

September 27<sup>th</sup> – 30<sup>th</sup>, 2023 Zuse Institute Berlin Takustr. 7, 14195 Berlin, Germany









### Welcome Address

Dear Participants,

It is with great pleasure that we extend a warm welcome to all of you to the Book of Abstracts of the 7<sup>th</sup> ZIB-IMI-ISM-NUS-MODAL Workshop. We are delighted to have you join us in this event.

The 7<sup>th</sup> Workshop, entitled *Workshop on Future Algorithms and Applications*, builds upon the successful collaborations established through the previous workshops organized by the Institute of Mathematics for Industry (IMI) of Kyushu University, the Institute of Statistical Mathematics (ISM) in Tokyo, and the Research Campus MODAL at the Zuse Institute Berlin (ZIB). Our 1<sup>st</sup> joint Workshop in 2017 focused on optimization and data-intensive high-performance computing, particularly emphasizing cooperation between research and industry. The 2<sup>nd</sup> Workshop continued this collaboration, with speakers from science and industry presenting their mathematical optimization and data analysis achievements. With the 6<sup>th</sup> Workshop, RIKEN and the National University of Singapore (NUS) joined our efforts. The 7<sup>th</sup> Workshop will explore new and innovative algorithms and applications, highlighting the commitment to collaborative research in applied mathematics and facilitating ongoing exchange between the participating institutes.

We want to express our deep gratitude to all the authors who have contributed valuable research to this book. Your dedication and commitment to advancing the field of applied mathematics are truly commendable. We also extend our heartfelt thanks to our sponsors, volunteers, and everyone who has played a crucial role in making this event a reality. As you explore the abstracts within these pages, we encourage you to engage in fruitful discussions, forge new collaborations, and contribute to the vibrant intellectual atmosphere of this Workshop. The research presented here will inspire innovation and further advance the boundaries of mathematical algorithms and their real-world applications.

Thank you for being an integral part of this exciting journey, and we look forward to the insightful exchanges and discoveries that the 7<sup>th</sup> ZIB-IMI-ISM-NUS-MODAL Workshop will undoubtedly bring. We hope you all have a fantastic time during the upcoming days.

With warm regards, the Organization Committee

(Katsuki Fujisawa, Satoshi Ito, Mirai Tanaka, Ying Chen, Ha Quang Minh, Yuji Shinano, Thorsten Koch, Thi Thai Le, Milena Petkovic, Janina Zittel, and Tim Kunt)

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### The approximate Carathéodory problem and an application to quantum mechanics

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Sebastian Pokutta

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The approximate Carathéodory theorem states that given a compact convex set P each point x in P can be approximated to  $\varepsilon$ -accuracy in the p-norm as the convex combination of  $O(pD_p^2/\varepsilon^2)$  vertices of P, where  $D_p$  is the diameter of P in the p-norm. We revisit the approximate Carathéodory problem by solving the primal problem via the Frank-Wolfe algorithm, providing a simplified analysis and leading to an efficient practical method. Furthermore, improved cardinality bounds are derived naturally using existing convergence rates of the Frank-Wolfe algorithm in different scenarios.

We then apply this approach to Bell scenarios with two outcomes per party. We algorithmically consider the two sides of the membership problem for the local polytope: constructing local models and deriving separating hyperplanes, that is, Bell inequalities. As an application, we study the threshold value for the nonlocality of two-qubit Werner states under projective measurements. Here, we improve on both the upper and lower bounds present in the literature and we establish refined bounds on the value of the Grothendieck constant of order three: We also demonstrate the efficiency of our approach in multipartite Bell scenarios, and present the first local models for all projective measurements with visibilities noticeably higher than the entanglement threshold.

### Optimization of measures from a unified perspective

Satoshi Ito

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Whether or not it is natural to do so, optimization problems can most often be viewed as optimization problems in some suitable measure space. In some cases, the "measure" appears directly as a (primal) decision variable, such as the problem of determining the optimal capacity (e.g., electrostatic capacity, communication channel capacity) or the problem of estimating a probability measure (e.g., the moment problem). However, in some other cases, such as infinite or semi-infinite optimization problems, two-level optimization problems, robust optimization problems, and optimal control problems with state inequality constraints, the "measure" appears implicitly as a dual variable. In this talk, we will look at such optimization problems of measures from a unified perspective.

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### Planning Berlin's Energy Transition: Multi-objective Portfolio Optimization for Decarbonized District Heating

Christoph Koch\* and Janina Zittel\*\*

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We are focusing on Berlin's district heating network, one of Western Europe's most complex systems. Our goal is to make this system free from fossil fuels, which involves addressing CO2 emissions, efficiency, and economic factors. To achieve this, we need advanced planning tools as the system becomes more diversified and decentralized. In our study, which is tailored to Berlin's district heating network transition, we propose a hierarchical mathematical model. This model decomposes the optimization process spanning up to 30 years from unit commitment to investment planning. Additionally, we evaluate two coordinating algorithms for a three-objective optimization, aiming to find the most accurate estimate of the Pareto surface. These algorithms successfully support multi-objective optimization, which is crucial for building sustainable, decarbonized energy systems in alignment with global climate goals.

### Collective Communication Scheduling on Optical Circuit Switch Networks with SmartNIC

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Nariaki Tateiwa

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Recent advances in machine learning have leveraged distributed machine learning (DML) for training large models across multiple GPUs. One of the main challenges of DML is network overhead, especially collective communications cause substantial bottlenecks in many DML workloads. To accelerate collective communication, we focused on optical circuit switch (OCS) networks, which offer advantages in terms of higher bandwidth, lower latency, and lower jitter compared to traditional electrical switch networks.

