

Identification, Simulation and Control of Complex Dynamical Systems from Data

 at

Schloss Ringberg in Tegernsee

May 8th-11th 2019

Wednesday, May 8

8:00	Bus departure (Treffpunkt: MPI entrance at 7:45)
18:30 - 19:30	Dinner
19:30 - 19:45	Opening remarks
Session 1	Chair: Roman Weinhandl
19:45 - 20:05	Jan Heiland (15+5 min) Riccati-based \mathcal{H}_{∞} controller for descriptor systems
20:05 - 20:25	Alexander Zuyev (15+5 min) Stabilization of the Euler equations with oscillating controls

20:30 - 22:00 **Poster session**

Thursday, May 9

8:00 - 9:00 E	Breakfast
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Session 2	Chair: Manuela Hund
9:00 - 9:45	Serkan Gugercin (40+5 min) Data-driven modeling for solving nonlinear eigenvalue prob- lems and estimating dispersion curves
9:45 - 10:05	Thanos Antoulas (15+5 min) The choice of interpolation points in the Loewner framework
10:05 - 10:25	Igor Pontes Duff (15+5 min) Automatic generation of minimal and reduced systems for structured parametric systems
10:25 - 10:45	Ion Victor Gosea (15+5 min) Data-driven identification and model reduction of nonlinear systems

10:45-11:15 **Coffee break**

Thursday, May 9 - Cont.

Session 3 Chair: Sridhar Chellappa

- 11:15 11:35 **Tim Mitchell** (15+5 min) Computing the Kreiss constant
- 11:35 12:50 Michael Hinze & Carmen Gräßle (65+10min) Tutorial: Adaptivity in simulation based model order reduction

12:50 Packed lunch

- 13:00 18:00 Hiking tour
- 18:30 22:00 Dinner Bavarian evening

Friday, May 10

8:00 - 9:00 Breakfast

Session 4	Chair: Manuel Baumann
9:00 - 9:30	Boris N. Khoromskij (25+5 min) Range-separated format for computation of electrostatics in many-particle systems
9:30 - 9:50	Cleophas Kweyu (15+5 min) Fast solution of the Poisson-Boltzmann equation using the reduced basis method and range-separated tensor format
9:50 - 10:10	Venera Khoromskaia (15+5 min) Fast ab-initio calculation of the optical spectra of molecules by using tensor-structured methods
10:10 - 10:30	Carolin Penke (15+5min) A structure-preserving divide and conquer method for the Bethe-Salpeter eigenvalue problem

Friday, May 10 - Cont.

Session 5	Chair: Carolin Penke
11:00 - 11:30	Patrick Kürschner (25+5 min) Tensor methods for finding roots of polynomials
11:30 - 12:00	Tobias Breiten (25+5min) A low-rank in time approach for the differential Riccati equa- tion
12:00 - 12:20	Tony Stillfjord (15+5min) Recent improvements, enhancements and generalizations in DREsplit: a package of splitting schemes for differential Ric- cati equations
12:20 - 12:40	Davide Palitta (15+5min) Matrix equation techniques for evolutionary partial differen- tial equations

12:40 - 14:00 Lunch

Session 6	Chair: Davide Palitta
14:00 - 14:30	Martin Stoll (25+5min) The graph Laplacian: Semi-supervised learning, PDEs, and eigenvectors
14:30 - 14:50	Pawan Goyal (15+5min) 3D Image reconstruction using small angle X-ray scattering tomography and application to bone
14:50 - 15:10	Lihong Feng (15+5min) New error estimator for MOR of linear parametric systems
15:10 - 15:30	Neeraj Sarna (15+5 min) Shifted PODs and Fourier transform for MOR of hyperbolic equations

15:30- 16:00 Coffee break

Friday, May 10 - Cont.

Session 7	Chair: Kirandeep Kour
16:00 - 16:20	Christian Himpe (15+5min) MORscore - Comparability of MOR algorithms
16:20 - 16:40	Yao Yue (15+5 min) An adaptive method for interpolating reduced-order models based on matching and continuation of poles
16:40 - 17:00	Manuela Hund (15+5 min) Parametric model order reduction based on $\mathcal{H}_2 \times L_2$ - optimality conditions
17:00 - 17:20	Petar Mlinarić (15+5 min) Model reduction for multi-agent systems
17:20 - 18:05	Tobias Damm (40+5 min) On the indefinite damping and gyroscopic stabilization

18:30 - 22:00 **Dinner**

Saturday, May 11

08:00 - 09:00 Br	eakfast
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09:30 Bus departure

