

## Knot Theory and Applications Special Session A2

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Knot theory is a very fertile branch of low-dimensional topology with ramifications in many other areas of mathematics and natural sciences. The goal of this special session is to enable an exchange of methods and ideas as well as exploration of fundamental research problems in the fields of knot theory and low-dimensional topology, from theory to applications in mathematics and science, and to provide high quality interactions across fields. The talks will touch upon the themes below:

- algebraic, categorical and combinatorial invariants in knot theory
- interplay between links and braids
- representations of knot theory in 3-manifolds
- use of knot theory in biological and biochemical models.

During the talks, discussion will be encouraged.

### Schedule and Abstracts

July 23, 2024

#### 11:00–11:45 Mock Alexander Polynomials

**Louis H. Kauffman (University of Illinois, USA)**

*Abstract.* We study generalizations of the Formal Knot Theory [1] state summation to general diagrammatic situations where the number of active regions in the diagram is equal to the number of crossings in the diagram. These situations include classical knot and link diagrams with non-adjacent starred regions (regions where the state sum is not evaluated and where the diagrams cannot move), knotoids, linkoids, knots and link diagrams in a torus and other configurations. The generalizations have many properties quite different from the classical Alexander polynomial and can often detect different species of chirality. Many examples will be given in the talk and we will discuss problems related to generalizing the Fox-Milnor Theorem and relationships with generalizations of the Dehn Presentation of the classical knot group.

Joint work with N. Gügümcü.

[1] L. H. Kauffman, Formal Knot Theory, *Princeton University Press* (1981).

#### 12:00–12:45 Hyperbolicity of Staked Links

**Colin Adams (Williams College, USA)**

*Abstract.* A staked link is obtained as a link diagram with finitely many points chosen in the complementary regions such that strands in the link diagram cannot pass over them. This is equivalent to taking a link in a handlebody. In this talk, we report on joint work as in the references. We focus on hyperbolicity of the complement of the link in the handlebody. In particular, we prove that every link can be staked to be hyperbolic, thereby implying every link in  $S^3$  has a minimal staked hyperbolic volume. We give a characterization of hyperbolicity when

the projection is alternating. We further discuss a version of composition and give a variety of results for specific classes of staked links, including volume bounds.

- [1] C. Adams, A. Bonat, M. Chande, J. Chen, M. Jiang, Z. Romrell, D. Santiago, B. Shapiro and D. Woodruff, Hyperbolic Knotoids, *preprint* (2022), ArXiv 2209.04556.
- [2] C. Adams, A. Bonat, M. Chande, J. Chen, M. Jiang, Z. Romrell, D. Santiago, B. Shapiro and D. Woodruff, Generalizations of Knotoids and Spatial Graphs, to appear in *Math. Proc. Cambridge Philos. Soc.* (2022), ArXiv 2209.01922.
- [3] C. Adams and J. Chen, Hyperbolicity of Alternating Links in Thickened Surfaces with Boundary, *preprint* (2023), ArXiv 2309.04999.
- [4] C. Adams and D. Santiago, Composition Properties of Hyperbolic Links in Handlebodies, *New York J. Math.* **29** (2023), 1097–1116.
- [5] C. Adams and E. High, Hyperbolicity of Staked Links, in preparation.

### **14:30–15:15 From the Kauffman bracket polynomial to cubic skein modules and beyond**

**Józef H. Przytycki (George Washington University and Georgetown University, USA)**

*Abstract.* The study of linear and quadratic skein modules over the last thirty-seven years has led to a very rich skein theory that is connected to many disciplines of mathematics and physics, such as algebraic geometry, hyperbolic geometry, Topological Quantum Field Theories (TQFT), and statistical mechanics. There is, however, another class of skein modules with more parameters than the linear and quadratic cases which, save for a few exceptions, have been largely neglected until now. The cubic skein module is the first object in this class which awaits exploration.

Joint work with Mathathoners VIII.

