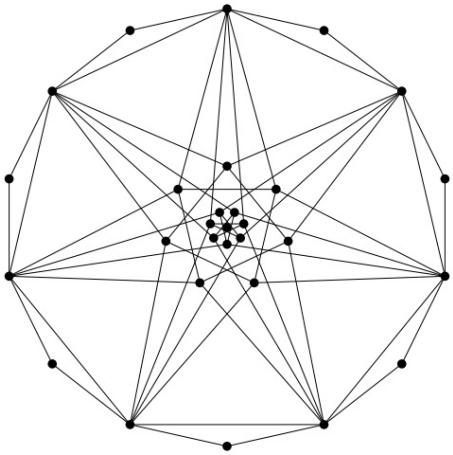

Abstracts of the Workshop

COMPUTERS IN SCIENTIFIC DISCOVERY 6 (CSD6)

Portorož, Slovenia, 21 – 25 August 2012

UP IAM
August 2012

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WELCOME

We thank all of you for coming and wish you a pleasant and successful workshop in Portorož.

Computers and Scientific Discovery 6 aims to continue the deliberately multidisciplinary emphasis of these conferences, provide space for collaborations and follow-up on results of the previous meetings, and expand even further the range of topics covered. As the first of the series to be held in Slovenia, CSD6 will benefit from the strong local tradition of research in pure and applied graph theory.

Much of the importance of interdisciplinary meetings comes from their influence in breaking down "language barriers" between fields, and in opening the eyes of researchers in one field to the expertise and challenges available in another. Our workshop format, which combines formal presentations from invited speakers with contributed talks, and builds in plenty of time for free discussion between active researchers, is designed to facilitate these aims.

Tomaž Pisanski
Klavdija Kutnar
Patrick Fowler

Portorož, August 21, 2012

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General Information

Computers in Scientific Discovery 6 (CSD6)
Portorož, Slovenia, 21 – 25 August 2012.

Organized by:
UP IAM *(Andrej Marušič Institute, University of Primorska)*.

In Collaboration with:
IMFM *(Institute of Mathematics, Physics and Mechanics)*,
UL FMF *(University of Ljubljana, Faculty of Mathematics and Physics)*,
UP FAMNIT *(University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies)*,
UP TURISTICA *(University of Primorska, Faculty of Tourism Studies)*.

Sponsored by:
ARRS *(Slovenian Research Agency)*,
ESF EUROCORES/EuroGIGA project GReGAS *(European Science Foundation, EUROCORES programme, EuroGIGA call, project GReGAS - Graphs in Geometry and Algorithms, Geometric representations and symmetries of graphs, maps and other discrete structures and applications in science)*,
ESRR KC Class *(European Regional Development Fund, competence center Cloud Assisted Services)*.

Scientific Committee:
Tomaž Pisanski (chair), Patrick Fowler, Klavdija Kutnar.

Organizing Committee:
Klavdija Kutnar (chair), Boštjan Frelih, Ademir Hujdurović, Alen Orbanić, Tomaž Pisanski.

Conference Venue:
University of Primorska, Faculty of Tourism Studies, Obala 11a, SI-6320 Portorož - Portorose, Slovenia.

Conference Website:
http://csd6.imfm.si

Conference Information:
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KEYNOTE SPEAKERS:
Oswin Aichholzer, *Graz University of Technology, Austria*
Alexandru Balaban, *Texas A&M University at Galveston, USA*
Gunnar Brinkmann, *Ghent University, Belgium*
Arnout Ceulemans, *K.U.Leuven, Belgium*
Kris Coolsaet, *Ghent University, Belgium*
Patrick Fowler, *University of Sheffield, UK*
Ante Graovac, *University of Split, Croatia*
Adalbert Kerber, *University of Bayreuth, Germany*
Harold Kroto, *The Florida State University, USA*
Bojan Mohar, *SFU, Canada & IMFM, Slovenia*
Milan Randić, *National Institute of Chemistry, Slovenia*
Dragan Stevanović, *University of Nis, Serbia & University of Primorska, Slovenia*
Ian Wanless, *Monash University, Australia*
Jure Zupan, *National Institute of Chemistry, Slovenia*

Special Events

Wednesday, August 22:

- Workshop Excursion.

Friday, August 24:

- Milestones: On the Development of Graph Theory in Slovenia, Boštjan Kuzman, University of Ljubljana and IMFM, Slovenia (poster exhibition).

  Since its very modest beginnings in the 1970's, Graph Theory in Slovenia has grown to become one of the most fruitful and internationally recognized branches of Slovenian scientific output today. The exhibition presents a set of posters, called Milestones. Each of them represents a certain step, either major or minor, in the development of the field in Slovenia: from the first lecture notes, scientific results, published papers and doctoral theses to international collaborations, celebrated publications, editorial positions, establishment of new institutions, scientific journals and other projects.

- Workshop Reception.

- Workshop Dinner.

PAST WORKSHOPS

This workshop is the sixth in a series that started in November 2001 with the Workshop of the DIMACS Working group on Computer-Generated Conjectures from Graph Theoretic and Chemical Databases, and and extends the earlier Discrete Mathematical Chemistry workshop (1998) also held at DIMACS. The events demonstrated the existence of an enthusiastic community of researchers on several continents active at the interfaces between chemistry, computer science and discrete mathematics.

Computers and Discovery (Workshop 2, Montreal, June 2004) concentrated on the nature of conjecture-making. Nevertheless, several chemical and mathematical software collaborative applications were initiated, such as the "House of Graphs" concept proposed by Pierre Hansen, which aims to align the efforts of groups working on implementing graph algorithms and developing user interfaces for automation of graph handling and conjecture making.

Computers and Scientific Discovery 3 (Ghent, 2006), the first of the series to take place in Europe, concentrated on computer implementation, with direct contact to potential scientific users. To keep developers of mathematical software in touch with their 'customers', theoretical/mathematical chemistry applications were emphasised, and the scope was extended to mathematical biology and bioinformatics.

The next meeting Computers and Scientific Discovery 4 (Shanghai, 2008) again moved to a new continent and carried forward the theme of the connections between the biosciences, mathematics and computer science.

Computers and Scientific Discovery 5 (Sheffield, 2010) kept up the strong connections and co-operations resulting from the previous workshops and made new contacts between those working on mathematical and software projects and potential users and applications in other fields. Contributions covered topics in graph theory, pure and applied, algorithms and software, and a ranges of applications drawn from chemistry, bioinformatics, physics, communications engineering and even basket weaving.

A FEW WORDS ABOUT THE UNIVERSITY OF PRIMORSKA

The University of Primorska (Univerza na Primorskem Universita del Litorale; UP) was established by the Slovenian parliament on January 29, 2003 and was registered at the District Court of the city Koper on **3 March, 2003** thus becoming a legal entity.