In this presentation, we introduce a method to optimize the collective communication schedule on OCS networks utilizing SmartNIC. The stream processing of SmartNIC supports communication without compromising the low latency and low jitter of OCS. Using our mixed integer linear programming (MILP) formulation, we could obtain schedules to maximize the stream processing capability of SmartNICs.

A pilot study conducted on a four-node cluster showed that our Allreduce colletctive communication schedule better tailored to the OCS network with SmartNIC than the conventional Ring-Allreduce, showcasing the potential for substantial DML performance enhancement.

### Construction of Demonstration Platforms for Realizing Digital Twins 27 Sept. 2023

Katsuki Fujisawa

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Efforts are being promoted to construct digital twins (bridging the physical (real world) and cyber space) by leveraging the latest mathematical and information technologies. This aims to address various challenges faced by cities, regions, and the industrial sector. Central to these efforts is the concept of Cyber-Physical Systems (CPS). Within CPS, optimization computations and simulations are conducted in cyber space based on real-world data (mobility of people, objects, money, information, etc.), and the results are reflected back into the real world. Such processes are expected to foster the creation of new industries, reduce costs and waste emissions, and improve work styles. These applications are garnering expectations from various sectors, including social infrastructure, manufacturing, and retail.

In this talk, we will provide an overview of the latest mathematical and information technologies, such as optimization algorithms for digital twins, and discuss their practical applications in industry. Additionally, we introduce ongoing projects that utilize quantum technology to construct smart factories.

### Process Flexibility and Supply Risk Mitigation: A New Methodology for Designing Resilient Supply Chains

Chou Cheng-Feng

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The global supply chain is undergoing significant changes as a result of recent international tensions and pandemic-related disruptions. To mitigate the uncertainties arising from these supply shocks, supply chain operators need to effectively cushion the supplyside risks while also hedging against demand uncertainties. In both theory and practice, process flexibility has been proven to be an effective supply chain strategy that enables timely and effective responses to demand uncertainties. This talk aims to shed light on how process flexibility can mitigate supply uncertainties, such as supply disruptions (e.g., unexpected reductions in production capacity during pandemic lockdowns) and price uncertainties (e.g., volatile production costs or commodity prices). We will introduce a new methodology for analyzing the resilience of a supply network and discuss its applications in designing a more resilient supply chain. By leveraging process flexibility and resilience analysis, supply chain operators can enhance their ability to respond to unforeseen events and adapt to changing market conditions, ultimately improving the efficiency and effectiveness of their operations.

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#### 27 Sept. 2023 Online Learning Algorithms for Wireless RIS Relay Communications

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Sherief Mostafa Salman Hashima

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Reconfigurable Intelligent surface (RIS) is a competitive relaying technology to widen the millimeter waves (mmWave) coverage range, as it offers an effective means of addressing blocking issues. However, selecting the optimal RIS relay for maximum attainable data rate is a time-consuming process, as it requires mmWave beamforming training (BT) to tune the phase shifts (PSs) for mmWave base station (mBS) and RIS relays. This paper proposes a self-learning based budgeted Multi armed bandit approaches for RIS relay probing to address this challenge. The BT time cost of probing the RIS relay is incorporated into the main bandit formulas. This enables the RIS relay to be chosen with the lowest BT time cost. Numerical results demonstrate the improved performance of the bandit aided RIS relaying technique regarding BT time consumption/cost, spectral efficiency, and attainable data rate when compared to other benchmarks.

### An efficient solver for multi-objective onshore wind farm siting and network integration

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Jaap Pedersen

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

Existing planning approaches for onshore wind farm siting and network integration often do not meet minimum cost solutions or social and environmental considerations. In this talk, we present an approach for the multi-objective optimization of turbine locations and their network connection using the Quota Steiner tree problem. Additionally, we demonstrate that contrary to many approaches for exclusive turbine siting, network integration must be simultaneously optimized in order to avoid excessive costs or landscape impacts in the course of a wind farm project.

### Optimal Market Making in a Multi-agent Market under Model Uncertainty: A Reinforcement Learning Approach

Yijiong Zhang

National University of Singapore, 21 Lower Kent Ridge Rd, 119077, Singapore

We study the optimal market making problem in order-driven electronic markets, with a focus on model uncertainty. We consider ambiguity in order arrival intensities and derive a robust strategy that can perform under various market conditions. To achieve this, we introduce a tractable model for the limit order book using Markov Decision Processes and intend to use Reinforcement Learning to solve the complex optimization problem. This approach enables us to accurately represent the order book dynamics with tick structures, as opposed to the usual price dynamics modeled in stochastic approaches. We conduct simulations as well as numerical studies to examine the effectiveness of different methods under our market setting.

Acknowledgement: This is a joint work with Ying Chen, Hoang Hai Tran and Julian Sester.

### **Realization of smart factories using IP**

Hiroki Ishikura

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Smart factories have become widely used for more efficient production activities recently. In collaboration with Rohto Pharmaceutical Co. (Rohto), we have conducted research to realize smart factories. In this talk, we will introduce mobility optimization related to automated warehouses. Rohto uses an automated warehouse to manage a large volume of various items. By optimizing the mobility of automated warehouses, production activities can be streamlined, and factory operations can be made more efficient.

