with successful generalization beyond the training time interval.

Poster Presentations / 53

Applications of operator inference for second-order systems

Author: Yevgeniya Filanova[None]

Co-authors: Igor Pontes Duff ; Peter Benner

Corresponding Author: filanova@mpi-magdeburg.mpg.de

Operator inference (OpInf) is a method for non-intrusive reduced modeling, i.e., identifying small surrogate models from data. In this poster, we consider second-order ODE systems, which are typically used to model mechanical vibrations. The variety of load cases requires specific adaptations of the OpInf method, taking into account different approaches to modeling the corresponding problems, as well as the characteristics of the output data. This poster shows extensions of the OpInf approach that allow us to preserve the structure of the system matrices, and thus the physical meaning and properties of the full-order system. Depending on the problem, the presented OpInf methods use semidefinite programming or parameterization of the unknown coefficients for structure preservation. In addition, a novel non-intrusive procedure for contact problems is presented that combines OpInf with classical intrusive substructuring approaches.
We present applications of the OpInf method to simple bending and rotating structures, such as beams and rotors, as well as to more complex systems, such as contact problems with a rigid obstacle. Using only data that stem from simplified simulations, the OpInf method allows efficient construction of reduced-order models, providing interpretable and meaningful results even for dynamic cases not included in the training data.

Poster Presentations / 31

A higher dimensional perspective on composite gas flow simulations in pipeline networks

Authors: Ashwin Nayak[1]; Sara Grundel[None]; Peter Benner[None]

[1] *CSC group*

Corresponding Author: anayak@mpi-magdeburg.mpg.de

Accurate simulations of gas flow within pipeline networks provide crucial insights for transmission and design operators. This importance intensifies with the growing integration of hydrogen-blended fuels in hydrogen-based energy systems. Existing models predominantly address single-component, one-dimensional flow within individual pipe segments, interconnected at network junctions. Recently, composite flow models within pipes, frequently employing mixture fraction methods, have garnered significant attention. These methods utilize a segregated approach to flow and composite transport, albeit within the limitations of one-dimensional modeling. Physically, hydrogen's low molecular weight can lead to complex and non-intuitive flow dynamics and advection patterns in blended gas mixtures which may not reflect in 1D models. Exploring higher-dimensional models can offer a more comprehensive understanding of the underlying physics. The talk focuses on developing 2D and 3D pipe flow models for composite gases, explore coupling frameworks and numerical discretizations for networks.

Poster Presentations / 40

Understanding the Mechanisms of Partially Observation by Mori-Zwanzig Formalism for Large-scale Systems

Authors: Fan Wang[1]; Jan Heiland[2]

[1] *MPI-Magdeburg*

[2] *Ilmenau University of Technology*

Corresponding Author: fwang@mpi-magdeburg.mpg.de

Model-order Reduction (MOR) is a technique used to reduce the complexity of high-dimensional dynamical systems while preserving their essential properties. It has been been successfully used in many scientific and engineering fields, such as Fluid Dynamics and Control Theory by methods like Proper Orthogonal Decomposition (POD), Autoencoder, Dynamic Mode decomposition (DMD) and so on. However, most MOR techniques assume that the full state is available which may not be the case, e.g. in molecular dynamics simulations and climate simulations. Hence techniques with partially observed states have been developed, since common MOR procedure cannot be applied.

Partial of the state space/observation is available of dynamical systems, unlike traditional MOR techniques mentioned above, there is not enough accessible information to build a ROM according to FOM. That is, we should propagate dynamics through the partially observed state space. The Mori-Zwanzig formalism (MZ) provides a powerful and systematic way to model the system by partially observed information by introducing a projection operator and memory kernel. The projection operator decomposes observed variables and observed variables to construct a model that only involves observed variables. We have implemented MZ in a large-scale linear system with partial observation, for which the matrix A of the dynamics $\dot{x} = Ax$ is partitioned into A_{11}, A_{12}, A_{21} and A_{22} corresponding to observed states, unobserved states and their interactions respectively. Our work demonstrates that the solution of the Mori-Zwanzig (MZ) formalism is quite accurate compared to the RK45 ODE solver in a large-scale linear system when a partial dimension (e.g., 5 out of 10) is observed. However, there is no free lunch; as a consequence of missing information about the unobserved dimensions, an integro-differential equation that includes a non-Markovian memory kernel must be solved. Consequently, the MZ approach suffers form high computational costs, especially when the integration time step is long. We plan to implement Neural Networks (NN) to approximate the memory kernel from data, thereby avoiding expensive on-the-fly computations. Subsequently, we intend to apply the MZ formalism to nonlinear large-scale systems to make it more widely applicable.

Poster Presentations / 68

Kinetically Consistent Coarse Graining using Kernel-based Extended Dynamic Mode Decomposition

Author: Vahid Nateghi[None]

Corresponding Author: nateghi@mpi-magdeburg.mpg.de

In this work, we show how kernel-based approximation to the Koopman generator –the kgEDMD algorithm –can be used to identify implied timescales and meta-stable sets in stochastic dynamical systems, and to learn a coarse-grained dynamics on reduced variables, which retains the essential kinetic properties of the full model. The centerpiece of this study is a learning method to identify an effective diffusion in coarse-grained space by leveraging the kgEMD model for the Koopman generator. By combining this method with force matching, a complete model for the effective dynamics can be inferred. Using a two-dimensional model system and molecular dynamics simulation data of alanine dipeptide and Chignolin, we demonstrate that the proposed method successfully and robustly recovers the essential theormodynamic and kinetic properties of the full model.