The UP is a **public institution**, financed by the Slovenian Government. The activities of the UP are focused on offering **high-quality study programs, active inclusion of students in research work and researchers in teaching, and on internationally comparable achievements in the fields of research and education**.

Members of the University of Primorska:

- Faculty of Built Environment;
- Faculty of Humanities;
- Faculty of Management;
- Faculty of Mathematics, Natural Sciences and Information Technologies;
- Faculty of Education;
- Faculty of Tourism Studies;
- Faculty of Health Care.

Two research institutes:

- Science and Research Centre;
- Andrej Marušič Institute.

- University Library;
- Students' Residence.

One associate member:

- College of Design Ljubljana.

International Cooperation

The UP strives to strengthen the international and cross-border cooperation and projects.

- Fields of project cooperation: research, education, applied sciences, student and faculty mobility.
- Themes of project cooperation: Intercultural dialogue, Languages, Cultural heritage, History, Anthropology, Geography, Education, Sociology, Management, Tourism, Environment, Agriculture, Health, Mathematics, Informatics, Kinesiology and Ergonomics, etc.
- Partner institutions from: Austria, Croatia, Denmark, Estonia, Finland, France, Germany, Hungary, Italy, Lithuania, Netherlands, Norway, Poland, Spain, UK, etc.

Keynote Talks

The Order Type Data Base

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Many Problems in Computational Geometry and geometric Graph Theory are based on the most simple geometric objects: points in the plane and straight line segments connecting them. Moreover, for most combinatorial questions in this area only the "discrete" properties of the underlying point set have to be considered. More precisely, the crossing properties of the complete straight line graph spanned by the point set completely determine all combinatorial characteristics. These intersection properties can be coded by the *order type* of a point set $\{p_1,...,p_n\}$, established by Goodman and Pollack in 1983 [1]. The order type is defined as a mapping that assigns to each ordered triple i,j,k in $\{1,...,n\}$ the orientation (clockwise or counterclockwise) of the triple (p_i,p_j,p_k). Two point sets have the same order type if there is a bijection π between these two sets such that for every triple p_i,p_j,p_k of the first set, the corresponding points $\pi(p_i),\pi(p_j)$, and $\pi(p_k)$ have the same orientation. This allows to reduce the "infinite" problem of considering "all sets of points of size n" to a finite, combinatorial problem, and thus, to make it accessible for computer investigations.

In recent years a complete order type data base for sets of cardinality $n \leq 11$ has been established, which is available online [2]. It has been shown that this data base is complete, that is, it contains all the realizable, nonequivalent order types for $n \leq 11$ points in general position (that is, no collinear triples). Moreover, each order type is presented as a realizing point set with small integer coordinates, such that computations can be performed efficiently and without numerical problems.

With the help of this data base – and partial extensions of it – already a vast number of problems from Computational Geometry and Graph Theory has been successfully investigated. Questions include intersection properties (crossing numbers), triangulations, perfect matchings, spanning trees and -paths, Erdős-Szekeres type questions like convex (empty) k-gons and generalizations of it, to just name a few. We will report on several of the obtained results as well as on the generation and extension of the data base.

Finally we will also discuss alternative versions of the order type, like colored versions, a globally directed order type, a geodesic order type, and applications of them.

References:

[1] J.E.Goodman, R.Pollack, *Multidimensional sorting.* SIAM J. Computing 12 (1983), 484-507.
[2] O. Aichholzer, *Enumerating Order Types for Small Point Sets with Applications.*
http://www.ist.tugraz.at/aichholzer/research/rp/triangulations/ordertypes/

Dualists of Two-Dimensional and Three-Dimensional Classes of Molecules: Benzenoids and Diamondoids

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The traditional allotropic forms of carbon, multilayer graphene and diamond, are "honorary hydrocarbons" with huge numbers of carbon atoms surrounded by a negligible number of hydrogen atoms. Enumerations of benzenoids should consider both definitions, including or excluding helicenes. Dualists offer simple classifications for catafusenes, perifusenes, and coronoids as having acyclic, triangular, or larger rings, respectively. Catafusenes can be encoded simply by means of numbers formed by digits $0, 1, 2$. Eric Clar developed a 'winner-takes-all' theory for aromatic sextets. Claromatics are the most stable among isomers. Biparametric correlations in terms of numbers of rings and of longest acene chains operate well in QSAR. Dias produced formula periodic tables for benzenoids based on two types of quaternary carbons. Diamondoids can be classified into catamantanes (regular or irregular), perimantanes, and coronamantanes according to their dualists, which are isomorphic to staggered alkane rotamers. The Balaban-Schleyer simple coding of catamantanes in terms of numbers formed by digits $1, 2, 3, 4$ is now generally accepted based on their dualists. Diamondoids can also be grouped in formula periodic tables using partitioned formulas according to quaternary, tertiary, and secondary CH_n groups ($n = 0, 1$, and 2, respectively), and information about their dualists. The table for regular catamantanes presents interesting symmetries, but for irregular ones the situation is more complicated and not fully understood. Invariants for dualists helped in assigning structures to chromatographically separated diamondoids from petroleum. A few computational challenges are listed.

Snarks – and Beyond?

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Klas Markström
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In this talk I will sketch an algorithm to generate Snarks – that is cubic cyclically 4-connected graphs with chromatic index 4. Snarks are especially interesting as for several conjectures it can be shown that if they wrong, the smallest counterexample is a Snark. I will also give some examples of conjectures that were refuted with the lists generated by the algorithm.

As we are now able to generate very large sets of snarks, the question arises whether it is possible to further restrict the class and still keep the property that the class contains smallest possible counterexamples for a lot of conjectures.

This is joint work with Jan Goedgebeur, Jonas Hägglund and Klas Markström.

The Jahn-Teller Theorem for Graphs

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Molecular stability and electronic degeneracy do not form an evident combination. In degenerate states of highly symmetric molecules, there is a mismatch between the symmetries of electronic and nuclear charge distributions. This imbalance gives rise to a spontaneous distortion of the nuclear frame to a lower symmetry, which lifts the degeneracy. The effect is known as the Jahn-Teller (JT) effect. Based on the analogy between molecules and graphs, the following conjecture was made: whenever the spectrum of a graph contains a set of bonding or anti-bonding degenerate eigenvalues, the roots of the Hamiltonian matrix over this set will show a linear dependence on edge distortions, which has the effect of lifting the degeneracy. When the degenerate level is non-bonding, distortions of vertex weights have to be included to obtain a full resolution of the eigenspace of the degeneracy [1].

