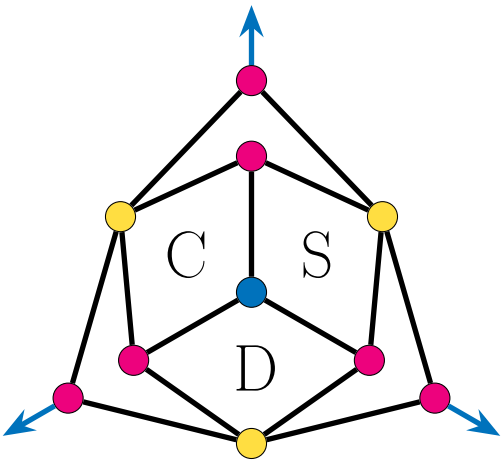
Abstracts of the

Computers in Scientific Discovery 11

Kranjska Gora, Slovenia, 4–8 May 2026



Slovenian Discrete and Applied Mathematics Society
May 2026

Abstracts of the Computers in Scientific Discovery 11
Kranjska Gora, Slovenia, 4–8 May, 2026

Editors: Nino Bašić, Patrick W. Fowler

Published by the
Slovenian Discrete and Applied Mathematics Society
Kettejeva 1, 6000 Koper

First online edition
Electronically available at https://csd11.si/book-of-abstracts.pdf
DOI: https://doi.org/10.26493/csd11.abstracts.2026

Koper, May 2026

Kataložni zapis o publikaciji (CIP) pripravili v Narodni in univerzitetni knjižnici v Ljubljani

COBISS.SI-ID 276208387
ISBN 978-961-95273-2-0 (PDF)

Introduction

Welcome to the 11th Conference on Computers in Scientific Discovery, held this year in Kranjska Gora, in the inspiring setting of the Slovenian Alps.

This meeting continues a tradition that started with two early DIMACS workshops around the turn of the millenium, and as before we aim to offer a focus for researchers working at the intersections between discrete mathematics, computer science, chemistry and other sciences.

Early CSD meetings already encompassed a wide range of activity in algorithmic graph theory, chemical applications, generation and curation of databases of mathematical objects and computer-assisted proofs. With this year's theme of *Computationally Intensive Methods in Mathematics: Applications in Chemistry and Beyond*, we hope to extend the scope even further.

As with its predecessors, CSD11 has a strong scientific programme of invited and contributed talks, but as always, a significant part of the meeting will be the discussions at social events and in the gaps between formal sessions. CSD has an excellent record of fostering interactions that lead to new multidisciplinary collaborations and unexpected ideas. In this connection, please note the opportunity to publish papers related to talks and topics from the meeting, in *Discrete Mathematical Chemistry* (DMC). The special proceedings issue will remain open until September 30, 2026. See https://dmc-journal.eu/ for further details, and contact the organisers with any questions.

Finally, we thank our sponsors, participants, speakers and committee members for their various contributions to the meeting, and, once more, wish everyone a stimulating, productive, and thoroughly enjoyable conference.

Kranjska Gora, May 2026

Scientific Committee of CSD11

Contents

General Information

Computers in Scientific Discovery 11 (CSD11)
Kranjska Gora, Slovenia, 4–8 May 2026

Organised by:
Slovenian Discrete and Applied Mathematics Society

In collaboration with:
University of Primorska, Slovenia
Institute of Mathematics, Physics and Mechanics, Slovenia
The European Mathematical Society

Scientific Committee:
Vesna Andova (Ss. Cyril and Methodius University in Skopje, North Macedonia)
Nino Bašić (University of Primorska & IMFM, Slovenia)
Patrick W. Fowler (University of Sheffield, United Kingdom)
Elizabeth J. Hartung (Massachusetts College of Liberal Arts, United States)
Craig E. Larson (Virginia Commonwealth University, United States)
Irene Sciriha Aquilina (University of Malta, Malta)

Organising Committee:
Nino Bašić (University of Primorska & IMFM, Slovenia)
Katja Berčič (University of Ljubljana & IMFM, Slovenia)
Ivan Damnjanović (University of Primorska, Slovenia & University of Niš, Serbia)
Andrés David Santamaria Galvis (IMFM, Slovenia)

Keynote speakers:
Marién Abreu (University of Basilicata, Italy)
Milica Anđelić (Kuwait University, Kuwait)
Marston Conder (University of Primorska, Slovenia &
University of Auckland, New Zealand)
Jan Goedgebeur (KU Leuven, Belgium)
Tatiana Jajcayová (Comenius University Bratislava, Slovakia)
Hadrien Mélot (University of Mons, Belgium)

Conference venue:
Hit Alpinea Hotels, Kranjska Gora, Slovenia

Conference website:
https://csd11.si

Past Conferences

The main theme of the 11th CSD conference is '*Computationally Intensive Methods in Mathematics: Applications in Chemistry and Beyond*'.

The Computers in Scientific Discovery (CSD) conference series is designed to bring together researchers whose work makes connections between mathematics, computer science, and natural sciences. In particular, the CSD meetings have concentrated on how algorithms, mathematical software and data are used in non-trivial ways to advance research in the mathematical and physical sciences. The conferences focus not only on applications, but also on mathematical foundations, philosophy and practicalities of the scientific discovery process, including conjecture-making, construction and the use of curated databases of mathematical objects, and computer-aided proofs.

The CSD series started at Rutgers University DIMACS centre with a workshop on Discrete Mathematical Chemistry (New Brunswick, United States, 1998) and the subsequent meeting on Computer-Generated Conjectures from Graph Theoretic and Chemical Databases (New Brunswick, United States, 2001). Subsequent conferences were in Montreal (Canada, 2004), Ghent (Belgium, 2006), Shanghai (P. R. China, 2008), Sheffield (United Kingdom, 2010), Portorož (Slovenia, 2012), Richmond (Virginia, United States, 2015), Mons (Belgium, 2017), Montreal (Canada, 2019), and Kortrijk (Belgium, 2024). These CSD conferences have demonstrated the existence of an enthusiastic community of researchers on several continents active at the interfaces between discrete and computational mathematics, computer science, chemistry and physics.

These CSD conferences have demonstrated the existence of an enthusiastic community of researchers on several continents active at the interfaces between chemistry, computer science and discrete mathematics. In this 11th meeting we will continue the deliberately multidisciplinary emphasis of these conferences, provide space for collaboration and follow-up on results of the previous meetings, and expand even further the range of topics covered.

Previous Editions

- Computers in Scientific Discovery 10 (Kortrijk, Belgium, 2024), https://csd10.be/
- Computers in Scientific Discovery 9 (Montreal, Canada, 2019)
- Computers in Scientific Discovery 8 (Mons, Belgium, 2017)

- Computers in Scientific Discovery 7
  (Richmond, Virginia, United States, 2015)
- Computers in Scientific Discovery 6 (Portorož, Slovenia, 2012)
- Computers in Scientific Discovery 5 (Sheffield, United Kingdom, 2010),
  https://caagt.ugent.be/csd5/
- Computers in Scientific Discovery 4 (Shanghai, P. R. China, 2008)
- Computers in Scientific Discovery 3 (Ghent, Belgium, 2006),
  https://caagt.ugent.be/csd3/
- Computers and Discovery (Montreal, Canada, 2004)
- Computer-Generated Conjectures from Graph Theoretic and Chemical
  Databases I (New Brunswick, New Jersey, United States, 2001)
- DIMACS Workshop on Discrete Mathematical Chemistry
  (New Brunswick, New Jersey, United States, 1998)

Keynote Talks

Factors and hamiltonicity in regular graphs

Marién Abreu [1], *R. E. L. Aldred* [2], *A. A. Diwan* [3], *M. Funk* [4], *J. Goedgebeur* [5], *B. Jackson* [6], *J. Jooken* [5], *D. Labbate* [4], *R. Rizzi* [7], *F. Romaniello* [4], *J. Sheehan* [8], *T. Van den Eede* [5]

[1] Dipartimento di Scienze di Base ed Applicate, Università degli Studi della Basilicata, Italy
[2] University of Otago, Dunedin, New Zealand
[3] Indian Institute of Technology, Mumbai, India
[4] Università degli Studi della Basilicata, Italy
[5] KU Leuven Campus Kulak-Kortrijk, Kortrijk, Belgium
[6] School of Mathematical Sciences, Queen Mary College, London, United Kingdom
[7] Università degli Studi di Verona, Verona, Italy
[8] Department of Mathematical Sciences, King's College, Old Aberdeen, United Kingdom

Graphs in which all vertices have the same degree r are called *r-regular*. An r-regular spanning subgraph of a graph is called an *r-factor*. Several kinds of problems that arise when studying 2-factors of regular graphs will be presented here. In particular, 2-factor hamiltonian; 2-factor isomorphic; pseudo 2-factor isomorphic graphs will be considered. These are respectively graphs in which all 2-factors are hamiltonian; all 2 factors are isomorphic (collection of cycles of same lengths); all 2-factors have the same parity of number of cycles. Partial solutions and infinite families with prescribed characteristics will be illustrated, sometimes in the special case of cubic graphs, together with old and new results.

