GOR
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GOR-AG: Praxis der Mathematischen Optimierung
Dr. Jens Schulz

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Herewith, we invite you to the 109th meeting of the GOR working group "Practice of Mathematical Optimization". This meeting is planned to be held in person (or virtually if circumstances require) with the topic

Global Optimization

The workshop takes place in the physics center Bad Honnef (DPG – Deutsche Physikalische Gesellschaft) **Thursday to Friday, March 27 & 28, 2025**.
The working language will be English to be inclusive for a non-German speaking audience.

Note that the participation in a GOR-AG-Workshop for non-members is subject to a registration fee, unless you are a speaker or a host. We strongly advise you to book your stay and travel acknowledging that cancellation of the on-site event may occur on short notice, and the organizers will waive the registration fee but will not refund any other cost.

Participation in the workshop is free for GOR members and 100 Euro for non-GOR members. Bachelor and master students can participate at zero charge for GOR student members and 50 Euro for non-GOR student members.

For accommodation and food/drinks, a service charge needs to be paid at physics center. Please, enter your selected stay during registration:

- Wednesday to Friday: 253 Euro
- Wednesday to Thursday: 164 Euro
- Thursday to Friday: 180 Euro
- Thursday only (no overnight stay): 91 Euro

Please, register here: https://www.redseat.de/pmo109/

The latest information on the meeting is available on the homepage of the GOR (http://www.gor-ev.de/arbeitsgruppen/praxis-der-mathematischen-optimierung/real-world-optimization).

Yours sincerely,

Jens Schulz, Julia Kallrath, Josef Kallrath

(GOR AG)

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Global Optimization

Specific aims

Global Optimization (GO) focuses on finding the global best solution to nonconvex, nonlinear, continuous, and mixed-integer nonlinear problems over the entire feasible domain. The field has advanced significantly in the last decades, driven by improved algorithms, computational power, and applications in various industries.

GO algorithms are divided into deterministic and stochastic methods. Deterministic methods, such as Branch and Bound, Interval Arithmetic, and Cutting Plane methods, guarantee convergence to the global optimum, albeit at a computational cost. Advances in convex relaxations and problem decomposition (e.g., Reformulation-Linearization Technique, RLT) have improved their efficiency. BARON, ANTIGONE, FICO Xpress, Gurobi, Lindoglobal, and SCIP are leading solvers in deterministic optimization. Meanwhile, hybrid methods that combine deterministic and heuristic techniques (e.g., global search coupled with local refinement) are emerging as practical alternatives.

GO problems occur in many practical applications such as chemical processing, energy systems, placement and design problems, health care, computational biochemistry and geometry, and finance.

We especially welcome presentations that deal with the practical aspects of modeling and solving such nonconvex problems.

While machines get more and more powerful, the running times for finding the global optimum are often still not competitive with local optimization procedures embedded in a clever search algorithm. Hence, presentations about enhancements to local optimization algorithms for nonconvex nonlinear problems and their comparison with global optimization approaches are welcome as well.

The core of this 2-day workshop will consist of an attractive schedule of talks covering a broad range of mathematical techniques, theoretical considerations and real world applications around global optimization. As usual, we will reserve plenty of time for informal exchange and networking.
In talks of 15+5min, 25+5min or 40+5min duration, experts from practice and research will address problems and solutions.

If you would like to contribute a talk, please feel free to contact any of the organizers.

Jens Schulz (schulz-gor ‘at’ gmx.net)
Josef Kallrath (josef.kallrath ‘at’ web.de)
Julia Kallrath (julia.kallrath ‘at’ h-da.de)

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The venue & accommodation

Venue

Deutsche Physikalische Gesellschaft (DPG)
https://www.dpg-physik.de/ueber-uns/physikzentrum-bad-honnef/kontakt-anfahrt
Physikzentrum Bad Honnef
Hauptstraße 5
53604 Bad Honnef

How to get there?
Bad Honnef has good train connection from Cologne, and a 10 minutes walk from the station to the venue.

Accommodation

The physics center offers accommodation for up to 50 participants. You can choose to stay in a hotel nearby. Please, select the appropriate option during registration.

Pre-conference get-together

For arrivals on Wednesday, we will arrange a table at a nearby restaurant.
Please, inform the organizers in case you want to attend. Everyone pays their bill themselves.
http://www.labruschetta-badhonnef.de/
Hauptstraße 47, 53604 Bad Honnef Wednesday 7pm

Conference dinner

The conference dinner will take place in physics center on Thursday evening 7pm.

