Conference:

Trends in Mathematical Modelling, Simulation and Optimisation: Theory and Applications

Talks and abstracts

Plenary talks

Prof. Dr. Peter Benner, Dr. Sara Grundel, Dr. Christian Himpe
Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, Deutschland

Reduced-order Modelling and Simulation of Gas Transportation Networks

In order to cope with the volatile nature of renewable energy sources, gas networks take a vital role. To ensure fulfillment of contracts under these new circumstances, a vast number of possible scenarios, incorporating uncertain supply and demand, has to be simulated ahead of time. This many-query task can be accelerated by model order reduction. Yet, large-scale, nonlinear, parametric, hyperbolic partial differential(-algebraic) equation systems, modeling gas transport, are a challenging application for model reduction algorithms. For this problem, we bring together the scientific computing topics of mathematical modeling of gas transportation networks, numerical simulation of hyperbolic partial differential equations, and model order reduction for nonlinear parametric systems. This research has resulted in the morgen (Model Order Reduction for Gas and Energy Networks) software platform, which enables modular testing of various combinations of models, solvers, and model reduction methods. In this talk, I will present the theoretical background on systemic modeling and structured, data-driven, system-theoretic model reduction for gas networks, as well as the implementation of morgen and associated numerical experiments testing model reduction adapted to gas network models.

Prof. Dr. Martine Labbé
Université Libre de Bruxelles, Belgium

Linear bilevel optimization: overview and recent results

A bilevel optimization problem consists in an optimization problem in which some of the constraints specify that a subset of variables must be an optimal solution to another optimization problem. This paradigm is particularly appropriate to model competition between agents, a leader and a follower, acting sequentially. In this talk I will focus on the simplest bilevel problems, those that are linear. I will present the main characteristics, properties and algorithms for these problems. Then, I will discuss some recent results showing that these problems are already extremely challenging.

Regular talks

Prof. Dr. Daniel Bienstock
Columbia University in the City of New York, Applied Physics and Applied Mathematics, USA

Title: Complexity and Exactness in Polynomial Optimization

Abstract: Polynomial optimization problems, that is to say, optimization problems whose constraint and objectives are multivariate polynomials, have acquired increased visibility in recent years due to their application in science and engineering. They are typically (highly) nonconvex and can be quite large, and, as a result, can prove very challenging. The methodology for solving such problems includes the development of relaxations that prove bounds, such relaxations are frequently described in a different space, of higher dimension, and often (almost always) only prove a bound on the objective value – the vector they output, often, cannot be easily converted into a feasible solution in the original space. At the other end, we have logarithmic barrier methods that seek to compute feasible solutions but without any guarantee of optimality. Software packages include an additional feature, branching, in order to guarantee (at least in principle) the computation of a near-optimal solution. The lower bounding and upper bounding techniques, both, can exhibit serious numerical issues. One point that is not widely understood is that in the presence of nonlinearities and nonconvexities, it is easy to obtain examples where 'a little infeasibility buys you a lot of optimality', or, in other words, solvers can (and do) output slightly

infeasible solutions that are very superoptimal.
In this talk, we examine classical issues regarding the solutions to polynomially constrained problems, or semi-algebraic sets as are known in the mathematics community. One example of the results we have is that, given a feasible system of quadratic inequalities with integer coefficients, it is strongly NP-hard to decide if the system has a rational feasible solution. And, given a system of quadratic inequalities which is known to have rational feasible solutions, it is strongly NP-hard to decide if the system has a rational feasible solution of polynomial-size (= number of bits). This is joint work with Alberto del Pia (U. of Wisconsin) and Robert Hildebrand (Virginia Tech).