In the course of the studies in this topic computers have been a very important companion and their rôle will be highlighted at each step of the way.

From equitable partitions to full spectra: A framework for symmetric graphs

Milica Anđelić [1]

[1] Kuwait University, Kuwait

An equitable partition of a graph is a powerful tool for extracting relevant spectral information. In particular, the spectral radius of the divisor matrix associated with any equitable partition is known to coincide with the spectral radius of the graph itself. For graphs exhibiting a high degree of symmetry, equitable partitions can be combined with the composition principle, originally developed by Edgar Heilbronner more than seven decades ago, to determine the full spectrum. We highlight how these methods can be employed both to compute the spectra of highly symmetric graphs and to construct families of graphs that share the same spectral radius.

Constructing databases of discrete objects with a high degree of symmetry

Marston Conder [1,2]

[1] University of Auckland, New Zealand

[2] University of Primorska, Slovenia

Symmetry has been a subject of human fascination for centuries, dating back to the ancient Greeks and even further, in art and architecture for example. More recently, the construction and analysis of discrete objects with a high degree of symmetry has developed into an important area of study, with obvious applications in chemistry and physics, but also with unexpected applications other fields of science and technology, such as coding, distribution networks, electrical circuits, graphics and quantum computing.

In this talk I'll describe how group theory and computation have enabled the construction of large databases of symmetric objects, including edge-transitive graphs, regular and chiral maps, regular and chiral polytopes, and compact Riemann surfaces with large automorphism group. For example, recent work with Primož Potočnik (Ljubljana) has resulted in lists of all arc-transitive and semi-symmetric 3-valent graphs with up to 10 000 vertices, and all orientably-regular maps on surfaces of genus 2 to 1501.

Also I'll describe some surprises that have resulted from such constructions over the last 40 years, including the fact that a focus on finding objects with a non-abelian simple group as the symmetry group has masked the importance of soluble groups, which appear to play a far more significant (if less fashionable) role.

An introduction to computational graph theory and generation algorithms

Jan Goedgebeur [1]

[1] KU Leuven, Belgium

Computers are often used in combinatorics to determine if combinatorial objects with given structural or extremal properties exist as these existence problems are often too complex to solve by hand. This is done by designing and implementing generation algorithms which construct combinatorial objects from a given class (typically avoiding the generation of isomorphic copies) and analysing the resulting objects.

In this talk we will give an introduction to computational graph theory and the design of generation algorithms in particular. We will also give concrete examples of how these generation algorithms have helped to gain new insights and solve problems in mathematics and in chemistry.

Computational aspects of interplay between global and local symmetries

Tatiana Jajcayová [1]

[1] Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, Slovakia

Exact complexity of finding the automorphism group of a graph is not known. Babai showed that it is subexponential. One approach to building automorphism groups of graphs is to use the k-dimensional Weisfeiler–Leman algorithm, that iteratively builds the orbits of the automorphism group. We propose to use another iterative approach using partial automorphisms of graphs.

A partial automorphism of a graph is an isomorphism between its induced subgraphs. The set of all partial automorphisms of a given graph forms an inverse monoid under composition of partial maps and taking partial inverses. In constrast to classical group theory approach to studying symmetries of graphs, where the automorphism group of a graph can be (and almost always is) trivial, the inverse monoid of partial automorphisms of a graph is never trivial and gives the full algebraic description of the graph. In our talk we will address some computational aspects of finding these inverse monoids.

In particular, we introduce the measures of asymmetric depth and asymmetric level of graphs defined through the rank of the largest nontrivial partial automorphism. We discuss bounds for these parameters and their implications in computing the inverse monoid of partial automorphisms. In joint work with Ján Pastorek, we were able to establish tight bound for asymmetric depth of any simple graph Γ of order n. Any graph achieving this bound must be a strongly regular graph with parameters $(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4})$ also known as conference graph.

A polyhedral journey through extremal chemical graphs

Hadrien Mélot [1], *Sébastien Bonte* [1], *Gauvain Devillez* [1], *Valentin Dusollier* [1], *Alain Hertz* [2], *David Schindl* [3]

[1] Université de Mons, Belgium
[2] Polytechnique Montréal
[3] Haute-Ecole de Gestion de Genève

Chemical graphs model molecules by representing atoms as vertices and bonds as edges. In this context, degree-based topological indices are widely used molecular descriptors to predict physicochemical properties. Finding the graphs that maximize or minimize these indices is a highly active area of research in mathematical chemistry, driving an extensive body of literature. This talk traces a cohesive research journey—progressing from empirical observations to a unifying geometric theory, and culminating in a practical software tool.

Our journey begins with a surprising discovery concerning one of the standard definitions of chemical graphs: those with a maximum degree $\Delta \leq 3$, which naturally model conjugated systems. For this established class of graphs, we observed that a mere five structural families are sufficient to characterize the extremal graphs for 29 out of 33 common indices. This strongly suggested that extremal behavior is remarkably consistent across diverse descriptors.

To uncover the underlying mathematical architecture, we developed a polyhedral framework. By mapping each chemical graph to a point in a three-dimensional space, we elegantly reduced the search for extremal values to linear optimization over a specific polyhedron. We proved that this polytope contains at most 10 facets and 16 extreme points, theoretically explaining why extremality is universally restricted to such a small subset of graph families.

This theoretical breakthrough led to `ChemicHull`, an online tool designed to automatically determine and visualize extremal chemical graphs. I will demonstrate how `ChemicHull` easily recovers established results and identifies counterexamples in existing literature, notably regarding the Randić index. Finally, I will conclude by exploring the open questions and exciting perspectives of extending this polyhedral approach to chemical graphs with larger maximum degrees ($\Delta > 3$).

Contributed Talks

Predicting lifetimes of metastable anions: A mathematical–chemical approach

Cate S. Anstöter [1], *Chiara Beldí* [2,1]

[1] University of Glasgow, United Kingdom

[2] University of Edinburgh, United Kingdom

Metastable electronic states play a central role in electron- and photon-driven chemistry. Whenever a molecule temporarily captures an electron or absorbs high-energy radiation, it can enter a short-lived state that either relaxes, fragments, or ejects the extra electron. These processes underpin radiation damage, plasma chemistry, atmospheric chemistry, and many catalytic cycles. They are especially critical in astrochemical environments such as the interstellar medium, planetary atmospheres, and cometary comae, where intense electron and photon bombardment occurs in the absence of a stabilising solvent.

Metastable anionic states are not truly bound. They possess finite lifetimes and are intrinsically susceptible to autodetachment of the excess electron. Theoretically, they fall outside the conventional Hermitian framework that underpins most quantum chemistry. Standard electronic structure methods are designed for bound states with real-valued energies. In contrast, metastable states must be described as resonances, characterised by complex energies whose imaginary component encodes the lifetime. This requires mathematical machinery (such as non-Hermitian quantum mechanics, complex scaling, or related techniques) that lies beyond the standard toolkit of many chemists.

