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Book of abstracts

Invited lectures

Unusual spectral properties of a class of Schrödinger operators

Pavel Exner

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The aim of this talk is to discuss several classes of Schrödinger operators with potentials that are below unbounded but their negative part is localized in narrow channels. A prototype of such a behavior can be found in Smilansky-Solomyak model devised to illustrate that an an irreversible behavior is possible even if the heat bath to which the systems is coupled has a finite number of degrees of freedom. We review its properties and analyze a regular version of this model, as well as another system in which $x^p y^p$ potential is amended by a negative radially symmetric term. All of them have the common property that they exhibit an abrupt parameter-dependent spectral transition: if the coupling constant exceeds a critical value the spectrum changes from a below bounded, partly or fully discrete, to the continuous one covering the whole real axis. We also discuss resonance effects in such models. The results come from a common work with Diana Barseghyan, Andrii Khrabustovskyi, Vladimir Lotoreichik and Miloš Tater.

Digital Signal Processing and Software-Defined Radios in Remote Attacks on GPS

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The possibility of position, velocity, and also time forging for the civil GPS service is a well-known implication of deliberately missing cryptographic protections of the L1 C/A satellite signal. Practical feasibility was already demonstrated several times, so is there anything new and interesting? It is in the massive rise of software-defined radio phenomenon that will soon allow even unskilled hackers to download the attack code from the internet and let it run. It is also interesting to see the mathematics behind the digital signal processing that enables software-defined radios to exist that in turn have such a strong effect on the risk associated with trustingly relaying on the "trustworthy" GPS service.

Contributed presentations

Copositive Optimization in Infinite Dimension

Claudia Adams
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Keywords: Copositive Optimization, Infinite Dimension, Duality, Functional Analysis

Many combinatorial optimization problems can be formulated as conic convex optimization problems (e.g. stable set, maximum clique, maximum cut). Especially NP-hard problems can be written as copositive programs. In this case the hardness is moved totally into the copositivity constraint.

We will show how to lift this theory to infinite dimension and we study operators in Hilbert spaces instead of matrices. For that purpose we develop a new theory of semidefinite and copositive optimization in infinite dimensional spaces. This new theory will use tools from functional analysis, but the restriction to finite dimensions provides the usual duality theory.

In this context we discuss some properties which are equivalent to the ones in finite dimension and we also point out differences. We will show some special cases for which the theory can be formulated very well and some cases for which it is not easy. Understanding these cases and special properties is essential for developing solution approaches for problems of that kind.

We will discuss an essential and popular norm in functional analysis, the symmetric projective norm, and its relevant properties. Furthermore we will explain its importance for our duality theory.

Multilevel optimal control of differential-algebraic systems

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Keywords: multilevel optimal control, dynamical systems, differential-algebraic systems

Optimal control tasks arise in a variety of applications from, e.g., mechanical or electrical engineering, where one wants to minimize a certain cost functional with respect to some input function and the resulting state trajectory. Usually, the systems describing the dynamical behavior of these applications are governed by ordinary differential equation.

However, the dynamics of such a system may be restricted to a manifold, and thus, one has to impose additional algebraic constraints which altogether constitute a so-called differential-algebraic system.

Furthermore, in certain applications, e.g. humanoid locomotion of robots or simulation of gas flows in gas networks, the cost functional and the system descriptions may depend on parameters. This introduces a second level of optimization.

In this talk I want to give a brief overview of multilevel optimal control problems and their numerical treatment. We point out difficulties that arise in this setting and present first approaches to deal with these problems.

MIP and Heuristics for Multiple Earth-Observing Satellites Scheduling Problem

Xiaoyu Chen

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Keywords: Satellite Constellation, Scheduling, MIP model, Heuristics, Optimization

Earth observing satellites play a significant role in resource exploration, disaster alert and environmental damage analysis. We address a problem of multiple satellites scheduling with limited observing ability, which is a highly combinatorial problem due to the large search space for potential solutions.

We decompose the problem into preprocessing and scheduling. By preprocessing it, we cope with some constraints, so that the input of the problem is only the available resources, the requested missions and the eligibility of resources for missions. By analyzing the distribution features of the visible time windows of missions and the contention degree of the available time interval on each resource, we construct a more exact mixed integer programming (MIP) optimization model for the satellites scheduling problem and solve it with Gurobi. We design several different kinds of instances to test the efficiency and applicability of the model. In comparison with some heuristic methods (including Greedy Techniques, and Evolutionary Algorithm), the results verify the correctness and efficiency of this scheduling model, indicating that the constructed algorithms are feasible.

