

# SCIP Workshop 2018

Aachen

March 6 – March 8, 2018

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## SCIP Introduction (Tuesday, March 6)

<i>Time</i>	<i>Speaker</i>	<i>Talk Title</i>
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*Session Intro – Chair: Matthias Walter*

09:30	Gregor Hendel	Introduction and Overview
11:00	Coffee break	
11:30	Team	Installation and testing of SCIP and GCG
12:30	Lunch break	
14:00	Team	Programming exercises
15:30	Coffee break	

## Workshop Day 1 (Wednesday, March 7)

*Time*      *Speaker*                      *Talk Title*

*Session 1 – Chair: Matthias Walter*

09:00	Marco Lübbecke	Welcome
09:10	Felipe Serrano	MINLP and stronger separation of bilinear terms
09:45	Stefan Vigerske	Introducing a new nonlinear expressions framework for SCIP
10:20	Pavlo Muts	Development of the new MINLP Solver Decogo using SCIP – Status Report
10:55	Coffee break	

*Session 2 – Chair: Ambros Gleixner*

11:30	Ruth Misener	Optimisation for Gradient Boosted Trees with Risk Control
12:40	Lunch break	

*Session 3 – Chair: Christopher Hojny*

14:00	Marc Pfetsch	Global optimization of ODE constrained network problems
14:45	Tristan Gally	Warmstarts and other improvements in SCIP-SDP
15:10	Leon Eifler	Proving cases of Chvatal’s conjecture using exact SCIP and VIPR
15:45	Coffee break	

*Session 4 – Chair: Jonas Witt*

16:15	Gregor Hendel	Using bandit algorithms for adaptive algorithmic decisions in SCIP
16:50	Saurabh Chandra	An MILP based hierarchical planning model for outbound automotive, maritime logistics system in India
17:25	Frederic Matter	Solving complex-valued $\ell_0$ minimization problems with con- stant modulus constraints
19:00	Workshop dinner	Restaurant <i>Elisenbrunnen</i> Friedrich-Wilhelm-Platz 14

## Workshop Day 2 (Thursday, March 8)

*Time*      *Speaker*                      *Talk Title*

*Session 5 – Chair: Stephen J. Maher*

09:15	Ambros Gleixner	Exact methods for recursive circle packing: “price-and-verify” with nonlinear subproblems
09:50	Markó Horváth	A branch-and-price method for the integrated multiple-depot vehicle and crew scheduling problem
10:25	Patrick Geman-der	Presolve Examples in SCIP
10:45	Coffee break	

*Session 6 – Chair: Jakob Witzig*

11:20	Michael Bastubbe	
11:55	Jonas Witt	Eliminating redundant columns from column generation subproblems using classical Benders’ cuts
12:40	Lunch break	

*Session 7 – Chair: Felipe Serrano*

14:00	Stephen J. Maher	Large Neighbourhood Benders’ Search
14:35	Matthias Walter	Solving Bulk-Robust Assignment Problems to Optimality
15:10	Jakob Witzig	Mixed-Integer Programming for Cycle Detection in Non-reversible Markov Processes
15:45	Coffee break	

## Plenary Talk

Ruth Misener (Imperial College London)

### Optimisation for Gradient Boosted Trees with Risk Control

Decision trees usefully represent the sparse, high dimensional and noisy nature of chemical data from experiments. Having learned a function from this data, we may want to thereafter optimise the function, e.g. for picking the best catalyst for a chemical process. This work studies a mixed-integer non-linear optimisation problem involving: (i) gradient boosted trees modelling catalyst behaviour, (ii) penalty functions mitigating risk, and (iii) penalties enforcing chemical composition constraints. We develop several heuristic methods to find feasible solutions, and an exact, branch and bound algorithm that leverages structural properties of the gradient boost trees and penalty functions. We computationally test our methods on an industrial instance from BASF.

This work was completed in collaboration with Mr Miten Mistry and Dr Dimitris Letsios at Imperial College London and Dr Robert Lee and Dr Gerhard Krennrich from BASF.

## Contributed Talks

Felipe Serrano (Zuse Institute Berlin)

### MINLP and stronger separation of bilinear terms

In this talk, we briefly introduce how SCIP solves mixed-integer nonlinear programs (MINLP) and show a technique for stronger separation of bilinear terms. The standard way of separating bilinear terms uses the convex envelope of the function  $f(x, y) = xy$  over the box  $B = [l_x, u_x] \times [l_y, u_y]$ , i.e., the given bounds of the variables. By projecting onto the  $x$ - $y$  space, we can obtain a polytope  $P$  strictly contained in  $B$ . Using the convex envelope of  $f$  over this polytope gives stronger separation of the bilinear term  $xy$ . We also show that computing  $P$  can naturally be integrated with OBBT, a procedure that SCIP uses when solving MINLPs.