### **Representation Learning for Protein Conformational Dynamics**

Tsuyoshi Ishizone Meiji University 1 Chome-1 Kanda Surugadai, Chiyoda City, Tokyo 101-0062, Japan

Protein is a macromolecule made of chains of amino acids that perform various bodily functions, including structural support, enzymatic reactions, gene regulation, and molecule transport. Protein dynamics exhibit phenomena on various time scales, and it is crucial to extract slow dynamics to understand biological functions. At the fast time scale (from femtoseconds to nanoseconds), proteins exhibit characteristic molecular vibrations and rapid conformational changes, including transitions between secondary structure motifs and local fluctuations of the protein backbone. At the slow time scale (from microseconds), proteins undergo global structural transitions and folding/unfolding events, which

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27 Sept. 2023 Wednesday Session 2 involve rearranging secondary structure elements and tertiary contacts. Slower dynamics are essential for protein dynamics because they allow for large-scale conformational changes and domain motions often required for biological function. To extract slower dynamics, we propose a new representation learning method which accerelate slowness in the representation space. Through the application of simulation sequence data, we quantitatively and qualitatively compare with the existing methods.

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#### **Rank-free Tensor Decomposition Using Energy-based Models**

Kazu Ghalamkari

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Tensor factorization has fundamental difficulties in rank tuning and optimization. To avoid these difficulties, we develop a rank-free energy-based tensor factorization, called many-body approximation, that allows intuitive modeling of tensors and global optimization. Our approach models tensors as distributions via the energy function, which describes interactions between modes, and a dually flat statistical manifold is induced. We visualize these interactions as tensor networks and reveal a nontrivial relationship between many-body approximation and low-rank approximation.

### Reducing Ising Model Sizes for Solving Permutation-Based Combinatorial Optimization through Dual-Matrix Domain-Wall Encoding

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An Ising model, represented by a quadratic formula of qubit variables taking values of -1 or +1, is a pivotal tool in quantum computing. Quantum annealers are designed to find optimal assignments of qubits that minimize Ising model values. Given the inherent limitations in quantum annealer sizes, it becomes crucial to minimize Ising model sizes. However, conventional one-hot encodings necessitate cubic-size Ising models to solve permutation-based optimization problems. In this study, we introduce the dual-matrix domain-wall encoding technique, which efficiently reduces Ising models for permutation-based problems to square sizes. By employing this technique, quantum annealers can effectively tackle larger permutation-based optimization problems with improved efficiency and feasibility.

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### **Quantum Optimization**

Stefan Wörner

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Quantum Optimization is a rapidly evolving field that seeks to use the power of Quantum Computers to solve optimization problems that are difficult to solve on classical computers. This talk will introduce IBM Quantum's roadmap towards useful Quantum Computing, spotlight key optimization algorithms and their viability on noisy quantum systems, and conclude with emerging directions and the key challenges towards a practically relevant advantage.

### Quantum and quantum-inspired algorithms for k-means and Lasso path problems

João Doriguello

National University of Singapore, 21 Lower Kent Ridge Rd, Singapore 119077

In this work we study two problems: high-dimensional linear regression with an  $\ell_1$  – *penalty* (Lasso path problem) and clustering of large datasets (*k*-means problem). On one hand, while classical algorithms are available for Lasso, our focus is on developing a quantum algorithm that offers new insights and speedup. Quadratic speedup is possible over the classical Homotopy (Least Angle Regression) method. In particular, we provide a general setup for Lasso solutions as the penalty term varies. On the other hand, one of the most popular clustering algorithms is Lloyd's iteration for k-means. This iteration takes N vectors and outputs k centroids; these partition the vectors into clusters based on which centroid is closest to a particular vector. We present an overall improved version of the "q-means" algorithm, the quantum algorithm originally proposed by Kerenidis, Landman, Luongo, and Prakash which is an approximate version of k-means clustering.

### A Short Tale from Industry: The Avoid-Vehicle's-Early-Arrival-Constraint -A Wolf in Sheep's Clothing

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Kai Hoppmann-Baum Delivery Hero, Oranienburger Str. 70, 10117 Berlin, Germany

The vehicle routing problem with pickups and deliveries (VRPPD) is one of the fundamental optimization problems in the (food) delivery business. Given a set of deliveries, each composed of a pickup location, i.e., the vendor, and a dropoff location, i.e., the customer, as well as a set of couriers, each associated with its current location, the goal is to determine routes for the latter such that every location pair is contained in exactly one of them. In this context, the pickup location must be visited before the dropoff. Finally, considering fixed travel times between the locations, a common goal is to minimize the sum of delivery times, i.e., the sum of the times it takes to visit the dropoff locations. In the following, let us consider an additional lower bound on when a pickup location can

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visited at the earliest, representing, for example, the time when the food is ready. Until recently, we at Delivery Hero allowed the courier to wait at the vendor's location. However, routes featuring long waiting times turned out to be inconvenient for both the vendor and the courier. Indeed, the vendors complained that the couriers occupy space in or in front of the restaurant or make the business look less attractive to potential customers. The couriers, on the other hand, had the feeling of wasting time and money. Thus, operations asked us to introduce an Avoid-Vehicle's-Early-Arrival-Constraint into the route-creating algorithm, limiting the waiting times. In this talk, I want to tell you the story of this simple-sounding requirement, which has led to heavy discussion across several different business units and is still ongoing.

### Fisher-Rao metric and infinite-dimensional divergences between Gaussian processes

Quang Minh Ha

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

Fisher-Rao metric is a fundamental object in information geometry and plays a crucial role in many areas of statistics and machine learning. In this talk, we present recent work on the generalization of Fisher-Rao metric from finite to infinite-dimensional settings, with a focus on the setting of infinite-dimensional Gaussian measures and Gaussian processes. In particular, we show that regularized versions of the Fisher-Rao distance and related divergences between Gaussian processes, including Kullback-Leibler and Renyi divergences, can be consistently estimated from finite-dimensional versions, with dimensionindependent sample complexities. The mathematical formulations will be illustrated with experiments on Gaussian processes.

