



# **Online Workshop on Applied Mathematics**

February 3-4, 2021 ZOOM: https://cesnet.zoom.us/j/99390308054?pwd=RVdFZ0Zzb0NDWHZ2OVpyMmtYaGFvZz09

## **Program**

### Wednesday February 3rd 2021

Morning Section: On Cages and Algebraic Graph Theory

Chairman: Petr Kovář

9<sup>00</sup> - 9<sup>50</sup> **Róbert Jajcay** - Algebraic constructions of cages

10<sup>00</sup> - 10<sup>50</sup> **Tatiana Jajcayová** - Partial automorphisms of graphs and algebraic tools to study them

11<sup>00</sup> - 11<sup>20</sup> Mária Mériová - Inverse monoids for certain classes of graphs

11<sup>30</sup> - 11<sup>55</sup> Slobodan Filipovski - On bipartite cages of excess 4

12<sup>00</sup> - 12<sup>20</sup> **Tom Raiman** - Conditions for vertex removal in (k,g)-graphs

Afternoon Section: Applied Statistics and Reliability

Chairman: Radim Briš

1345 - 1445 Frank Coolen - Survival Signature for Quantification of System Reliability

 $15^{00}$  -  $16^{00}$  Christophe Berenguer - On post-prognosis decision making for predictive maintenance and optimal operation of deteriorating system

#### **Thursday February 4th 2021**

Morning Section: Introduction to Quantum Computing

Chairman: Marek Lampart

8<sup>45</sup> - 9<sup>45</sup> **Piotr Gawron** - *Quantum neural networks -- a practical approach* 

10<sup>00</sup> - 11<sup>00</sup> Katarzyna Rycerz - Solving workflow scheduling problems with near-term quantum devices

11<sup>15</sup> - 12<sup>15</sup> Lukasz Pawela - Peeking inside the quantum black box -- quantum learning

Afternoon Section: Numerics

Chairman: David Horák

13<sup>45</sup> - 14<sup>30</sup> **Helmut A. Mayer** - Evolutionary Computation - Principles and Applications

14<sup>45</sup> - 15<sup>30</sup> **Helmut A. Mayer** - *Artificial Neural Networks - Principles and Applications* 

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# Abstracts and About speakers

Section: On Cages and Algebraic Graph Theory

**Róbert Jacay** - Algebraic constructions of cages Comenius University, Bratislava, Slovakia

<u>Abstract:</u> A cage with parameters (k,g) is a k-regular graph of girth g of the smallest possible order. Networks based on the use of cages often prove to be among the most efficient and reliable, and the search for cages (the Cage Problem) is an important part of Extremal Graph Theory as well as a widely studied optimization problem. Even though cages do not necessarily have to be algebraic objects, the majority of the known cages and of the smallest known (k,g)-graphs come from algebraic constructions. In our talk we will present a brief overview of the Cage Problem, describe some of the most successful algebraic constructions of small graphs of given degree and girth, and also address the question of the limitations of algebraic constructions.

**Róbert Jajcay** received his Master's degree at the Comenius University in Bratislava and his PhD. at the University of Nebraska-Lincoln. The main focus of his research is on the applications of symmetries in Discrete Mathematics, specifically in Algebraic, Topological and Extremal Graph Theory. Together with Geoff Exoo, he co-authored a dynamic survey on cages which serves as the main reference source for research devoted to the well-known Cage Problem. His research travels took him all around the world, he collaborates with researchers from many different countries, and he firmly believes in the collaborative nature of research in Mathematics.

**Tatiana Jajcayová** - Partial automorphisms of graphs and algebraic tools to study them Comenius University, Bratislava, Slovakia

<u>Abstract:</u> The problem of determining the full automorphism group of a graph is one of the well-known hard problems. The focus of our recent joint project with Maria Szendrei, Nora Szakacs, and Robert Jajcay is on an extension of the automorphism group problem to that of inverse monoid problem. The full inverse monoid of partial automorphisms of a combinatorial structure is a much richer algebraical structure that contains more detailed local information about the underlying object. The goal is to apply the algebraic methods of partial permutation semigroup theory to the class of structures that admit none or only very few automorphisms and typically resist the use of methods from permutation group theory. The results involving partial automorphisms and use of inverse monoids may offer new insights into some well known and long open problems from Graph Theory, as we will illustrate with some examples.