Why revisit this problem now? Many of the seminal theoretical approaches to electronic resonances were developed over thirty years ago, when computational resources severely limited their applicability. These methods were often benchmarked on small atomic or diatomic systems and may not transfer reliably to larger, chemically relevant molecular anions. Today, vastly increased computational power, improved numerical algorithms, and modern mathematical insights create an opportunity to reassess and improve how metastable states are modelled. By refining how we describe metastable anions, we aim to unlock a largely inaccessible sector of redox chemistry and provide new theoretical tools for understanding electron-driven processes in chemistry and space.

A curious family of point-covering, plane-filling curves

Jörg Arndt [1], *Mark Legradi*

[1] Technische Hochschule Nürnberg, Germany

We describe a family of plane-filling curves on the square grid with a curious property: the shape of each curve is a lattice tile. These curves are point-covering, all point of a disk of any size are covered by a high enough iterate of the curve. Our exposition is driven by illustrated examples.

Computation and conjectures: Skew morphisms of finite cyclic groups

Martin Bachratý [1], *Michal Hagara*

[1] Slovak University of Technology, Slovakia

A skew morphism of a finite group G is an element φ of $\mathrm{Sym}(G)$ preserving the identity element of G and having the property that for each $a \in G$ there exists a non-negative integer i_a such that $\varphi(ab) = \varphi(a)\varphi^{i_a}(b)$ for all $b \in G$. Skew morphisms arise naturally in the study of regular Cayley maps, permutation group factorizations, and related combinatorial structures. Their classification for finite cyclic groups is notoriously hard, and no complete classification is available to date.

In this talk, I will explain how we systematically extended the census of skew morphisms of all cyclic groups of orders up to 60 to all cyclic groups of orders up to 2000. This was accomplished through an iterative process in which extensive computational lists of skew morphisms were used to formulate and verify new conjectures, which in turn enabled the generation of even larger datasets. Our work illustrates the usefulness of this iterative interplay between computation and theory.

The author acknowledges funding from the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00272.

ILP/CP-SAT does it again: Construction of d-regular nut graphs with practical efficiency

Nino Bašić [1,2]

[1] University of Primorska, Slovenia

[2] IMFM, Slovenia

A nut graph is a simple graph whose adjacency matrix has nullity one, such that non-trivial kernel eigenvectors have no zero entries. This class of graphs was introduced in 1998 by Sciriha and Gutman [1].

The order–degree existence problem for regular nut graphs was initiated by Gauci et al. in [2]. Let $\mathfrak{N}_d$ denote the set of orders attainable by a d-regular nut graph. The problem is to determine $\mathfrak{N}_d$ for a given integer d. Gauci et al. have shown that $\mathfrak{N}_3 = \{12\} \cup \{n \in \mathbb{N} : n \text{ is even and } n \geq 18\}$ and $\mathfrak{N}_4 = \{8, 10, 12\} \cup \{n \in \mathbb{N} : n \geq 14\}$. In the same paper, they described the Fowler construction, which plays a central role in these developments: it produces a d-regular nut graph of order $n + 2d$ from a d-regular nut graph of order n. The sets $\mathfrak{N}_5, \mathfrak{N}_6, \ldots, \mathfrak{N}_{11}$ were determined by Fowler et al. [3], and the set $\mathfrak{N}_{12}$ was determined in [4].

In [5], it was shown that infinitely many d-regular nut graphs exist for each degree $d \geq 3$. Consequently, $\mathfrak{N}_d$ is infinite for every $d \geq 3$, although these sets have not been completely determined.

In this talk, we formulate the search for d-regular nut graphs of order n as an integer linear programming (ILP) problem by prescribing an integer kernel eigenvector and encoding adjacency via binary variables. The model includes linear constraints enforcing d-regularity and ensuring that the prescribed vector lies in the nullspace of the adjacency matrix.

This approach is highly effective in practice: we determined $\mathfrak{N}_d$ for all $d \leq 100$. These computations can be extended further with a modest additional investment of computational resources. We provide an implementation supporting both `Gurobi` [6] and and the CP-SAT solver from `OR-Tools` [7].

References

[1] I. Sciriha and I. Gutman, Nut graphs: Maximally extending cores, *Util. Math.* **54** (1998), 257–272.

[2] J. B. Gauci, T. Pisanski and I. Sciriha, Existence of regular nut graphs and the Fowler construction, *Appl. Anal. Discrete Math.* **17** (2023), 321–333.

[3] P. W. Fowler, J. B. Gauci, J. Goedgebeur, T. Pisanski and I. Sciriha, Existence of regular nut graphs for degree at most 11, *Discuss. Math. Graph Theory* **40** (2020), 533–557.

[4] N. Bašić, M. Knor and R. Škrekovski, On 12-regular nut graphs, *Art Discrete Appl. Math.* **5** (2022), #P2.01.

[5] N. Bašić, I. Damnjanović, P. W. Fowler, On the degrees of regular nut graphs and Cayley nut graphs, *Ars Math. Contemp.*, in press.

[6] Gurobi Optimization, LLC, Gurobi Optimizer Reference Manual, 2026, https://www.gurobi.com.

[7] L. Perron and V. Furnon, OR-Tools, Version v9.15, Google, 2026, https://developers.google.com/optimization/.

Collections of mathematical objects

Katja Berčič [1]

[1] University of Ljubljana and IMFM, Slovenia

The landscape of mathematical data, including collections of mathematical objects and properties, remains fragmented and undercharted, yet has been gaining visibility thanks to rapid advances in formalized mathematics and AI.

We take stock of what currently exists: what kinds of mathematical knowledge these collections encode, how they relate to each other, and where significant gaps remain. Along the way, we examine different types of collections and their potential with respect to formalization and AI. We also touch on practical questions of data models, curation, and long-term sustainability: challenges familiar to anyone who has tried to build or maintain a mathematical dataset.

We close with a call for greater coordination around shared standards and discovery infrastructure, all the more urgent as formal methods and AI raise both the stakes and the possibilities for mathematical data at scale.

Distinct vertex-edge spectral labelling for threshold graphs

James L. Borg [1], *Irene Sciriha* [1], *Zoia Sherman* [1]

[1] University of Malta, Malta

A *vertex labelling* of a graph is defined as an injective function between the vertex set of the graph and the nonnegative integers. A *square difference* (*SD*) *labelling* of a graph is a vertex labelling that assigns a value $|(f(u))^2 - (f(v))^2|$ equal to the difference of the squares of the vertex labels $f(u)$ and $f(v)$ on each edge labelled $\{u, v\}$, which induces an injective function between the edge set of the graph and the nonnegative integers.

Threshold graphs have the remarkable property that all graphs of the same order share a common integer Laplacian eigenbasis. There is a one-to-one correspondence between the vertices of a threshold graph, labelled according to its creation sequence, and the eigenvectors of its Laplacian matrix. Hence, we can use this bijection to define a valid vertex labelling supported by the Laplacian geometry of the graph, which we name the Laplacian Eigenvector Labelling (LEL) of the threshold graph.

There is an infinite family of threshold graphs for which the LEL is not an SD labelling. We give an algorithm by which a threshold graph for which the LEL labelling is not an SD labelling can be transformed into a SD-feasible threshold graph on the same number of vertices such that the vertex labelling inherited from the original threshold graph is a valid SD labelling.

Reinforcement learning meets graph theory: A new framework

Ivan Damnjanović [1,2], *Uroš Milivojević* [2], *Irena Đorđević* [2], *Dragan Stevanović* [3]

[1] University of Primorska, Slovenia
[2] University of Niš, Serbia
[3] Abdullah Al Salem University, Kuwait

Reinforcement learning (RL) is a branch of machine learning concerned with designing models that can learn effective decision-making strategies through interaction and experience. In a recent influential paper, Wagner showed that the Deep Cross-Entropy method from RL can be used to address problems in extremal graph theory by reformulating them as combinatorial optimization tasks. This idea sparked growing interest in the community, leading to a range of refinements and extensions of Wagner's original framework, as well as the development of RL environments specialized for graph theory. As a result, several problems in extremal graph theory have already been successfully approached using RL techniques.

