





ESF-EMS-CRM-Pi

International Conference on

Knots and Links: From Form to Function

Centro di Ricerca Matematica (CRM) "Ennio De Giorgi" Scuola Normale Superiore, Pisa, Italy

2-8 July, 2011

SPEAKERS' ABSTRACTS AND REFERENCES







SURNAME: Adams FIRST NAME: Colin

ABSTRACT TITLE:

Indicatrices, Stick Index and Superinvariants for Knots

ABSTRACT (maximum 200 words):

In 1985, Kuiper introduced superbridge index for knots, which has allowed for the determination of the least number of sticks for certain knots. In this talk, we will consider superbridge index and a variety of other superinvariants, and see how they relate to the tangent, normal and binormal indicatrices for a conformation of a knot.

- Kuiper, Nicolaas, A new knot invariant, Math. Ann. 278 (1987), no. 1-4, 193-209.
- Adams, Colin, Collins, Dan, Hawkins, Katherine, Sia, Charmaine, Silversmith, Rob, Tshishiku, Bena, Duality Properties of Indicatrices of Knots, preprint.

SURNAME: Barenghi **FIRST NAME:** Carlo F.

ABSTRACT TITLE:

Vortex knots and vortex tangles in quantum fluids

ABSTRACT (maximum 200 words):

Turbulent flows contain eddies and swirls, regions of vertical motion. A natural question to ask is what is the topology of the turbulence. This talk is concerned with a special class of fluids in which turbulence is simpler, at least in principle: quantum fluids. Quantum fluids (superfluid helium, atomic Bose-Einstein condensates) are characterized by a macroscopic quantum mechanical wavefunction Ψ . The existence of Ψ requires that the vorticity is concentrated in discrete thin vortex filaments, sort of elementary mini-tornadoes; on the contrary, in ordinary fluids eddies have any shape and strength. Recent progress in visualizing and controlling quantum vortices may open the way to a better understanding of the topology of turbulence. The aim of the talk is to introduce the subject of quantum vortices, and to present recent results on the dynamics of simple vortex structures, from vortex rings to vortex knots.

- C.F. Barenghi "Is the Reynolds number infinite in superfluid turbulence ?", Physica D, 237, 2195 (2008).
 - J.L. Helm, C.F. Barenghi, and A.J. Youd, "Slowing down of vortex rings in atomic Bose-Einstein condensates", Phys. Rev. A 83, 045601 (2011)

The writhe of open curves: theory and applications

ABSTRACT (maximum 200 words):

Many natural objects have a ribbon or tube-like shape, but with endpoints. Defining the geometric and topological properties of such objects is not always straightforward. This talk will review the measures of twist and writhe, for applications in astrophysics and biomolecules.

The magnetic helicity of a thin magnetic flux element can be decomposed into contributions from twist (proportional to the parallel electric current) and writhe (a measure of kinking). The local twist is difficult to observe; generally we see a projection of the three-dimensional shape of the axis.

This projection is insufficient to determine the writhe. We also give examples where two loops with the same projected S shape (but different heights) can have different signs of writhe.

An interesting question is whether magnetic flux ropes with a similar shape will always have the same helicity. To help answer this question, we analyze the twist and writhe content of individual field lines within a force—free field. We find that the total helicity of a thin flux element is always the same sign as the helicity of the field as a whole, although the writhe can sometimes be of opposite sign. Additionally we show that much of the interesting morphological behaviour occurs for field lines located next to separatrix boundaries.

SURNAME: Blasco FIRST NAME: Fernando

ABSTRACT TITLE:

Mathematical magic with knots

ABSTRACT (maximum 200 words):

The documented relation between maths and magic begins in the 16th century since Luca Pacioli wrote the first description of a card magic trick in "The Viribus Quantitatis". In that book also appears a puzzle, that can be easily converted into a magic trick, involving a ring and a rope. It can be considered the first one among lots of magic tricks involving ropes.

In this talk we will perform and teach a few magic tricks based on knot and link properties. The tricks can serve as a good introduction to knot theory to non specialists. We will focus our attention in both the mathematics underlying the tricks and the presentation of them.

- Gardner, Martin. Mathematics, magic and mystery. Dover. 1956.
- Fulves, Karl. Self-working rope magic. Dover. 1990.
- Hiéronymus. Nouveaux tours extraordinaries de mathémagique. Ellipses. 2009.