In this lecture we will establish the strict analogy between JT instabilities in molecules and graphs for the special case of the simplex structures, represented by the complete graphs, K_n. The proof is based on the irreducible representations of the symmetric group, S_n, and consists of two parts: a molecular part in which the simplex is treated as a geometric structure, consisting of equivalent sites, which can undergo distortions, and a graph-theoretical part, which derives the symmetries of changes of the edge weigths.

The complete graph is found to represent the ideal case, where the Jahn-Teller effect is 'symmetry-precise'. Deviations from the ideal case may be 'symmetry- deficient'. This is the case when not all of the coupling operators that give rise to the lifting of the degeneracy, have a counterpart in the space of edge distortions. Symmetry-deficiency raises intriguing questions about the distortivity of graphs with degenerate eigenvalues.

References:

[1] Ceulemans, A.; Lijnen, E.; Fowler, P. W.; Mallion, R. B.; Pisanski, T., *Graph theory and the Jahn-Teller theorem.* Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, vol. 468, issue 2140, pp. 971-989 (2012)

Classifying the Complete Arcs in Small Projective Planes

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Heide Sticker
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An arc is a set of points in a projective plane with the property that no three of them are on the same line. An arc is called complete if no point can be added to it so that it still remains an arc. The conic serves as the standard example of a complete arc, but many other constructions are known.

Although arcs are relatively small (at most $q+2$ points in a finite projective plane of order q and at most $q+1$ if q is odd), only for really small values of q (say, $q < 10$) it is possible to find all complete arcs in a plane by hand, and classify them up to isomorphism.

Until five years ago, a full (computer) classification of the complete arcs in Desarguesian projective planes was only known for $q < 20$. We managed to extend this bound to $q = 29$. The algorithm we have used is based on the well-known process of 'canonical augmentation', introduced in the 1980's by Brendan McKay. In this talk I will give a sketch of the algorithm as it was applied to our problem.

Instead of generating all complete arcs, it is also of interest to focus on certain special cases, for example, arcs that have a 'large' number of points ($q-1$ in particular). It was proved that for $q > 89$, q odd, an arc of size $q-1$ can always be extended to a conic, and except for two sporadic examples ($q = 7, 13$), it is believed that this property holds for all (odd) values of q.

I shall describe an algorithm that might be used to settle the remaining cases within reasonable time, by classifying the larger arcs without having to generate all the smaller arcs as well.

Molecular Currents, Harmonics, Conjugated Circuits and Aromaticity

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Aromaticity is an elusive chemical concept, with many definitions, but it does have at least one clear manifestation in 'ring currents' induced in planar unsaturated molecules by perpendicular magnetic fields. Efficient ab initio calculation of such currents is now a practical possibility. The resulting current-density maps allow us to visualise aromaticity and to develop interpretations and test simpler mathematical models. It turns out that surprisingly simple models give clues about molecular electronic structure and help us identify new classes of aromatics. Most models are counting something (electrons, nodal lines in cylindrical harmonics, conjugated circuits, benzene-like hexagonal rings, ...) and all have different insights to offer. This contribution discusses some ways in which combinatorics and graph theory can be applied to the theory of molecular currents in chemistry.

The talk includes work done in collaboration with computer scientists (Wendy Myrvold and William Bird, University of Victoria, Canada) and with chemistry research groups in Utrecht (Jenneskens), Groningen (Havenith), Leuven (Ceulemans) and Melbourne (Soncini).

On Topology Versus Geometry in Molecules

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Graphs can be drawn in an infinite number of ways. However, by analysis of eigenvectors of adjacency and Laplacian matrices of molecular graphs one is able to get drawings which reproduce rather well geometries in some classes of molecules like fullerenes, nanotubes and their junctions. The results obtained up to now will be discussed and possible new routes to generalize graph drawing techniques will be discussed.

This presentation is a result of collaboration with Istvan Laszlo (Budapest) and Tomaž Pisanski (Ljubljana).

Computers in Chemistry: Molecular Structure Generation and Applications

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The standard model of molecule (on the topological level of abstraction) is an unlabeled colored multigraph, expressing by its nodes the atoms, by its (multiple) edges the covalent bonds. The nodes are colored by atom names and states. But there are problems, the model expresses pairwise interactions only, so the notion of aromaticity shows that it should be generalized, maybe to a hypergraphic model. Since the graphs are unlabeled, they are orbits of a specific action of a symmetric group. MOLGEN generates such structural formulas, and it can be used in order to construct molecular libraries, for example patent libraries in such a way that two of them can easily be compared according to patent violations. Another important application is molecular structure elucidation.

Science, Lost in Translation?

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Fluency in a language is fundamental to an understanding of any culture and the struggle to develop the language of the Sciences, mathematics and related symbolism, proved to be unnaturally difficult. In fact Science was born around the time of the 16th Century as a consequence of a new philosophical approach which required evidence for the validation of all claims without exception. This way of thinking suddenly uncovered the fact that the common-sense attitudes that are necessary for basic survival are actually quite unreliable when it comes to understanding how the Universe works. So Natural Philosophy, which is the only philosophical construct we have to determine truth with any degree of reliability, was born. The Enlightenment was the byproduct of this philosophical breakthrough and Science its Prodigal Son. From the moment of birth this philosophy has engendered conflict with those who claimed authority, and indeed still hold great sway over society, on the basis of unsubstantiated and unsubstantiatable dogma. This conflict continues to this day as mystical and other dogma-based attitudes are intrinsically impervious to rational argument and will, almost certainly, lead to serious consequences for the human race in the future. Science, arguably the most influential factor in shaping the modern world, has been so incredibly successful that most no longer need even common sense (at least in the developed world) to survive.

Although there have been negative consequences most people would feel that society has in general benefited greatly from the application of scientific advances ie Technology. However this very usefulness has obscured the fact that Science, aka Natural Philosophy, is actually a supremely cultural, intellectual and, most importantly, an intrinsically ethical activity, particularly with regard to deciding what is or can be true. As so few people are mathematically literate it is not surprising that there is little real understanding of what Science is or how scientific advances are made. This is a dangerous situation as this illiteracy applies to almost all politicians and administrators who have responsibility for making socio-economic decisions involving scientific and technological matters. Furthermore The Enlightenment, which can only survive in a democratic environment, is under threat as those who arrogate their power and influence through dogma, mystical dogma in particular, are conspiring to drag humanity back into a Second Dark Age.