A partial automorphism of a graph is an isomorphism between its induced subgraphs. The set of all partial automorphisms of a given structure forms an inverse monoid under composition of partial maps. In our presentation, we describe the algebraic structure of such inverse monoids by the means of the standard tools of inverse semigroup theory, and give a characterization of inverse monoids which arise as inverse monoids of partial graph (digraph and edge-colored digraph) automorphisms.

**Tatiana Jajcayová** completed her undergraduate studies at the Comenius University in Bratislava, and her doctoral studies, completed by her PhD. degree in Mathematics with minor in Computer Science, at the University of Nebraska. Her research interests are in Computational, Algorithmic and Combinatorial Algebra. She worked for many years at Universities in the USA, and had long research visits at several Universities (Japan, Italy). She enjoys interdisciplinary connections between Mathematics and Computer Science, and most of all interpersonal connections working on research with her colleagues in Bratislava and around the world.





**Mária Mériová** - Inverse monoids for certain classes of graphs Comenius University, Bratislava, Slovakia

<u>Abstract:</u> In order to better understand a specific combinatorial structure (for instance a graph) it is recommended to study, investigate and analyze the symmetries of this combinatorial structure. Up to recently, the main tools to study these symmetries were tools of Group Theory, that is full automorphisms and groups of full automorphisms. In cases where

structures have no global symmetries and full automorphisms can not be used, these tools are rather limited. But the structures may still exhibit some local symmetries and thus their partial automorphisms are interesting. Based on theoretical results published about local symmetries, we know that induced subgraphs need to be studied for graphs, and we have developed software that makes a list and analyzes the induced subgraphs of a given graph. Then, using these induced subgraphs, we studied the structure of inverse monoids related to the partial automorphisms of these graphs. At the beginning of our project, we have dealt with simple families of graphs: paths, cycles and trees, but we believe that our results can be generalized to other classes of graphs as well. As J. Nešetřil, M. Konečný et al. research suggests, another interesting class of graphs could be tournaments.

**Mária Mériová** is a doctoral student at Comenius University, she obtained her Master's degree at the same university. During her undergraduate studies, she had an extended scientific stay in Budapest, at Eötvös Loránd University. In her doctoral studies, she works in the area of the Computational Algebraic Combinatorics, specifically the partial symmetries of combinatorial structures.

**Slobodan Filipovski** - On bipartite cages of excess 4 University of Primorska, Koper, Slovenia

**Abstract:** The Moore bound M(k,g) is a lower bound on the order of k-regular graphs of girth g (denoted (k,g)-graphs). The excess e of a (k,g)-graph of order n is the difference n-M(k,g). In this talk we consider the existence of (k,g)-bipartite graphs of excess 4 via studying spectral properties of their adjacency matrices.

**Slobodan Filipovski** finished his PhD at University of Primorska in Koper, Slovenia, 2018, and post-doc at Comenius University in Bratislava, 2020. His research area is graph theory, (extremal graph theory, spectral graph theory).

**Tom Raiman** - Conditions for vertex removal in (k,g)-graphs VŠB - Technical University of Ostrava, Czech Republic

**Abstract:** For almost sixty years there has been thorough research about properties of (k,g)-graphs and (k,g)-cages. There have been a lot of attempts to improve lower and upper bounds for (k,g)-graphs given some qualities of these graphs. We want to show new ideas how to find smaller (k,g)-graphs from existing ones, while preserving the regularity and girth and show how these ideas may help to find new upper bounds that could be smaller than the existing ones.

