Topology, Physics, and Chemistry of Soft Matter: Eutopia-IV

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About

Topology, Physics, and Chemistry of Soft Matter

The last few years have witnessed remarkable advances in our understanding of the emergence and consequences of topological constraints in bio- and soft matter, thanks to technological progress and the integration of experiments with increasingly sophisticated numerical simulations. Examples are abundant and cover seemingly distant topics, ranging from knotted proteins to genome organization and the interplay between topological and physical properties in complex fluids. As a consequence, topological bio- and soft matter is becoming a vibrant area of research attracting scientists from a broad range of disciplines.

The aim of this meeting, sponsored by the European Topology Interdisciplinary Action (EUTOPIA COST Action), is to bring together scientists from biology, chemistry, physics, and mathematics to discuss the most recent results in topological soft and bio-materials and share ideas with an interdisciplinary community.

The main topics of the conference comprise both (a) the modeling of complex systems and the emergence of collective behavior, as well as (b) the analysis of complex data sets in order to infer the underlying structure and functionality of networks. Particular focus will be put on oscillatory phenomena in neuroscience.

Organizing committee

Luca Tubiana (IT) Raffaello Potestio (IT) Franco Ferrari (PL)

Scientific committee

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Franco Ferrari (PL)
Achille Giacometti (IT)
Davide Michieletto (UK)
Joanna Sulkowska (PL)

Timetable

CT: Contributed Talk, IS: Invited Speaker, KL: Keynote Lecture, IT: Invited Talk.

Monday, 5 of September

8:40–9:20	**Registration**		
9:20–9:40	**Welcome remarks**		
9:40–10:00	CT	**Ferrari** Szczecin, Poland	Some recent advancement in the characterization of polymer systems and circularized polycatenanes in the presence of topological constraints
10:00–10:30	CT	**Piatek** Szczecin, Poland	Knots – gauge theory correspondence, and integrable conformations of polymer rings
10:30–10:50	CT	**Gabrovsek** Ljubljana, Slovenia	Bonded knotoids and linkoids
10:50–11:10	CT	**Dabrowksi-Tumanski** Warsaw, Poland	The statistical properties of entangled spatial graphs
11:10–11:50	KL	**Nedebock** Stellenbosch, South Africa	Closed polymer loops: simulated annealing of topology conserving planar crossing dynamics
11:50–14:10	**Lunch**		
14:10–14:30	IS	**Ioannidou** Thessaloniki, Greece	A Novel Discrete Algebra
14:30–14:50	CT	**Azote** Venice, Italy	Coarse-Grained Modelling of Biological polymers: proteins with ellipsoidal side chain
14:50–15:10	CT	**Skrbic** Venice, Italy	TBA
15:10–15:50	KL	**Liwo** Gdansk, Poland	Recent developments and applications of the UNICORN coarse-grained model of biological macromolecules
15:50–16:20	**Coffee break**		
16:20-16:40	CT	**Virnau** Mainz, Germany	AlphaFold predicts the most complex protein knot and composite protein knots
16:40-17:00	CT	**Andonovic** Skopje, North Macedonia	Mathematical analysis in characterization of carbon nanotubes (CNTs)
17:00-17:20	CT	**Dimitrov** Skopje, North Macedonia	Optimal selection of parameters for production of Multiwall Carbon Nanotubes (MWCNTs) by electrolysis in molten salts using machine learning
17:20-17:40	CT	**Palese** Turin, Italy	Second order Lagrangians for (2+1)-dimensional generalized Boussinesq equations and an extension of the Krupka-Betounes equivalent
17:40-18:00	CT	**Zappone** Lecce, Italy	Strength from defects: Topological barriers to defect nucleation generate large mechanical forces in a liquid crystal

Tuesday, 6 of September

8:40–9:00	**Registration**		
9:00–9:20	CT	**Fischer** Bayreuth, Germany	Topological control of colloids on magnetic patterns
9:20–9:40	CT	**Salamon** Budapest, Hungary	Topology and thermohydrodynamics in a ferroelectric nematic liquid crystal
9:40–10:00	IS	**Komineas** Crete, Greece	Breathing skyrmions in chiral magnets
10:00–10:30	**Coffee break**		
10:30–10:50	CT	**Grelet** Bordeaux, France	Topological Defects at the Colloidal Scale: Visualization, Structure and Role in Chirality Amplification
10:50–11:10	CT	**Travasso** Coimbra, Portugal	Adhesion modulates cell migration and endothelial cell dynamics
11:10–11:50	KL	**Lopez-Leon** Paris, France	TBA
11:50–14:10	**Lunch**		
14:10–14:30	IS	**Provan** Paris, France	Topological assignment of DNA knots and catenanes by high resolution Atomic Force Microscopy
14:30–14:50	CT	**Skoruppa** Leuven, Belgium	DNA fluctuations reveal the size of topological domains
14:50–15:10	CT	**Suma** Bari, Italy	Nonequilibrium thermodynamics of DNA nanopore unzipping
15:10–15:50	KL	**Japaridze** Delft, The Netherlands	Role of DNA sequence and topology in regulating nucleoprotein complexes
15:50–16:20	**Coffee break**		
16:20-16:40	CT	**Guzman** Ljubljana, Slovenia	Nanomechanical crowding at the interface between RNA and soft surfaces
16:40-17:00	CT	**Rosa** Trieste, Italy	Statistical mechanics of RNA as a branched polymer
17:00-17:20	IS	**Pasquali** Paris, France	TBA
17:20–18:30	Discussion		