There is only one hope and this resides in a massive global educational offensive to improve the general level of knowledge and thinking. Although knowledge cannot guarantee good decisions, common sense suggests that wisdom is an unlikely consequence of ignorance. Fortunately there has been a major advance in that the birth of the Internet offers the second most important advance in education since the invention of the printing press. I would argue that Wikipedia is an amazing example of what can be achieved. Our GEOSET programme (www.geoset.info see also www.vega.org.uk) is a related project which aims to harness the efforts of educators via the Internet in a synergistic exercise to improve the knowledge and understanding of people wherever they are in the World and in particular help teachers achieve this end.

Large Eigenvalues of Graphs

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How many large eigenvalues can a graph have? An answer depends on the interpretation of what it means for en eigenvalue to be large. This question and some related problems in extremal algebraic graph theory will be discussed.

Recent Developments in Chemical Graph Theory and Graphical Bioinformatics

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Chemical Graph Theory is concerned with analysis of chemical data using Discrete Mathematics and Graph Theory. Graphical Bioinformatics approaches problems of Bioinformatics by representing input data graphically and follows with their numerical analysis. We will consider recent developments in these areas including: (1) Novel graph matrices and novel graph invariants; (2) Graph theoretical calculation of ring currents in molecules; (3) Comparative study of maps focusing on proteomics maps; (4) Analytical solution to DNA and protein sequence alignments. RE 1: Novel graph matrices include the DMAX, the elements of which are the largest entries (entry) in each row and column of the distance matrix; and the Common Vertex matrix, the elements of which are given by the number of vertices at equal distance from vertices (i, j). Novel invariants include the ordered row sums and the sum over all atoms of the quotients of path/walk counts of the same length. RE 2: We will illustrate how enumerations of contributions of π-electron currents in conjugates circuits, which are of opposite direction in $4n+2$ and $4n$ circuits, give results that are comparable to ab initio quantum chemical calculations of π-current densities. This opens fundamental question: How can discrete and continuous models yield similar results? RE 3: We consider the problem of canonical labels for map elements and will illustrate how information contained in a triplet (x, y, z) can be graphically represented as a 2D map using weighted Voronoi domains. Finally, RE 4: We will outline VESPA (Very Efficient Search for Protein Alignment) and VESNA (Very Efficient Search for Nucleotide Alignment), very recent exact analytical solutions to protein and DNA alignments, respectively, which awaited over 40 years to be found. All hitherto obtained solutions to the protein and DNA alignments have been based on use of computer algorithms, starting with: Needleman–Wunsch algorithm (1970), followed by Smith–Waterman algorithm (1981), and more efficient algorithms FASTA of David J. Lipman and William R. Pearson (1985) and BLAST (Basic Local Alignment Search Tool) by David J. Lipman et al. (1990).

Spectral Approaches to Community Detection

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Community detection is an important part of the analysis of naturally occuring networks. The quality of division into communities is measured mostly by modularity, representing the difference from the expected number of edges occuring within and between the communities. Here we reinterpret modularity within a more general framework for measuring the quality of community division and discuss on real-world examples a few related community division measures, related to the eigenvectors of the extremal eigenvalues of the adjacency and the normalized Laplacian matrices of network's complement. Due to expected large size of naturally occuring networks, we further study the result of using a new local search method for improving the quality of spectral division as opposed to the standard Kernighan-Lin heuristic.

Symmetries of Latin Squares

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A Latin square of order n is an $n \times n$ matrix containing n different symbols (often the numbers $1,\ldots,n$), positioned in such a way that each symbol occurs exactly once in each row and exactly once in each column. Latin squares have numerous applications in design of experiments, schedules for sporting tournaments, codes for communication and so on. In this talk I will consider, from a pure mathematical perspective, the possible symmetries of Latin squares. Consider the following examples:

$$A = \begin{pmatrix} 3 & 6 & 1 & 2 & 5 & 4 \\ 4 & 1 & 2 & 3 & 6 & 5 \\ 5 & 2 & 3 & 4 & 1 & 6 \\ 6 & 3 & 4 & 5 & 2 & 1 \\ 1 & 4 & 5 & 6 & 3 & 2 \\ 2 & 5 & 6 & 1 & 4 & 3 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 6 & 5 & 2 & 3 & 4 & 7 \\ 6 & 2 & 7 & 3 & 5 & 1 & 4 \\ 5 & 7 & 3 & 1 & 4 & 6 & 2 \\ 2 & 3 & 1 & 4 & 7 & 5 & 6 \\ 7 & 4 & 2 & 6 & 1 & 3 & 5 \\ 3 & 5 & 4 & 7 & 6 & 2 & 1 \\ 4 & 1 & 6 & 5 & 2 & 7 & 3 \end{pmatrix}$$

The square A has an obvious pattern whereby the numbers occur in the same cyclic order in each column. Mathematically, we capture this idea by saying it has a symmetry that applies the cyclic permutation (123456) to the rows, and the same permutation to the symbols. The square B has a less obvious symmetry that applies the permutation (123)(4)(567) to the rows, columns and symbols at the same time.

Given 3 permutations α,β,γ, does there exist a Latin square which has a symmetry whereby α is applied to the rows, β is applied to the columns and γ is applied to the symbols, but overall the square is unchanged? If so then (α,β,γ) is called an *autotopism*. The special case when $\alpha=\beta=\gamma$ (as it did in example B above), is known as *automorphism*.

I will consider the question of which permutations can be used to build autotopisms and automorphisms. The (partial) answers that I provide will be a nice blend of theory and computation, with both aspects facilitating each other.

Computers and Linguistics

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One of the promising fields in linguistics deals with the 'meanings' of sentences and words. In the present talk two cases will be discussed to show how various computer methods can be applied to the linguistic problems. The first case shows is the use of Kohonen Self-organizing maps- SOM (a special method of Artificial neural networks (ANNs) for studying and comparison of different styles of writers and poets, while the second case will show how a large scale hierarchical network organized around the concept of 'meanings' of words can be used for the corpuses of text.

In the frame of the first case two examples will be shown. In both examples 2D Kohonen SOM mapping of a) six to seven short texts of seven authors and b) 30 poems of 3 different Slovenian poets will be shown and the results discussed. As the second case, the general scheme of a hierarchical network of 'meanings' of words will be discussed. As an example a network of 15,000 Slovenian verbs will be explained in detail with the reference to its use of 'context' retrieval from large corpuses.

Other Talks

Digenes, a New Tool Using Genetic Algorithms for Directed Extremal Graph Theory

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There are nowadays many automated systems [3] helping researchers in graph theory, such as Graffiti (1987) [2], AutoGraphiX (AGX) (2000) [1] and Graphedron (2008) [4]. However, no system has been developed for directed graphs. Moreover, as most of existing systems use exact (and costly in time) algorithms, new approaches are needed. We introduce here Digenes, a new tool for directed extremal graph theory using genetic algorithms. This system has three main features. Firstly, given a class of graphs and a graph invariant, it allows to automatically find supposed extremal graphs for this invariant, using genetic algorithms. Moreover, given a graph transformation and a property, the system is able to heuristically check whether the property is hold before and after the transformation. Finally, Digenes is able to track invariant evolution under graph transformation.