Stefan Vigerske (GAMS Berlin)

### **Introducing a new nonlinear expressions framework for SCIP**

We discuss current work on renovating the handling of (continuous) nonlinear constraints in SCIP. The new framework replaces the five existing constraint handlers by a single one, thereby reducing the amount of duplicate code and focusing more on the use of a single expression graph to represent the nonlinear part of an optimization problem. The new design aims to improve numerical robustness and performance and simplifies the addition of new mathematical operators and structure-specific solution algorithms (convexification, bound tightening, etc.).

Pavlo Muts (HAW Hamburg)

### **Development of the new MINLP Solver Decogo using SCIP – Status Report**

Traditional deterministic global optimization methods are often based on a branch-and-bound tree, which may grow rapidly, preventing the method to find a good solution. Motivated by column generation methods for solving transport scheduling problems with over 100 million variables, we present a new deterministic global optimization approach, called Decomposition-based Inner- and Outer-Refinement (DIOR), which is not based on branch-and-bound. DIOR can be applied to general modular and/or sparse optimization models. It is based on a block-separable reformulation of the model into sub-models, which can be solved in parallel. In the first phase, the algorithm generates inner- and outer-approximations using column generation. In the second phase, it refines a nonconvex outer approximation based on a convex-concave reformulation of sub-problems. We present preliminary numerical results with Decogo, a new DIOR-based MINLP solver implemented in Python and Pyomo.

Marc Pfetsch (TU Darmstadt)

### **Global optimization of ODE constrained network problems**

This talk considers a global optimization approach to solve mixed integer nonlinear optimization problems with ordinary differential equation constraints in network problems. We combine techniques from mixed-integer nonlinear programming with an adaptive discretization of differential equations within a spatial branch-and-bound framework. We show that certain discretization schemes allow to construct lower and upper convex relaxations for the ODE constraints, which are then used to construct linear relaxations. This approach does not need to introduce additional variables for the different discretization nodes. We will illustrate our approach on the example of stationary gas transport and will present computational results.

Tristan Gally (TU Darmstadt)

### **Warmstarts and other improvements in SCIP-SDP**

Mixed-integer semidefinite programming (MISDP) has received increasing attention in recent years. MISDPs appear in many applications either by adding combinatorial decisions to non-linear problems with natural SDP-formulations or by reformulating combinatorial optimization problems to incorporate stronger SDP-relaxations. In this talk we will present SCIP-SDP, an open source MISDP-solver using SCIP. After a general introduction, we will focus on the recently added functionality to warmstart the interior-point SDP-solvers. We will give an overview of different ways to create sufficiently interior initial points and discuss their implementation within SCIP-SDP. Finally, we will talk about future plans for SCIP-SDP, including a dedicated handling of SDP-knapsack constraints.

Leon Eifler (Zuse Institute Berlin)

### **Proving cases of Chvátal's conjecture using exact SCIP and VIPR.**

Chvátal's conjecture in extremal combinatorics states a property of decreasing families over finite sets. We use this conjecture as an example to demonstrate how such problems can be translated into an optimization problem. We formulate a MIP that is equivalent to the correctness of the conjecture in the sense that the MIP is infeasible if and only if the conjecture holds. Floating point MIP solvers are unfit to solve such a problem, as the use of tolerances and inexact data cannot lead to a certain proof. To overcome this problem, exact SCIP uses a mix of exact rational arithmetic and safe dual bounding methods for floating point arithmetic. However, the possibility of algorithmic or programming errors remains. The VIPR certificate format presents a possibility to validate results of branch-and-cut solvers externally, using simple inference rules.

Gregor Hendel (Zuse Institute Berlin)

### **Using bandit algorithms for adaptive algorithmic decisions in SCIP**

Modern MIP solvers like SCIP implement numerous algorithmic components that use very similar techniques to find solutions. A classic example are the expensive class of Large Neighborhood Search (LNS) primal heuristics, which solve an auxiliary MIP problem and translate potential solutions back into the original problem. Since little can be predicted a priori about the performance of such heuristics for a particular instance, it is desirable for the solver to quickly adapt its choice of LNS techniques to the instance at hand.