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### **Spectral Sparsification of Hypergraphs**

Tasuku Soma

Institute of Statistical Mathematics, 10-3 Midoricho, Tachikawa, Tokyo 190-0014, Japan

Spectral sparsification is a technique to approximate dense objects (e.g., weighted graphs and matrices) with sparse objects while preserving the original spectral information (e.g., eigenvalues and energy functions). This concept has been the cornerstone for developing faster algorithms for fast algorithms for continuous/combinatorial optimization and numerical linear algebra. In this talk, I will discuss recent results of spectral sparsification for hypergraphs. Since hypergraph energy functions are no longer quadratic, spectral sparsification presents additional challenges compared to the existing spectral sparsification and requires more advanced tools. I will present simple edge-sampling sparsification algorithms and the analysis. Furthermore, I will also present recent joint work on online spectral sparsification of hypergraphs.

# Convex optimization techniques for mixed-integer nonlinear problems

Mathieu Besançon

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

Nonlinear and mixed-integer optimization have long remained separate fields with their own techniques, representations, and algorithms. In this talk, we will introduce a novel approach leveraging first-order methods for convex optimization based on the Frank-Wolfe algorithm. First-order methods are the usual choices for large-scale smooth optimization but are typically not prime candidates in branch-and-bound algorithms because of their slower convergence and lower accuracy, which does not systematically provide a safe dual bound necessary to prune nodes in a branch-and-bound framework. We will show how we designed a convex mixed-integer algorithm leveraging techniques and algorithms both from the first-order convex and mixed-integer literature, challenging the status quo on first-order methods in the mixed-integer setting.

### Classification from Positive and Unlabeled Data and Its Application in Audio Signal Enhancement

Masashi Sugiyama

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Supervised classification is aimed at learning a boundary between classes from labeled training data. However, obtaining labels is often costly or even impossible in real-world applications. Positive-Unlabeled (PU) classification is aimed at learning a boundary between positive and negative classes only from positive and unlabeled training data without negative data. In this talk, I will give an overview of PU classification and its extensions to a variety of weakly supervised classification problems. Then we show that PU classification can be successfully employed in audio signal enhancement.

#### References

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- Ito, N. & Sugiyama, M. Audio signal enhancement with learning from positive and unlabeled data. In Proceedings of 2023 IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP2023), pp. 1-5, Rhodes Island, Greece, Jun. 4-10, 2023. (Best Paper Award)

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### Optimisation of submarine power cable systems

Jakub Tomczyk

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Submarine power cable systems are close to breaking the 1,000 kilometers in length this decade. Currently, the world's longest subsea interconnector is North Sea Link, 720 km, which brings together electricity systems of the UK and Norway. There are two projects in planning stages, which will move the world record by almost an order of magnitude, i.e., Australia-Asia PowerLink project and the Xlinks Morocco-UK Power Project. While optimisation related to short interconnectors is relatively easy due to the low number of feasible solutions, optimising subsea cable systems over routes, which are approx. 4,000 kilometers involves many decisions, which require appropriate mathematical formulations. The projects face conductor, armour and route optimisation problems, which need to be viewed in the context of costs, thermal behaviours, laying and maintenance activities, and risk. We will propose a modelling framework, which captures key driving variables and allows one to make informed decisions, which balance risk and returns.

# Data analytics and machine Learning for creating high impact in Mckinsey

Xiuqin Xu

McKinsey, One Raffles Quay, Level 24, South Tower, 048583, Singapore

In today's data-driven world, businesses are seeking to leverage the power of data analytics and machine learning to create high impact. At QuantumBlack, AI by McKinsey, we have developed reliable and scalable assets to help our clients achieve this goal. In this talk, we will introduce two open-source Python packages that we have developed: Kedro and Causalnex. Kedro is a powerful package that allows you to create reusable and standardized end-to-end data science pipelines that can scale with your data. Causalnex, on the other hand, is a package designed to help you analyze causal relationships in your data. By leveraging these assets, we can streamline the data science workflow, create production-ready code, uncover hidden insights, and drive higher business value.

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### **Revisiting GenéLive! for Rhythm Action Generation**

Daisuke Sakurai

Institute of Mathematics for Industry, Kyushu University 744 Motooka, Nishi-ku, Fukuoka-shi, Fukuoka, 819-0395 JAPAN

This talk re-visits our recent deep neural network model GenéLive! that was in operation to aid professional music game developments. The model helps game creators build rhythm action games, which challenge the player to perform certain actions, such as tapping game pad button, in sync with the background music. Indeed, the GenéLive! is based on the famous Dance Dance Convolution model, with original improvements like multiscale analysis and additional timing labels. After a general introduction to the model, I would like to focus somewhat on the application perspective if time permits.

### Understanding microbiome dynamics via interpretable graph representation learning

Tim Conrad

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

In this presentation, we address the challenges of deciphering complex interactions within large-scale networks, using the human microbiome as a case study. The primary challenge lies in understanding the intricate relationships represented by a large number of interactions. To tackle this, we introduce a novel computational approach based on the deep-learning transformer architecture. We show how to use this approach to model these interactions as a time-evolving graph, where nodes denote individual entities, and edges signify their interactions. Our key contribution is the development of an interpretable method that captures a low-dimensional representation of this time-evolving graph, ensuring the retention of essential dynamics from the original high-dimensional space. The generalizability of our method is showcased by its performance on both synthetic and real-world datasets, indicating its potential utility in diverse fields beyond the biological context.

Reference: https://doi.org/10.1038/s41598-023-29098-7

### Cutting Plane Selection for Mixed-Integer Linear Programming

Mark Turner

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In this talk, we present some recent advancements of cutting plane selection for mixedinteger programming. We show how cutting plane selection can be used to improve branching decisions, and how information from other solving processes can be used to improve cutting plane selection. All work is performed within the mixed-integer programming solver SCIP, with performance results presented on MIPLIB 2017.