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[2] FAJTLOWICZ , S. Written on the Wall. A regulary updated file accessible from
http://www.math.uh.edu/ clarson/

[3] HANSEN , P., and MÉLOT, H. Computers and Discovery in Algebraic Graph Theory. Linear Algebra and its Applications 356 (2002), 211 – 230.

[4] MÉLOT, H. Facet defining inequalities among graph invariants : the system GraPHedron. Discrete Appl. Math. 156 (2008), 1875–1891

Bootstrap Percolation and Cube Dismantling

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An $n \times n \times n$ cube is made from n^3 unit cubes. Two such cubes are neighbours if they touch along a face. In each step of a dismantling process, we may remove a small cube that has precisely three neighbours. A move is *balanced* if the three neighbours are in three orthogonal directions. In the extremal case, there are n^2 independent small cubes left at the end of the dismantling. We call this set of cubes a *solution*. If a solution is projected in three orthogonal directions and we get the entire $n \times n$ square in each direction, then the solution is *perfect*.

We show that it is possible to use a greedy algorithm to test whether a set of cubes forms a solution. For every $n \geq 2$ we find at least n perfect solutions, and we use our greedy algorithm to count the perfect solutions for $n \leq 6$. Perfect solutions turn out to be precisely those which can be reached using only balanced moves. Every perfect solution corresponds naturally to a Latin square.

If our dismantling process is reversed we get a build-up process very closely related to well-studied models of bootstrap percolation. We show that in an important special case our build-up reaches the same maximal position as bootstrap percolation.

There are several computational aspects in the above discoveries. We will highlight these segments in our presentation.

Realizability of $(12_4, 16_3)$ Configurations

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A *combinatorial configuration* (v_r, b_k) is an incidence structure with v points and b blocks (called lines) such that each point is incident with r lines, each line is incident with k points and two distinct lines are incident with at most one common point. When $v = b$ (and consequently $r = k$) we speak of *symmetric* or *balanced* (v_r) configurations.

One of the oldest problems studied in this field is possibility of a *realization* of points and lines of a combinatorial configuration with points and lines in the Euclidean plane. Most of the research was done on (v_3) configurations. In this case we can reduce the problem of realization to looking for (non-trivial) solutions of a single polynomial equation.

In this talk we focus on $(12_4, 16_3)$ configurations. This is, after the single $(9_4, 12_3)$ configuration (affine plane of order three), the smallest possible case for (v_4, b_3) configurations. Although such configurations were first studied more than 150 years ago, there are still many unresolved questions, in particular, the problem of realizability remains almost untouched. We show that the problem of realizability of $(12_4, 16_3)$ configurations involves solving a system of three polynomial equations. Each of 574 $(12_4, 16_3)$ configurations is considered by solving the corresponding system of equations by a polynomial homotopy, using the PHCpack solver. An analysis of the results will be presented.

Network Analysis of Publications on Topological Indices

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In chemical graph theory a topological index is a molecular descriptor that is calculated on the basis of molecular graph of a chemical compound. They are used for example in QSAR approach in which the biological activity of molecules is correlated with their chemical structure.

The bibliographic data on topological indices were obtained from Web of Science, an online citation database for scientific works. We transformed them into corresponding networks: the citation network and two-mode networks of works x authors, works x journals and works x keywords and the partition of works by the publication year. We present the results of analysis of these networks. We identified the most important authors, works, subtopics and keywords and also important relations between them. We also determined the main citation and critical path, main subthemes on citation path based on keywords, the most prominent islands of citing authors, important journals and citing of works between them, journals preferred by authors and hierarchy of similar collaborating authors with respect to keywords they use.

Network Analysis of Collaboration in Mathematics

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The Zentralblatt MATH Database stores metadata about mathematical papers and books. It is maintained by the Berlin editorial ooffice of FIZ Karlsruhe in cooperation with European academies and mathematical institutes. We analyzed the ZB data about scientific works published within the period 1990 to 2010.

The raw data were converted into four 2-mode networks: works x authors, works x journals, works x keywords and works x MSCs, and a partition of works by publication year. Networks were analyzed separately and in combination with each other using Pajek, a computer program for analysis and visualization of large networks.

To reveal the structure of collaboration among mathematicians, we analyzed the collaboration network that was produced from the network works x authors by multiplication of networks. Different normalization of the so obtained network are considered. Groups of collaborating mathematicians can be identifed by generalized cores. Another way of grouping authors is by using line islands. They partition the authors geographically or by mathematical disciplines. We also investigate how the collaboration is changing through time and the interactions between different disciplines (as determined by the MSCs).

Computer Visualization in Search for Geometric (n_k) Configurations and Incidence Theorems

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In the simplest case, a geometric (n_k) configuration is a set of n points and n lines such that each of the points is incident with precisely k of the lines and each of the lines is incident with precisely k of the points. Instead of lines, the second subset can consist of planes, hyperplanes, circles, ellipses, etc. We present some new classes of highly symmetric spatial point-line configurations, and of planar point-circle configurations. In constructing these configurations computer visualization played an important heuristic role. The same is valid for certain new incidence statements which we also briefly discuss.

These results have been obtained partly in joint work with Tomaž Pisanski.

Fast Generation of Fullerenes

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We describe a new algorithm for the efficient generation of fullerenes. The algorithm generates all non-isomorphic fullerenes using the construction operations from [1]. We will describe the construction, provide details on the way isomorphism rejection is handled, and give some optimizations. Our implementation of this algorithm is more than 3 times faster than previous generators for fullerenes.

Using this new generator we were able to enumerate all fullerenes up to 400 vertices. This also allowed us to determine the smallest fullerene that does not allow a face spiral code: it has 380 vertices (see [2]).

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Computers and the Classification of Configurations

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This talk will discuss the construction and classification of configurations by computers. Results and conjectures will be presented. An early result was obtained for cubic graphs on 10 vertices (which were needed for applications in chemistry) in the 1960s by Balaban and Imrich. The same result had already be obtained at the end of the 19th century in the language of configurations, of course without a computer. Mainly symmetric configurations will be discussed, but also e.g. the configurations $(12_4, 16_3)$ will be considered. At the end, the focus will be on spatial configurations and other lambda-configurations.