### **15:30–15:50 Non-triviality of welded knots and the ribbon torus knots**

**Rama Mishra (Indian Institute of Science Education and Research, Pune, INDIA)**

*Abstract.* In this paper we study welded knots and their invariants. We focus on generating examples of non-trivial knotted ribbon tori as the tube of welded knots that are obtained from classical knot diagrams by welding some of the crossings. Non-triviality is shown by determining the fundamental group of the concerned welded knot. Sample examples under consideration are the standard diagrams of the family of  $(2, q)$  torus knots and the twist knots. Standard diagrams of knots from Rolfsen’s tables with 6 crossings are also discussed which are not in the family of torus and twist knots.

### **16:00–16:20 The Roger-Yang Skein Algebra of the $n$ -punctured torus**

**Rhea Palak Bakshi (ETH Zürich, SWITZERLAND)**

*Abstract.* Skein modules were introduced by Przytycki in [2] with the goal of building an algebraic topology based on knots, generalising the skein theory for links in  $S^3$  to arbitrary 3-manifolds. Turaev introduced the Conway and Kauffman skein modules independently in [3]. The Kauffman bracket skein module, which serves as the generalisation of the Kauffman bracket polynomial, has a natural algebra structure given by the stacking of skeins (elements in the skein module) when the 3-manifold is a thickened surface. This algebra, known as the Kauffman bracket skein algebra, has deep connections with algebraic and hyperbolic geometry. The Roger-Yang skein algebra is a generalisation of the Kauffman bracket skein algebra for punctured surfaces, allowing framed arcs between punctures [4]. It is known that this new algebra is related to the decorated Teichmüller space introduced by Penner [1]. Further study of the Roger-Yang skein algebra will help better understand the connections between hyperbolic geometry and quantum topology. In this talk, we give a presentation of the Roger-Yang skein algebra of the  $n$ -punctured torus,  $n > 0$ .

Joint work with H-B. Moon.

The speaker acknowledges the support of Dr. Max Rössler, the Walter Haefner Foundation, and the ETH Zürich Foundation.

- [1] R. C. Penner, The decorated Teichmüller space of punctured surfaces, *Comm. Math. Phys.* **113** (1987), 299–339.
- [2] J. H. Przytycki, Skein modules of 3-manifolds, *Bull. Polish Acad. Sci. Math.* **39** (1991), 91–100.
- [3] V. G. Turaev, The Conway and Kauffman modules of a solid torus, *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)* 167 (1988), Issled. Topol. 6, 79–89, 190; translation in *J. Soviet Math.* **52** (1990), 2799–2805.
- [4] J. Roger and T. Yang, The skein algebra of arcs and links and the decorated Teichmüller space, *J. Differential Geom.* **96** (2014), 95–140.

### 17:00–17:45 Relations between knot invariants

**Radmila Sazdanovic (North Carolina State University, USA)**

*Abstract.* Ernst and Sumners’ theorem [2], affirming that knots constitute a form of big data, coupled with the comprehensive knot tabulation by Burton, Hoste, Thistlethwaite, and Weeks, along with numerous computations of knot invariants, establishes the groundwork for employing big data methodologies such as machine learning in knot theory [1,3,4,5]. Utilizing dimension reduction and machine learning methods, such as Ball Mapper and other techniques inspired by the topological data analysis (TDA), yields valuable insights into the statistical characteristics of knots, offers compelling means to visually represent and analyze relations between knot invariants [2, 6]. Invariants in focus include the Jones, Alexander, HOMFLYPT and Khovanov polynomials and numerical invariants such as signature and Rasmussen s-invariant.

