

GOR-AG: Praxis der Mathematischen Optimierung Dr. Jens Schulz Fontaneweg 15 D-16547 Birkenwerder

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Herewith, we invite you to the 104th meeting of the GOR working group "Real World Optimization" jointly organized with **DLR (German Aerospace Center)**. This meeting is held as a virtual event with the topic

Quantum Computing and Mathematical Optimization

The workshop takes place on March 18th & 19th, 2021 on Thursday and Friday.

The working language will be English. This will be a fully virtual event hosted by FICO. You can register for the webinar by clicking on this link: https://fico.zoom.us/webinar/register/8016116103273/WN HyPEpOUbRBigkPSJYND0jA

The registration will be possible until mid of March 2021. The latest information on the meeting is available on the homepage of the working group: http://www.gor-ev.de/arbeitsgruppen/praxis-der-mathematischen-optimierung (German)

http://www.gor-ev.de/arbeitsgruppen/praxis-der-mathematischen-optimierung/real-worldoptimization (English)

Yours sincerely,

Jens Schulz, Julia Kallrath, Josef Kallrath

(GOR AG)

Elisabeth Lobe

(DLR)



Quantum Computing and Mathematical Optimization

Specific aims

This virtual event is intended to be a forum to learn and exchange about Quantum Computing methods for Mathematical Optimization problems and is a follow on to our working group meeting held in 2017 at DLR Braunschweig.

A computer works by manipulating bits and bytes where each can be set to either 0 or 1. In contrast, a quantum computer employs quantum bits (qubits) that can be both 0 and 1 at the same time. As it is able to contain multiple states simultaneously, it exploits an inherent parallelism which has the potential to be millions of times more powerful than today's most powerful bit-based supercomputers.

Huge investments of large companies into quantum computing show the underlying long-term hope for practical use cases. Recent advances in Adiabatic Quantum Computing and first commercial adiabatic quantum computers being able to handle 5,000 qubits, show the tremendous progress in that area. What will be the role of quantum computing technology in the upcoming years, what is the role of mathematical optimization techniques in the light of quantum computing, will hybrid approaches of these enable us to solve even larger real-world problems – possibly in real-time applications? What are the challenges ahead?

The first day of this workshop is devoted to the foundations of quantum computing and adiabatic quantum computing. It provides the basics and insights for those not yet familiar with the new technology. Day 2 covers examples from industry and research how (adiabatic) quantum computing can be used in conjunction with mathematical optimization or other techniques to solve mathematical optimization problems. We will hold open discussion forums and a plenary round table.

In talks of 25+5min, 40+5min or 50+10min duration, experts from practice and research will share their knowledge and learnings.

If you are willing to contribute a talk, please feel free to contact one of the organizers.

Jens Schulz (schulz-gor 'at' gmx.net)



Speakers and titles

David E. Bernal (Carnegie Mellon University) Modern Computational Approaches to Nonlinear Discrete Optimization

Bettina Just (Technische Hochschule Mittelhessen) How Quantum Computing works

Matthias Koch (DB Systel) & William Steadman (DB Netz AG) (30min) **Quantum optimization for the train timetable problem**

Wolfgang Lechner (University Innsbruck, ParityQC) Parity Quantum Computing - Encoding Real-World Problems in Near-Term Quantum Devices

Martin Leib (Volkswagen AG) Beating classical heuristics for the binary paint shop problem with the quantum approximate optimization algorithm

Elisabeth Lobe (DLR) Solving combinatorial optimization problems with a quantum annealer

Pavel Lugovski (Amazon Braket) Exploring Optimization Problems with Quantum Computers on AWS

Mark Mattingley-Scott (IBM) Quantum Computing Perspectives

Marika Svensson (Jeppesen) Quantum Computing and Airline Planning



Program

Times may be subject to changes and slight adaptations during the workshop to tackle technical issues and to leave room for discussion. All time slots are given in CET (UTC+1).