Martina Cerulli
Laboratoire d'Informatique de l'X (LIX), CNRS & École Polytechnique, Institut Polytechnique de Paris, France

Title: Reformulating particular bilevel programs with quadratic lower level

Abstract: We focus on a particular class of bilevel programs with a quadratic lower level, which can be obtained reformulating semi-infinite problems with an infinite number of quadratically parametrized constraints. We propose a new approach to solve this class of bilevel programs, based on the dual of the lower level problem and which can lead to a convex or a semidefinite programming problem depending on the parametrization of the lower level with respect to the upper level variables. This approach is compared with is a tailored cutting-plane algorithm. We test these two methods on several instances of two applications: the constrained quadratic regression and a zero-sum game with cubic payoff.

Sandrine Charousset-Brignol
Électricité de France, R&D, Paris, France

Title: Solving European Electricity System Optimization problems using the latest Modelling and Optimisation methods advances

Co-authors: Wim van Ackooij, Nadia Oudjane, Antonio Frangioni, Rafael Lobato Durbano, Ali Ghezelsoflu, Niccolo Iardella

Abstract: The 2030 and 2050 EU's carbon reduction targets are calling for significant changes in our electricity system. These changes, especially the emergence of a high share of intermittent renewable energy sources in the energy system, create new challenges. In particular, the volatile character of generation from renewable energy sources and the dependency on weather conditions increases the need for flexibility.
Within the H2020 plan4res project, we are implementing state-of-the-art optimization and modelling tools aiming at filling the gaps between the increasing complexity of the future energy system planning and operational problems, and the currently available system analysis tools. In particular, we are implementing a new European electricity system model, combining generation, transmission and storage optimization and simulation, considering the major short-term and long-term uncertainties affecting the energy system: electricity demand (including meteorological uncertainties and long-term trends such as electrification of transport), renewable sources generation, water inflows and technical failures, and including modelling of various kinds of flexibilities, involving generation, storage and consumption, such as dynamic operation constraints of power plants (ramping constraints, minimum shut-down duration) or dynamic operation of storages (including battery-like storages and complex hydro-valleys modeling).
In this talk, I will detail how the system is modelled and implementing within the SMS++ modelling and solving framework, and which optimization methods are used to solve this big size problems.
This work was supported by the project plan4res which has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 773897and benefited from the support of the FMJH 'Program Gaspard Monge for optimization and operations research and their interactions with data science', and from the support from EDF.

Prof. Dr. Claudia d'Ambrosio
Laboratoire d'Informatique de l'X (LIX), CNRS & École Polytechnique, Institut Polytechnique de Paris, France

Title: Mathematical Optimization for Tactical Deconfliction in Urban Air Mobility

Urban Air Mobility is a new, challenging way to transport people, which several municipalities around the world plan to offer in the next few years. It will exploit the third dimension to help smooth ground traffic in densely populated areas, thanks to the use of electric vertical take-off and landing vehicles. In this talk, we introduce the problem of tactical deconfliction in UAM and propose a mathematical optimization model to solve it. The aim is to minimize the deviation from flight schedules while correcting conflicting trajectories via speed changes when some disruption occurs. We present preliminary computational results considering three different disruption scenarios: i. delays occurring in the planning; ii. priority flight has to be accommodated; iii. intruder. The results show that our method is very fast and could in practice be used as a decision-making support tool for air traffic controllers. (Joint work with R. Delmas, Y. Hamadi, M. Pelegrín)

Prof. Dr. Santanu Dey
Georgia Institute of Technology, H. Milton Stewart School of Industrial and Systems Engineering, Atlanta, USA