In this talk, I will first present the Adaptive Large Neighborhood Search (ALNS), which com-

bines different LNS techniques into a single heuristic with an adaptive neighborhood selection, guided by different randomized algorithms for the Multi-Armed Bandit Problem. Second, I will discuss analogous selection problems for two other interesting classes of solving components, namely diving heuristics and the LP pricing strategy, where the goal for the LP pricing strategy is not to produce more solutions, but to be the fastest among its competitors. Experimental results confirm the learning success and the computational benefit of the ALNS framework, as well as the performance gain of an adaptive selection of the LP pricing strategy.

Throughout the talk, I will give some implementation details about the involved plugins.

Saurabh Chandra (Indian Institute of Management Indore)

**An MILP based hierarchical planning model for outbound automotive, maritime logistics system in India**

India has a long coastline, which makes it amenable to usage of coastal shipping for bulk movement of cargo as an environmentally friendly mode of transportation. Automotive manufacturing clusters have evolved in Northern, Western and Southern parts of India. The automotive manufacturers primarily use road transportation as a means of outbound logistics of finished vehicles from the factories to the dealers. With rising social and environmental cost of road transportation due to increasing road congestion, the government of India has been trying to promote coastal shipping. Under these circumstances, some companies have started coastal shipping based intermodal transportation of finished automobiles from their factories to the dealers or customers. To this end, we propose a hierarchical mixed integer programming based optimization model to suggest on a strategic maritime logistics system design for outbound automotive distribution in India. A master model is used to suggest best route options, and ship types suitable for the trade and a submodel tries to find the optimal inventory allocation to different locations in a given time frame. The simulations of this model are expected to yield strategic insights into storage capacities at different ports, expected cost reduction for companies and handling different variants with different demand characteristics for the firm using the same logistics system.

Frederic Matter (TU Darmstadt)

**Solving complex-valued  $\ell_0$  minimization problems with constant modulus constraints**

We consider the problem of finding complex-valued least squares solutions with the additional constraint that each entry of the solution is either zero or has a constant modulus of one. As a generalization of compressed sensing, we are interested in sparse solutions that fulfill a given bound for the least squares error. We use an  $\ell_0$ -term as objective function and add the bound for the least squares error as a constraint. This problem can be cast as a real-valued MINLP and we use a spatial branch-and-cut approach to solve it with the framework SCIP. As the constant modulus constraints are non-convex, we develop a specialized branching and propagation method to efficiently handle these constraints. In order to find a good initial primal solution, we present a heuristic. For a demonstration of the effectiveness of our method, we look at the problem of joint antenna selection and phase-only beamforming and present numerical results for this application. We also discuss some details of the implementation of the heuristic and the constraint handler as plugins for SCIP.

Ambros Gleixner (Zuse Institute Berlin)

**Exact methods for recursive circle packing: “price-and-verify” with nonlinear subproblems**

A large fraction of the total costs in tube industry arises from delivery inside rectangular containers. The problem of minimizing the number of containers to transport a set of different tubes can be modeled as a nonconvex MINLP: the recursive circle packing problem (RCPP), which is practically unsolvable for any state-of-the-art MINLP solver. We present a branch-and-price algorithm that handles recursiveness in the master problem and solves nonconvex MINLPs for column generation. The performance of the method is enhanced by enumerating a subset of the packing patterns in advance and verifying their feasibility via nonconvex NLP solves on the fly. Our computational results using the MINLP solver SCIP show that this algorithm solves small-sized instances to proven optimality and produces better solutions than the best known heuristic for larger RCPP instances.

Markó Horváth (Hungarian Academy of Sciences)

**A branch-and-price method for the integrated multiple-depot vehicle and crew scheduling problem**

In the integrated multiple-depot vehicle and crew scheduling problem, vehicle and crew schedules are to be determined simultaneously in order to satisfy a given set of trips over time. The vehicles and the crew are assigned to depots, and a number of rules have to be observed in the course of constructing feasible schedules. In this talk we introduce our novel mathematical formulation for the problem, and present our branch-and-price based solution approach. We also give some details on how we used the SCIP Optimization Suite to implement our solution method.

Patrick Gemander (FAU Erlangen)

**Presolve Examples in SCIP**

No abstract available.