Collection of posters

Hussam Al Daas

Coarse spaces and multilevel additive Schwarz

Björn Baran

 $Recent\ advances\ at\ Riccati-feedback\ control\ of\ a\ two-phase\ Stefan\ problem$

Manuel Baumann

Surrogate models for coupled microgrids

Sridhar Chellappa

An approach to deal with high-dimensional parameter spaces in the context of model reduction $\$

Sergey Dolgov Tensor product approximation of high-dimensional HJB equations

Sara Grundel Isothermal Euler and discretisation

Dimitrios Karachalios

Data-driven identification and model reduction of nonlinear systems

Martin Köhler Fast direct solvers for Sylvester-type matrix equations

Kirandeep Kour

Structure preserving kernelized tensor train classification model with application in neuroimaging

Li-Gang (Charles) Lin

Nonlinear optimal control using a state-dependent (differential) Riccati equation

Petar Mlinarić

System-Theoretic Model Reduction in pyMOR

Shaimaa Monem Abdelhafez

Parameterized POD-reduction for syngas production

Jens Saak

Model reduction for an artificial fishtail: A comparison

Roman Weinhandl

 $Low\-rank\ methods\ for\ parameter\-dependent\ fluid\-structure\ interaction\ discretizations$

Steffen Werner

Calm, smooth and smart – Structure-preserving model reduction for dissipative mechanical systems

Invited speakers abstracts

Boris N. Khoromskij

Range-separated tensor format for computation of electrostatics in many-particle systems

Tensor numerical methods allow to construct computational schemes for solving ddimensional PDEs with the linear complexity scaling in dimension, (B. Khoromskij, 2018; V. Khoromskaia et al., 2018). We discuss on how the tensor numerical methods apply to calculation of electrostatic potential of many-particle systems by using the novel Range Separated (RS) tensor format (P. Benner et al., 2018). The particular application of the RS tensor representation for numerical modeling of electrostatics in large bio-molecular systems via the Poisson-Boltzmann equation will be discussed [P. Benner et al., 2019; C. Kweyu et al, 2019]. The approach is based on appli- cation of the RS tensor decomposition of the Dirac delta (B. Khoromskij. et al., 2019). The numerical illustrations will be presented. This talk is based on the joint works with P. Benner, V. Khoromskaia, C. Kweyu and M. Stein.

Tobias Damm

On indefinite damping and gyroscopic stabilization

We consider linear vibrational systems with positive definite stiffness matrix K and indefinite damping matrix D. For the system to be stabilizable by gyroscopic forces it is necessary that both the trace of D and the trace of $K^{-1}D$ is negative. In the present talk we discuss sufficiency of this condition. As tools we derive results on hollow matrices and symplectic transformations

Patrick Kürschner

Tensor methods for finding roots of polynomials

We discuss the problem of finding roots of systems of multivariate polynomials. The goal is to show how this problem in numerical polynomial algebra has natural connections to certain problems in numerical multilinear algebra. To this end, we consider two possibilities for the treatment of the root finding problem: first via multilinear systems of equations and second via the so called Macaulay matrix framework. In both ways, the solutions of interest can be represented by tensor decompositions, for which specialized numerical approaches are available.

Sergey Dolgov

$Tensor\ product\ approximation\ of\ high-dimensional\ HJB\ equations$

It was dynamic programming that motivated Richard Bellman to coin the term "curse of dimensionality", referring to an exponential growth of the number of unknowns in a numerical solution with the number of independent coordinates in a system. Specifically, we consider optimal feedback control of a dynamical system, assuming no knowledge of the initial state. This is useful when certain objectives (e.g. stabilisation) must be achieved for a system subject to stochastic perturbation. Optimal control for any current state of the system can be produced from the value function, which satisfies the Hamilton-Jacobi-Bellman (HJB) equation. However, the latter is a high-dimensional PDE with the number of coordinates being equal to the state dimension of the original dynamical system. Straightforward numerical discretization of the HJB equation can thus go out of memory for fewer than ten dimensions.

Traditional approach to the optimal feedback control problem relies on a linear approximation of a system, solution of a (low-dimensional) Riccati equation for the so-called Linear Quadratic Regulator (LQR), and higher-order nonlinear perturbations where necessary (T. Breiten et al., 2018). Recently a polynomial ansatz with a bounded total degree was used successfully for a direct numerical solution of a moderate dimensional HJB equation (D. Kalise et al., 2018). However, it still suffers from a rapid growth of complexity for larger systems.

In this talk, I will discuss our alternative approach of applying low-rank tensor decompositions to a high-dimensional HJB equation for optimal feedback control of a PDE system. For linear systems, low ranks of the value tensor can be backed up by low mosaic ranks of the Riccati solution. However, numerical evidence suggests that some strongly nonlinear PDEs admit also a low-rank value function, which can be approximated efficiently by low-rank tensor algorithms, and which can deliver a much lower running cost than LQR.