Excursion

This time, we will do an excursion on Friday morning to reserve time for speakers on Thursday.

Talks

Introduction and Overview on NLP, MINLP and Deterministic Global Optimization
Josef Kallrath (GOR AG PMO)

The workshop begins with an introduction to the field of nonconvex nonlinear optimization, its applications, and the various methods used. We start with the fundamentals of local nonlinear programming (NLP), covering essential concepts such as objective functions, constraints, and optimality conditions. Special attention is given to the challenges posed by nonconvex NLP problems, including the existence of multiple local optima due to lack of convexity, and the difficulties in ensuring global optimality.

Building on this foundation, we explore mixed-integer nonlinear programming (MINLP), which extends NLP by incorporating discrete decision variables. The discussion highlights the increased complexity introduced by integer variables, the combinatorial nature of MINLP problems, and their importance in real-world applications such as engineering design, logistics, and process optimization.

Finally, we discuss deterministic global optimization techniques for solving nonconvex NLP and MINLP problems. We discuss the combination of branch-and-bound and convex relaxation strategies provide participants with a comprehensive understanding of the mathematical and computational strategies used to solve complex optimization problems with guaranteed global optimality.

Cracking a Cracker System: nonlinear expressions in matrix forms passed on and on
Claude-Philippe Medard (SAP SE)

We look at testing a solver for a system of crackers that involves many yield matrices, separation matrix, and post processing matrix, in view to find out what optimal feed stocks the system handles, subject to chemical formulas and capacity constraints, and what output chemical semi-finished products can be yielded (tons/hr). Results are required to be found within the second mark, in view to support long range planning scenarios for production planning and other Distillation plant models (also nonlinear by virtue of blendings).

Global Optimization for Disk Placement Problems: Non-Overlapping, Area Coverage, and Discrete Point Coverage Models
Josef Kallrath (University of Florida)

In this talk, we present a geometric optimization framework that addresses three disk-placement problems within a bounded planar region. First, we formulate the Maximal Non-Overlapping Disk Packing Problem (P1), which seeks to position *n* non-overlapping, equal-sized disks within a given region, maximizing their radii -- this is formulated as a nonlinear programming (NLP) problem. The simplest example is when the region is a circle. The most general case is when the region is prescribed by its perimeter represented by a set of points. Second, we present the Discrete Point Set Covering Problem with Heterogeneous Disks (P2), which focusses on computing the center positions and radii for n disks to cover a given finite set of target points. This is modeled as a mixed integer nonlinear programming (MINLP) problem. Third, we propose the Variable-Radius Area Coverage Problem (P3), which allows

disks of different sizes to overlap freely, with the objective of achieving coverage of a prescribed area using exactly *n* disks. This leads to a semi-infinite programming (SIP) problem with a finite number of variables and an infinite number of constraints (continuum). We approach this by discretizing the area to be covered by a finite number of points and obtain problem P2.

We explore the limits of deterministic global optimization techniques using the Branch & Reduce Optimization Navigator (*BARON*) solver called from *GAMS* and outline heuristic algorithms for each problem. Application areas for proposed models are spatial design, network coverage planning, and resource-efficient spatial allocation.

Josef Kallrath obtained his PhD in astrophysics from Bonn University (Germany) in 1989. He is a professor at the University of (Gainesville, FL), and for 35 years has been solving real-world problems in industry using a broad spectrum of methods in scientific computing, from modeling physical systems to supporting decisions processes by mathematical optimization. He has written review articles on the subject, about 150 research papers in astronomy and applied mathematics, and several books on mixed integer optimization, as well as one on eclipsing binary stars.

With Jens Schulz and Julia Kallrath in charge, he leads the “Practice of MathOpt” Working Group of the German Operations Research Society. Among his current research interests are multi-precision and exact arithmetic in optimization, geometry and optimization, and polylithic modeling and solution approaches to solve large-scale or difficult optimization problems, for instance, by decomposition techniques such as column generation, or hybrid methods.

An abstract framework for unifying nonconvex constrained optimization
Charlie Vanaret (Argonne & ZIB)

SQP and interior-point methods for nonconvex constrained optimization, also referred to as Lagrange-Newton methods, typically share key algorithmic components, such as strategies for computing descent directions and mechanisms that promote global convergence. Building on this insight, we introduce an abstract framework with 8 building blocks that unifies the workflows of Lagrange-Newton methods. We then present Uno, a modern software implementation that enables the automatic generation of a wide range of strategy combinations, and is competitive against state-of-the-art solvers such as IPOPT and filterSQP. This is joint work with Sven Leyffer (Argonne).