A Few Families of Non-Schurian Association Schemes

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Association schemes are background combinatorial objects in the area of Algebraic Graph Theory (AGT). The main well-known origin of models for association schemes, the so-called Schurian association schemes, appears from transitive permutation groups by taking their 2-orbits (orbitals). All association schemes of order up to 14 can be obtained in this manner. It turns out that not all association schemes are Schurian. The construction of wide classes of non-Schurian association schemes still creates a challenge for experts in the area of AGT.

It is known (from the catalogue of small association schemes) that there are exactly two different non-Schurian association schemes of order 18. First, we will describe them in the terms of biaffine planes, i.e., we are giving a computer-free interpretation of these objects. Second, starting with the automorphism groups of these two schemes and with the corresponding coherent configurations (CC), we arranged a successful computer aided experimentation (for a few initial prime numbers p), looking for fusion schemes in the considered CC.

Basing on the earned observations we are able to prove the existence of at least four infinite families of non-Schurian association schemes of order $2p^2$, where $p > 3$ is a prime.

Moreover, with the aid of a computer, especially by the using of the computer packages COCO and COCO II (S. Reichard), we described (for initial values of p) their combinatorial, algebraic and color groups of automorphisms. Also more properties of these schemes were explored in the same computational fashion and later on rigorously proved with the aid of theoretical tools of AGT.

We will also show, how these association schemes are related to some well-known objects from the extremal graph theory.

Cloud Computing in Scientific Discovery for the Industry

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Cloud computing is fundamentally changing how computing resources are being delivered. The end-users increasingly access cloud-based applications using remote web-services, standard web browsers or "native applications" that just pretend to be more than a web browser. Infrastructure, databases and software are being deployed in a way that can be used as a service (rented) when needed. At the same time, cloud computing challenges several research fields with problems arising from topics such as: privacy and security, standards, resource sharing, scalability, distributed file systems, computational and data-intensive requirements (e.g. big data, big networks, parallelization, visualization), interoperability, accountability etc. In this presentation, several results of Competence center CLoud ASsisted Services (KC CLASS) will be presented with emphasis on industrial problems arising from the following topics: logistics, economy, health, environment and education.

On Positivity of Principal Minors of Bivariate Bezier Collocation Matrix

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In approximation theory, it is well known that the bivariate polynomial interpolation problem at domain points of a triangle is correct. Thus the corresponding interpolation matrix M is nonsingular. L.L. Schumaker stated the conjecture, that the determinant of M and all principal minors of M are positive. This result would solve the constrained interpolation problem.

In this talk, the basic conjecture for the matrix M, the conjecture on minors of polynomials for degree ≤ 17 and for some particular configurations of domain points are confirmed.

The Rank of Hadamard Powers of Euclidean Distance Matrices

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A matrix $A \in \mathbb{R}^{n\times n}$ is a Euclidean distance matrix (EDM) if there exist points $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$, such that $a_{ij} = \|x_i - x_j\|^2$. The minimal possible d is called the embedding dimension. A well known result states that the rank of an EDM is $d+2$ for the points in a general position, and $d+1$ if the points lie on a $d-1$ dimensional hypersphere.

In this talk, we extend the result to k-th Hadamard power of an EDM. The rank will be given in a closed form and is independent of the matrix size n, provided that n is not too small. The result was obtained in the context of researching DNA descriptors for determining the degree of similarity of DNA sequences.

Minimum Genus of Cartesian Products of Graphs

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The minimum genus problem is a classical, but NP-complete problem in topological graph theory. Minimum genus of cartesian products is closely related to the minimum genus of a group, the minimum among genera of all Cayley graphs of the given group. For abelian groups, the most difficult case arises when the group contains a Z_3 factor in its canonical decomposition. In this talk we focus mainly on the genus of G_n, the cartesian product of n triangles, which is the Cayley graph of the direct product of n copies of Z_3. Characteristic features of the problem are a significant level of symmetry of the underlying graphs, very large problem space, and an absence of readily available methods.

To determine the minimum genus of Z_3 we used both theoretical and computational approach. In this talk we focus on our practical experience with heuristics developed to obtain upper bounds, that is, low genus embeddings of G_n. In particular, we present currently the best upper bounds, which are quite irregular.

This is a joint work with T. Pisanski.

Geometric Nodal Domains and Trees with Minimal k-th Laplacian and Dirichlet Eigenvalues

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We investigate the structure of trees that have minimal k-th Laplacian and Dirichlet Eigenvalues among all trees with a given degree sequence.

Molecular Dynamics Simulation of Carbon Nanostructures

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Molecular dynamics calculations can reveal the physical and chemical properties of various carbon nanostructures or can help to devise the possible formation pathways. In our days the most well known carbon nanostructures are the fullerenes and the nanotubes. They can be thought of as being formed from graphene sheets, i.e. single layers of carbon atoms arranged in a honeycomb lattice. Usually the nature does not follow the mathematical constructions. An ideal nanotube can be thought of as a hexagonal network of carbon atoms that has been rolled up to make a cylinder. There is not any theory of carbon nanotube formation which is based on this construction. Although the first time the C60 and C70 were constructed by laser irradiated graphite, the fullerene formation theories are based on various fragments of carbon chains, and networks of pentagonal and hexagonal rings. In the present talk various formation pathways for carbon nanostructure formations will be studied in the frame work of molecular dynamics calculations. Suggestions will be given for practical experimental realizations.

GReGAS Atlas - Encyclopedia of Graphs

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Encyclopedia of Graphs (http://atlas.gregas.eu/) is an online encyclopedia of graph collections aiming to help researchers find and use data about different families of graphs. It has been created as a part of the ESF funded GreGAS project with the goal of becoming a general reference and repository of graphs and graph-like structures offered to all scientists and researchers for use and to provide new contributions.

At the talk the functionality of the Encyclopedia with be presented with the goal of getting feedback and ideas on possible new collection to be included.

What Kirchhoff Really Did

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In 1845, as a 21-year-old undergraduate, Gustav Robert Kirchhoff (writing under the pseudonym 'Studiosus' Kirchhoff) published, as 'Mitglied des physikalischen Seminars zu Königsberg' at the Albertina University, a classic paper [1] in which he stated his Laws I and II of electrical circuits — laws which, for more than a century, have been 'well-known to every schoolboy'. Two years later, in a second paper [2] in the Analen der Physik und Chemie, he examined the mathematical foundations of these laws and it is this paper which is still of interest to modern Graph Theorists. This is because it has deep implications for the theory of linear equations [3], and it was also the first paper to consider, if only implicitly, the idea of the spanning trees of a graph [4,5]. The speaker has long had an interest the enumeration of spanning trees [6,7] and this talk evaluates what Kirchhoff actually did in his much-cited paper of 1847, and how this relates to modern work [5–7].