### Global Optimization of Mixed-Integer Nonlinear Programs with SCIP 8

Stefan Vigerske

GAMS Software GmbH, Augustinusstraße 11B, 50226 Frechen, Germany

For over ten years, the constraint integer programming framework SCIP has been extended by capabilities for the solution of convex and nonconvex mixed-integer nonlinear programs (MINLPs). With version 8, these capabilities have been largely reworked and extended. This talk is a reminiscence of this work and gives a short overview on the state of MINLP solving in SCIP 8.

For a detailed overview, see https://arxiv.org/abs/2301.00587.

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### **SCIP beyond 8.0**

Ksenia Bestuzheva

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

SCIP is currently among the leading solvers for mixed-integer nonlinear programming (MINLP). It implements a spatial branch-and-bound algorithm to solve MINLPs to global optimality, and the framework for handling nonlinear constraints added in release 8.0 ensures numerically safe handling of extended formulations. In this talk we will give an overview of MINLP solving in SCIP and present the latest techniques added to SCIP, including features that will be part of the future SCIP 9.0 release.

## Solving nonconvex MINLPs to global optimality with FICO Xpress Global

Leona Gottwald

FICO, Takustr. 7, 14195 Berlin, Germany

This talk introduces FICO Xpress Global, the latest addition to the Xpress optimization suite, which allows to solve general mixed-integer nonlinear problems to global optimality. We will discuss how existing features of the MILP and local NLP solvers are used and explain several different extensions for, e.g., spatial branching and convexification cuts, and their performance implications.

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### Combining Machine Learning with Optimization using Gurobi-machine learning

**Roland Wunderling** 

GUROBI Optimization LLC 251 Little Falls Drive, Wilmington, New Castle, DE 19808, USA

Machine Learning is viewed as the solution to everything these days, but is it really? In this presentation we will highlight some shortcomings and how to use optimization with gurobi-machinelearning to identify and/or overcome those. This leads to MIPs that can be solved with the gurobi solver.

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### **Recent advances in the Cardinal Optimizer**

Gerald Gamrath

COPT GmbH, Englerallee 19, 14195 Berlin, Germany

In this talk, we present the recent developments in the Cardinal Optimizer (COPT) and give an overview of the different problems classes that can be solved with COPT. We discuss some key techniques that contributed to the performance improvements of our MIP solver and present preliminary performance numbers for the upcoming COPT release.

### Chance Constrained Probability Measure Optimization: Problem Formulation, Equivalent Reduction, and Sample-based Approximation

Shen Xun

29 Sept. 2023 Friday Session 3

Osaka University, 1-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Choosing decision variables deterministically (deterministic decision-making) can be regarded as a particular case of choosing decision variables probabilistically (probabilistic decision-making). It is necessary to investigate whether probabilistic decision-making can further improve the expected decision-making performance than deterministic decisionmaking when chance constraint exists. The problem formulation of optimizing a probabilistic decision under chance constraint has not been formally investigated. In this paper, for the first time, the problem formulation of Chance Constrained Probability Measure Optimization (CCPMO) is presented towards realizing optimal probabilistic decisionmaking under chance constraint. We first prove the existence of the optimal solution to CCPMO. It is further shown that there is an optimal solution of CCPMO with the probability measure concentrated on two decisions, leading to an equivalently reduced problem of CCPMO. The reduced problem still has chance constraints due to the existence of random variables for model uncertainties. We then extend the sample-based smooth approximation method to solve the reduced problem. Samples of model uncertainties are used to establish an approximate problem of the reduced problem. General nonlinear programming problems can solve the approximate problem. The solution of the approximate problem is an approximate solution of CCPMO. A numerical example of controlling a quadrotor in turbulent conditions has been conducted to validate the proposed probabilistic decision-making under chance constraint.

### Mapping High-resolution Land Cover Product Anywhere

Junshi Xia

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

OpenEarthMap has emerged as a benchmark dataset for global high-resolution land cover mapping. In this talk, we will delve into the remarkable features of OpenEarthMap and its significance in high-resolution land cover mapping. We will highlight the global reach of OpenEarthMap, covering diverse regions and continents. This comprehensive geographic coverage enables the creation of land cover mapping models that exhibit remarkable generalization capabilities. The models trained on OpenEarthMap can accurately classify land cover types in regions not explicitly included in the dataset, making them invaluable global land cover analysis tools. Furthermore, we will discuss the potential applications of these off-the-shelf land cover mapping models derived from OpenEarthMap.

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### **Categorification of Disentangled Representation Learning**

Yivan Zhang

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

Disentangling the factors of variation in data is an important task in machine learning, aiming to break down complex and compositional input into simpler and meaningful parts. Despite the numerous empirical studies, more theoretical research is needed to fully understand the defining properties of disentanglement and how different definitions relate to each other. This work presents a meta-analysis of disentanglement definitions using category theory as a unifying framework. We propose the cartesian and monoidal products as core concepts and explore their manifestations in the categories of functions, equivariant maps, relations, and stochastic maps. Overall, our meta-analysis deepens our understanding of compositionality and disentanglement and can help researchers navigate different definitions and choose the most appropriate one for their specific context.

**Robust Contrastive Learning and Its Applications** 

Shuo Chen

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

Self-supervised contrastive learning has recently become a popular and powerful unsupervised learning approach. In this talk, we will first review the classical contrastive learning methods in terms of self-supervisory information and feature encoder structure. After that, we will present our recent work to solve the issues caused by inaccurate self-supervisory information and high-dimensional features. Finally, we will discuss some novel and challenging applications of contrastive learning in real-world tasks, e.g., zero-shot recognition, multi-view classification, and cross-modal learning.