**Tom Raiman** is a doctoral student of Robert Jajcay. He studies at Technical University of Ostrava. His main focus of research is in the area of (k,g)-graphs, where he has published together with Robert Jajcay some results about (k,g)-graphs.

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**Section:** Applied Statistics and Reliability

**Frank Coolen** - Survival Signature for Quantification of System Reliability Department of Mathematical Sciences, Durham University, UK

**Abstract:** The system structure function is central to much of the theory and methods for quantification of system reliability. It describes the state of the system as function of the states of the individual components. For binary systems with n components, this function has 2^n inputs, so it quickly becomes problematic to use for large systems. In 2012, we introduced the survival signature as a summary of the survival signature, which is sufficient to derive the system reliability function, and through that several metrics of main interest. It is useful if the system has components of multiple types, but not too many different types.

I will present an introductory overview to the survival signature, with discussion of several recent contributions and related research challenges.

**Frank Coolen** is Professor of Statistics at the Department of Mathematical Sciences, Durham University, UK. He completed his PhD at Eindhoven University of Technology in The Netherlands in 1994, after which he joined Durham University. His main areas of research are Nonparametric Predictive Inference, Imprecise Probability Theory, and System Reliability. He has published about 250 journal and conference papers. He is member of the editorial boards of 9 journals in Statistics and Reliability, and has supervised about 20 PhD students to completion, with about 10 further students working under his supervision at the moment. He regularly serves on Conference Committees and Research Funding Panels.

**Christophe Berenguer** - On post-prognosis decision making for predictive maintenance and optimal operation of deteriorating system

Univ. Grenoble Alpes, Grenoble INP, GIPSA-lab, France

<u>Abstract:</u> "Post-prognosis decision making", "reliability-adaptive smart systems", "RUL control algorithms", "load sharing and deterioration management", all these subjects develop a new vision on how to use monitoring information on a deteriorating system to optimally operate it beyond "classical" condition-based or predictive maintenance.

The objective of this presentation is to give some insights on how monitoring information on deteriorating system can be used to jointly make decision on maintenance & operation to better manage systems' health, considered either individually or as part of fleet. We explore the complete processing chain for a system, from deterioration monitoring and health status assessment, to remaining useful life estimation (RUL), right through to online decision-making for predictive maintenance optimization and remaining useful life control and health & deterioration management, using e.g. system "derating", load sharing or system reconfiguration.

The presentation overviews some recent results, but it focuses more on open problems and challenges ahead than worked-out solutions.

Christophe Berenguer is Professor of Reliability & Maintenance, Monitoring and Control Systems at Univ. Grenoble Alpes, Grenoble Institute of Technology, France and researcher at Gipsa-lab since 2011. From 1995 to 2011, he was a Professor at Troyes University of Technology, France. He graduated from Compiègne University of Technology (M.Eng BioEngineering; M.Sc. Control Systems, 1990) and University of Nice Sophia-Antipolis (PhD, 1994). His research interests include stochastic modelling of systems and structures

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deterioration and lifetime, performance assessment models of dynamic maintenance policies, methods for systems & structure health management and RUL control, reliability models for probabilistic safety assessment and reliability of safety instrumented systems. He is involved in several collaborative research projects both with academics and industry partners. He is chair of the ESRA Technical Committee on Maintenance Modelling and Applications. He is (or has been) member of the Editorial Boards of Reliability Engineering and System Safety, Journal of Risk and Reliability (Associate Editor), Eksploatacja i Niezawodnosc – Maintenance and Reliability and he regularly serves for the main conferences on reliability, maintenance and safety (ESREL, RAMS, SAFEPROCESS).

He has published about 80 journal papers and 170 international conference papers. He has supervised 27 PhD students and 7 PhD students are currently working under his supervision.