Sparse PSD approximation of the PSD cone

While semidefinite programming (SDP) problems are polynomially solvable in theory, it is often difficult to solve large SDP instances in practice. One computational technique used to address this issue is to relax the global positive-semidefiniteness (PSD) constraint and only enforce PSD-ness on smaller $k \times k$ principal submatrices — we call this the sparse SDP relaxation. Surprisingly, it has been observed empirically that in some cases this approach appears to produce bounds that are close to the optimal objective function value of the original SDP. In this talk, we formally attempt to compare the strength of the sparse SDP relaxation vis-à-vis the original SDP from a theoretical perspective. In order to simplify the question, we arrive at a data independent version of it, where we compare the sizes of SDP cone and the k-PSD closure, which is the cone of matrices where PSDness is enforced on all $k \times k$ principal submatrices. In particular, we investigate the question of how far a matrix of unit Frobenius norm in the

k-PSD closure can be from the SDP cone. We provide two incomparable upper bounds on this farthest distance as a function of k and n. We also provide matching lower bounds, which show that the upper bounds are tight within a constant in different regimes of k and n.
This is joint work with Grigoriy Blekherman, Marco Molinaro, Kevin Shu, and Shengding Sun.

Prof. Dr. Simone Göttlich
Universität Mannheim, Wirtschaftsinformatik und Wirtschaftsmathematik, Deutschland

Modeling and simulation of sector-coupled energy networks

The gas dynamics within each pipeline of the considered gas networks are modeled by the isentropic Euler equations, supplemented with equality-of pressure coupling or Bernoulli-coupling and suitable boundary conditions. For the power grid we apply the well-known Powerflow equations. The first kind of coupling between gas and power networks at gas-fired power plants is modeled by (algebraic) demand-dependent gas consumption terms. The second kind of coupling is done via gas production in power-to-gas facilities paired with the power plants, which is again modeled with algebraic conditions. While for the Powerflow equations no further discretization scheme is necessary, we apply an implicit box scheme to the isentropic Euler equations, which allows the application of large time steps. The entire discretized system is solved with Newton's method. Data for the gas network is taken from the GasLib library, namely GasLib-134 with 86 pipes, while the power grid is adapted from the IEEE 300 bus system.

Julia Grübel
Friedrich-Alexander-Universität Erlangen-Nürnberg, Deutschland

Existence of Equilibria in Energy Markets with Convex and Nonconvex Players

Abstract: We consider a special type of market equilibrium problem (MEP) involving players with nonconvex strategy spaces or objective functions.This type of problem naturally occurs in transportation networks. We propose an algorithm that decides the existence of an equilibrium for MEPs ofthis type and returns a market equilibrium in case of existence. Moreover,we provide a uniqueness/nonexistence result for strictly convex players. Finally,

we test the proposed algorithm on well-known literature instances6 from the field of energy market modeling. There, nonconvexities arisemainly from considering the Transmission System Operator (TSO) as anadditional player who, e.g., switches lines or faces nonlinear physical laws.Preliminary results indicate that an equilibrium usually exists, especiallyfor the case of nonlinearities.

Dr. Utz-Uwe Haus
Cray EMEA Research Lab, HPE, Bern, Switzerland

The brave new world of Exascale computing: Computation is free, Data Movement is not

High-Performance computing has always been about pushing the boundaries of technology to apply it to the most challenging problems in science and technology. For the most part, this meant increasing the computational power as measured in FLOPs generation after generation, by with Moore's law and Denard scaling. As we move towards the Exascale era we are facing a new challenge: the data access and data transfer bandwidth does not keep up with the computational power, and while storage capacity and computational capacity will reach Exa-FLOPs and Exa-Bytes ranges, algorithms will need rethinking in order to reduce data movement and energy usage in order to make use of these systems, and middleware layers need to become smarter to shield users from these complications. We discuss old and new challenges, and opportunities for operations research approaches in this context.

Dr. Jean Maeght
Reseau de Transport d'Electricité – R&D Division, France

Recent methods for Optimal Power Flow with discrete variables

Alternative Current Optimal Power Flow (ACOPF) is known as a nonconvex polynomial problem. Solving continuous ACOPF to global optimality remains a challenge when classic convex relaxations are not exact. After an introduction to OPF and review of recent advances towards global optimality, we will present our own work. We use Semi-Definite Programming to reformulate ACOPF into a quadratic relaxation and get some convexity properties. To solve the gap between Interior Point (feasible, good) solution and quadratic convex relaxation, we are using a branch-and-bound algorithm. Thanks to optimal quadratic reformulation, the initial lower bound (at root node) is very good since it is the same as the SDP relaxation which is known to be tight. This approach may be extended to ACOPF with binary variables : SDP relaxations are straightforward, and finding feasible solutions is now possible with the introduction on MPEC constraints in Interior Point Solver.