The Classification of Rational Tangle Adjacencies, with Applications to Complex Nucleoprotein Assemblies

ABSTRACT (maximum 200 words):

Author: Dorothy Buck Author: Ken Baker

Abstract: Many proteins cleave and ligate DNA molecules in precisely orchestrated ways. Modelling these reactions has often relied on the underlying DNA molecule being covalently closed, so these cut-and-seal mechanisms can be tracked by corresponding changes in the knot type of the DNA axis. However, in the (common) case when the DNA molecule is linear, or the enzyme action does not manifest itself as a change in knot type, or the knots types are not 'standard', these knot theoretic models are less germane.

Here we give a taxonomy of local DNA axis configurations. We endow this classification with a distance: that determines how many enzyme reactions of a particular type (corresponding to steps of a specified size) are needed to proceed from one local conformation to another. We discuss a variety of applications of this categorization, including type-II topoisomerase, site-specific recombinase, and transposase-mediated reactions.

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Integrable evolution of closed vortex filaments: finite-gap solutions and their linear stability

ABSTRACT (maximum 200 words):

The Localized Induction Approximation (LIA), describing the self-induced motion of a vortex filament in a perfect fluid, is a simple but important example of integrable curve dynamics, and one in which knotted curves arise as solutions of a differential equation possessing a rich geometrical structure.

The connection between the LIA and the cubic focusing nonlinear Schrödinger (NLS) equation through the well-known Hasimoto transformation allows the use of many of the tools of soliton theory to study properties of its solutions. In this talk I will focus on three areas: The construction of closed finite-gap filaments using the classical Baker-Akhiezer eigenfunction approach developed by Krichever for the NLS equation. The use of isoperiodic deformations of spectral data for constructing families of periodic small amplitude finite-gap solutions of increasingly high genus, and the complete description of their knot types in terms of spectral data. The relation between the linearizations of the LIA and the NLS equation, and the role of squared eigenfunctions in determining the stability properties of LIA solutions in terms of those of the associated NLS potentials.

- Finite-gap solutions of the Vortex Filament Equation: Isoperiodic Deformations. (with T. Ivey) Journal of Nonlinear Science, Vol. 17, no. 6 (2007)
- Stability of Small-Amplitude Torus Knot Solutions of the Localized Induction Approximation. (with T. Ivey) Submitted (2011)
- Squared Eigenfunctions and Linear Stability Properties of Closed Vortex Filaments. (with S. Lafortune and S.F. Keith) Submitted (2011)

New Computational Approaches to Exploring Polygon and Knot Spaces

ABSTRACT (maximum 200 words):

After devoting a significant effort to finding ropelength-critical configurations of knots using a version of gradient descent, we are ready to face a different question: what is the best way to explore the space of knotted polygons to understand its topology and geometry and search for alternate (or tighter!) critical configurations?

In this talk, we discuss some large-scale experiments performed finding critical configurations for more than 500 composite knot types and some new computational approaches motivated by different geometric and topological structures on polygon space. In particular, the symplectic structure proposed by Millson and Kapovich seems to yield a very promising approach to constructing new alternatives to the ``crankshaft" and ``folding" moves now commonly used in exploring polygon spaces.

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SURNAME: Nafaa FIRST NAME: Chbili

ABSTRACT TITLE:

Form symmetry of knots to symmetry of spatial graphs

ABSTRACT (maximum 200 words):

In this talk, we start by a brief review on how the polynomial invariants of knots and links have been used successfully to study the symmetry of knots and links in the three dimensional space. Then, we explain how to extend these techniques to study the problem of symmetry in a more general setting where we consider spatial graphs instead of knots and links.

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SURNAME: Darcy FIRST NAME: Isabel

ABSTRACT TITLE:

Tangle analysis of protein-DNA complexes

ABSTRACT (maximum 200 words):

Some proteins will cut DNA and change the DNA configuration before resealing the DNA. Thus, if the DNA is circular, the DNA can become knotted. When modelling protein-DNA reactions, one would like to know how to draw the DNA. For example, are there any crossings trapped by the protein complex? How do the DNA strands exit the complex? Is there significant bending? Topological analysis cannot determine the exact geometry of the protein-bound DNA, but it can determine the overall entanglement of this DNA, after which other techniques may be used to more precisely determine the geometry.