Thursday CET (UTC+1)

11:00-11:30	Jens Schulz, Julia Kallrath (GOR) and Elisabeth Lobe (DLR)
11:30-12:15	Bettina Just (THM)
	How Quantum Computing works
12:15-13:00	Mark Mattingley-Scott (IBM)
	Quantum Computing Perspectives
	Break
13:30-15:00	Elisabeth Lobe (DLR)
	Solving Combinatorial Optimization Problems using a Quantum
	Annealer
15:15-16:00	Wolfgang Lechner (University Innsbruck)
	Parity Quantum Computing - Encoding Real-World Problems in Near-
	Term Quantum Devices
16:15-17:00	David E. Bernal (Carnegie Mellon University)
	Modern Computational Approaches to Nonlinear Discrete
	Optimization
17:00-17:30	Room for open discussion

Friday CET (UTC+1)

11:00-11:15	Elisabeth Lobe (DLR) and Jens Schulz (GOR, FICO) Welcome to second day
11:15-11:45	Marika Svensson (Jeppesen)
	Quantum Computing and Airline Planning
11:45-12:30	Matthias Koch (DB Systel) & William Steadman (DB Netz AG)
	Quantum optimization for the train timetable problem
	Break
13:00-13:45	Martin Leib (Volkswagen AG)
	Beating classical heuristics for the binary paint shop problem with the quantum approximate optimization algorithm
13.45-14.30	the - due to cancellation
15.45-14.50	tha
	iba Breek
11.15 15.20	Povol Lugovski (Amazon Brakat)
14.45-15.50	Exploring Optimization Broblems with Quantum Computers on AWS
45.00 40.00	Exploring Optimization Problems with Quantum Computers on AWS
15:30-16:00	Discussion round

Please, register here for the event: https://fico.zoom.us/webinar/register/8016116103273/WN_HyPEpOUbRBigkPSJYND0ja



Speakers

David E. Bernal is a Ph.D. Candidate at Carnegie Mellon University working in nonlinear discrete optimization. His research has been related to the development and implementation of algorithms to solve these optimization problems. During his Ph.D. he was awarded the Feynman Quantum Academy Fellowhip from the University Space Research Association (USRA) to work on the NASA Quantum and Artificial Intelligence Laboratory. He designed a brand new course on Quantum Integer Programming at CMU together with Prof. Sridhar Tayur and Dr. Davide Venturelli.

Bettina Just studied mathematics and computer science and got her Ph.D. in theoretical computer science at the J.W. Goethe University Frankfurt. For allmost 20 years she held various positions in German and European insurance industry. Since 2010 she is a full professor for mathematics and computer science at the THM - Technische Hochschule Mittelhessen. She is the author of the book "Quantum computing compact" published by Springer in 2020. It explains the basic ideas of quantum computing to readers without mathematical, physical or IT background.

Matthias Koch obtained his Diploma in Physics at Freie Universität Berlin in 2009 and received his PhD in 2013 at Fritz-Haber-Institut der Max-Planck-Gesellschaft about "Growth and characterization of single molecular wires on metal surfaces". He has been PostDoc at University of New South Wales (Sydney) from 2014 onwards focused on "Process development for 3D device fabrication for scalable ph-silicon quantum computers". After 2017 he has been group leader at Fritz-Haber-Institute der Max-Planck-Gesellschaft: "Multiprobe experiments on nano-objects". In 2020, he joined DB Systel as Research Engineer in the project "Evaluating the use of quantum algorithms inside the Deutsche Bahn".

Wolfgang Lechner is an Associate Professor at the University of Innsbruck and CEO of ParityQC. His research group is dedicated to quantum optimization with near term quantum devices, the development of novel quantum algorithms and their implementation. He is recognized for the invention of the parity transformation known as the Lechner-Hauke-Zoller mapping. https://www.uibk.ac.at/th-physik/quantum-optimization/

Martin Leib studied theoretical physics at the University of Konstanz. He finished his PhD in the group of Prof. Hartmann at the TU Munich on the theory of superconducting qubits, one of the leading hardware platforms for quantum computing. After his PhD he held three postdoc positions in Tokyo at RIKEN, in Scotland at Heriot-Watt and finally at the IQOQI in Innsbruck. During his time as a postdoctoral researcher his interest shifted from the underlying hardware to the software of quantum computers. He is currently employed at the Volkswagen Data:Lab and responsible for the development and research of quantum uses cases for the VW group.