Parametrized Sylvester Equations in Model Order Reduction

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Keywords: Sylvester equation, parametric model order reduction, linear time-invariant system, orthogonal polynomials, moment matching

Various mathematical and physical processes can be modeled as linear time-invariant (LTI) input-output systems. Since these systems often have a huge number of degrees of freedom, numerical simulations might be too expensive or even impossible caused by the computational time and memory requirements. Nevertheless, these LTI systems can be solved fast and sufficiently accurate if they are reduced to LTI systems of much smaller order, such that structural properties are preserved and the error between these systems or system outputs is small in a suitable norm.

There are several model order reduction (MOR) techniques to reduce the order of a given LTI system. The basic idea of linear MOR is to project the given matrices of the system onto a much lower dimensional subspace, that computes the dynamics in the state space sufficiently well.

In my talk I will present a projection method, that samples the time-dependent dynamics by orthogonal polynomials. The projection matrix is directly obtained from a sparse-dense Sylvester equation, which is a system of equations resulting in a solution matrix instead of a solution vector. Here, sparse-dense means that the matrices have a special structure, i.e. matrices multiplied from the left to the solution matrix are large and sparse and matrices multiplied from the right are small and dense. I will furthermore show two possibilities to obtain a parametrized Sylvester equation.

On the one hand, we can parametrize the small and dense matrices containing information about the orthogonal polynomials. It is known, that the above mentioned time-domain MOR is related to another MOR method, moment matching. The goal of the latter procedure is to match the moments of the transfer function describing the relation of the input and the output of the original system. Therefor so-called expansion points are needed. Due to the equivalence it is known, that these expansion points are given by the spectrum of the small and dense matrices. Thus to obtain a broader spectrum, we can use parametrized families of Jacobi polynomials, such that the Sylvester equation gets parametrized in the small matrices.

On the other hand, considering a system with parameter-dependent matrices, we are seeking for a well-approximating reduced system. A good indicator for this is measuring the error between their transfer functions in the $\mathcal{H}_2$ norm, which is an important system norm describing the influence of the inputs on the outputs. In the non-parametric case it is known, that the $\mathcal{H}_2$-optimality can be guaranteed by solving the Wilson conditions, that are given by Sylvester equations. Our final goal is to solve this $\mathcal{H}_2$-optimal parametric MOR problem via a fixed point iteration on the Wilson conditions along the lines of the two sided iterative approximation (TSIA) algorithm. Considering non-parametric systems, where the input and output are given by vectors instead of matrices, it is known, that the TSIA algorithm computes the same subspace resulting in the same projection matrix as the iterative rational

Krylov algorithm (IRKA). The latter one can be seen as a generalization of moment matching, since each iteration of this algorithm is moment matching with expansion points, that are adapted on-the-fly resulting in locally optimally placed expansion points for the system in the sense of $\mathcal{H}_2$ optimal approximation. Thus our idea could in turn serve as an alternative $\mathcal{H}_2$-optimal MOR algorithm to the “parametric IRKA”, which is an extension of IRKA for parametric systems by interpolating the parameter space.

In my talk, I will present first results towards this goal.

The Computation of the Discriminant of a Mass Action Network

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Keywords: Chemical reaction networks, Polynomials, Discriminants

The steady states of a mass-action network are the non-negative real solutions to a parametric system of polynomial equations. It is a central problem to classify the number of isolated real solutions of such a system in certain linear subspaces. One approach to this problem is the computation of discriminants. We exemplify this method on the dual-site phosphorylation network.

Subset selection and regression problems

Dennis Kreber

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Keywords: Subset selection, Sparse regression, Feature selection, Mixed integer programming, Discrete optimization

Sparsity is an often desired property in regression and an extensively examined area of research. One of the most prominent methods to select relevant variables is the Lasso method. Sufficient conditions on the data under which Lasso generates a predictive, sparse solution are well known, however they are hard to verify. Thus, if those conditions are not satisfied, Lasso can exclude predictive variables or can fail at producing sparsity.

To avoid these disadvantages, instead of a regularization term, a cardinality-constrained subset selection formulation is used to limit the number of non-zero regression coefficients. The resulting problem is NP-hard and can be solved via mixed integer quadratic programming.

We present an equivalent mixed integer linear formulation for this problem and show properties of the subset selection, which can be useful to find a solution more efficiently.