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SURNAME: Deguchi FIRST NAME: Tetsuo

ABSTRACT TITLE:

Probability distribution function of distance between two segments of random knots with an analytic expression of the scattering function

ABSTRACT (maximum 200 words):

We evaluate two-point correlation functions of a ring polymer with fixed topology in a theta solution by simulation, and show novel critical behaviour for such ring polymers. Here the solvent satisfies the theta conditions of the corresponding linear polymers. We introduce an empirical formula for the probability distribution function of distance between two segments of a ring polymer with a fixed knot type K consisting of N statistical segments. It holds independently of the number of statistical segments, N, such as for N=300, 800 and 1000. Through simulation we show that the formula also gives good fitting curves to the end-to-end distance distribution of self-avoiding walks (SAW). From the large-distance behaviour of the distribution function and the large-q behaviour of the scattering function we suggest that ring polymers in the theta solvent should have new critical behaviour, which is an intermediate one between the Gaussian criticality and that of SAW, and is rather close to the Gaussian one.

- A. Yao, et al, J. Phys. A: Math. Gen. Vol. 37 (2004) pp. 7993-8006
- T. Deguchi et al., OCAMI Studies Vol. 1 (2007) pp. 165 -- 178,
- T. Deguchi et al, Bussei-Kenkyu 92-1 (2009) pp. 131--134.

Fibred knots in laser beams

ABSTRACT (maximum 200 words):

Coherent light fields are physical manifestations of maps from R^3 to C, as, at each point in physical space, the light beam has an intensity (modulus squared) and phase (argument). When light beams interfere, they generically produce three-dimensional nodal lines (phase singularities, optical vortices) along which the phase is physically undetermined [1].

By carefully controlling the interference of specific laser modes, it is possible to create physical light beams with nodal configurations that are knotted and linked. These beams are effectively realizations of fibred knots, where the fibre surfaces in the rest of space are the wavefronts, twisting around the knotted nodal lines. Explicit details of the laser knot construction, and descriptions of the experimental realization will be given [2].

- [1] M R Dennis, K O'Holleran and M J Padgett, "Singular Optics: Optical Vortices and Polarization Singularities", Progress in Optics 53 (2009) 293-363
- [2] M R Dennis, R P King, B Jack, K O'Holleran and M J Padgett "Isolated Optical Vortex Knots" Nature Physics 6 (2010) 118-121

Random polygons and random links in a confined volume

ABSTRACT (maximum 200 words):

In this talk I will discuss several issues regarding random polygons generated in a confined volume that includes model developments, generating algorithms, knotting and linking probability problems and the quantification of various geometric measures of these objects.

- Y. Diao, C. Ernst, K. Hinson and U. Ziegler, The mean squared writhe of alternating random knot diagrams, J. Phys. A: Math. Theor. 43, doi: 10.1088/1751-8113/43/49/495202 (2010).
- J. Portillo, J. Arsuaga, Y. Diao, R. Scharein and M. Vazquez, On the mean and variance of the writhe of random polygons, to appear in J. Phys. A: Math. Theor.
- T. Blackstone, R. Scharein, B. Borgo, R. Varela, Y. Diao and J. Arsuaga, Modeling of chromosome intermingling by partially overlapping uniform random polygons, J. Math. Biology 62(3), 371-389 (2011).

SURNAME: Dietler FIRST NAME: Giovanni

ABSTRACT TITLE:

Interplay between topology and bubble formation in double-stranded DNA

ABSTRACT (maximum 200 words):

Here we present a quantitative study of local DNA unwinding based on extensive single DNA plasmid imaging and discuss the interplay between topology and bubble formation in double-stranded circular DNA. The results presented herein strongly underlines the important role of denaturation bubbles in negatively supercoiled DNA for transcription and replication initiation in vivo. Bubble formation is a primary requirement for the initiation of DNA transcription and replication in both prokaryotic and eukaryotic cells: DNA unwinding provides access to the core of the base-pairs and thus the reactive groups of the nucleobases. Local unwinding of the DNA double-strand may be spontaneously effected by thermal fluctuations. Also a statistical physics treatment of the interplay between topology and bubble formation is presented. Additionally the temperature regulation of the bubble formation by controlling the linking number is discussed and experimental results are presented.