Michael Bastubbe (RWTH Aachen University)

### **Modular Detection of Model Structure in Integer Programming**

Dantzig-Wolfe reformulation applied to specially structured mixed integer programming models is well-known to provide strong dual bounds, though one of many requirements for implementing this method is structural problem knowledge. This is typically a reordering of the coefficient matrix to singly bordered block diagonal form. While searching such forms we pursue two goals: (a) try to retrieve what the modeler had in mind when building the model, and (b) find a vast variety of promising decompositions to facilitate studies on decomposition quality measures. In this talk we present a new modular, iterative algorithm to detect model structures in general mixed integer programming models aiming for these goals. After a predetection step, where constraints and variables are classified in various ways, we iteratively build a tree of successively more completed (refined) decompositions where each leaf is a complete decomposition. We demonstrate manifold refinement procedures, based on the predetected classifications, isomorphism detection algorithms, (hyper-)graph partitioning algorithms, and user given meta data. Finally we present computational results of our implementation integrated in the generic branch-and-price solver GCG.

Jonas Witt (RWTH Aachen University)

### **Eliminating redundant columns from column generation subproblems using classical Benders' cuts**

When solving the linear programming (LP) relaxation of a mixed-integer program (MIP) with column generation, columns might be generated although there exists an integer optimal solution of the MIP that can be expressed without these columns. Such columns are called redundant and the dual bound obtained by solving the LP relaxation is potentially stronger if (some) redundant columns are not generated. To avoid generating redundant columns, we introduce a sufficient condition, which can be checked by solving a compact LP. If the sufficient condition is fulfilled, we can use a dual solution of this compact LP to generate classical Benders' cuts that eliminate redundant columns from the column generation subproblem. We implemented the elimination of redundant columns in the branch-price-and-cut solver GCG and present computational results on structured as well as unstructured MIPs from the literature. Furthermore, we analyze the effect of this approach and discuss promising applications.

Stephen J. Maher (Lancaster University)

### **Large Neighbourhood Benders' Search**

A general enhancement of the Benders' decomposition algorithm can be achieved through the improved use of large neighbourhood search heuristics within mixed-integer programming solvers. While mixed-integer programming solvers are endowed with an array of large neighbourhood search heuristics, their use is typically limited to finding solutions to the Benders' decomposition master problem, which may be of poor quality for the original problem or even infeasible. Given the lack of general frameworks for Benders' decomposition, only ad hoc approaches have been developed to enhance Benders' decomposition through the use of large neighbourhood search heuristics. Within the solver SCIP, a Benders' decomposition framework has been developed to achieve a greater integration with the internal large neighbourhood search heuristics. Benders' decomposition is employed to solve the auxiliary problems of all large neighbourhood search heuristics, the Large Neighbourhood Benders' Search, to improve the quality of the identified solutions and generate additional cuts that can be used to accelerate the convergence of the main solution algorithm. The computational results demonstrate the performance improvements achieved by this general enhancement technique for Benders' decomposition.

Matthias Walter (RWTH Aachen University )

### **Solving Bulk-Robust Assignment Problems to Optimality**

We consider the bulk-robust assignment problem in which we are given a bipartite graph, edge costs, an integer  $k$  and a list of failure (edge) sets. The goal is to find minimum-cost subset of edges such that after the removal of any failure set, the remaining subgraph still contains a matching of size  $k$ . A recent result is an approximation algorithm for the case in which failures consist of single edges. We discuss a straight-forward integer programming model, improve the tractability of its LP relaxation, present cutting planes that are very strong and discuss the associated separation problem. Preliminary computational results for solving these problems to optimality are presented. They indicate effectiveness for such structured instances, whereas the LP relaxations for instances with random failure sets are rather weak.

Jakob Witzig (Zuse Institute Berlin)

### **Mixed-Integer Programming for Cycle Detection in Non-reversible Markov Processes**

In the field of computational molecular design a frequently asked question is about the different states of the molecules during the whole biological process, e.g., a catalyst. If the underlying Markov process is non-reversible, i.e., forward and backward probability between two states are different, there is – to the best of our knowledge – no established method to determine a clustering of the different states of molecules, which describe the different states of the catalyst itself, that can be proven to be optimal. In this talk, we present a new, optimization-based method to exhibit cyclic behavior in these non-reversible stochastic processes. We address this task using a mixed-integer programming model that allows us to compute a cycle of clusters with maximum net flow, i.e., large forward and small backward probability which can be interpreted as the effectiveness of the catalyst. This optimization problem turned out to be very hard to solve for both commercial and non-commercial MIP solvers. In order to tackle this problem, we studied valid inequalities and were able to prove which are facet defining for the corresponding cycle-clustering polytope. An implementation of these techniques within the academic MIP solver SCIP led to a reduction of solving time by a factor of 3.