In this work, we introduce Reinforcement Learning for Graph Theory (RLGT), a new framework that unifies and organizes these previous efforts. RLGT is designed to handle both undirected and directed graphs, optionally allowing loops and supporting an arbitrary number of edge colors. The framework provides efficient graph representations and is intended to support future research in RL-based extremal graph theory through improved computational efficiency and a modular architecture.

Metric dimension of some structured graph families: Exact values and explicit bases

Akbar Davoodi [1], *Mohsen Jannesari* [2]

[1] University of Southern Denmark, Denmark

[2] University of Isfahan, Iran

The metric dimension of a connected graph is the minimum size of a resolving set, namely a set of landmark vertices whose distance vectors distinguish all vertices.

In this talk, we will discuss recent exact results for some structured graph families, focusing on sharp formulas and explicit metric bases. The arguments bring out several recurring themes: symmetry, twin vertices, product structure, and constructive or optimization-based methods that make exact computation possible in nontrivial cases. We will also touch on fault-tolerant variants, where the resolving property must persist under the loss of a landmark.

Overall, the talk shows how concrete families of graphs provide a natural setting for studying resolvability, robustness, and efficient landmark placement in structured networks.

Knowledge management in House of Graphs

Gauvain Devillez [1], *Sven D'hondt* [2], *Jan Goedgebeur* [2,3]

[1] Computer Science Department, University of Mons, Belgium
[2] Department of Computer Science, KU Leuven Kulak, Belgium
[3] Department of Mathematics, Computer Science and Statistics, Ghent University, Belgium

The House of Graphs is an online database of graphs which can be accessed at https://houseofgraphs.org/. It serves as a central repository for complete lists of graphs for various graph classes. However, its main feature is a searchable database of so-called "interesting" graphs. The development of the original House of Graphs started in 2010 and it was completely rebuilt in 2021–2022.

Each graph in the database is accompanied by a significant amount of metadata such as a name, drawings, precomputed graph invariants, and comments. Given this volume of information and the importance of reliability in the scientific world, robust data management is essential to ensure accuracy and consistency across the database.

In this talk, we therefore focus on knowledge management in the House of Graphs and describe the inner workings of the House of Graphs and how we ensure that its data is coherent, qualitative and stable.

PHOEG Again?! Yes, but this time we're catching Al Capone!

Valentin Dusollier [1], *Sébastien Bonte* [1], *Gauvain Devillez* [1], *Hadrien Mélot* [1]

[1] University of Mons, Belgium

PHOEG is a discovery system, based on a large database of small graphs and their invariant values, using a geometric approach to discover inequalities between graph invariants. This tool was first introduced at *Computers in Scientific Discovery 8* (Mons, 2017), and its accessible web interface was recently presented at *CSD10* (Kortrijk, 2024). So, you might ask: "PHOEG again?!" You are right, but this time, we are catching Al Capone! In this talk, we will introduce new features of PHOEG and explore on how PHOEG can be used in education.

We will briefly recall the concepts and the geometric approach of PHOEG. Then, we will try to catch Al Capone by investigating his alibi with PHOEG. We will also look at how students can use this tool to formulate conjectures and discover "new" results in graph theory. This demonstrates to students the open-ended nature of scientific research.

An example of graph theory in molecular design: Polyhedral carbon-nitrogen cages

Patrick W. Fowler [1], *Peter Portius* [2], *Wendy Myrvold* [3], *Joseph Mowll-Clarke* [4], *Tom M. Black* [4], *Rory M. Campbell* [4]

[1] Chemistry, School of Mathematical and Physical Sciences, University of Sheffield, United Kingdom
[2] University of Birmingham, United Kingdom
[3] University of Victoria, Canada
[4] University of Sheffield, United Kingdom

A problem motivated by chemical synthesis is to find a cubic polyhedron that supports a vertex colouring such that all vertices are marked as either nitrogen (N) or singly hydrogenated carbon (C), with the N centres forming an independent dominating set and the CC edges a perfect matching of the N-deleted graph. Call such a polyhedron an NCH polyhedron. Each distinct decoration constructed according to these rules corresponds to an isomer of a hypothetical cage-like molecule of formula $N_{4q}((CH)_2)_{3q}$, an '*azapolyhedrane*'. If the restriction to polyhedral parent graphs is relaxed, open nanotube, toroidal and 2D sheet analogues of the NCH polyhedra can be envisaged.

Properties and constructions to be discussed:

(i) NCH polyhedra exist for all orders $10q$ with $q \geq 1$, with multiple NCH polyhedra at every allowed order;
(ii) NCH polyhedra typically have only one decoration (modulo symmetry and enantiomerism), but NCH polyhedra with exponentially many (each potentially corresponding to a molecule) can be constructed;
(iii) Exactly 11 fullerenes (cubic polyhedra with pentagonal and hexagons faces only) are NCH, each corresponding to one molecular solution (an '*azafullerane*'). Allowed orders for NCH fullerenes are 20, 40, 50 (1 isomer each) and 60 (8 fullerene isomers).

Estimates of total energy from quantum chemical calculations will be used to comment on likely trends in overall stability of azapolyhedranes.

Autocatalytic cores in reaction networks with explicit catalysis

Richard Golnik [1,2], *Thomas Gatter* [1], *Peter F. Stadler* [1,2,3,4,5,6,7], *Nicola Vassena* [1]

[1] Bioinformatics Group, Department of Computer Science & Interdisciplinary Center for Bioinformatics, Leipzig University, Germany

[2] School of Embedded Composite Artificial Intelligence, Leipzig University, Germany

[3] Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, Leipzig University, Germany

[4] Max Planck Institute for Mathematics in the Sciences, Germany

[5] Department of Theoretical Chemistry, University of Vienna, Austria

[6] Facultad de Ciencias, Universidad National de Colombia, Bogota, Colombia

[7] Santa Fe Institute, United States

Autocatalytic cores are the minimal units in reaction networks (RNs) responsible for the emergence of autocatalysis. In the absence of explicit catalysis, i.e., when an entity appears both as a reactant and a product in the same reaction, they are known to be encoded by square submatrices of the stoichiometric matrix whose columns can be reordered as an irreducible child-selection (CS) matrix with negative diagonal and nonnegative off-diagonal (Metzler matrix). In the bipartite König graph representing the RN, these CS matrices can be identified by *fluffles*, i.e., strong blocks with an identical number of metabolite and reaction vertices, and such that the metabolite vertices have out-degree 1 and the reaction vertices have in-degree 1.

Here, we adapt the concepts derived for autocatalytic cores to RNs with explicitly catalyzed reactions, which emerge as *digons*, i.e., elementary circuits in the König graph of length 2. In this setting, we confirm that an inspection of the stoichiometric matrix alone is inconclusive concerning the presence and number of autocatalytic cores, and that a more delicate algebraic analysis is required. Nevertheless, this generalization preserves both the graph representation of autocatalytic cores as fluffles and their matrix representation as irreducible Metzler CS matrices, although the diagonal is no longer necessarily strictly negative.

Finally, we consider the case of trivial stoichiometries and show that every autocatalytic core can be constructed as the superposition of at most two elementary circuits in the König graph. In particular, autocatalytic cores involving explicitly catalyzed reactions always contain a spanning subgraph consisting of a single elementary circuit together with a simple metabolite-to-reaction chord. Moreover, we identify the essentially unique example for which at least two circuits are required.

The p-anionic Clar structures of a fullerene

Elizabeth J. Hartung [1], *Jack E. Graver* [2], *Aaron Slobodin* [3]

[1] Massachusetts College of Liberal Arts, United States
[2] Syracuse University, United States
[3] University of Victoria, Canada

A *fullerene* is a pure carbon molecule and corresponds with a 3-regular plane graph whose faces have degree 5 or 6. For a fixed integer p, a p-anionic resonance structure (F, M) of a fullerene G is a set of faces, $F \subseteq F(G)$, and a matching, $M \subseteq E(G)$, such that F contains exactly p pentagons (the remaining faces are hexagons) and each vertex of G is incident with exactly one element of $F \cup M$.