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Topological Ring-Currents in Some 'Super-Ring' Molecules

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The Hückel–London–Pople–McWeeny (HLPM) ('Topological') approach [1–4] for calculating π-electron ring-currents and bond-currents in conjugated systems is applied to a series of structures that have been called 'super-ring' molecules [5]. These consist of an outer ring of carbon atoms (of perimeter length either $[4n]$ or $[4n+2]$) connected by internal C–C bonds to an inner, central ring, which is likewise of length either $[4n]$ or $[4n+2]$. In none of the cases considered is the original 'annulene-within-an-annulene' (AWA) model [6] respected. An alternative criterion is suggested — what we have named the 'Ring-Current AWA', based on ring currents rather than bond currents — whose provisions ostensibly have a greater probability of being fulfilled by any given structure. This new rule requires (a) that diamagnetic ring-currents should be manifested in all peripheral rings that form part of a $[4n+2]$-membered outer rim, as well as in any $[4n+2]$-membered inner- ring; and (b) that paramagnetic ring-currents should be evident in all peripheral rings that form part of a $[4n]$-membered outer-rim, as well as in any $[4n]$-membered inner-ring. This model is respected by almost all the examples studied here and elsewhere; however, a counter-example ([9]-coronaphene]) is identified even to this more-restricted AWA rule. Accordingly, it is concluded that that neither form of the AWA rule can generally be regarded as reliable.

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An Open Database of Interesting Graphs : The House of Graphs

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House of Graphs (http://hog.grinvin.org) is a searchable database of graphs. It offers lists of graphs and generators but also a special list of graphs that turned out to be interesting or relevant in the study of graph theoretic problems or as counterexamples to conjectures. A prototype of this project was first presented in the previous edition of CSD (Computers in Scientific Discovery 5, Sheffield, 2010). Since then the House of Graphs has evolved and is now also open to graphs that are submitted by users. In this talk, we present the current features of the House of Graphs and explain how graphs were initially selected to be in the database.

Homo-Lumo Gaps in Zigzag Carbon Nanotubes with Stone-Wales Defect

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An interesting aspect of finite-length carbon nanotubes (CNTs) is the quantum finite-size effects of the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). It has been shown that the HOMO- LUMO gaps in the zigzag CNTs show the oscillation depending on the number of hexagons around the peripheral circuits. We have shown that this HOMO-LUMO gap oscillation arises from the existence of 4k-membered conjugated circuits in (n,0)m zigzag CNTs. Various kinds of defects are known to be present in carbon nanotubes, which have significant influence on electronic, mechanical, and transport properties of the tubes. The Stone-Wales defect plays a key role, enabling large-scale structural rearrangements in graphitic networks. It creates two pentagons and two heptagons. In this paper we evaluate the effects of SW defect on the HOMO-LUMO gaps in zigzag CNTs by using semiempirical PM3 method.

There are two types of SW defect with different configurations. We call the two types of SW defect, H-type and V-type, respectively. The results of PM3 calculations showed that (n,0)m zigzag CNTs with SW defect have larger energies than pristine zigzag CNTs, regardless of types of SW defect. This implies that the formation energies of SW defect are positive, regardless of types of SW defect. The formation energies of SW defect of V-type are larger than those of H-type.

The V-type SW defects increase the magnitudes of HOMO-LUMO gaps in pristine zigzag CNTs at each radius n, implying that zigzag CNTs with V-type SW defects are chemically more stable than pristine zigzag CNTs. On the other hand H-type SW defects do not significantly affect HOMO-LUMO gaps. The HOMO-LUMO gaps in the zigzag CNTs with SW defects of H-type and V-type exhibit similar oscillation with period two depending on the number of hexagons around the peripheral circuits to those in the pristine zigzag CNTs.

Independent Sets of Fullerenes

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A *fullerene* is an all carbon molecule that can be represented by a 3-regular planar graph with face sizes five or six. A subset S of the vertices of a graph forms an *independent set* if the vertices of S are pairwise non-adjacent. This talk describes chemical applications for independent sets of fullerenes and algorithms for generating them.

Carbon Clusters with Tetrahedral Symmetry

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Carbon cages which violate the isolated pentagon rule or have an open-shell electronic system can be stabilized to be isolable by an appropriate endohedral or exohedral functionalization. Such an example is the observation of the C28 cluster with Td symmetry with an encapsulated uranium atom. A systematic study of classical fullerenes, i.e. containing only pentagons and hexagons, with tetrahedral (Td or T) topological symmetry to construct the corresponding tetrahedral carbon nanotube junctions revealed that a structural analogy exists between them. On this basis the carbon cages can be sorted into three groups. DFT method was employed to study the equilibrium geometries and electronic structure of the tetrahedral carbon nanostructures. It was found that total energies show a linear relationship. Because some of the fullerenes have an open shell electronic structure the stability was evaluated in different states, as charged species and lower symmetry structures have also been considered.

A Computer Tool in Logistics Operations Research

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Several optimization techniques have been developed in the past for optimizing various real-life problems we encounter during logistic operations. The quality and applicability of the results depend on the quality of input data as the famous saying "garbage in - garbage out" applies here more than anywhere. With input data we consider here quality of digital maps, accessibility and quality of GPS samples from vehicles in a fleet and in detail knowledge about processes and anomalies that can occur during daily operations. We shall present the results of the on-going applied research project where we have managed to establish a research and technological platform that enables quality research and applications on a real life problems of road maintenance, snow plowing and road salting logistic activities, as well as some results of analyses and optimizations.

Constructive Classification of Strongly Regular Designs

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Coherent configurations (Higman, Weisfeiler-Leman) are a central notion in Algebraic Graph Theory. An important class of coherent configurations - the so-called Schurian configurations - are obtained from the 2-orbits of permutation groups of finite degree. However in general, coherent configurations are non-Schurian.

Important invariants of coherent configurations are their types; they include information on the number and sizes of the fibers, which are the combinatorial analogues of the simplest characteristics for the orbits of permutation groups. Configurations with a single fiber are known as association schemes, and they have been studied extensively, leading to complete catalogues for moderately small orders (Hanaki-Miyamoto). This is in contrast to the situation of coherent configurations in general. Until recently, no such catalogues existed even for the smallest orders.

Recently we started first attempts towards the systematical enumeration of small coherent configurations. In this presentation we restrict ourselves to a particular class of two-fiber configurations, namely strongly regular designs (Higman). (We extend Higman's definition by removing a rather artificial condition, namely that the graphs induced on each fiber be primitive.)