Elisabeth Lobe received her Master's degree in Mathematics at the Otto von Guericke University of Magdeburg, Germany. Now she is a research associate at the German Aerospace Center in the Institute for Software Technology, working in the field of quantum computing and optimization. Together with Prof. Volker Kaibel from the OvGU Magdeburg she is doing her Ph.D. on the capabilities of solving combinatorial optimization problems using quantum annealing technologies.



Pavel Lougovski is a principal quantum solutions architect with Amazon Braket. Pavel did his PhD at Max Planck Institute for Quantum Optics (Garching, Germany) where he studied quantum information processing protocols with atomic systems. After graduating in 2004, Pavel spent 9 years in various academic and industry roles developing novel methods and algorithms to process and communicate quantum and classical information. He then joined U.S. DOE Oak Ridge National Lab (ORNL) as a staff scientist in 2013. At ORNL, Pavel established a research program in quantum algorithms and applications, directing multiple US DOE-funded quantum computing projects. He joined Amazon Braket team in 2020 and helps customers all over the world with adoption of quantum computing.

Mark Mattingley-Scott holds a Doctor of Philosophy on the subject of Code Division Multiple Access Local Area Networks from the University of Durham, combined with 36 years experience in the commercial exploitation of technology and research. As a Principal at IBM he is specialised in the identification, nurturing and development of technological innovation, with a primary focus on Big Data Analytics, Neuromorphic Computing and Quantum Computing, and became IBM Quantum Business Leader in 2020.

He currently teaches human & machine learning and quantum computing at the Institute for Cognitive Science at the University of Osnabrück and quantum computing at the Kirchoff Institute at the University of Heidelberg. He is a director of the Frankfurt Institute for New Media and a senior member of the IEEE, having founded the German chapter of the Systems, Man and Cybernetics Society, a member of the IEEE European Public Policy Committee, a member of the Board of Disruptive Technologists, a member of the Advisory Board of the Graduate School in Cognitive Science at the university of Osnabrück, the Chairman of the Big Data working group and co-Chairman of the HPC and Quantum Computing working group at BITKOM, the German IT and Telecommunication Industry Association.

William Steadman holds a B.S in Mathematics at MIT in Cambridge, USA (2012). From 2014-2016 he worked as Algorithm Developer at Kiwigrd GmbH in Dresden where he scheduled EV charging using Viterbi algorithm and ML forecasts of photovoltaic production. From 2016-2018 he has been Data Team Co-Lead at Spire Global Inc in Boulder, USA where he developed multi-objective mixed integer model for scheduling satellite and ground-station network. Since 2020 he is Operations Research Expert at DB Netz in Berlin developing a mixed integer model and evaluating integrating quantum algorithms.

Marika Svensson holds an Engineering Physics master's degree from Chalmers University of Technology (2011-2016). Afterwards she worked as Antenna Designer at RUAG space (2016), Systems Analyst at Jeppesen (2017-2019) and is currently Industrial PhD student at Jeppesen since 2019.



Abstracts

Title: Modern Computational Approaches to Nonlinear Discrete Optimization Speaker: David E. Bernal

Optimization problems arise in different areas of Process Systems Engineering (PSE), and solving these problems efficiently is essential for addressing important industrial applications.

Quantum computers have the potential to efficiently solve challenging nonlinear and combinatorial problems. However, available quantum computers cannot solve practical problems; they are limited to small sizes, and do not handle constraints well. In this talk, we propose hybrid classical-quantum algorithms to solve mixed integer nonlinear problems (MINLP) and apply decomposition strategies to break down MINLPs into Quadratic Unconstrained Binary Optimization (QUBO) subproblems that can be solved by quantum computers. We will also cover different approaches to solving Quadratic Unconstrained Binary Optimization (QUBO) problems through unconventional computation methods, including but not limited to Quantum algorithms, and discuss how these approaches lead to algorithms able to outperform classical solution approaches.

Title: How Quantum Computing works Speaker: Bettina Just

In the lecture we pass from physical to logical qubits and therefore enter the world of quantum circuits and quantum algorithms. The functionality of quantum circuits is presented. The analysis of quantum circuits using unitary matrices will be presented, and also illustrated in a geometric way. As an example, the algorithm for teleportation is examined in detail. The lecture also reports on the basic ideas of others quantum algorithms and adiabatic quantum computing.