## Section: Introduction to Quantum Computing

**Piotr Gawron** - Quantum neural networks -- a practical approach AtroCeNT, Particle Astrophysics Science and Technology Centre International, Research Agenda, Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences, Poland

<u>Abstract</u>: With the recent success of artificial neural networks and emergence of Near Intermediate Scale Quantum computers a new field of quantum machine learning was established. There is hope that quantum computers will be able to build better and faster machine learning models. While many approaches are being studied, during this lecture we will focus on the class of machine learning models derived from variational quantum algorithms. These models are called quantum neural networks. This approach is interesting because it allows embedding quantum computers into classical neural network processing graphs.

**Piotr Gawron** is a scientist working in the area of quantum computation and machine learning.

In the years 2001-2019 he was a member of Quantum Systems of Informatics group of the Institute of Theoretical and Applied Informatics, Polish Academy of Sciences. Since 2019 he leads the Scientific Computing and Information Technology Group at AstroCeNT—Particle Astrophysics Science and Technology Centre International Research Agenda, Nicolaus Copernicus Astronomical Center Polish Academy of Sciences.

In the past he has been working on quantum game theory, study of influence of quantum noise on quantum algorithms, quantum walks, quantum Markov models, quantum control theory, mathematical tools of quantum information, quantum annealing. Outside quantum information / computation area he worked on image and signal processing, compression and classification. Currently, his group work focusses on applications machine learning techniques for gravitational wave prediction and detection.

He has obtained the following degrees:

- MSc of informatics (2003), master thesis "Simulation of quantum computers", Silesian University of Technology, Poland.
- PhD in the field of informatics, (2008), dissertation: "High level programming in quantum computer science", Institute of Theoretical and Applied Informatics, Polish Academy of Sciences.
- DSc in the field of informatics, (2014), dissertation: Influence of the environment on quantum information processes, Silesian University of Technology, Poland.

Katarzyna Rycerz - Solving workflow scheduling problems with near-term quantum devices Institute of Computer Science, AGH University of Science and Technology, Kraków, Poland

**Abstract:** The subject of this talk focuses on exploring the possibility of solving a popular optimization problem, workflow scheduling [1], using quantum computers. In the model of scientific computations, called scientific workflow, computations are expressed as a graph of many (often thousands) computational tasks, which must be performed in a strictly defined order. Many important computational problems in the field of astronomy, bioinformatics, high energy physics or computational medicine can be expressed in that way.

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We particularly focus on the problem of assigning workflow tasks to machines in a cloud environment. In this talk, we will present a formal problem description, its transformation into a form acceptable by quantum computers (Ising Hamiltonian and QUBO) and discussion of experimental results. We present two different approaches for small problem instances. First, using D-Wave quantum annealer [2] and second using hybrid Variational Quantum Eigensolver (VQE) [3] algorithm run on IBM-Q. We will also discuss limitations of such approaches, the existing solutions and point possible future work.

[1] Deelman, E., Gannon, D., Shields, M., Taylor, I.: Workflows and e-science: An overview of workflow system features and capabilities. Future Generation Computer Systems 25(5), 528–540 (2009)

[2] D. Tomasiewicz, M. Pawlik, M. Malawski, K. Rycerz: Foundations for workflow application scheduling on D-Wave system. Computational Science - ICCS 2020: 20th International Conference: Amsterdam, The Netherlands, June 3–5, 2020:

[3] Alberto Peruzzo, Jarrod McClean et al.: A variational eigenvalue solver on a photonic quantum processor. Nature Communications 5, 4213 (2014)

**Katarzyna Rycerz** received her PhD in computer science from UvA, Amsterdam in 2006. Currently works as an assistant professor at the Department of Computer Science AGH, Kraków, Poland and is a co-author of over 50 international publications in the area of distributed computing, environments for multiscale simulations, quantum computing simulation and support for scientific applications. She was involved in the EU ICT projects: CrossGrid (the Architecture Team member), CoreGRID and MAPPER (WP leader). Currently, she is interested in quantum computation, in particular solving HPC and Cloud related problems using existing quantum computers. She is also interested in quantum games.