- [1] A. Davies, A. Juhász, M. Lackenby, N. Tomasev, The signature and cusp geometry of hyperbolic knots, *preprint* (2021), ArXiv 2111.15323.
- [2] C. Ernst, D. W. Sumners, The Growth of the Number of Prime Knots, *Math. Proc. Cambridge Philos. Soc.* **102** (1987), 303–315.
- [3] P. Dłotko, D. Gurnari, R. Sazdanovic, Mapper–type algorithms for complex data and relations, *J. of Computational and Graphical Statistics* (2024), 1–18.
- [4] S. Gukov, J. Halverson, C. Manolescu, F. Ruehle, P. Sułkowski, Learning to unknot, *Machine Learning: Science and Technology* **2(2)** (2021), 025035.
- [5] S. Gukov, J. Halverson, C. Manolescu, F. Ruehle, Searching for ribbons with machine learning, *preprint* (2023), ArXiv 2304.09304.
- [6] J. Craven, M. Hughes, V. Jejjala, A. Kar, Illuminating new and known relations between knot invariants, *preprint* (2022), ArXiv 2211.01404.
- [7] J.S. Levitt, M. Hajij, R. Sazdanovic, Big data approaches to knot theory: understanding the structure of the Jones polynomial, *J. of Knot Theory and Its Ramifications* **31.13** (2022), 2250095.

July 24, 2024

### 11:30–12:15 Dynamics and mechanics of knotted DNA and RNAs

**Cristian Micheletti (SISSA - Scuola Internazionale di Studi Superiori Avanzati, ITALY)**

*Abstract.* I will report on a series of theoretical and computational studies of DNA and RNAs that present knots and other forms of structural entanglement [1]. I will first consider model bacterial DNAs that are both knotted and supercoiled, and discuss how the simultaneous presence of knots and supercoiling creates long-lived multi-strand interlockings that might be relevant for the simplifying action of topoisomerases. I next consider how entangled nucleic acids behave when driven through narrow pores [2-4], a setting that models translocation through the lumen of enzymes, and discuss the biological implication for a certain class of viral RNAs [4].

- [1] L. Coronel, A. Suma and C. Micheletti, Dynamics of supercoiled DNA with complex knots, *Nucleic Acids Res.* **46** (2018), 7533.
- [2] A. Suma, V. Carnevale and C. Micheletti, Nonequilibrium thermodynamics of DNA nanopore unzipping, *Phys. Rev. Lett.* **130** (2023), 048101.

- [3] A. Suma, A. Rosa and C. Micheletti, Pore translocation of knotted polymer chains: how friction depends on knot complexity, *ACS Macro Letters* **4** (2015), 1420-1424.
- [4] A. Suma, L. Coronel, G. Bussi and C. Micheletti, Directional translocation resistance of Zika xrRNA, *Nature Communications* **11** (2020), art no. 3749.

### 12:30–12:50 Identifying knots and theta-curves via neural networks

**Boštjan Gabrovšek (University of Ljubljana, SLOVENIA)**

*Abstract.* We show that Long Short-Term Memory (LSTM) based Neural Networks can be applied to successfully predict the knot type and theta-curve type of entangled curves in 3D space. The model is 99% successful at detecting the knot type of open polymeric chains resembling real proteins. In the case of native protein structures predicted by AlphaFold 2, the model can distinguish between trivial and non-trivial knot type with an accuracy of 93% [1].

Joint work with F. Bruno, I. Sulkowska and others.

- [1] F. Bruno, B. Gabrovšek, J. I. Sulkowska, et al., Knots and  $\Theta$ -Curves Identification in Polymeric Chains and Native Proteins Using Neural Networks, *Macromolecules* (2024), 10.1021/acs.macromol.3c02479.

### 14:30–15:15 Vortex knot cascade by geodesic flows in a knot polynomial space

**Renzo L. Ricca (University of Milano-Bicocca, ITALY)**

*Abstract.* It is well known that topologically complex tangles of superfluid vortex knots and links tend to decay through a topological cascade producing a system of unlinked vortex loops [1-2]. Here we propose a geometric interpretation of this unlinking process by geodesic flows in an abstract knot polynomial space [3]. By taking advantage of the re-formulation of the Jones polynomial in terms of helicity contributions [4] we introduce a discrete metric space, whose points represent different knot types, and show that optimal unlinking paths in this space can describe some fundamental features of the topological decaying process observed in superfluid simulations.