Dr. Kurt Majewski
Siemens AG RDA BAM ORD-DE München, Deutschland

Some aspects of optimized energy dispatching and trading

Smart grids planning and operation poses mathematical optimization problems on various levels, different types and arbitrary sizes. In this talk we present three applications of mixed-integer linear programming in this area: Firstly a linearization technique for cyclic battery aging, secondly, a heuristic for solving small energy dispatch problems based on decomposition, and, thirdly, a glance over optimizing bids of a virtual power plant in multiple markets.

Riccardo Morandin
Technische Universität Berlin, Deutschland

A hierarchy of port-Hamiltonian models for gas networks

Abstract: Port-Hamiltonian (pH) systems are energy-based equations that are in some sense an extension of Hamiltonian systems, introducing interaction with the environment in the form of dissipation or exchange of energy. One of the main advantages of pH systems is that they directly provide stability and passivity properties from their structure. Other advantages include structure-preserving interconnection, discretization schemes and model order reduction methods, and robust representations.
In this talk we introduce a port-Hamiltonian formulation for partial-differential equations with algebraic constraints and boundary control (pHDAE). We then proceed by presenting a hierarchy of gas pipe models in pH form. The advantage of working with a hierarchy of models is being able to choose which model to use, depending on the application, required degree of accuracy, and current state of the system. We then show how to use the common structure of all models to interconnect a network of gas pipes in a power-preserving manner, i.e., while preserving the pH structure without extra loss of energy.

Prof. Dr. Gabriel Peyré
CNRS and DMA,École Normale Supérieure, Paris, France

Scaling Optimal Transport for High dimensional Learning

Optimal transport (OT) has recently gained lot of interest in machine learning. It is a natural tool to compare in a geometrically faithful way probability distributions. It finds applications in both supervised learning (using geometric loss functions) and unsupervised learning (to perform generative model fitting). OT is however plagued by the curse of dimensionality, since it might require a number of samples which grows exponentially with the dimension. In this talk, I will explain how to leverage entropic regularization methods to define computationally efficient loss functions, approximating OT with a better sample complexity. More information and references can be found on the website of our book "Computational Optimal Transport" `https://optimaltransport.github.io/`

Nora Philippi
Technische Universität Darmstadt, Deutschland

An asymptotic preserving Galerkin scheme for instationary gas transport in pipe networks

Abstract: Gas transport in one-dimensional pipe networks can be describedas an abstract dissipative Hamiltonian system, for which quantitative stability bounds can be derived by means of relative energy estimates. This allowsus to conclude stability of solutions to subsonic flow problems with respectto perturbations in initial and boundary data as well as model parameters.In addition, we can prove convergence to the parabolic limit problem in thepractically relevant high friction regime. Furthermore, the stability estimates are inherited almost verbatim by variational discretization schemes,like mixed finite elements in space and the implicit Euler method in time,leading to order optimal convergence rates and asymptotic stability in thelimiting high friction regime. The results will be explained in detail for theflow on a single pipe, but in the spirit of the port-Hamiltonian formalism,they naturally extend to pipe networks.

Prof. Dr. Nikolaos Sahinidis
Georgia Institute of Technology, H. Milton Stewart School of Industrial & Systems Engineering and School of Chemical & Biomolecular Engineering, Atlanta, USA

Spectral relaxations for global optimization of mixed-integer quadratic programs

We consider the global optimization of mixed-integer quadratic programs. We present convex quadratic relaxations derived by convexifying nonconvex quadratic functions through perturbations of the quadratic matrix. We investigate theoretical properties of these quadratic relaxations and relationships to certain semidefinite programs. We report computational results with the implementation of these relaxations in the solver BARON, demonstrating very significant reductions in BARON's computational times. This is joint work with Carlos Nohra and Arvind Raghunathan.