Charlie Vanaret is an assistant computational mathematician at Argonne National Laboratory (remote) and Zuse-Institut Berlin, where he develops the nonconvex optimization solver Uno. He earned his PhD in 2015 from Toulouse INP (France), specializing in interval global optimization, before working as a postdoc at IRT Saint Exupéry (France), Argonne (USA), Fraunhofer ITWM, TU Berlin, and ZIB (Germany). In his spare time, he is a passionate bass player and landscape photographer.

Efficient Deterministic Global Optimization: Adaptive Time Grids for Dynamic Challenges
Tim Varelmann (Bluebird Optimization)

Global optimization is notoriously challenging due to the exponential worst-case runtime of branch-and-bound schemes.
Dynamic optimization problems that require to model transient system behavior introduce an additional complication to maintaining tractable problem scales.

Recent successes with reduced-order models highlight the importance of minimizing decision variables, a principle we extend to dynamic optimization through adaptive time grids. This allows to solve such problems with a coarse initial time discretization and then automatically refine only those parts of the time grid that have a crucial impact on the solution quality. Case studies in chemical engineering demonstrate how adaptive time grids not only deliver high-quality solutions but also uncover structural insights inaccessible with traditional equidistant grids.

Dr. Tim Varelmann studied Computational Engineering Science at RWTH Aachen, University of Queensland, and MIT from 2013 to 2018. He subsequently completed his doctorate in process systems engineering at RWTH and UT Austin.
As a freelancer, he contributes his expertise in efficient modeling and tailor-made decomposition algorithms to industries such as energy, supply chain management and production planning with his own brand ‘Bluebird Optimization’ since 2022. Tim likes to spend his spare time on the football pitch, with strategy games, or cooking and eating delicious dishes in good company.

Solving MINLPs to global optimality with FICO Xpress
Tristan Gally (FICO)

In this talk we will introduce the global optimization capability within FICO Xpress Solver, which allows to solve general mixed-integer nonlinear problems to global optimality. We will discuss how the global solver incorporates existing capabilities like the parallel branch-and-bound framework and the local solver SLP and report on the performance impact of different components of the solver like presolve, cutting, branching, heuristics and parallelization. Furthermore, we will describe differences between our local and global optimization capabilities and typical use cases for a global optimization solver.

Tristan Gally is a Principal Engineer at Fair Isaac Services Limited, working as a developer on both the global optimization solver as well as the local solver SLP within the Xpress Solver team. Before joining FICO in 2019, he completed a PhD at TU Darmstadt on Computational Mixed-Integer Semidefinite Programming, working within the Collaborative Research Center SFB 805 "Control of Uncertainty in Load-Carrying Structures in Mechanical Engineering".

Modeling and solving global optimization problems with Gurobi
Robert Luce (Gurobi)

In this talk, we provide an overview of Gurobi's algorithmic components for solving nonlinear optimization problems to globaloptimality. In essence, we extend our existing mixed-integer programming (MIP) framework to handle such problems. This includes our presolve algorithms, an extension of the branch-and-bound method utilizing spatial relaxations, and an interior point algorithm for nonlinear problems, which serves as a primal heuristic to find high-quality solutions. As a result, we can compute solutions to nonlinear optimization problems along with certificates for global optimality.

Finally, we have extended gurobipy to facilitate the easy formulation of expression-based nonlinear optimization problems in Python. Gurobi's nonlinear solver applies to explicit expression-based constraints and does not require the supply of derivative data.

Robert Luce is an experienced researcher in applied mathematics, and author of numerous publications in the fields of numerical linear algebra and optimization. He's currently Principal Developer at Gurobi optimization with a focus on continuous optimization.

Burak Usul (GAMS)
Global vs. Local Optimization in Machine Learning: Striking the Right Balance

There are several compelling reasons to embed neural networks into optimization models. For example, in chemical engineering, surrogate models (sometimes neural networks) are commonly used to approximate complex systems. Making decisions over neural networks requires embedding them into your optimization models.

Another key motivation is the verification problem. Neural networks operate as black-box learners, making it crucial to verify their behavior before deploying them in mission-critical systems. While mixed-integer programming (MIP) and mixed-integer nonlinear programming (MINLP) are among the slower approaches, they remain valuable tools for ML specialists to rigorously verify neural networks.
However, the inherent nonlinearities in many neural networks pose challenges to optimization. In this talk, we will explore the interplay between global and local optimization, demonstrating how they complement each other to enhance problem-solving capabilities.