Joint work with X. Liu and X-F. Li.

- [1] D. Kleckner, L.H. Kauffman, W.T.M. Irvine, How superfluid vortex knots untie, *Nature Physics* **12** (2016), 650–655.
- [2] R.G. Cooper, M. Mesgarnezhad, A.W. Baggaley, C.F. Barenghi, Knot spectrum of turbulence, *Scientific Reports* **9** (2019), 10545.
- [3] X. Liu, R.L. Ricca, X-F. Li, Minimal unlinking pathways as geodesics in knot polynomial space, *Nature Comm. Physics* **3** (2020), 136.
- [4] X. Liu, R.L. Ricca, The Jones polynomial for fluid knots from helicity, *J. Phys. A: Math. & Theor.* **45** (2012), 205501.

### 15:30–15:50 Everything AlphaFold tells us about protein knots

**Joanna I. Sulkowska (University of Warsaw, Centre of New Technology, POLAND)**

*Abstract.* I will report on a series of numerical and experimental studies to demonstrate a new type of knots [1,2] and lassos discovered in proteins based on AI methods (data are deposited in AlphaKnot [3] and AlphaLasso [4] databases). Next, I will concentrate on proteins with non-twist type of knot [5] and discuss how such proteins can fold with just one threading across the topological barrier.

Finally, I will present a cross-proteome-wide big data analysis of topologically knotted protein structures based on the AlphaFold and ESMFold predictions that essentially cover >90% of known genomic open reading frames. Using this approach, we found that there are approx. 700,000 protein structures. Next, I will show that the  $3_1$  knot type is the most prevalent in all proteomes, and the knotted proteins account for 0.4% of all tested proteomes regardless of their evolutionary and habitat differences. Thus, although knotted proteins make up only approx. 0.4% of the proteome, are ubiquitous throughout all kingdoms of life. Finally I will show that all organisms contain at least one knotted protein [6].

- [1] A.P. Perlinska, W.H. Niemyska, B.A. Gren, M. Bukowicki, S. Nowakowski, P. Rubach, J.I. Sulkowska, AlphaFold predicts novel human proteins with knots, *Protein Science* **32(5)** (2023).
- [2] M. Sikora, D. Sramková, D. Uchal, E. Klimentova, A.P. Perlinska, M.L. Nguyen, M. Korpacz, R. Malinowska, P. Rubach, P. Simecek, J.I. Sulkowska, Knot or Not? Identifying unknotted proteins in knotted families with sequence-based ML mode, *Protein Science* (2024), 10.1002/pro.4998.
- [3] P. Rubach, M. Sikora, A.I. Jarmolinska, A.P. Perlinska and J.I. Sulkowska, AlphaKnot 2.0 – a web server for the visualization of proteins’ knotting and a database of knotted AlphaFold-predicted models, *Nucleic Acids Research* (2024).
- [4] P. Rubach, J. Plonka, B.A. Gren, F. Bruno da Silva, J.I. Sulkowska, AlphaLasso – a database of lasso proteins AlphaFold-predicted models, under review.
- [5] M. Sikora, E. Flapan, H. Wong, P. Rubach, W. Garstka, S. Niewieczerzal, E.J. Rawdon, J.I. Sulkowska, Proteins containing 6-crossing knot types and their folding pathways, *preprint* (2023), bioRxiv DOI 10.1101/2023.06.16.545156.
- [6] M. Sikora, A.P. Perlinska, J.I. Sulkowska, Everything AlphaFold tells us about protein knots, under review.