The p-anionic Clar number $C_p(G)$ of a fullerene G is the maximum value of $|F|$ over all possible p-anionic resonance structures for G. This parameter generalizes the Clar number and is motivated by the observation that in fullerene anions (negatively charged fullerenes), pentagons can compete with hexagons to host 'Clar sextets' of six electrons.

In this talk, we describe properties of p-anionic resonance structures in fullerenes, and show that the edges of M decompose into 'chains'. We introduce tools to find the p-anionic Clar numbers of fullerenes and find bounds on the p-anionic Clar numbers for families of highly symmetric fullerenes.

`Rust`-based symbolic framework for symmetry in quantum chemistry

Bang C. Huynh [1]

[1] New College, Physical and Theoretical Chemistry Laboratory, University of Oxford, United Kingdom

Symmetry provides a powerful machinery to classify, interpret, and understand quantum-mechanical theories and results. However, most contemporary quantum chemistry packages lack the ability to handle degeneracy and symmetry breaking effects, especially in non-Abelian groups, nor are they able to characterise 'exotic' symmetry under unconventional conditions, such as in the presence of an external magnetic field or when relativistic phenomena are considered. This is chiefly because these packages hard-code real-valued character tables for a limited number of point groups (mostly boolean groups) and are only capable of performing symmetry transformations in an ad hoc manner for a restricted range of quantum-chemical quantities such as molecular orbitals.

In this talk, I will introduce the symmetry framework of `QSym`^{2} (https://www.qsym2.dev) [1] that has been designed to tackle the above limitations. I will in particular describe how the powerful abstract and algebraic type system in the `Rust` programming language enables the full exploitation of the group-theoretic nature of symmetry in order for character tables of any arbitrary group to be generated analytically and symbolically using modular arithmetic [2, 3]. I will then show how this general approach paves the way for the insightful interpretation of electronic states in chemical systems involving projective symmetries that arise from the inherent coupling of spin and spatial degrees of freedom in relativistic quantum theories [4, 5], or magnetic symmetries that result from antiunitary operations when magnetic fields and time reversal are considered [6, 7], or a combination of both. If time permits, I will also illustrate the use of symmetry-assisted non-orthogonal configuration interaction to restore any broken symmetry to yield physically meaningful wavefunctions that capture static electron correlation effects and that can be attributed to actual ground and excited electronic states [8].

References

[1] B. C. Huynh, M. Wibowo-Teale and A. M. Wibowo-Teale, QSym^2: A Quantum Symbolic Symmetry Analysis Program for Electronic Structure, *J. Chem. Theory Comput.* **20** (2024), 114–133.

[2] J. D. Dixon, High speed computation of group characters, *Numer. Math.* **10** (1967), 446–450.

[3] L. C. Grove, *Groups and Characters*, Wiley, New York, 1997.

[4] T. Saue, Relativistic Hamiltonians for Chemistry: A Primer, *Chem. Phys. Chem.* **12** (2011), 3077–3094.

[5] W. Liu, Ideas of relativistic quantum chemistry, *Mol. Phys.* **108** (2010), 1679–1706.

[6] C. J. Bradley and B. L. Davies, Magnetic Groups and Their Corepresentations, *Rev. Mod. Phys.* **40** (1968), 359–379.

[7] M. Wibowo-Teale, B. C. Huynh, A. M. Wibowo-Teale, F. De Proft and P. Geerlings, Symmetry and reactivity of π-systems in electric and magnetic fields: a perspective from conceptual DFT, *Phys. Chem. Chem. Phys.* **26** (2024), 15156–15180.

[8] B. C. Huynh and A. J. W. Thom, Symmetry in Multiple Self-Consistent-Field Solutions of Transition-Metal Complexes, *J. Chem. Theory Comput.* **16** (2019), 904–930.

Searching for hypergraphs with prescribed regular automorphism groups of small orders

Robert Jajcay [1], *Isabel Hubard* [2], *Tatiana Jajcayová* [1]

[1] Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, Slovakia

[2] Institute of Mathematics, National Autonomous University of Mexico (IM UNAM), Mexico

A *k-uniform hypergraph* is a pair $(V, \mathcal{B})$ of *vertices* V paired with a family of k-subsets of V called *hyperedges*. The automorphism group of a k-uniform hypergraph $(V, \mathcal{B})$ consists of all permutations $\varphi \in \mathbb{S}_V$ that preserve the hyperedges in $\mathcal{B}$, i.e., in their induced action on the k-subsets in $\mathcal{B}$, they map the k-subsets in $\mathcal{B}$ to k-subsets in $\mathcal{B}$.

As a part of a classification project of finite groups G for which there exists a k-uniform hypergraph $(V, \mathcal{B})$ whose automorphism group is isomorphic to G and acts regularly on V, we had to resolve the problem of searching for such k-uniform hypergraphs for a given finite (small) group G. Even though the problem might appear exponential in the order of G, we have discovered several ways of making the search more efficient, and we intend to discuss these discoveries in our presentation.

Symmetry-preserving operations and the genus of graphs

Oscar Jocqué [1], *Heidi Van Den Camp*

[1] Ghent University, Belgium

Lopsp-operations, or "local orientation-preserving symmetry-preserving operations", are a general framework using which one can investigate large classes of operations on graph embeddings. Well-known examples of such operations are Dual and Truncation.

We present our research on the effect of lopsp-operations on the genus of graphs. We have been able to characterize the operations that preserve the genus on polyhedral embeddings. In addition, we present some possibly surprising results, such as the fact that the operation Dual can reduce the genus from an arbitrary high number to zero.

How symmetric do you wish your graph to be?

Pavol Kollár [1]

[1] Comenius University, Bratislava, Slovakia

The most natural interpretation of "a graph being symmetric" is that it "looks the same, no matter which vertex we are looking from." This notion is commonly known as vertex-transitivity and it is a property that is highly studied and researched in theoretical graph theory, while still having practical applications.

Cayley graphs are graphs that stem from group theory and they are always vertex-transitive, which can be seen by having the group, from which the graph was constructed, act on itself. However, not all vertex-transitive graphs are Cayley; the famous Petersen graph is the smallest example of such a "non-Cayley" graph. Having the class of vertex-transitive graphs be more granularly split has already been studied and researched by Gauyacq as well as Jajcay and Jones in their papers.

In this talk, we combine their approaches and study what is known as an "r-regular family of graph automorphisms" with the goal to create a hierarchy within the class of vertex-transitive graphs. Furthermore, we will find a number of extremal graphs, which are related to this notion.

Fractional matching extendability of Cayley graphs of Abelian groups

Boštjan Kuzman [1], *Primož Šparl* [1]

[1] University of Ljubljana, Slovenia

A fractional matching of a graph $\Gamma = (V, E)$ is a function $f\colon E \to [0, 1]$ with the property that for each vertex $v \in V$, the sum of f-values of all the edges incident to v is at most 1. When this sum equals 1 for each vertex v, the fractional matching is perfect. A graph of order at least $2t + 1$ is fractional t-extendable if it contains a matching of size t and if each such matching M can be extended to a fractional perfect matching in the sense that the corresponding function f assigns value 1 to each edge of M.

In this talk, we present results on fractional matching extendability of Cayley graphs of Abelian groups that extend the classification of 2-extendable (in the classical sense) connected Cayley graphs of Abelian groups of even order by Chan, Chen and Yu (1995).

`graphotaxy`: A graph classification system

Anthony Labarre [1]

[1] LIGM, Université Gustave Eiffel, France

The graph recognition problem involves determining whether a given graph belongs to a specific graph class. This concept naturally extends to the graph classification problem, which seeks to identify all graph classes to which a given set of graphs belongs. Such problems are relevant in various fields, including:

- Algorithms, where structural properties of input graphs are critical for the design of efficient algorithms: some NP-complete problems may become solvable in polynomial time for specific graph classes, or could allow for efficient parameterised algorithms for others.
- Structural graph theory, where researchers investigate the relationships between graph classes, aiming to discern whether two classes are equivalent or if one is a subset of another.
- Extremal graph theory, which focuses on identifying graphs that optimise specific invariants and potentially characterising extremal families of graphs.