Symmetric Factorization of Saddle-point Matrices in Nonlinear Optimization and Reusing Pivots

Jan Kuřátko

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Keywords: saddle-point matrix, nonlinear optimization, symmetric indefinite factorization, sequential quadratic programming

Iterative methods for nonlinear optimization usually solve a sequence of linear systems. In this talk we will address the application of direct methods in solving linear systems where the matrix is symmetric and indefinite. Moreover, we assume that the matrices from that sequence of linear systems are related such that the structure of blocks and bands of nonzero elements remains the same.

We solve the linear system by the symmetric indefinite factorization that is by Bunch-Parlett or Bunch-Kaufman methods. We will describe how to use the knowledge of the pattern of 1x1 and 2x2 pivots from one iteration in the next iteration of the optimization method. We will describe our strategy for monitoring the pivots and the stability of the factorization. According to our strategy we either skip searching for pivots or update the permutation matrix if needed.

In addition, we will present our method that adaptively switches from the signed Cholesky factorization to Bunch-Parlett or Bunch-Kaufman. We will show on examples that this monitoring strategy reduces the time spent on searching the matrix for pivots.

Fast Solution of the Poisson-Boltzman Equation by the Reduced Basis Method and Range-Separated tensor format

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Keywords: Poisson-Boltzmann equation, biomolecular modeling, electrostatic potential, range-separated tensor format, singularities, reduced basis method, low-dimension, many-query context

The Poisson-Boltzmann equation (PBE) is a nonlinear elliptic parametrized partial differential equation that arises in biomolecular modeling and is a fundamental tool for structural biology. It is used to calculate electrostatic potentials around an ensemble of fixed charges immersed in an ionic solution. Efficient numerical computation of the PBE yields a high number of degrees of freedom in the resultant algebraic system of equations, ranging from several hundred thousands to millions. Coupled with the fact that in most cases the PBE requires to be solved multiple times for a large number of system configurations, this poses great computational challenges to conventional numerical techniques. To accelerate such computations, we here present the new range-separated tensor format for purposes of modifying the PBE in order to eliminate the terms related to singularities and also to obtain affine parametric dependence in the resultant algebraic system. Then we apply the reduced basis method (RBM) which further reduces the computational complexity by constructing a reduced order model of typically low dimension. The end results are reduced storage space and improved computational speed-up which enable the PBE simulations in a many-query context.

End to End Learning for DeepDriving with leveraging available scene segmentation side tasks to improve performance under a privileged learning paradigm and Robust Exponential Stability of Periodic Solutions for Static Recurrent Neural Networks with Delays

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Keywords: Robust Exponential Stability, Static Recurrent Neural Networks, End to End Learning, Behavior reflex approach

In this paper we reference to other scientists using Deep Q-Networks as the refinement step in Inverse Reinforcement Learning approaches. This enabled us to extract the rewards in scenarios with large state spaces such as driving, given expert demonstrations. The aim of this work was to extend the general approach to IRL. Exploring more advanced methods like Maximum Entropy IRL and the support for nonlinear reward functions is currently under investigation. We also give a proof of the mathematical aspects of the theory used in this paper. The static recursive neural network with Markovian modulation and the time-delay static recurrent neural network model considering both random perturbation and Markovian switching are studied. The linear matrix inequality, the finite state space Markov chain property and the Lyapunov-krasovskii function , The judgment condition of the global exponential stability of the system is obtained. Firstly, the global exponential stability problem of quasi - static neural neural network with time - delay and recursive neural network is studied by using the generalized Halanay inequality. Then the stability of the Markovian response sporadic static recurrent neural network is studied by combining the properties of Markov chain.Our paper draws on a novel FCN-LSTM architecture, which can be learned from large-scale crowd-sourced vehicle action data, and leverages available scene segmentation side tasks to improve performance under a privileged learning paradigm.

On Optimization of Stabilized Methods in FEM

Petr Lukáš
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Keywords: numerical mathematics, FEM, optimization, stabilized methods, SUPG, SOLD

In stabilized methods in FEM we typically use h-adaptivity or p-adaptivity. We will introduce a new approach to optimization. The optimization procedure is based on minimizing an error functional which we call error indicator. Numerical results will be provided.

The Separation Problem for 1-Wheel Inequalities and Extended Formulations

Bernd Perscheid
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Keywords: Stable Set, Wheel Inequalities, Extended Formulation, Product Graph

Finding a maximum stable set in a graph is NP-hard. Therefore, it is out of reach to describe the convex hull of incidence vectors by a polynomial system of inequalities. The cycle inequalities are an exponential class of valid stable set inequalities. Yannakakis (1991) shows how the separation problem for cycles can be solved with an extended formulation.

We focus on solving the 1-wheel separation problem for stable sets in polynomial time. Our efficient and compact extended formulation can be used to avoid the application of shortest path algorithms. The construction relies on satisfying sufficient conditions for a given vector x in product graphs. These conditions are implicitly represented by adding polynomially many inequalities.