### 16:00–16:20 On the Jones polynomial of quasi-alternating links

**Khaled Qazaqzeh (Yarmouk University, JORDAN)**

*Abstract.* We use graph theoretical approach to extend the result of Thistlethwaite in [3] on the structure of the Jones polynomial of alternating links to the wider class of quasi-alternating links defined for the first time in [2]. In particular, we prove that the Jones polynomial of any prime quasi-alternating link that is not a  $(2, n)$ -torus link has no gap and this gives an affirmative answer to [1, Conjecture 2.3]. As an application, we show that the differential grading of the Khovanov homology of any prime quasi-alternating link that is not a  $(2, n)$ -torus link has no gap. Also, we show that the determinant is an upper bound for the breadth of the Jones polynomial for any quasi-alternating link. Finally, we prove that the Jones polynomial of any non-prime quasi-alternating link  $L$  has more than one gap if and only if  $L$  is a connected sum of Hopf links.

Joint work with A. Al-Rhayyel, N. Chbili.

- [1] N. Chbili, and K. Qazaqzeh, On the Jones polynomial of quasi-alternating links, *Topol. Appl.* **264** (2019), 1–11.
- [2] P. Ozsváth and Z. Szabó, On the Heegaard Floer homology of branched double-covers, *Adv. Math.* **194(1)** (2005), 1–33.
- [3] M. Thistlethwaite, A spanning tree expansion of the Jones polynomial, *Topology* **26** (1988), 297–309.

### 17:00–17:20 Congruence subgroups of braid groups and crystallographic quotients

**Paolo Bellingeri (University of Caen Normandy, FRANCE)**

*Abstract.* This talk delves into the relationship between two families of groups, respectively subgroups and quotients of classical braid groups: congruence subgroups of braid groups and crystallographic braid groups, respectively introduced Arnol’d and Tits. We recall and introduce some elements belonging to congruence braid groups and we establish some (iso)-morphisms between crystallographic braid groups and corresponding quotients of congruence braid groups. Finally, we study the lower central series of congruence braid groups related to the braid group  $B_3$ , showing in particular that corresponding quotients are all *almost* crystallographic.

Joint work with C. Damiani, O. Ocampo, and C. Stylianakis.

### 17:30–17:50 From Kirby diagrams to triangulations of PL 4-manifolds

**Paola Cristofori (Università degli Studi di Modena e Reggio Emilia, ITALY)**

*Abstract.* Kirby diagrams, i.e. links in the 3-sphere equipped with integers associated to some components, are a classical representation method for compact PL 4-manifolds encoding their handle decompositions.

On the other hand, regular edge-colored graphs have proved to be, in many ways, an useful combinatorial tool to encode triangulations and so represent compact PL manifolds of any dimension.

We present an algorithm which, given a suitable Kirby diagram  $(L, d)$  of a compact PL 4-manifold  $M$ , produces an edge-colored graph  $\Gamma(L, d)$  representing  $M$  and directly “drawn” over a planar diagram of the link ([2]).

As a consequence, the combinatorial structure of  $\Gamma(L, d)$  allows to obtain upper bounds for the value of some invariants of  $M$  ([2], [3]). In particular, for any closed orientable PL 4-manifold  $M$ , an estimation can be given, in terms of combinatorial properties of  $L$ , for the *trisection genus* of  $M$ , an invariant defined within the theory of *trisections*, which were introduced in [4] as a generalization to dimension 4 of the classical concept of Heegaard splitting of a 3-manifold, and are currently intensively studied.

Moreover, the presented algorithm turns out to be an useful tool in the study of triangulations of exotic pairs of 4-manifolds; in fact, most examples of such pairs are known only through their representation by Kirby diagrams, while explicit triangulations can be rarely found in literature.

Actually, as shown in [1], the implementation of our algorithm in the *Regina* software package produced several examples of triangulations of exotic pairs as well as the first known triangulations of some Akbulut’s corks, thus opening the possibility to gain an insight into their structural features.

Joint work with M.R.Casali.

This work was supported by GNSAGA of INDAM and by the University of Modena and Reggio Emilia, project: “*Discrete Methods in Combinatorial Geometry and Geometric Topology*”.