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Random linking

ABSTRACT (maximum 200 words):

We consider the Gauss linking number of pairs of closed curves in three-dimensional space, or of closed manifolds in higher-dimensional space. The kinematic integral of its square over the group of relative displacements of the curves (or manifolds) is shown to be given by the scalar product of two pairs of characteristic functions of the curves (or manifolds). This factorization theorem is generalized to the cyclic product of linking numbers of a set of curves (manifolds), moving at random in ambient space, and successively linked in a chain-like fashion. Applications include the calculation of the topological second virial coefficient of a gas of non-linked circles (or higher-dimensional spheres). The factorization theorem directly allows for randomization over the curves' (manifolds') shapes, with application to the topological interaction of random ring polymers.

SURNAME: Guadagnini FIRST NAME: Enore

ABSTRACT TITLE:

Knots and quantum field theory

ABSTRACT (maximum 200 words):

Applications of quantum field theory methods in the computation of link invariants will be illustrated.

- E. Guadagnini and F. Thuiller, Deligne-Beilinson Cohomology and Abelian Link Invariants, SIGMA 4 (2008) 078, 30 pages, arXiv:0801.1445
- E. Guadagnini and F. Mancarella, Abelian link invariants and homology, J. Math. Phys. 51 (2010) 062301, arXiv:1004.5211v1

An equivalence between two theories of `non-realizable' links

ABSTRACT (maximum 200 words):

One can consider Euler tours on a connected link and construct the intersection graph corresponding to an Euler tour. There are simple graphs which are not intersection graphs for any Euler tour. Defining Reidemeister moves on intersection graphs and extending them on all graphs we obtain new theories. We show that it is enough to consider only rotating circuits, i.e. Euler tours rotating at each classical crossing and each theory of `non-realizable' graphs is equivalent the theory constructed by using only rotating circuits. Also we discuss how one can define an orientation on graph-links with many components. This work is partially supported by RFBR grants 10-01-00748-a.

- D.P.Ilyutko, V.O.Manturov, Graph-links, arXiv:math.GT/1001.0384.
- D.P.Ilyutko, Framed 4-Valent Graphs: Euler Tours, Gauss Circuits and Rotating Circuits, arXiv:math.CO/0911.5504.
- D.P.Ilyutko, An Equivalence between the Set of Graph-knots and the Set of Homotopy Classes of Looped Graphs, arXiv:math.GT/1001.0360.

SURNAME: Kusner FIRST NAME: Robert

ABSTRACT TITLE:

Knots and Links as Ropes, Bands and Branched Coverings

ABSTRACT (maximum 200 words):

What is the geometry of tightly knotted rope? How, for example, is its length related to combinatorial or algebraic knot invariants? And what shapes are typical of tight knots or links? We'll discuss recent progress on such ropelength growth-rate and criticality issues, relating them to some simpler, potentially more computable, ideal geometric models, including one realizing knots or links as "fattest" (i.e. maximum modulus) annuli on Riemann surfaces branched covering the two-sphere.

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Framization of knot algebras

ABSTRACT (maximum 200 words):

We introduce the concept of modular framization. The idea originates from the Yokonuma--Hecke algebra, built from the classical Hecke algebra by adding framing generators and replacing the Hecke algebra quadratic relation by a new quadratic relation involving the framing generators. Using a Markov trace by Juyumaya we have constructed invariants for oriented framed knots, classical knots and singular knots. In this talk we shall present the above and we will show how to construct the framization $F_{d,n}$ of the Birman--Wenzl--Murakami algebra. The framization has been also applied to the Temperley--Lieb algebra, and it can be applied to other knot algebras having generators whose behaviour involves braid relations and polynomial relations, such as the singular Hecke algebra, the Hecke algebras of type \$B\$, et cetera.

(Joint work with Jesus Juyumaya)

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Knot polynomials in topological fluid mechanics

ABSTRACT (maximum 200 words):

The Kauffman bracket, Jones and \$S_L\$ polynomials have been constructed in topological fluid mechanics in terms of helicity of fluid flows. A direct relationship is established between classical fluid mechanics and knot algebraic polynomial topological invariants.

- Moffatt H.K.: J. Fluid Mech. 35 (1969) 117.
- Ricca R.L.: Lect. Notes Math. 1973 (2009) 167.
- Kauffman L.H.: Knots and Physics, 3rd ed., World Scientific Co., Singapore, 2001.