Surface Face Graphs and Their Tightness

Qays Shakir
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Keywords: Rigidity Theory, Framework, Sparsity and tightness of graphs, Surface graphs, Girth inequality

Geometric rigidity theory is a tool which is designed to decide whether a framework (typically bar and joint) is rigid or flexible. Geometric and combinatoric mathematical aspects are used to build such theory.

Combinatorially, Lamans theorem gives a complete answer for the rigidity status of a framework in two dimensions using (2,3)-tightness. In three dimensions, if a framework is minimally 3-rigid then its abstract graph is (3,6)-tight while the converse is not true in general; the double banana graph is a typical counterexample.

Such observation motivated us to study (3,6)-tightness via various surfaces . The main theorem which is proved in this project is:

Theorem: Let G be a Σ-face graph. If G has at least one triangle then G is (3,6)-tight if and only if every proper ∂-curve (c, U_c) in G satisfies the girth inequality.

Multi-Leader-Follower Games

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Keywords: Game Theory, Nonsmooth Analysis, EPEC, Nash Equilibrium Problem

The multi-leader-follower game is a particular subset of classical game theory. These models serve as an analytical tool to study the strategic behavior of individuals on a noncooperative manner. In particular, the individuals (players) are divided into two groups, namely the leaders and the followers, according to their position in the game.

Mathematically, this leads optimization problems with optimization problems as constraints.

Most recently, such type of models gains an increasing interest among mathematicians as well as scientists of other fields such as operations research, robotics and computer sciences. However, compared to the knowledge of other classical game models so far only very little is known concerning existence and uniqueness theory as well as suitable numerical solution methods.

In this talk, we give an introduction to multi-leader-follower games where we formulate them as equilibrium problems with equilibrium constraints (EPEC). Furthermore, we illustrate challenges and present early results.

Posters

On pairing between exact and finite-precision short recurrences

Tomáš Gergelits

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Keywords: Krylov subspace, CGL, MINRES, finite-precision computations, loss of orthogonality, delay of convergence, Lanczos vectors

Krylov subspace methods often rely mathematically on computation of an orthonormal basis of the associated Krylov subspaces. For a symmetric matrix, a sequence of the basis vectors can be computed by short recurrences, in particular by the Lanczos tridiagonalization.

Due to the effect of rounding errors, however, the use of short recurrences in practical computations inevitably leads to the loss of global orthogonality and even to the loss of linear independence among the generated vectors. Consequently, the generated susbpaces become rank-deficient, which may cause a significant delay of convergence.

In this contribution, we investigate whether, in which sense, and how accurately, the first k steps of the finite precision arithmetic computation can be related to the first l steps of the exact computation with the same matrix and starting vector. This allows to compare not only the convergence curves, but also the computed approximations, the corresponding residuals, or the nearness of the generated subspaces with exact Krylov subspaces.

Joint work with Iveta Hnětynková and Marie Kubínová.

Noise representation in residuals of LSQR, LSMR, and CRAIG regularization

Marie Kubínová

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Keywords: ill-posed problems, regularization, Golub-Kahan iterative bidiagonalization, LSQR, LSMR, CRAIG

Golub-Kahan iterative bidiagonalization represents the core algorithm in several regularization methods for solving large linear noise-polluted ill-posed problems. We consider a general noise setting and derive explicit relations between (noise contaminated) bidiagonalization vectors and the residuals of bidiagonalization-based regularization methods LSQR, LSMR, and CRAIG.

Joint work with Iveta Hnětynková and Martin Plešinger.

On a Navier-Stokes-Fourier-like system capturing a transition between viscid and inviscid fluid regimes and between no slip and perfect slip boundary conditions

Erika Maringová

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Keywords: implicit constitutive relations, non-Newtoninan fluid

We study a model with implicit constitutive relations that captures non-Newtonian fluids with temperature-dependent coefficients, in particular those which are able to describe the threshold slip phenomenon with the temperature-dependent activation criteria. Such a model is able to describe all states of the fluid from the yield stress, through the Newtonian fluid up to the inviscid case only by the temperature change. Also, concerning the boundary conditions, we are able to capture the standard Naviers slip, but also the threshold slip case, i.e. the stick-slip or the perfect slip-slip condition. These models always include the activation, however, the standard constitutive relations (yield stress, inviscid fluid, no slip or perfect slip boundary conditions) are the limit cases when certain activating coefficient tends to infinity for some temperature. Finally, also the large-data and the long-time existence analysis is provided.