Despite the recognised need for efficient recognition algorithms, a practical tool for tackling the classification problem has yet to emerge. In this talk, I will introduce `graphotaxy`, a software tool designed to fill that void. `graphotaxy` targets all classes in the ISGCI (`https://graphclasses.org`) that can be recognised in polynomial time and currently features 1 000 recognition algorithms. The software offers two primary modes of operation:

- For a single input graph, it outputs all minimal classes (in terms of graph class inclusion) to which the graph belongs.
- For multiple input graphs, it provides a list of all minimal classes associated with at least one input graph, along with the percentage of graphs belonging to each class, sorted by decreasing prevalence.

Maximum nullity of benzenoid graphs

Craig Eric Larson [1]

[1] Virginia Commonwealth University, United States

The nullity ν of a graph is the number of 0-eigenvalues in the spectrum of its adjacency matrix. In chemical terms this is the number of non-bonding π molecular orbitals. We will investigate the question of which benzenoids in the class of benzenoids with h hexagonal faces maximize their nullity. We will prove that ν is no more than $\lfloor \frac{h}{3} \rfloor$. Computational experiments suggest that large numbers of hexagons achieve this maximum (there are, for instance, 300 086 benzenoids with 10 hexagonal faces and 39 of these achieve a maximum nullity of 3). We will present conjectures towards the goal of characterizing these extremal benzenoids.

Self separable sets

Maruša Lekše [1], *Marco Barbieri,*
Primož Potočnik, Kamilla Rekvényi

[1] IMFM, Slovenia

In this talk, we will discuss a graph-theoretic problem and its permutation group generalization. Namely, a subset of a domain is self-separable if there exists a group element mapping it into a disjoint subset. We will be interested in the parameter sep(G), which represents the size of the smallest non-self-separable subset for a permutation group G. With the help of computational methods, we determine the groups that meet the upper and lower bounds for the parameter sep. Finally we give some graph-theoretic corollaries of studying this parameter.

On r-regular families of permutations

Martin Mačaj [1], *Pavol Kollár* [1]

[1] Comenius University, Slovakia

G. Gauyacq in 1997 introduced the notion of quasi-Cayley graphs to determine which vertex transitive non-Cayley graphs are "very close" to being Cayley. R. Jajcay and G. Jones in 2019 generalize the quasi-Cayley graphs to r-regular families of permutations where quasi-Cayley graphs are those which admit an 1-regular family of automorphisms.

By means of constructive enumeration F. Kerák in his bachelor thesis in 2020 determined the exact number of r-regular families on four points for each r and 2- and 3-regular families on five points. Using multidimensional generating functions and corresponding Fourier transformations P. Kollár and M. Mačaj in 2024 derived an upper bound on the total number of r-regular families on five points and conjectured that this bound is close to the exact value.

Further improving the above methods and using high performance cluster CLARA at Comenius University in Bratislava we determine the exact number of r-regular families of permutations on five points for each r.

Total colouring of Halin graphs

Matúš Matok [1], *František Kardoš* [2]

[1] Comenius University, Bratislava, Slovakia
[2] University of Bordeaux, Bordeaux, France

A Halin graph is a planar graph consisting of a tree with at least three leaves and an additional cycle connecting all the leaves in such manner that no two edges are crossing. We will be interested in cubic Halin graphs, i.e. graphs with all vertices of degree three. Total colouring of a graph is a mapping from the set of vertices and edges to a set of colours such that no two neighbouring objects receive the same colour.

Besides K_4 there were only 3 known cubic Halin graphs with total chromatic index greater than 4, which we managed to prove is the complete set.

The proof involves computer assistance based on the following approach. A Halin graph can be dissected into tripoles, which are Halin graphs with precisely three dangling edges, called semiedges. For each tripole we can observe what colours are admissible on the objects around semiedges. The full collection of such colourings for a given tripole is called a palette. Thanks to the tree-like structure of Halin graphs, we can compute the palette of a tripole from the palettes of its subtripoles. Moreover, it can be done in constant time, which we implemented by elementary operations over a small binary matrix. This way, we can compute the set of all realisable palettes, which allows us to precisely characterise the set of Halin graphs with total chromatic index 5.

Finding and enumerating abnormal digraphs

Maxine M. McCarthy [1], *Clara C. Wanjura* [1]

[1] Max Planck Institute for the Science of Light, Germany

An abnormal digraph is a weighted directed graph that has defective eigenvalues for almost all arc weights. This is because the network topology protects defective eigenvalues, making them robust to any changes in arc weights. Consequently the 'abnormality' of a digraph is a graph invariant.

In non-Hermitian physics, graphs with defective eigenvalues have unusual topological properties and are a promising source of potential applications to enhanced sensing, resulting from having higher order poles in their Green's functions. Typically, multiple parameters of a directed graph must be adjusted to ensure some of its eigenvalues are defective; in physics such a point is called an exceptional point. However, due to the enhanced sensitivity at an exceptional point, it is difficult in an experiment to maintain parameters that keep a physical system at a point of defective eigenvalues. This makes such devices fragile to inevitable imperfections in the physical system, and has contributed to significant controversy on the sensing application of such digraphs. One solution is to design a device using an abnormal digraph.

Despite the utility of abnormal digraphs, relatively few examples are known. We construct the set A of non-isomorphic abnormal digraphs, using a map f from an efficiently computable subset of directed graphs R. Then, using the symmetries of graphs in R, enumerate all the non-isomorphic abnormal digraphs on n vertices. In addition, we discuss properties of f, such as its preimage (including why any nut digraph in R is not in this preimage), and how the symmetries of a graph are altered under the action f.

Faithfulness in maniplexes

Antonio Montero [1]

[1] University of Ljubljana, Slovenia

Although not stated in the title, this talk is about abstract polytopes and, more specifically, how far a maniplex can be from being an abstract polytope. An abstract polytope is a flagged partially ordered set that generalises, in a purely combinatorial way, classical geometric objects such as convex polytopes, tilings of Euclidean and hyperbolic spaces, and maps on surfaces. The flag graph of a polytope is a maniplex, that is, a properly edge-coloured graph satisfying certain natural conditions. Conversely, every maniplex M has an associated incidence poset $\mathrm{Pos}(M)$. If M is the flag graph of a polytope P, then $\mathrm{Pos}(M)$ is isomorphic to P, and the flag graph of $\mathrm{Pos}(M)$ is isomorphic to M.

However, not every maniplex arises from a polytope, and there are several ways in which this correspondence can fail. Of particular interest is the notion of a faithful maniplex, for which the poset $\mathrm{Pos}(M)$ retains enough combinatorial information from M. We discuss the possible obstructions and explain how the `GAP` package `RAMP` (Research Assistant for Maps and Polytopes) was used in the development of these results.

Extremely asymmetric graphs and partial automorphisms

Ján Pastorek [1]

[1] Department of Applied Informatics, Faculty of Mathematics, Physics and Informatics, Comenius University, Slovakia

Although almost all (fullerene) graphs are asymmetric (having no nontrivial global automorphisms), they may still possess local symmetries in the form of isomorphisms between induced subgraphs, i.e., partial automorphisms. We study such local symmetries via *asymmetric depth*, defined in terms of the maximum rank of a nontrivial partial automorphism.

We prove a tight upper bound on asymmetric depth in the class of (planar) graphs and identify (planar) graphs attaining the extremal value. It turns out that these extremely asymmetric graphs can belong to interesting graphs classes.

We demonstrate that any graph achieving general upper bound for asymmetric depth must be a strongly regular graph with parameters $(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4})$ also known as a *conference graph*. We identified an asymmetric conference graph on 37 vertices that attains these bounds, thereby proving their tightness. It is a graph of the smallest possible order that attains the general bounds.

Furthermore, we restate the general bound in terms of the number of edges, which yields stronger bound for sparse graphs. It turns out that duals of IPR fullerenes of C_{90} on 47 vertices can attain maximum asymmetric depth for planar graphs.