We propose a strategy for their enumeration and present our results, which in particular include a complete list of such designs with at most 24 points and blocks.We also give computer-free models of a few newly discovered designs, as well as new descriptions of some classical objects like Reye's configuration and 24-cell. Keywords: Coherent configuration, strongly regular graph, equitable partition, exhaustive search

Parallel-ProBiS: Fast Parallel Algorithm for Local Structural Comparison of Protein Structures and Binding Sites

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We present a new parallelized algorithm, Parallel-ProBiS, for detecting similar binding sites on clusters of computers. This is a new algorithm that calcu- lates the local similarity metric between protein structures, and is especially suited to efficient execution on multiple CPUs. The obtained speedups of the parallel ProBiS scale almost ideally with the number of computing cores up to about 64 computing cores. Scaling is better for larger than for smaller query proteins. For a protein with almost 600 amino acids, the maximum speedup of 180 was achieved on two interconnected clusters with 248 computing cores. Source code of Parallel-ProBiS is available for download free for academic users at http://probis.cmm.ki.si/download.

Generation of Delaney-Dress Symbols

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A Delaney-Dress symbol is a structure that encodes an equivariant tiling, i.e. tilings together with their symmetry groups. In this talk we will describe a generator for Delaney-Dress symbols and thus for tilings. We will give an introduction to Delaney-Dress symbols and discuss the structural properties that are used by the generation algorithm. We will also present some results already obtained at this point of the development.

Poster Presentations

Using Weighted Voronoi Diagrams to Describe Proteomic Maps

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In this work we investigate the problem of numerical characterization of two dimensional proteomics maps based on construction of Voronoi regions. To enable for the taking into account of the concentrations of proteins on the proteomic map, we have used the process which gives greater weights to spots representing proteins with greater abundance. As we have shown, the shapes of the resulting Voronoi regions are sensitive to relative abundances of the proteins spots. In this work the spot abundances are naturally incorporated in the numerical analysis, as a partitioning of the plane. We investigated a series of proteomic maps, where experimental animals being administered the same peroxisome proliferator, albeit in different concentrations, we explore the properties of the dual graph of the partitioning of the plane and compare the results of this novel method with approaches encountered in the literature. In doing this we have observed a J-shaped dose-response curve, typical of hormesis, similar to the results published previously but using a method that is independent.

Lower and upper Bound for Roman Domination Number on Cardinal Product of Paths

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For a graph $G=(V,E)$, *a Roman dominating function* (RDF) is a function $f\colon V\to\{0,1,2\}$ satisfying the condition that every vertex u for which $f(u)=0$ is adjacent to at least one vertex v for which $f(v)=2$. The weight of an RDF equals $w(f)=\sum_{v\in V}f(v)=|V_1|+2|V_2|$. An RDF for which $w(f)$ achieves its minimum is called *a γ_R-function* and its weight, denoted by $\gamma_R(G)$, is called *a Roman domination number*.
We studied the Roman domination on cardinal product of two paths $P_m\times P_n$ and determined the lower and the upper bound for $\gamma_R(P_m\times P_n)$ as well as the exact value of $\lim_{m,n\to\infty}\frac{P_m\times P_n}{mn}$.

Effect of H-Bonding on Aromaticity of Purine Tautomers

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Purine, as a mother template of important nucleobases, is the good model system to study such properties of these systems as pi-electron delocalization and interactions with acidic or basic partners. For this purpose, modeling of equilibrium H-bond formation of the types N...HF and NH...F– was used [1]. H-bonded complexes of purine (four complexes for each tautomer: 1-H, 3-H, 7-H and 9-H purines) were studied [2]. In the case of NH...F– interactions, a proton is transferred to fluoride and hydrofluoric acid is formed. In consequence, two types of H-bonds were considered: conventional, N...HF, and charge-assisted, N–...HF. For all complexes optimized structural parameters, relative energies and strengths of H-bonds were calculated at the B3LYP/6-311++G** level theory. Detection and classification of the observed hydrogen bonds were performed by means the Quantum Theory of Atoms in Molecules. The Popelier's criteria were applied to the critical point (CP) describing H-bond formation. These criteria were fulfilled by all H-bonds for the studied complexes. Moreover, the negative value of the total energy density at CP suggested partially covalent character of all intermolecular interactions. The ionic H-bonds, N–...HF, are stronger by 10 kcal/mol than the neutral ones. For all N...HF interactions in a particular purine tautomer, the greatest basicity (and, thus, the strongest H-bonding) is observed if basic and acidic centers belong to different rings. To study the effect of H-bond formation on pi-electron delocalization two aromaticity indices (HOMA and NICS) were applied. The H-bonded complexes for 7-H and 9-H tautomers are characterized by higher aromaticity (HOMAtot) and a much lower range of HOMA variability. The 6-membered rings without NH group (in 7-H and 9-H tautomers) exhibit higher aromaticity (mean HOMA6 is equal to 0.971), whereas for 1-H and 3-H tautomers, the aromaticity is lower (mean HOMA6 = 0.742). To the contrary, in the 5-membered rings, the presence of NH favors aromaticity. The HOMA index calculated for 7-H and 9-H tautomers (mean HOMA5 = 0.833) is higher than the corresponding HOMA value obtained for 1-H and 3-H (mean HOMA5 = 0.720). Similar trends are observed for NICS values, since there is an acceptable linear regression between NICS and HOMA.

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MD Methods in Evaluating Aromaticity Changes by Environment

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Aromaticity is an important and widely used concept characterizing properties and structure of many organic and inorganic chemical compounds [1–3]. Environmental effects can lead to significant structural alterations of molecules directly exposed to environment. Such changes are of particular interest in molecules important from a biochemical perspective. All nucleobases and four amino acid residues possess aromatic rings that can be affected by the environmental heterogeneity. These influences can be as different as explicit solvent molecules, dense packing in solids, particular molecular surroundings in polymeric neighborhoods and a variety of organic or inorganic ligands directly interact with the solute. Straightforward contacts between molecules in the closest proximity, or chemical modification or indirect influence via intermolecular interactions can lead to sizable alterations of physico-chemical properties including aromaticity. The aim of this study was the quantitative analysis of π-electron delocalization in aromatic ring of phenol (as a model system), nucleobases and amino acids in explicit and implicit water solvation. The conformations of these systems were obtained via quenching Molecular Dynamics (MD) method followed by QM/MM [4] hybrid molecular-mechanics/quantum-chemical geometry optimization using AMBER forcefield [5,6].

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Mathchem Python Package

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Mathchem is a free open source Python package for calculating topological indices and other invariants of molecular graphs. For performance reasons we use here concept of lazy calculations. This means that we calculate data only when it is needed and then we save the results. Mathchem can be installed either as Python or as Sage module. Since the package contains no compiled code it is cross-platform and could be used in any operating system compatible with Python. The poster represents functionality of the package, its usage examples, installation process, structure and features with samples of code.

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