Tobias Breiten

A low-rank in time approach for the differential Riccati equation

Optimal feedback laws for linear quadratic control problems are intimately connected with the differential Riccati equation (DRE). Due to the curse of dimensionality, an explicit computation of the time-varying matrix valued unknown is infeasible for problems related to partial differential equations. A common remedy is to combine low-rank methods with an ODE integration scheme. While this allows to efficiently compute the solution at each individual time instance, the temporal complexity is still tied to the ODE integration scheme. We propose an alternative procedure that is based on a full space-time discretization of the DRE. For the resulting nonlinear system, we discuss a tensor structured Newton iteration. Based on numerical examples, we evaluate the performance of the method for several PDE constrained control problems.

Martin Stoll The Graph Laplacian: Semi-supervised learning, PDEs, and eigenvectors

The graph Laplacian plays a crucial role in many data science applications. We give a quick review of some of its properties and then show how techniques borrow from materials science can be used for semi-supervised learning. Namely, we will use a phase field scheme formulated on the graph domain to illustrate how the process of inpainting can find its analogue in classification. Additionally, we will show how the eigenvectors of the graph Laplacian can be approximated efficiently.

Venera Khoromskaia

Fast ab-initio calculation of the optical spectra of molecules by using tensor-structured methods

The Bethe-Salpeter equation (BSE) is a reliable model for estimating the absorption spectra in molecules and solids on the basis of accurate calculation of the excitation energies from first principles. The prerequisites for generation of matrices in the BSE system are ab-initio ground state energy calculations. Our tensor-structured Hartree-Fock solver (V. Khoromskaia, 2014) provides all data for application of the BSE model: a full set of molecular orbitals and eigenvalues, and an efficient low-rank Cholesky factorization for the 4th order tensor of two-electron integrals (TEI) (V.Khoromskaia et al., 2013; P. Benner et al., 2016). Using this factorization of TEI in a molecular orbitals basis, we developed a new approach (P. Benner et al., 2016; P. Benner et al., 2017) to computation of the Bethe-Salpeter excitation energies which relaxes the numerical costs to $O(N^3)$ in size of atomic orbitals basis set, N, instead of practically intractable $O(N^6)$ for conventional diagonalization of the BSE matrix. The diagonal plus lowrank tensor approximations to the fully populated blocks in the large BSE matrix are constructed gaining from the low-rank form of TEI, thus enabling easier partial eigenvalue solver for a large auxiliary system but with a simplified block structure. An economical method is introduced in (P.Benner et al., 2019) for calculating the density of states for the optical spectra of molecules by taking advantage of the block-diagonal plus low-rank matrix structure of the system Hamiltonian. Thus, we developed an efficient scheme for computing the excitation energies of molecules starting from the ab-initio ground state energy calculations. Numerical examples for compact molecules are presented.

Serkan Gugercin

Data-driven modeling for solving nonlinear eigenvalue problems and estimating dispersion curves

Projection-based methods are a common approach to model reduction in which reducedorder quantities are obtained via explicit use of full-order quantities. However, these full-order quantities are not always accessible and instead a large-set of input/output data, e.g., in the form of transfer function evaluations, are available. In this talk, we will focus on both interpolation (Loewner) and least-squares (Vector Fitting) frameworks to construct reduced-models directly from data. In the former case, we will connect the data-driven modeling framework to nonlinear eigenvalue problems and discuss how the classical realization theory gives further insights into certain classes of methods for nonlinear eigenvalue computations. In the Vector Fitting framework, we will show how one can use data-driven modeling in estimating dispersion curves in structural materials.

Michael Hinze & Carmen Gräßle

$\label{eq:thm:total} \textit{Tutorial section: Adaptivity in simulation based model order} \textit{reduction}$

In this talk, we are concerned with simulation based model order reduction, where the goal is to replace a high-fidelity system by a low-dimensional approximation. This surrogate model is built upon snapshot data generated by numerical simulations. In order to construct a reduced-order model which is sufficiently accurate with respect to the true solution, we require 'good' snapshots. Having recalled basic concepts of POD-MOR, we focus on offline adaptive strategies in order to generate snapshots efficiently and sufficiently accurate. On the one hand, we introduce a residual-based adaptive time discretization for POD-MOR in optimal control which is based on a reformulation of the optimality system into a biharmonic equation. On the other hand, we combine spaceadapted snapshots with the usual POD framework and address additional challenges in optimal control and incompressible flow. We provide numerical examples and give an outlook to future research perspectives.