LCF codes for chemical graphs

Tomaž Pisanski [1], *Nino Bašić* [1], *Leah W. Berman* [2],
Gábor Gévay [3], *Patrick W. Fowler* [4]

[1] University of Primorska and IMFM, Slovenia
[2] University of Alaska Fairbanks, United States
[3] University of Szeged, Hungary
[4] The University of Sheffield, United Kingdom

Chemical graphs, i.e. subcubic graphs, with a specified Hamilton cycle admit an elegant description via an LCF code that is a generalisation of the well-known LCF code for cubic graphs. In this talk we discuss some properties of such LCF codes. Hamilton cycles in cubic graphs can be classified into 11 distinct types, depending on symmetry and on the presence of main diagonals. In case of chemical graphs, the number of types increases by five.

What makes a graph interesting?

Michiel Provoost [1], *Gauvain Devillez* [2],
Jan Goedgebeur [1], *Jorik Jooken* [1]

[1] KU Leuven KULAK, Kortrijk, Belgium
[2] University of Mons, Mons, Belgium

House of Graphs (https://houseofgraphs.org/) is an online graph database. It is widely used within the graph theory community to visualize and analyze specific graphs and graph classes. This work investigates which graph properties are associated with high community interest on House of Graphs, aiming to understand why certain graphs are used frequently and what makes them "interesting" to researchers.

In this work the entirety of the House of Graphs database is analyzed, combining all available graph properties with metrics of user interaction. To this large instance set an instance space analysis methodology is applied using the MATILDA tool chain (Smith-Miles and Muñoz, 2023, see [1]) to project graph instances into a two dimensional space. Building on the patterns observed in these projections, statistical tests were performed to verify correlations between graph properties and user interest metrics.

By identifying which properties correlate with high user interest on House of Graphs, we provide researchers with guidance on what makes a graph a promising candidate for further study, independent of any specific research context. Using the previously described techniques insight is given into what makes a graph "interesting" for the broader research community.

References

[1] K. Smith-Miles and M. A. Muñoz, Instance Space Analysis for Algorithm Testing: Methodology and Software Tools, *ACM Comput. Surv.* **55** (2023), Article No. 255, https://doi.org/10.1145/3572895.

Nut graphs with two vertex and three edge orbits

Ksenija Rozman [1,2], *Primož Šparl* [1,3,4]

[1] Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia
[2] University of Primorska, FAMNIT, Koper, Slovenia
[3] University of Ljubljana, Faculty of Education, Ljubljana, Slovenia
[4] University of Primorska, Institute Andrej Marušič, Koper, Slovenia

A nut graph is a graph whose adjacency matrix is singular with one-dimensional null space spanned by a vector with no zero entries. In a recent paper, Bašić, Fowler and Pisanski proved that the automorphism group of a nut graph has more edge orbits than vertex orbits. They classified all orders for which a vertex-transitive nut graph with precisely two edge orbits exists, and conjectured that a nut graph with two vertex and three edge orbits exists for each non-prime order $n \geq 9$. They also confirmed the conjecture for all even n but it remained largely unsolved for odd n.

In this talk, we present some properties of nut graphs of odd order admitting a subgroup of automorphisms with two vertex and three edge orbits. Starting from a very general construction of graphs of odd order admitting such a subgroup of automorphisms, we derive several infinite families of nut graphs with precisely two vertex and three edge orbits. These families provided the foundation for an extensive computational search. The resulting computations show that members of these infinite families confirm the above conjecture for all odd non-prime orders up to 2 500 and for at least 99.8 percent of all odd non-prime orders up to one million.

Constructing partitioning schemes for d-dimensional manifolds

Andrés David Santamaria Galvis [1], *Russ Woodroofe* [2]

[1] IMFM, Ljubljana, Slovenia

[2] FAMNIT, University of Primorska, Slovenia

The connection between shellability and partitionability has been understood since the 1970s, with many triangulations of balls and spheres known to satisfy these properties. In this talk, we consider partitionability for other d-manifolds and present constructive tools to produce new partitionable complexes. As a particular example, we show that the dodecahedral spaces—namely the 3-dimensional projective space, the Poincaré homology sphere, and the Seifert–Weber space—admit partitionable triangulations. Our approach makes use of computational tools to decide partitionability and shellability for manageable complexes.

Walks and nut graphs in uniform threshold hypergraphs

Irene Sciriha [1], *Miriam Abdon* [2]

[1] Department of Mathematics, Faculty of Science, University of Malta, Malta
[2] Department of Mathematics, Fluminense Federal University, Brasil

A threshold graph is a special type of split graph in which the open neighborhoods of the coclique (independent) vertices lie within the clique subset forming a nested family of sets. Similarly, the closed neighborhoods of the clique vertices also form a nested set family. Threshold graphs can be constructed iteratively, starting from a single isolated vertex and adding one vertex at a time through either the disjoint union or join operation. A creative sequence is a binary string of length n that encodes a threshold graph on n vertices, where a 0 represents the addition of an isolated vertex and a 1 represents the addition of a dominating vertex.

In a k-uniform hypergraph, every edge (that is, a hyperedge) contains exactly k vertices. A k-uniform threshold hypergraph on n vertices can likewise be encoded by a binary string of length n. Notably, when $k = 2$, the k-uniform hypergraph reduces to the classical (simple) threshold graph with edge weights of 1. Thus, the spectral theory of k-uniform threshold hypergraphs elegantly generalizes the spectral theory of threshold graphs.

We show that a k-uniform threshold hypergraph and its underlying threshold graph, which share the same creative sequence, are closely connected. Specifically, the adjacency matrix $\mathbf{A}$ of a k-uniform threshold hypergraph, with appropriate edge weights, reveals a structure that mirrors the intricate properties of the threshold graph. Furthermore, we demonstrate how key aspects of spectral theory, such as main eigenvalues, walks and equitable vertex partitions, naturally extend to the setting of k-uniform threshold hypergraphs.

We show that the image of the walk matrix associated with the weighted graph of $\mathbf{A}$ coincides with the main eigenspace. For $k > 2$, each main eigenvalue μ of $\mathbf{A}$ has an eigenspace of dimension one. Moreover, we show that for each main eigenvalue μ and for $k > 2$, $\mathbf{A}$ is the adjacency matrix of a μ-nut weighted graph, that is, the μ-eigenspace is of dimension one, generated by a vector with no zero entries.

References

[1] M. Abdón, L. Portugal, R. Del-Vecchio and R. de Freitas, On the spectra of k-uniform threshold hypergraphs, 2026, to appear.

[2] R. A. Brualdi and E. Solheid, On the spectral radius of connected graphs, *Publ. Inst. Math.* **53** (1986), 45–54.

[3] V. Chvátal and P. L. Hammer, Aggregation of inequalities in integer programming, in: P. L. Hammer, E. L. Johnson, B. Korte and G. L. Nemhauser (eds.), *Studies in Integer Programming*, North-Holland, Amsterdam, volume 1 of *Annals of Discrete Mathematics*, pp. 145–162, 1977, proceedings of a Workshop held in Bonn, September 8–12, 1975.

[4] I. Damnjanović, On the maximum spectral radius of connected graphs with a prescribed order and size, *Filomat* **39** (2025), 12281–12297.

[5] R. L. Graham, D. E. Knuth and O. Patashnik, *Concrete Mathematics: A Foundation for Computer Science*, Addison-Wesley, Reading, MA, 2nd edition, 1994. See Section 5.3 for the Hockey–Stick Identity.

[6] P. Rowlinson, The main eigenvalues of a graph: A survey, *Appl. Anal. Discrete Math.* **1** (2007), 445–471.

[7] I. Sciriha and S. Farrugia, On the spectrum of threshold graphs, *ISRN Discrete Math.* **2011** (2011), 108509.

[8] I. Sciriha and I. Gutman, Nut graphs: Maximally extending cores, *Util. Math.* **54** (1998), 257–272.