Geometrical and topological entanglement in ring polymers under spherical confinement

ABSTRACT (maximum 200 words):

The interplay of geometrical and topological entanglement in semiflexible polymer rings inside a spherical cavity is investigated using advanced numerical methods. In particular, we consider trefoil-knotted rings with a wide range of contour lengths and degree of confinement. By using stringent and robust algorithms for knot location, we characterize how the knot length, I_k (the arclength of ring portion accommodating the knot) depends on the ring contour length, L_c and the radius of the confining sphere, R_c. In the no- and strongconfinement cases it is observed weak knot localization and complete knot delocalization, respectively. We show that the complex interplay of I_k, L_c and R_c that seamlessly bridges these two limits can be encompassed by a simple scaling argument based on Odjik's deflection theory for semiflexible rings. The same argument is used to rationalise the increasing level of entanglement found in in progressively confined rings. The implications of the results in contexts of general interests, from viral genome entanglement to dense polymer phases is finally discussed.

Measures of Polymer Shape

ABSTRACT (maximum 200 words):

Polymers, both linear and ring, have long been know to have, on average, asymettrical features. We will explore several ways to methods to capture the scale of conformations and the degree of asymmetry. These will be employed in the study of influence of knotting on scale and shape.

- The effect of knotting on the shape of polymers, Macromolecules 41, 21, 2008, 8281-8287
- Effect of knotting on polymer shapes and their enveloping ellipsoids, J. P. Chem, 130, 2009, 1651041-8
- Symmetry-breaking in cumulative measures of shapes of polymer models, J. Chem Physics, 133, 2010, 1541131-4

Relaxation to topologically complex equilibria

ABSTRACT (maximum 200 words):

The method of 'magnetic relaxation' to magnetostatic states in which magnetic flux tubes may be knotted and/or linked in arbitrarily prescribed manner will be reviewed, with particular attention to the tangential discontinuities that inevitably appear in this process. The parallel problem of evolution of a minimum area soap-film in response to slow boundary deformation, and the topological jumps to which such films are subject, will also be discussed.

- Moffatt, H.K. 1985 Magnetostatic equilibria and analogous Euler flows of arbitrarily complex topology Part 1, Fundamentals. *J. Fluid Mech.* **159**, 359–378.
- Moffatt, H.K. 1990 The energy spectrum of knots and links. *Nature* **347**, 367–369 [see also *News and Views*, p.332].
- Goldstein, R.E., Moffatt, H.K., Pesci, A.I. & Ricca, R.L. 2010 Soap-film Möbius soap-film changes topology with a twist singularity. *PNAS*, **107** no. 51, 21979–21984.

Phase transitions in membranes of high genus

ABSTRACT (maximum 200 words):

The geometrical method describing phase transitions in membranes with nontrivial topology is elaborated. This approach based on the possibility to represent real membranes (Willmore-Helfrich surfaces) as minimal surfaces embedded in \$S ^3\$. The change of genus of membrane corresponds to creating holes in associated minimal surface. In the frame of mean field theory we describing phase transitions in membranes in terms of crystallization of holes. From this point of view we study the phase transition from cubic to sponge phase. We also describe the conformal modes , Moduli space and defects of membranes.

- E.Kats, M.Monastyrsky, Minimal Surfaces and Fluctuations of Membranes with nontrivial Topology, JETP V91, N6 (2000), 1279-1285
- E.Kats, M.Monastyrsky, Phase Transitons in membranes with high genus, Marinov Memorial Volume, World Scientific, 718-728, (2002)
- D. Jakobson, M. Monastyrsky , Stability of minimal surfaces (in preparation, 2011)

SURNAME: O'Hara FIRST NAME: Jun

ABSTRACT TITLE:

M\"obius invariant energies and average linking with circles (with Gil Solanes)

ABSTRACT (maximum 200 words):

We introduce a renormalized potential of a compact planar domain. By integrating it on the domain and then by renormalization, we can define a M\"obius invariant energy of planar domains, which can be considered as a functional for the simple closed planar curves. It can be generalized for the closed space curves, which turns out to be the renormalization of the average of squared linking number with random circles. This generalization is a M\"obius version of Banchoff-Pohl's notion of area enclosed by a space curve.

- Jun O'Hara and Gil Solanes, Möbius invariant energies and average linking with circles, arXiv:1010.3764v1
- Jun O'Hara, Renormalized \$r^{\bullet}\$-potentials and generalized centers of a domain, arXiv:1008.2731

Exceptional Dehn surgeries on the minimally twisted 5-chain link

ABSTRACT (maximum 200 words):

I will outline the general problem of understanding the exceptional (non-hyperbolic) Dehn surgeries on a hyperbolic link, and more generally the exceptional fillings of a cusped hyperbolic manifold, and I will state some consequences of the classification of all such fillings on a specific example, that displays a wealth of interesting phenomena. This is joint work with Martelli and Roukema.