#### Lukasz Pawela - QLearning

Institute of Theoretical and Applied Informatics, Polish Academy of Sciences, Gliwice, Poland

Abstract: It is a well established fact that arbitrary, unknown quantum states can not be copied perfectly - this is known as the no-cloning theorem. A similar result holds for programming quantum devices: a universal machine able to perform any quantum operation on an arbitrary input state of fixed size, programming the desired action in a quantum register inside the machine can not exist. Instead, we asked a related question: given a black-box, containing an unknown quantum operation and the ability to use the black-box today an arbitrary number of times, what is the correct procedure to approximate the action of the black box tomorrow. As it turns out, the answer to the question is non-trivial and depends on the initial promise (i.e. the type of operation stored in the black box). Finally we can study different approaches to this problem: we can have perfect recreation of the black-box, but with some finite probability or we can have imperfect recreation with certainty. These problems will be introduced and potential solutions will be shown during the lecture.

Łukasz Pawela is working in the area of quantum computation, machine learning and random matrix theory. Since 2011 he is a member of Quantum Systems of Informatics group of the Institute of Theoretical and Applied Informatics, Polish Academy of Sciences. During this time (2017-2018) he was also a postdoc in the National Quantum Information Centre in Gdańsk in Karol Horodecki's group.

Currently he works in two research groups: Quantum Machine Learning, which he co-leads, and Quantum Simulation and Emulation group, which he leads. His research interest involve integrating cutting-edge numerical (e.g. tensor networks), mathematical (e.g. random matrix theory) and machine learning methods into quantum science.

He has obtained the following degrees:

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- MSc of physics (2011), master thesis "Simulation of logical operations in low-dimensional magnetic structures", Silesian University of Technology, Poland.
- PhD in the field of informatics, (2017), dissertation: "Open systems in quantum informatics", Institute of Theoretical and Applied Informatics, Polish Academy of Sciences.
- DSc in the field of informatics, (2020), dissertation: "Application of probabilistic methods in quantum information theory", Silesian University of Technology, Poland.

Section: Numerics

**Helmut A. Mayer** - Evolutionary Computation - Principles and Applications Department of Computer Sciences, University of Salzburg, Austria

<u>Abstract:</u> In this talk we give an introduction to Evolutionary Computation, a branch of computer science, which employs basic concepts of Darwinian Evolution in order to tackle problems in science, engineering, and business. Basically, an Evolutionary Algorithm generates a large number of (initially) random solutions to a problem, which are selected according to their fitness defined by a quality function. In this process candidate solutions are recombined and mutated potentially generating improved solutions. In a variety of applications these nature-inspired procedures have created solutions, which are equal to or even better than those developed by human engineers. In order to demonstrate the potential of these Computational Intelligence techniques we discuss some applications including own research.

**Helmut A. Mayer** - Artificial Neural Networks - Principles and Applications Department of Computer Sciences, University of Salzburg, Austria

<u>Abstract:</u> Biological neural networks having been shaped in billions of years of evolution are the source of numerous, complex capabilities of living organisms. Especially, the form of intelligence attributed to humans has inspired computer scientists to model artificial neural networks in order to achieve learning in computers. In a general form learning is equivalent to controlled changes in the complex neural circuitry of the brain. In the artificial model the control mechanisms governing the adaptation of neural parameters are built into training algorithms being an important area of research in artificial neural networks. We will summarize the basic ideas of artificial neural networks, discuss the recent advances in deep learning, and illustrate these achievements by various applications including own research.

**Helmut A. Mayer** is an associate professor at the Department of Computer Sciences at the University of Salzburg. After completing his master degree in electrical engineering at the Technical University Vienna in 1987 he worked for five years as a software engineer for automation and control systems. In 1997 he received his PhD in computer science from the University of Salzburg, where he also completed his habilitation in informatics in 2004. His main areas of research are: Evolutionary Computation, Artificial Neural Networks, Evolutionary Robotics, ANN Game Playing, and Industrial Applications of Computational Intelligence.

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