Spectral properties of large fullerenes, graphene and nanotubes

Evgeny Spodarev [1], *Artur Bille* [1], *Victor Buchstaber* [2], *Simon Coste* [3], *Pavel Ievlev* [4], *Svyatoslav Novikov* [4], *Satoshi Kuriki* [5]

[1] Ulm University, Germany
[2] Steklov Mathematical Institute, Moscow, Russian Federation
[3] Université de Paris VII, France
[4] University of Lausanne, Switzerland
[5] Institute of Statistical Mathematics, Tokyo, Japan

This talk presents recent results on the spectral theory of carbon allotropes, with emphasis on adjacency spectra, closed walk counts, and limiting spectral distributions.

We begin with the spectral clustering of fullerene isomers. Fullerenes are finite 3-regular planar graphs with exactly twelve pentagons and $n/2 - 10$ hexagons. Using adjacency spectra and Newton polynomials, we analyze structural similarity between isomers and show how spectral data reflect the combinatorics of their facet graphs. This raises asymptotic questions on the empirical spectral distributions of large fullerenes.

We then pass to the infinite hexagonal lattice (graphene) and its dual triangular lattice. The number μ_k of closed walks of length k at a vertex forms the moment sequence of a probability measure, interpreted as the spectral measure (random eigenvalue) of the lattice. We derive explicit formulas for the corresponding density, characteristic function, and moment generating function. The analysis relies on a new integral identity for the series $\sum_{n\in\mathbb{Z}} I_n(2x)^3$ of modified Bessel functions and establishes connections with planar random flights and ergodic averages.

Next, we consider infinite dual (p, q)-nanotubes obtained by periodic identifications of the triangular lattice. We obtain explicit representations of their random eigenvalues as functions of independent uniform random variables, compute moments and MGFs, and prove weak convergence of their spectral distributions to that of graphene as $p + q \to \infty$.

We conclude with open problems, including the conjectured Benjamini–Schramm convergence of random fullerenes to the hexagonal lattice and the resulting convergence of empirical spectral distributions.

Algorithms for the generation of snarks

Steven Van Overberghe [1], *Gunnar Brinkmann* [1]

[1] Ghent University, Belgium

Snarks are cubic, cyclically 4-edge-connected graphs that are not 3-edge-colourable. They are significant in graph theory as potential minimal counterexamples to several conjectures. Consequently, complete lists of snarks are desirable. However, developing efficient algorithms for their generation remains a computational challenge.

We present two new algorithms to exhaustively generate all snarks of fixed order. The first uses the canonical construction path method, and targets snarks with girth exactly 4. It was utilized to generate complete lists of such graphs up to 40 vertices. The second algorithm is based on the technique of orderly generation, and generates snarks with girth at least 5. It was used to produce all such graphs up to 38 vertices.

Computer-assisted determination of stability of chemical compounds

Henryk Witek [1]

[1] Department of Applied Chemistry, National Yang Ming Chiao Tung University, Taiwan

Quantum chemical determination of molecular properties relies on computer codes derived from quantum mechanics. Recent years show that many results of such calculations can be obtained in a cheaper way from appropriately-parameterized machine-learning models based on molecular descriptors, often related to the topology of chemical connections inside the studied molecules. It is natural to represent the bond topology as a graph, and the resulting molecular descriptors, as the corresponding graph invariants, making a natural connection between computational chemistry, graph theory, and enumerative combinatorics.

In my talk, I will discuss several aspects of such connections, including the problem of finding appropriate molecular quantum chemical descriptors, computer-assisted determination of Clar covers for polycyclic aromatic hydrocarbons and fullerenes, combinatorial techniques for enumeration of Clar covers, the automatized computer codes developed in my group for such enumerative combinatorics problems, and their applicability in quantum chemical modeling. Most of these results could not have been obtained without `ZZPolyCalc` and `ZZDecomposer`, the automatized graphical interface for proof-oriented combinatorial computer environment developed in our group.

References

[1] R. Podeszwa, H. A. Witek and C. P. Chou, ZZPolyCalc: An open-source code with fragment caching for determination of Zhang-Zhang polynomials of carbon nanostructures, *Comput. Phys. Commun.* **301** (2024), 109210.

[2] Hendra and H. A. Witek, Energy decomposition scheme for rectangular graphene flakes, *Nanomaterials* **14** (2024), 181.

[3] J. Langner and H. A. Witek, ZZ polynomials of regular m-tier benzenoid strips as extended strict order polynomials of associated posets. Part 2. Guide to practical computations, *MATCH Commun. Math. Comput. Chem.* **88** (2022), 109–130.

[4] C. P. Chou and H. A. Witek, ZZDecomposer: A graphical toolkit for analyzing the Zhang-Zhang polynomials of benzenoid structures, *MATCH Commun. Math. Comput. Chem.* **71** (2014), 741–764.

List of Participants

Marién Abreu, *Università degli Studi della Basilicata – DiSBA, Italy*

Milica Anđelić, *Kuwait University, Kuwait*

Vesna Andova, *Ss. Cyril and Methodius University, North Macedonia*

Cate S. Anstöter, *University of Glasgow, Scotland*

Jörg Arndt, *Technische Hochschule Nürnberg, Germany*

Martin Bachratý, *Slovak University of Technology, Slovakia*

Nino Bašić, *University of Primorska and IMFM, Slovenia*

Katja Berčič, *University of Ljubljana and IMFM, Slovenia*

James L. Borg, *University of Malta, Malta*

Marston Conder, *University of Auckland, New Zealand, and University of Primorska, Slovenia*

Ivan Damnjanović, *University of Primorska, Slovenia, and University of Niš, Serbia*

Akbar Davoodi, *University of Southern Denmark, Denmark*

Gauvain Devillez, *University of Mons, Belgium*

Timothy K. Dickens, *Peterhouse, Cambridge, United Kingdom*

Valentin Dusollier, *University of Mons, Belgium*

Patrick W. Fowler, *University of Sheffield, United Kingdom*

Jan Goedgebeur, *KU Leuven, Belgium*

Richard Golnik, *Leipzig University, Germany*

Elizabeth J. Hartung, *Massachusetts College of Liberal Arts, United States*

Bang Huynh, *New College, Physical and Theoretical Chemistry Laboratory, University of Oxford, United Kingdom*

Robert Jajcay, *Faculty of Mathematics, Physics and Informatics of the Comenius University in Bratislava, Slovakia*

Tatiana Jajcayová, *Comenius University, Bratislava, Slovakia*

Oscar Jocqué, *University of Ghent, Belgium*

Pavol Kollár, *Comenius University, Bratislava, Slovakia*

Boštjan Kuzman, *University of Ljubljana, Slovenija*

Anthony Labarre, *LIGM (Université Gustave Eiffel), France*

Craig E. Larson, *Virginia Commonwealth University, United States*

Márk Légrádi, *Hungary*

Maruša Lekše, *IMFM, Slovenia*

Martin Mačaj, *Comenius University, Slovakia*

Matúš Matok, *Comenius University, Slovakia*

Maxine M. McCarthy, *Max Planck Institute for the Science of Light, Germany*

Elías Mochán, *Northeastern University, United States*

Antonio Montero, *University of Ljubljana, Slovenia*

Hadrien Mélot, *Université de Mons, Belgium*

Ján Pastorek, *Comenius University in Bratislava, Slovakia*

Tomaž Pisanski, *University of Primorska and IMFM, Slovenia*

Primož Potočnik, *University of Ljubljana, Slovenia*

Michiel Provoost, *KU Leuven KULAK, Belgium*

Ksenija Rozman, *IMFM, Slovenia*

Andrés David Santamaría Galvis, *IMFM, Slovenia*

Kocherlakota Satya Pritam, *Pandit Deendayal Energy University, India*

Irene Sciriha, *Dept of Mathematics, Faculty of Science, University of Malta, Malta*

Evgeny Spodarev, *Ulm University, Germany*

Nico Van Cleemput, *Ghent University, Belgium*

Steven Van Overberghe, *Ghent University, Belgium*

Henryk Witek, *NYCU, Taiwan*

Speaker Index

Inštitut za matematiko, fiziko in mehaniko