Burak Usul is a senior software engineer at GAMS working there since about 6 years. He received his Master's degree from TU Braunschweig in Data Science in 2023. Currently, he is actively working on providing fast and convenient ways of embedding neural networks and other ML constructs to GAMSPy. He is a passionate chess player.

Container shape optimization for packing Irregular objects
Tetyana Romanova (University of Leeds, UK & IPMach, National Academy of Sciences of Ukraine & Kharkiv National University of Radio Electronics, Kharkiv, Ukraine)

Packing irregular polygons into a shape-optimized (soft) convex polygonal container is considered. Polygonal objects refer to a special class of two-dimensional canonically closed sets bounded by line segments, rays, or lines (called phi-polygons). Each polygonal object can be freely translated and rotated. The container is represented by a convex polygon with at most m unknown vertices, while the side lengths of the container can be bounded. The convexity and metric conditions for the container are formulated, as well as the non-overlapping and containment constraints for arbitrary polygonal objects. The objective function to be minimized is either the area of the soft container or the length of its perimeter. A corresponding nonlinear programming (NLP) problem is formulated, and a multi-start heuristic based on the local NLP solver IPOPT is proposed. Computational results are reported to demonstrate the efficiency of the proposed approach. For small problem instances global solutions obtained by BARON and FICO Xpress Global are provided.

Joint work with J. Bennell , J. Kallrath, I. Litvinchev, O. Pankratov, Y. Wei

Tetyana Romanova (Professor) received her M.Sc. degree in Applied Mathematics from Kharkiv National University of Radio Electronics (KNURE), Ukraine; Ph.D. and Dr.Sci. (Habilitation) in Mathematical Modeling and Computational Methods from the Institute of Cybernetics of the National Academy of Sciences of Ukraine, Kyiv. She is a leading scientist of the Institute for Mechanical Engineering Problems of the National Academy of Sciences of Ukraine and visiting professor of the University of Leeds. She is an author of numerous research papers focused on the development of geometric tools, mathematical models and optimization algorithms for solving packing, cutting, layout and covering problems.

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Global Optimization

Thursday, March, 27 2025: 09:30 – 18:00

09:00-09:30 *Welcome coffee, take a seat and have first chats*

09:30-09:45 **Opening and Welcome** (Jens Schulz & Julia Kallrath & Josef Kallrath)

09:45-10:30 **Introduction and Overview on NLP, MINLP and Global Optimization**
Josef Kallrath (GOR AG PMO, University of Florida)

10:30-11:15 **Cracking a Cracker System: nonlinear expressions in matrix forms passed on and on**
Claude-Philippe Medard (SAP SE)

11:15-12:00 **Efficient Deterministic Global Optimization: Adaptive Time Grids for Dynamic Challenges**
Tim Varelmann (Bluebird Optimization)

12:00-13:00 ---------- Lunch Break ----------
---------- Taking a Group Photo for the OR News and Press ----------

13:00-13:45 **Solving MINLPs to global optimality with FICO Xpress**
Tristan Gally (FICO)

13:45-14:30 **Modeling and solving global optimization problems with Gurobi**
Robert Luce (Gurobi)

14:30-15:15 **Burak Usul (GAMS)**
Global vs. Local Optimization in Machine Learning: Striking the Right Balance

15:15-15:45 ---------- coffee break ----------

15:45-16:30 **An abstract framework for unifying nonconvex constrained optimization**
Charlie Vanaret (Argonne & ZIB)

16:30-17:15 **Global Optimization for Disk Placement Problems: Non-Overlapping, Area Coverage, and Discrete Point Coverage Models**
Josef Kallrath (University of Florida)

17:15-17:45 **Container shape optimization for packing Irregular objects**
Tetyana Romanova (Leeds, UK & Ukraine)

19:00-21:00 **Conference Dinner at physics center**

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Friday, March, 28 2025: 09:30 – 12:00

09:30-10:00 ----- *Excursion: Physics center; starting in meeting room (Victor Gomer)* -------

10:15-11:00 **Last speaker slot (tba)**

11:00-11:45 **Discussion round: The future of Global Optimization**
Josef Kallrath (GOR AG PMO, University of Florida)

12:00-13:00 ---------- Lunch Break ----------