Plenary talk / 35

Optimal control for a class of linear transport-dominated systems via the shifted proper orthogonal decomposition

Author: Tobias Breiten[1]

[1] *Technische Universität Berlin*

Corresponding Author: tobias.breiten@tu-berlin.de

Solving optimal control problems for transport-dominated partial differential equations (PDEs) can become computationally expensive, especially when dealing with high-dimensional systems. To overcome this challenge, we focus on developing and deriving reduced-order models that can replace the full PDE when solving the optimal control problem.
Specifically, we explore the use of the shifted proper orthogonal decomposition (sPOD) as a reduced-order model, which is particularly effective for capturing high-fidelity, low-dimensional representations of transport-dominated phenomena.
Furthermore, we propose two distinct frameworks for addressing these problems: one where the reduced-order model is constructed first, followed by optimization of the reduced system, and another where the original PDE system is optimized first, with the reduced-order model subsequently applied to the optimality system. We consider a 1D linear advection equation problem and compare the computational performance of the shifted POD method against conventional methods like the standard POD when the reduced-order models are used as surrogates within a backtracking line search.

This is joint work with S. Burela and P. Schulze from TU Berlin.

Plenary talk / 44

Preservation of Algebraic Stability Domains in Reduced Models

Author: Tobias Damm[1]

Co-author: Tobias Breiten

[1] *RPTU Kaiserslautern-Landau*

Corresponding Author: tdamm@rptu.de

For linear control systems, we study algebraic stability domains which are defined by polynomial inequalities in the complex plane. Based on Kharitonov's characterization via generalized Lyapunov matrix inequalities, we define a suitable pair of Gramians and a balancing transformation. Then we analyze the preservation of these stability domains by balanced truncation. For domains bounded by conic sections we obtain positive results, while for some other types of domains counterexamples are presented.

Plenary talk / 70

A reduced basis method for parabolic PDEs based on a least squares space-time formulation

Author: Michael Hinze[1]

[1] *Universitat Koblenz*

Corresponding Author: hinze@uni-koblenz.de

We propose a least-squares formulation for parabolic PDEs in the natural $L^2(0,T;V^*) \times H$ norm which avoids regularity assumptions on the data of the problem, which e.g. appear in the recently proposed First Order System Least Squares (FOSLS) method. For abstract parabolic equations the resulting bilinear form then is symmetric, continuous, and coercive. This among other things paves the ground for classical space-time a priori and a posteriori Galerkin frameworks for the numerical approximation of this problem class.

The approach is applicable for parameterized parabolic equations as well and we introduce a model order reduction technique that takes over all advantages from well-known elliptic settings. We introduce a POD-greedy method in some space-time energy norm at hand with absolute and relative error bounds. Numerical examples illustrate the performance of the method.

This is joint work with Christian Kahle and Michael Stahl from the University of Koblenz.

Contibuted Talk / 30

System Norms for LPV Approximations

Author: Jan Heiland[None]

Corresponding Author: heiland@mpi-magdeburg.mpg.de

The computation of system norms is an important part of system-theoretic model order reduction (MOR). For linear time-invariant (LTI) systems, norms are well-defined and accessible formulas are available and one may well say that the handling of the relevant system norms is what makes the popular MOR methods Balanced Truncation and IRKA performant.

Beyond LTI systems, already the definition of the system norms comes with several theoretical difficulties and there only exists a few heuristic computational approaches to their evaluation.

In this work, we review the basic concepts of system norms and how they have been used for measuring linear parameter-varying (LPV) systems. We consider simplifying structures in the parameter dependencies, we comment on their applicability for the quantification of approximation errors, and propose reformulations for the efficient numerical evaluation of the norms.

Contibuted Talk / 38

On classical and sampling strategies in the stabilization problem under nonlinear controllability conditions

Author: Alexander Zuyev[None]

Corresponding Author: zuyev@mpi-magdeburg.mpg.de

This talk addresses the stabilization problem for essentially nonlinear control-affine systems under the Lie Algebra Rank Condition (LARC). Previously, a family of oscillating feedback controls was proposed to stabilize the equilibrium of a driftless system under higher-order controllability assumptions. This stabilization scheme relies on a sampling process, which differs from the classical definition of solutions to the closed-loop system or the definition in the sense of Carathéodory.
In the present talk, we refine the design of feedback controllers by presenting sufficient conditions for the exponential and polynomial convergence of classical solutions of the closed-loop system to the stabilized target.

Contibuted Talk / 33

Reduced-Order Models for Fluid Flow: A Physics-Preserving Approach

Author: Yongho Kim[1]

Co-authors: Jan Heiland [1]; Peter Benner [1]

[1] *Max Planck Institute for Dynamics of Complex Technical System*

Corresponding Author: ykim@mpi-magdeburg.mpg.de

Model order reduction (MOR) is a method designed to simplify high-dimensional systems by representing their states using a low-dimensional parametrization. It enhances computational efficiency and reduces memory usage but can lead to reduced simulation accuracy and difficulties in preserving system properties, such as sparsity, positivity, and incompressibility. Consequently, choosing an appropriate MOR approach with an optimal latent dimension is critical to achieving a balance between accuracy and efficiency.

In this work, we introduce autoencoders that reconstruct latent states using actual states sampled from a dataset. This method is compared against two well-known approaches: proper orthogonal decomposition and proper CUR decomposition. We develop reduced-order models of the wake flow around a single cylinder, governed by the incompressible Navier-Stokes equations, and evaluate their simulation accuracy and ability to preserve fundamental physical principles such as incompressibility.