This is a joint work with J. Žabenský.

Multiscale modeling of aortic media

Marek Netušil
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Keywords: composite materials, nonlinear homogenization, finite elements

Homogenization is a popular and modern approach to modelling of composite materials. Arterial tissue is an example of such kind of material, consisting of several constituents forming a complex three-dimensional structure. While there has been done a lot in the field of linear PDEs, homogenization in large deformations is still an open problem.

We introduce a simplified representative volume element for the aortic media and a way to approximately attack the problem of nonlinear homogenization will be presented. This approach is based on the linearization of the PDE during the Newton iterative method used in the finite element approximation.

Multi-phase modelling of a reactive flow in fluidized bed reactors heated by internal tubes

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Keywords: multi-phase modelling, multiphase system, phase-change mechanisms

We investigate a model of fluidized bed reactor where a solution of liquid formic acid is decomposed to a gaseous mixture of carbon dioxide and hydrogen in the presence of solid catalytic particles. We describe the system, contained in a fixed control volume, as a multiphase system composed of the nine constituents possessing several phase-change mechanisms such as endothermic chemical reaction and evaporation. For the individual mixture components, we distinguish partial densities and momenta while we only consider one common temperature field for the mixture as a whole. The system is, under certain assumptions, reduced to a three-phase system.

The liquid mixture phase is considered as a compressible non-Newtoian fluid with density and viscosity depending on both the temperature and the volume fraction of the catalyst particles. Physical interaction between the phases is modelled by Euler-Lagrange approach. The chemical rates satisfy the mass-action law and follow the Arrhenius kinetics.

In addition to inner reactor body simulation, we model also the heating system which is composed of several hollow metal tubes heated by passing oil flow driven by thermostat pump. We proceed the CFD analysis of the system, determinate a bottleneck and propose improvements. The model was implemented numerically in COMSOL Multiphysics.

Joint work with Ondřej Souček and Peter Čendula

GPU-Accelerated Implementation of the Storage-Efficient QR Decomposition

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Keywords: GPU Acceleration, QR Decomposition, Numerical Linear Algebra, Storage Efficiency, Block Algorithm

The LAPACK routines `GEQRT2` and `GEQRT3` can be used to compute the QR decomposition of a matrix of size $m \times n$ as well as the storage-efficient representation of the orthogonal factor $Q = I - VTV^T$. A GPU-accelerated algorithm is presented that expands a blocked CPU-GPU hybrid QR decomposition to compute the triangular matrix T. The storage-efficient representation is used in particular to access blocks of the matrix Q without having to generate all of it. The algorithm runs on one GPU and aims to use memory efficiently in order to process matrices as large as possible. Via the reuse of intermediate results the amount of necessary operations can be reduced significantly. As a result the algorithm outperforms the standard LAPACK routine by a factor of 3 for square matrices.

Experimental Characterization of Fatigue Crack Initiation of Mineralized AA320 Alloy under CTC & ML during Four Point Rotating and Bending Fatigue Testing Machine

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Keywords: Fatigue, Initiation, SN Curve

Initiation of crack during fatigue of casting alloys are noticed mainly on the basis of experimental results. Crack initiation and strength of fatigue of AA320 alloy mineralized with silicon are summarized here. Load sequence effect is applied to notify initiation phase life. Effect of mineralization on crack initiation at notch root and fatigue life is studied under single & two step mechanical loading (ML) with and without combined thermal cycling (CTC). The composition of silicon is increased for this purpose from 5.48 to 14.5%. An Experimental setup is proposed to create the working temperature as per alloy applications. S-N curves are plotted and a comparison is made between crack initiation leading to failure under different ML with & without thermal loading (TL).

Sparsity and tightness of graphs Surface graphs

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Keywords: Rigidity Theory, Framework, Sparsity and tightness of graphs, Surface graphs Girth inequality

Geometric rigidity theory is a tool which is designed to decide whether a framework (typically bar and joint) is rigid or flexible. Geometric and combinatoric mathematical aspects are used to build such theory. Combinatorially, Lamans theorem gives a complete answer for the rigidity status of a framework in two dimensions using (2,3)-tightness. In three dimensions, if a framework is minimally 3-rigid then its abstract graph is (3,6)-tight while the converse is not true in general; the double banana graph is a typical counterexample. Such observation motivated us to study (3,6)-tightness via various surfaces . The main theorem which is proved in this project is:

Theorem: Let G be a Σ-face graph. If G has at least one triangle then G is (3,6)-tight if and only if every proper ∂-curve (c, U_c) in G satisfies the girth inequality.