- [1] R.A.Burke, Practical software for triangulating and simplifying 4-manifolds, *preprint* (2024), ArXiv 2402.15087.
- [2] M.R.Casali, P. Cristofori, Kirby diagrams and 5-colored graphs representing compact 4-manifolds, *Rev. Mat. Complut.* **36** (2023), 899–931.
- [3] M.R.Casali, P. Cristofori, Trisections of PL 4-manifolds arising from colored triangulations, *preprint* (2024), ArXiv 2312.01902.
- [4] D. Gay, R. Kirby, *Trisecting 4-manifolds*, *Geom. Topol.*, **20** (2016), 3097–3132.

## 18:00–18:20 A New Combinatorial Invariant of Doubly Periodic Tangles

**Sofia Lambropoulou (National Technical University of Athens, GREECE)**

*Abstract.* Doubly periodic tangles, or *DP tangles*, are complex entangled structures consisting of curves embedded in the thickened plane  $\mathbb{E}^2 \times I$ , so can be defined as lifts of links in the thickened torus,  $T^2 \times I$ . They serve as a significant framework for analyzing and understanding the topological properties of interwoven filament systems across micro-, meso- and macro-scales, including, but not limited to, polymer melts, fabric-like structures, molecular chemistry, and cosmic filaments. The topological classification of DP tangles is at least as hard a problem as the full classification of knots and links in the three-space and is approached by constructing topological invariants. To reduce the complexity of this problem, the idea is to consider the quotient of a DP diagram under a periodic lattice, namely a link diagram in the (flat) torus  $T^2$  that we call *(flat) motif*. This approach leads to a diagrammatic theory of the topological equivalence of DP tangles, which has been established in [1] on the level of motifs, and that generalizes works initiated by Grishanov et al. related to textiles [4-5].

In this talk we introduce new topological invariants of DP tangles. We will, in particular, present the notion of *axis-motif*, that is a set of arcs in the flat torus which can be viewed as a blueprint of a DP tangle capturing the different directions along which its components are organized. This will lead to the definition of the *directional type* of the DP tangle, which constitutes a topological invariant of DP tangles [2]. We will then introduce the concept of *density* of a motif  $\tau$ , defined in terms of the total number of arcs of the axis-motif of  $\tau$ , which gives rise to a new invariant called *density of the DP tangle*  $\tau_\infty$ , defined as the minimal density over all axis-motifs of  $\tau_\infty$ . However, we will note that this topological invariant is not strong enough to distinguish two DP tangles of different directional types. Thus, by using the fact that the set of arcs of an axis-motif of a motif  $\tau$  can be partitioned into a specific triple of integers,

that we call *arc-triple* of  $\tau$ , we will present a stronger invariant of DP tangles, called *minimal arc-triple*. This notion leads to a characterization of the directional type of a DP tangle by its minimal arc-triple. All the above invariants of DP tangles are measures that naturally inform on their topological complexity, they refer to global topological properties of theirs, and they add to the list of the existing invariants. In the end of this talk we will present examples of computations of our invariants on several DP tangles, comparing them with some known numerical invariants.

Joint work with I. Diamantis and S. Mahmoudi.

- [1] I. Diamantis, S. Lambropoulou, S. Mahmoudi, Equivalences of doubly periodic tangles, *preprint* (2023), ArXiv 2310.00822.
- [2] I. Diamantis, S. Lambropoulou, S. Mahmoudi, Directional invariants of doubly periodic tangles, *preprint* (2024), ArXiv 2404.05092.
- [3] I. Diamantis, S. Lambropoulou, S. Mahmoudi, On the combinatorics of doubly periodic tangles, in preparation.
- [4] S.A. Grishanov, V.R. Meshkov, A.V. Omel'Chenko, Kauffman-type polynomial invariants for doubly periodic structures, *J. Knot Theory Ramifications* **16** (2007), 779–788.
- [5] H.R. Morton, S.A. Grishanov, Doubly periodic textile structures, *J. Knot Theory Ramifications* **18** (2009), 1597–1622.