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Session 3

### **Continuous Learning in Both Medical and General Domains**

Lin Gu

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

Community has spent much efforts in designing cutting edge techniques in artificial intelligence. However, it is equally important to leverage AI for practical applications. During the presentation, Dr. Lin Gu will discuss the application of continious learning in both medical and general domains.

### Picking winners: Diversification through portfolio optimization

Chung-Piaw Teo

National University of Singapore, 21 Lower Kent Ridge Rd, 119077, Singapore

We develop a general framework for selecting a small pool of candidate solutions to maximize the chances that one will be optimal to a combinatorial optimization problem, under a linear and additive random payoff function. We formulate this problem using a twostage distributionally robust model, with a mixed 0-1 semidefinite program. This approach allows us to exploit the "diversification" effect inherent in the problem, to address how different candidate solutions can be selected to improve the chances that one will attain ahigh ex-post payoff. More interestingly, using this distributionally robust optimization approach, our model recovers the "evil twin" strategy, well-known in the field of football pool betting, under appropriate settings. We also address the computational challenges of scaling up our approach to construct a moderate number of candidate solutions to increase the chances of finding one that performs well. To this end, we develop a sequential optimization approach based on a compact semidefinite programming reformulation of the problem. Extensive numerical results show the superiority of our approach over existing methods. This talk is based on joint work with Liu Changchun (SIA-NUS Digital Aviation Corp lab) and Liu Ju (NUS Chongqing Research Institute).

### Game of Trains - Recent Success Stories of Railway Optimization

30 Sept. 2023 Saturday Plenary Talk

Thomas Schlechte LBW Optimization GmbH, Englerallee 19, 14195 Berlin

For many years, planning tasks in the railway industry were performed manually. The absence of mathematical optimization technology and standardized processes in those planning tasks can be mainly attributed to the high complexity of railway operations, and the lack of performance from existing algorithms of the time. This has changed significantly over the last decade however, with more and more successful decision support tools going into production, which directly aid and assist in railway applications. In particular, classical resource optimization for crew and rolling stock has become a necessity for any railway operator of the current day. This talk reviews the recent progress in these applications with a focus on future timetabling for moving block systems.

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Session 1

### **Blockchain & DeFi Security**

Dabin Wang

JP Morgan, Taunustor 1, Frankfurt am Main, 60310, Germany

Blockchain & DeFi Security: Algorithms and Applications. Blockchain based DeFi ecosystem is a great innovation for creating efficiencies and new business models. In this talk, we cover blockchain security consideration under DeFi reference framework (network, consensus, smart contract, Defi protocol, auxiliary services); cryptography fundamentals; post-Quantum Computing applications for blockchain security and new technology and algorithm towards Blockchain-based application for 5G, 6G UIoT network.

### Yet Another Implementation of Automatic Differentiation Software: Utilization of Spatial Locality

Hiroshige Dan

Kansai University, 3 Chome-3-35 Yamatecho, Suita, Osaka 564-8680, Japan

Automatic differentiation (also known as algorithmic differentiation, AD) is a technique used to compute the partial derivative values of target functions. The fundamental principle behind AD is the chain rule of composite functions, making it highly intuitive and thus resulting in numerous AD implementations. In this presentation, we will explain the details of our AD software implementation. Our approach focuses on optimizing spatial locality, a property where accessing a specific memory location also involves accessing nearby memory locations. This property plays a crucial role in accelerating computations, as data from nearby memory is efficiently fetched into the cache. Throughout the presentation, we will elucidate our strategies for leveraging spatial locality for indexed variables and functions.

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#### **Improving Kidney Exchange Programs**

João Pedroso

University of of Porto, Praça de Gomes Teixeira, 4099-002 Porto, Portugal

Renal diseases affect thousands of patients who, to survive, must incur in dialysis – a costly treatment with many negative implications in their quality of life. As an alternative, patients may enter a waiting list for receiving a kidney from a deceased donor; however, waiting times are typically very long. For reducing the waiting time, another alternative in some countries is to find a healthy living donor – usually, a relative of a person emotionally connected – who volunteers to cede one of their kidneys. However, in some situations transplantation is not possible due to blood, or tissue-level incompatibility. In these cases, a donor-patient pair may enter a pool of pairs in the same situation, in the hope of finding compatibility in crossed transplants. The problem has been studied under different perspectives, but the most commonly used objective is maximizing the number of patients in the pool for which a crossed transplant is possible. We propose to change this objective by that of maximizing the cumulative patient survival times. This model departs from the previous deterministic setting, putting into play a method for predicting survival time based on historical data.

### Problems of fluid interface instabilities in Energy Systems

Thi Thai Le

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

Fluid interface instabilities are critical in various energy systems, particularly hydrogen gas production, storage, and transportation. Our research delves into the challenges associated with fluid interface instabilities within energy systems, emphasizing hydrogen's interface stability when in contact with other co-existing gases in storage. Our particular interest comes from the transition of natural gas storage to hydrogen. The storage is already a mixture of gases, particularly some unwanted toxic components, so-called *cushion gas*, that always remain in the storage. The interface between the remaining natural gas, hydrogen, and cushion gas is essential for assessing the storage capacity during and after the transition. The stability of the interface in a tangential-velocity discontinuity provides us with the exact velocity rate for injecting and withdrawing natural gases effectively. Understanding and controlling these instabilities is crucial for hydrogen's safe and efficient injection and withdrawal processes into/from storage. In this talk, we introduce our mathematical model to analyze these instabilities and provide a better understanding of the physical stability mechanism.