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High resolution portrait of the ideal trefoil knot. New morphology details and new conjectures.

ABSTRACT (maximum 200 words):

An extremely high resolution picture of the trefoil knot tightened on the perfect rope will be presented and confronted with similar images obtained by other authors. It will be shown that high precision of the portrait allow us to formulate new conjectures concerning the shape of the ideal trefoil, in particular, its curvature and torsion.

Presented results are based on the Finite Elements Method simulations performed by Sylwester Przybył.

- Sylwester Przybył, *Poszukiwanie węzłów idealnych i ich własności*, Ph.D. thesis, Poznan University of Technology, Poznań 2001.
- Henryk Gerlach, *Ideal Knots and Other Packing Problems of Tubes*, Ph.D. thesis, EPFL, Lausanne 2010.
- T. Ashton, J. Cantarella, M. Piatek and E. J. Rawdon, Exp. Math., 20, 57 (2011)

Knotted Arcs

ABSTRACT (maximum 200 words):

The recent discovery of knotting in some proteins is both exhilarating and mysterious. However, these are not traditional mathematical knots. The proteins have free ends and from a strictly topological perspective all such curves are equivalent to a straight line (and, therefore, not knotted). Several different definitions for knotting within open arcs have been proposed. We consider one definition (in our opinion, the most stable of the definitions), due to Dobay, Millett and Stasiak, and analyze the subarc knot types seen within knotted closed configurations, concentrating on ropelength-minimized knots and random freely jointed chains. This is joint work with Ken Millett and Andrzej Stasiak.

REFERENCES (maximum 3):

 Kenneth Millett, Akos Dobay, and Andrzej Stasiak, Linear Random Knots and Their Scaling Behavior, Macromolecules, 38(2):601—606 (2005).

On the groundstate energy spectrum of magnetic knots

ABSTRACT (maximum 200 words):

In this talk we present new results on the groundstate energy spectrum of magnetic knots and links in ideal magnetohydrodynamics. By using classical results of Arnold (1974), Moffatt (1990) and Freedman and He (1991), we prove that the topology of magnetic knots and links provides a lower bound on the magnetic energy of the system [2]. By using standard relaxation techniques of the magnetic field, the groundstate energy of tight knots is determined [1], The relationship between this energy, topological crossing number and ropelength are examined. Groundstate energy spectra for the first 250 prime knots and links are determined and compared and new upper bounds for ropelength and tight braid energy are presented.

These results may find useful applications in astrophysical flows, and provide further grounds to establish a mathematical foundation for the classification of physical knots and links based on a one-to-one correspondence between energy and topology [3].

- [1] Maggioni F. & Ricca, R.L. On the groundstate energy of tight knots. *Proc. R. Soc.* A **465**, 2761-2783.
- [2] Ricca, R.L. Topology bounds energy of knots and links. Proc. R. Soc. A 464, 293-300 (2008).
- [3] Ricca, R.L. (Ed.) *Lectures on Topological Fluid Mechanics.* Lecture Notes in Mathematics **1973**, Springer-Verlag, Heidelberg (2009).

SURNAME: Scharein FIRST NAME: Robert

ABSTRACT TITLE:

Investigating Knots and Tangles in Physical Systems

ABSTRACT (maximum 200 words):

A large body of research has been devoted to understanding knots found in molecular biology, for example in DNA knotting. We apply these powerful visualization and computational tools to knots found in larger scale physical systems, such as in fluid flow and magnetohydrodynamic simulations.

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Tightening of DNA knots by supercoiling facilitates their unknotting by type II DNA topoisomerases

ABSTRACT (maximum 200 words):

Using numerical simulations, we compare properties of knotted DNA molecules that are either torsionally relaxed or supercoiled. We observe that DNA supercoiling tightens knotted portions of DNA molecules and accentuates the difference in curvature between knotted and unknotted regions. The increased curvature of knotted regions is expected to make them preferential substrates of type IIA topoisomerases because various earlier experiments have concluded that type IIA DNA topoisomerases preferentially interact with highly curved DNA regions. The supercoiling-induced tightening of DNA knots observed here shows that torsional tension in DNA may serve to expose DNA knots to the unknotting action of type IIA topoisomerases, and thus explains how these topoisomerases could maintain a low knotting equilibrium in vivo, even for long DNA molecules.