Title: Quantum optimization for the train timetable problem Speaker: Matthias Koch & William Steadman

The need of optimization in railway industry is tremendous, which also reflects in the active research community. Here, we focus on timetable problems, i.e. the assignment of trains to times and routes through the track infrastructure while respecting all operational and capacity constraints. We use a path-based formulation to formulate this as a quadratic unconstrained binary optimization (QUBO) model and examine techniques to improve the problem structure for embedding on NISQ quantum devices. We will discuss upcoming plans to integrate with the dual prices from a mixed integer model or formulating the problem as a more general lsing spin glass model.



Title: Parity Quantum Computing - Encoding Real-World Problems in Near-Term Quantum Devices Presenter: Wolfgang Lechner

Optimization problems are omnipresent in Industry, Science and Technology. In this talk I will give an overview about the parity architecture, an architecture that allows for an efficient encoding of optimization problems in near term quantum devices. Real-world problems are hard to encode, because they can contain higher-order terms and constraints. The parity transformation allows to encode such problems on current hardware with a scaling advantage in number of qubits compared to the standard encoding.

Title: Beating classical heuristics for the binary paint shop problem with the quantum approximate optimization algorithm Presenter: Martin Leib

The binary paint shop problem (BPSP) is an APX-hard optimization problem of the automotive industry. In this work, we show how to use the Quantum Approximate Optimization Algorithm (QAOA) to find solutions of the BPSP and demonstrate that QAOA with constant depth is able to beat classical heuristics on average in the infinite size limit $n\rightarrow\infty$. For the BPSP, it is known that no classical algorithm can exist which approximates the problem in polynomial runtime. We introduce a BPSP instance which is hard to solve with QAOA, and numerically investigate its performance and discuss QAOA's ability to generate approximate solutions. We complete our studies by running first experiments of small-sized instances on a trapped-ion quantum computer through AWS Braket.

Title: Solving Combinatorial Optimization Problems using a Quantum Annealer Presenter: Elisabeth Lobe

In this talk we will start with a brief introduction of the rough concept of quantum annealing and how it can be used for combinatorial optimization. In the following we mainly focus on the steps that are necessary to transform an arbitrary discrete optimization problem to the specific class of problems D-Wave's quantum annealer is able to process, which are, in general, quadratic unconstrained binary optimization problems (QUBO) respectively so-called Ising models. We will summarize some established transformation steps, such as encoding and reduction.

However, due to several physical limitations the class of problems that can be solved on the machine is further restricted. E.g. by graph minor embedding we need to overcome the non-complete hardware connectivity. Afterwards the weight of an original node needs to be distributed over several hardware nodes in a certain way to enforce the equivalence of the solutions. We will show the accompanying difficulties and some first approaches to tackle them.



Title: Exploring Optimization Problems with Quantum Computers on AWS Presenter: Pavel Lugovski

Optimization problems are common across many industries including telecommunications, supply chain logistics, and financial services. Finding the optimal approach from a set of alternatives can overwhelm classical computers as the number of possible combinations drives up complexity. Quantum computing has the potential to address a wide range of these problems. In this talk we will demonstrate how to approach Quadratic Unconstrained Binary Optimization (QUBO) problems, and run them on Amazon Braket, using different types of quantum computers including a D-Wave quantum annealer and IonQ and Rigetti gate-based machines.

Title: Quantum Computing Perspectives Presenter: Mark Mattingley-Scott

Quantum computing is a very hot topic, and many amazing claims have been made about it but what is speculation, what is reality and what is fantasy? in my talk I will shed some light on this fascinating and disruptive technology and provide you with a foundation on which to gain deeper understanding if so inclined.

Title: Quantum Computing and Airline Industry Presenter: Marika Svensson

Real world airline planning problems such as Crew Rostering, Crew Pairing and Tail Assignment fall into the class of large-scale Integer Linear Programs (ILPs) and are very hard to solve due to their size and combinatorial nature combined with very complex rules. In this talk we will present Ising spin glass models for such optimization problems and what quantum algorithms can be suitable choices for NISQ computers. Finally, we present possible limitations for applying quantum algorithms.