### Large-Scale Dynamic Portfolio Optimization with Quantum Algorithms

Hanqiu Peng

National University of Singapore, 21 Lower Kent Ridge Rd, 119077, Singapore

We introduce a quantum framework that utilizes Quadratic Unconstrained Binary Optimization (QUBO) to optimize dynamic trading strategies, taking into account transaction costs, integer restrictions, and scalability. While dynamic trading strategies in modern portfolio optimization have been extensively studied, their practical implementation often faces considerable challenges due to market frictions and computing limitations, which adversely affect computational efficiency. In light of this, our work explores the potential of quantum solutions to transform the field of portfolio optimization. We present a uniquely equipped quantum algorithm that can tackle the complexities of real-world portfolio optimization and ensure optimal results. By doing so, we aim to bridge the gap between quantum finance and practical portfolio optimization.

This is a joint work with Ying Chen, Thorsten Koch and Hongrui Zhang.

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### **Discovering Optimal Tensor Network Architectures: An Exploration** of Tensor Network Structure Search (TN-SS)

Chao Li

RIKEN Center for Advanced Intelligence Project (AIP) 15F, Mitsui Building Nihonbashi 1-chome, 1 Chome-4-1, Nihonbashi, Chuo City, Tokyo, 103-0027, Japan

In this talk, we delve into the dynamic domain of Tensor Network Structure Search, an innovative approach to discerning optimal tensor network architectures. The talk will first demystify the concept of TN-SS, providing a comprehensive understanding of its formulation and application in modern data science. Subsequently, we introduce and dissect three state-of-the-art algorithms - TNGA (ICML'20), TNLS (ICML'22), and TnALE (ICML'23) - each contributing uniquely to resolving TN-SS efficiently. Through this exploration, we aim to elucidate the journey of these sophisticated algorithms, highlighting their impact in shaping the future of tensor networks.

### Fredholm integral equations for the training of shallow neural networks

Patrick Gelß

Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

We present a novel approach for the training of single-hidden-layer neural networks, based on the approximate solution of associated Fredholm integral equations of the 1. kind by Ritz-Galerkin methods. We show how quantum-inspired tensor formats and Tikhonov regularization can be used to construct continuous counterparts of discrete neural networks with an infinitely large hidden layer. The efficiency and reliability of the introduced approach is illustrated by the practical application to several supervised learning problems.

Saturday Session 2

### Efficient machine learning with tensor networks

Qibin Zhao

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Tensor Networks (TNs) are factorizations of high dimensional tensors into networks of many low-dimensional tensors, which have been studied in quantum physics, high-performance computing, and applied mathematics. In recent years, TNs have been increasingly investigated and applied to machine learning and signal processing, due to its significant advances in handling large-scale and high-dimensional problems, model compression in deep neural networks, and efficient computations for learning algorithms. This talk aims to present some recent progress of TNs technology applied to machine learning from perspectives of basic principle and algorithms, novel approaches in unsupervised learning, tensor completion, multi-model learning and various applications in DNN, CNN, RNN and etc.

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### Current situation of transportation networks in Thailand

Piang-or Loahavilai

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The rail sector in Thailand has experienced significant growth and transformation in recent years, driven by the nation's commitment to modernizing its transportation infrastructure and promoting sustainable development. This abstract provides an overview of the key developments and initiatives in Thailand's rail sector, highlighting the economic, environmental, and social benefits of these efforts.

Thailand's rail sector has evolved from a modest transportation system into a pivotal component of the country's modern infrastructure. The Thai government, in collaboration with private sector partners, has undertaken an ambitious agenda to expand and enhance the rail network. This includes investments in high-speed rail, urban transit systems, and freight transportation, connecting major cities and regions across the country. Key initiatives within Thailand's rail sector development include the construction of high-speed rail lines connecting major cities like Bangkok, Chiang Mai, and Nong Khai, as well as the expansion of urban transit systems in cities like Bangkok and the other major cities. These projects not only improve connectivity but also reduce travel times, making rail a more attractive and convenient mode of transportation. Additionally, Thailand has focused on modernizing its existing rail infrastructure, upgrading tracks, signaling systems, and stations to ensure safety and efficiency. Public-private partnerships play a crucial role in funding and implementing these projects, ensuring a sustainable and cost-effective approach to rail development.

In conclusion, Thailand's rail sector development represents a significant step toward achieving a more sustainable, efficient, and integrated transportation system. The commitment to expanding and modernizing rail networks not only benefits the economy but also contributes to environmental conservation and improved quality of life for the population. As Thailand continues to invest in its rail sector, it positions itself as a regional leader in sustainable transportation and paves the way for a more connected and prosperous future.

### The agenda for developing rail traffic in Thailand

30 Sept. 2023 Saturday Session 2

Rail Technology Research and Development Agency 110/1 KX Building, Banglamphulang, Klongsan, Bangkok, 10600, Thailand

Santi Charoenpornpattana

Thailand's rail technology development has witnessed a remarkable evolution in recent years, reflecting the nation's commitment to enhancing its transportation infrastructure, promoting sustainable mobility, and embracing cutting-edge innovations. This abstract provides an overview of the key technological advancements and initiatives driving the transformation of Thailand's rail sector.

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The rail sector in Thailand has undergone a profound transformation as the government and industry stakeholders harness advanced rail technologies to address pressing challenges and meet the growing demands of the modern economy. These efforts encompass a range of technological innovations, including high-speed rail systems, digital signaling and communication, electrification, and smart transportation solutions. For example, electrification initiatives have played a pivotal role in reducing the environmental footprint of the rail sector. Thailand's transition to electric and hybrid rail systems not only reduces greenhouse gas emissions but also decreases noise pollution and promotes energy efficiency. These developments align with the country's sustainability goals and commitments to eco-friendly transportation solutions. Smart transportation solutions have been integrated into Thailand's rail networks to enhance passenger experiences and operational efficiency. Digital ticketing, passenger information systems, and mobile apps provide commuters with real-time updates, ticket booking convenience, and seamless connectivity to other modes of transportation. These innovations transform rail travel into an integrated and user-friendly experience.