- Witz, G., Dietler, G. & Stasiak, A. Tightening of DNA knots by supercoiling facilitates their unknotting by type II DNA topoisomerases. PNAS, 108, 3608-3611, 2011.
- Witz, G., Dietler, G. & Stasiak, A. DNA knots and DNA supercoiling. Cell Cycle, 10, published on line 10.03.2011, <u>http://www.landesbioscience.com/journals/cc/article/15293/</u>

Geometric curvature energies for curves: an overview of analytic and knot-theoretic properties.

ABSTRACT (maximum 200 words):

We shall discuss several geometrically defined curvatures, related to Menger curvature for rectifiable sets (a soft potential, defined by means of a triple integral over the set) and to global curvature (a hard steric constraint, introduced more than a decade ago by Gonzalez and Maddocks). In fact, we consider several families of energies, interpolating between these In several works, written in various configurations together with Heiko von der Mosel and Marta Szumanska, we obtain a series of results that - seen from a certain perspective - allow one to show precisely in what sense the energies in question allow one to control the bending of a curve and the speed of changes of its tangent vector. We obtain also compactness results and can use them to control the number of knot classes below a given energy level.

We shall finish with a list of open problems related both to `physical' knot theory and to analysis.

- P. Strzelecki, H. von der Mosel: On rectifiable curves with L^p-bounds on global curvature: Self-avoidance, regularity, and minimizing knots. Math. Z. 257 (2007), 107-130.
 P. Strzelecki, M. Szumanska, H. von der Mosel: Regularizing and self-avoidance effects of integral Menger curvature. Ann. Scuola Norm. Sup. di Pisa 9 (2010), 145-187
 P. Strzelecki, H. von der Mosel: Tangent-point self-avoidance energies for curves. Preprint, avoidable on the arXiv converse arXiv 1006 1566
- available on the arXiv server, see arXiv:1006.4566

Ropelength Criticality

ABSTRACT (maximum 200 words):

What is the shape of a knot tied tight in rope?

The ropelength problem asks us to minimize the length of a knot or link in space, subject to a thickness constraint that keeps a unit tube around the curve embedded.

We derive a Balance Criterion giving necessary and sufficient conditions for a space curve to be ropelength-critical.

Our approach is modeled on rigidity theory for frameworks and uses a new infinite-dimensional version of the Kuhn-Tucker theorem.

In terms of the core curve, the thickness constraint has two parts:

an upper bound on curvature and a self-contact condition.

The curvature bound is especially difficult to handle, as the curve may fail to be twice differentiable.

In the end, we express thickness as the minimum of a compact family of smooth functions in order to apply Clarke's theorem on the derivative of such a minimum.

Using our balance criterion, we can give explicit descriptions of several tight links. The tight configuration of the Borromean rings, for instance, is piecewise smooth with 42 pieces. Even two simply clasped ropes surprising geometric behavior:

there is a slight gap between them when they are pulled tight.

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DNA Topology: Experiments and Analysis

ABSTRACT (maximum 200 words):

Cellular DNA is a long, thread-like molecule with remarkably complex topology. Enzymes that manipulate the geometry and topology of cellular DNA perform many vital cellular processes (including segregation of daughter chromosomes, gene regulation, DNA repair, and generation of antibody diversity). Some enzymes pass DNA through itself via enzyme-bridged transient breaks in the DNA; other enzymes break the DNA apart and reconnect it to different ends. In the topological approach to enzymology, circular DNA is incubated with an enzyme, producing an enzyme signature in the form of DNA knots and links. By observing the changes in DNA geometry (supercoiling) and topology (knotting and linking) due to enzyme action, the enzyme binding and mechanism can often be characterized. This tolk will give an overview of the use of knot theory in the analysis of experiments on circular DNA.

- **D.W. Sumners.** DNA Topology: Experiments and Analysis. In *Knot Theory for Scientific Objects, Proceedings of the International Workshop on Knot Theory for Scientific Objects,* A. Kawauchi, ed., OCAMI Studies 1 (2), 213-237 (2007).
- **D.W. Sumners**. Random Knotting: Theorems, Simulations and Applications. In *Lectures on Topological Fluid Mechanics*, Springer-CIME Lecture Notes in Mathematics 1973, R. Ricca, ed. (2009), 187-217.