Dr. Mathias Sirvent
d-fine GmbH, Grünwald, Deutschland

d-fine your future - Data Science, Technology, and Mathematical Modeling in an European Consulting Company

This presentation consists of two parts. In the first half, we want to give an overview of the successful european consulting company d-fine. We present our DNA, our fields of competence, our way of working and our typical range of customers. Moreover, we specify the key qualifications and abilities that our employees need and why physicists, mathematicians, and computer scientists are the ones that we are looking for. In the second half, we show interesting details about typical d-fine projects and how mathematical modeling and optimization comes into play. In this way, we show how theoretical research results are used in real-world applications.

Lucas Slot
Centrum Wiskunde & Informatica (CWI), Amsterdam, Niederlande

Sum-of-squares hierarchies for binary polynomial optimization

We consider the hierarchy of sum-of-squares approximations for the problem of computing the minimum value of a polynomial f over the n-dimensional boolean hypercube. This hierarchy provides lower bounds for each order r and is known to be exact at (roughly) order $\frac{n+d}{2}$, where d is the degree of f. We provide an asymptotic analysis for the quality of the bound in the regime where the order r is approximately equal to $t * n$ for some scalar $0 < t < \frac{1}{2}$, showing that the relative error is in the order $\frac{1}{2} - \sqrt{t(1-t)}$. Our analysis relies on constructing suitable feasible solutions using polynomial kernels, which we obtain by exploiting symmetry and Fourier analysis on the Boolean cube. A crucial tool is relating the sum-of-squares hierarchy to another hierarchy of measure-based *upper* bounds (also introduced by Lasserre), and to exploit a link to extremal roots of orthogonal polynomials (in this case the Krawtchouk polynomials). Our error analysis in fact also applies to this second hierarchy.
This is based on joined work with Monique Laurent.

Prof. Dr. Stefan Steinerberger
University of Washington, Department of Mathematics, Seattle, USA

Sampling a Graph: finding the important vertices

Someone gives you a (possibly) large graphon which something interesting happens. Unfortunately it's so large that it's hard to keep track, you only have enough resources to observe what happens in k specific vertices. Which vertices do you pick? I will discuss a very interesting approach that is quite pretty, relates to classical sampling theory, produces nice pictures and is numerically best approached via a certain suitable quadratic program. It also comes with a large number of open problems.

Johannes Thürauf
Friedrich-Alexander-Universität Erlangen-Nürnberg, Deutschland

Title: Maximal Uncertainty Sets in Robust Optimization

Abstract: The radius of robust feasibility (RRF) determines a value for the maximal "size" of the uncertainty set such that robust feasibility of the considered uncertain optimization problem can be guaranteed. In this talk, we focus on the RRF for mixed-integer problems (MIPs). We first analyze relations between the RRF of a MIP and its continuous linear (LP) relaxation and derive conditions under which a MIP and its LP relaxation have the same RRF. In contrast to the setting commonly used in the literature, we then consider a potentially different uncertainty set for every constraint that is not necessarily full-dimensional. Thus, we extend the RRF to include "safe" variables and constraints, i.e., uncertainties do not affect certain variables or constraints. This allows for the RRF to be applied to a large variety of optimization problems and uncertainty sets. We then present first methods for computing the RRF of LPs as well as of MIPs with safe variables and constraints and successfully apply them to instances of the MIPLIB for computing the RRF. We conclude this talk by first insights into computing maximal uncertainty sets within the European entry-exit gas market, which can be seen as a further problem-specific development of the RRF and illustrates possibilities for future research regarding the RRF. This is joint work with Frauke Liers and Lars Schewe.