In conclusion, Thailand's rail technology development signifies a paradigm shift in the country's transportation landscape. By adopting advanced rail technologies, Thailand aims to meet the demands of its growing population, reduce congestion on roadways, and lower carbon emissions. These efforts position Thailand as a regional leader in rail innovation and create opportunities for economic growth while ensuring a sustainable and efficient transportation future.

### Diversified Adversarial Attacks based on Conjugate Gradient Method

Keiichiro Yamamura

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Deep learning models are vulnerable to adversarial examples, and adversarial attacks used to generate such examples have attracted considerable research interest. Although existing methods based on the steepest descent have achieved high attack success rates, ill-conditioned problems occasionally reduce their performance. To address this limitation, we utilize the conjugate gradient (CG) method, which is effective for this type of problem, and propose a novel attack algorithm inspired by the CG method, named the Auto Conjugate Gradient (ACG) attack. The results of large-scale evaluation experiments conducted on the latest robust models show that, for most models, ACG was able to find more adversarial examples with fewer iterations than the existing SOTA algorithm Auto-PGD (APGD). We investigated the difference in search performance between ACG and APGD in terms of diversification and intensification, and define a measure called Diversity Index (DI) to quantify the degree of diversity. From the analysis of the diversity using this index, we show that the more diverse search of the proposed method remarkably improves its attack success rate.

## Improvement of black-box adversarial attacks based on discrete optimization using Superpixel

Issa Oe

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Deep learning models have recently been considered for applications to safety-critical tasks, such as automatic driving and face recognition. This situation necessitates research into the robustness and vulnerability of deep learning models. Adversarial attacks aim to cause misclassification by adding appropriate perturbations to the model input, such as images. These attacks are used to assess vulnerabilities by evaluating the misclassification rate post-attack. They also contribute to developing models that are robust to small perturbations. Adversarial attacks are attributed to high-dimensional nonlinear optimization problems. They are computationally intensive, especially black-box adversarial attacks, which operate under the assumption of no access to model gradients. This presentation introduces a new attack method that transforms this problem into a discrete optimization problem and uses an image processing technique called Superpixel. This presentation also provides numerical results demonstrating its performance.

### **Towards Continuous Adaptation in Non-stationary Environments**

Zhen-Yu Zhang

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Adapting to distribution changes is a critical challenge in modern machine learning. Many test-time adaptation methods have shown promising results in adapting a model to a new fixed testing distribution. However, in many real-world applications, testing data are collected in non-stationary environments and continuously accumulated in the form of a stream. This paper investigates the problem of sequentially adapting the model to non-stationary environments, where the data distribution continuously shifts, and only a few unlabeled data are available at each time. In order to handle the unknown distribution shifts within the unlabeled streams, we will introduce our recent research that explores varying lengths of the stream while ensuring alignment of representations with the initial well-trained model.

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### Influence of the construction of China – Thailand railway on logistics and economic trade between China – Yunnan and Thailand

Fan Zhai

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China-Thailand's railway can help make Thailand, ASEAN countries, and China interoperable and promote regional economic co-development. China-Thailand's railway cooperation is an excellent help for Thailand to be a better role as the central hub for land transportation and geographical advantages, accept more foreign tourist passengers, raise local employment, and capital income driven by tourism development. Moreover, to promote the country's economic development and improve people's living standards. This project can deepen international trade to Thailand, Laos, and China, Soas to drive the Thai economy. With the continuous growth of international commerce due to China and surrounding countries, the transportation and train systems have become much more vital for improving international commerce. The train transportation of China has seen vast growth as a primary strategy of commerce. With the completion of the Bang Sue Railway Station, the central hub of the Trans – Asian Railway, at the end of 2021, the central international corridor of the China- Thailand Railway will affect the development of trade between Yunnan and Thailand.

By consulting information and data, this article analyzed the development of trade between Yunnan Province and Thailand in recent years; compared the situation and development of logistics infrastructure; and used SWOT analysis to analyze railways from advantages and disadvantages opportunities qualitatively and threats. After the opening, the impact on Yunnan Province and Thailand and results were analyzed, relevant suggestions were provided to promote the development of the China-Thailand railway logistics trade.

Keywords:Trans-Asian' Railway, China-Thailand' Railway, Commerce, Logistics trade development

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### **Domain-Independent Dynamic Programming**

Ryo Kuroiwa University of Toronto 27 King's College Cir, Toronto, ON M5S 1A1, Canada

In a model-based paradigm for combinatorial optimization, such as mixed-integer programming (MIP) and constraint programming (CP), a problem is defined as a declarative mathematical model, and then the model is solved by general-purpose solvers. Due to their flexibility, model-based paradigms are widely used for various problems in academia and industry. To complement existing paradigms, I am developing domain-independent dynamic programming (DIDP), a novel model-based paradigm based on dynamic programming. In existing popular model-based paradigms, including MIP and CP, a model is described as a set of constraints that must be satisfied by decision variables. In contrast, in DIDP, a model is described by a state transition system. In this talk, I will first introduce the notion of DIDP and its Python-based modeling interface. Then, I will explain general-purpose DIDP solvers developed so far, including anytime and multi-thread solvers, and show that they outperform MIP and CP on six combinatorial optimization problems.

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