Wednesday, 7 of September

8:40–9:00	**Registration**		
9:00–9:20	CT	**Racko** Bratislava, Slovakia	Channels with Helical Modulation Display Stereospecific Sensitivity for Chiral Superstructures
9:20–9:40	CT	**Cifra** Bratislava, Slovakia	Pressure of semi-flexible linear and ring polymers inside a spherical cavity
9:40-10:00	CT	**Milchev** Sofia, Bulgaria	Translocation kinetics of vesicles through narrow pores
10:00–10:30	**Coffee break**		
10:30–10:50	CT	**Novotna** Prague, Czech Republic	Defect structures in cholesterics with extremely short pitch and in the twist-grain boundary (TGB) phases characterized by various experimental technique.
10:50–11:10	CT	**Ferrarini** Padova, Italy	Spontaneous twisting of hard rod nematics
11:10–11:50	KL	**Copar** Ljubljana, Slovenia	Topology of equilibrium and flowing nematics
11:50–14:10	**Lunch**		
14:10–14:30	CT	**Bozeman** Cospicua, Malta	Probabilistic and topological approaches to potential Z-DNA genomic sequences
14:30–14:50	CT	**Kaplan** Haifa, Israel	Reorganizing the somatic genome with sperm proteins
14:50–15:10	IS	**Zippo** Trento, Italy	TBA
15:10–15:50	KL	**Di Stefano** Montpellier, France	TBA
15:50–16:20	**Coffee**		
16:20–18:30	MC Meeting/Poster session I		

Thursday, 8 of September

8:40–9:00	**Registration**		
9:00–9:20	CT	**Lamura** Bari, Italy	Active semiflexible polymer under shear flow
9:20–9:40	CT	**Locatelli** Padova, Italy	Interplay between topology and confinement in active polymers
9:40–10:00	CT	**Mandal** Darmstat, Germany	Crowding-Enhanced Diffusion for Highly Entangled Self-Propelled Stiff Filaments
10:00–10:30	**Coffee break**		
10:30–10:50	IS	**Salminen**	TBA
10:50–11:10	CT	**Coluzza** Bilbao, Spain	pH-antenna residues trigger large-scale conformational change in proteins
11:10–11:50	KL	**Jackson** Cambridge, United Kingdom	TBA
11:50–14:10	**Lunch**		
14:10–14:30	CT	**Rubach** Warsaw, Poland	AlphaKnot - efficient distributed knot detection for Alphafold-solved protein models
14:30–14:50	CT	**Niemyska** Warsaw, Poland	New knots in human proteome
14:50–15:10	IS	**Faccioli** Trento, Italy	A new therapeutic strategy from protein folding simulations
15:10–15:50	KL	**Sulkowska** Warsaw, Poland	How entangled proteins can be? Prediction and in vitro verification.
15:50–16:20	**Coffee**		
16:20-16:40	CT	**Zhao** Darmstadt, Germany	Regulatory effects of proline isomerization on the phase behavior of intrinsically disordered proteins
16:40-17:00	CT	**Lyu** Dublin, Ireland	Mechanism Study of Radical Homopolymerization of Multivinyl Monomers: Applicability of Flory-Stockmayer Theory
17:00–18:30	Poster session II		

Friday, 9 of September

8:40–9:00	**Registration**		
9:00–9:20	CT	**Papale** Paris, France	The role of topology in the nanorheology of active–passive polymer mixtures
9:20–9:40	CT	**Liu** Paris, France	A single-chain model for the linear viscoelasticity of unentangled melts of associating polymers
9:40–10:00	CT	**Stefanou** Limassol, Cyprus	Introducing a variable entanglement density constitutive rheological model based on principles of non-equilibrium thermodynamics
10:00–10:30	**Coffee break**		
10:30–10:50	CT	**Ubertini** Trieste, Italy	Computer simulations of melts of ring polymers with non-conserved topology
10:50–11:10	CT	**Zapata** Spain	Hypergraph and Hypermatrix Models for Higher-Order Connectivity
11:10–11:50	KL	**Leigh** Manchester, United Kingdom	Orderly Molecular Entanglements
11:50–14:10	**Lunch**		
14:10–14:30	IS	**Fosado** Edinburgh, UK	Programmable degradation of DNA hydrogels
14:30–14:50	IS	**Lappala** Cambridge, USA	Cooperative Motions and Topology-Driven Dynamical Arrest in Prime Knots
14:50–15:10	CT	**Sulkowski** Warsaw, Poland	Knots and AI – Learning to Unknot
15:10–16:30	Discussion and Farewell		

List of Abstracts – Talks

Monday 5th

Some recent advancement in the characterization of polymer systems and circularized polycatenanes in the presence of topological constraints

F. Ferrari[1]

[1] University of szczecin, Szczecin, Poland

In this contribution a few recent advances in characterizing certain soft matter systems in the presence of topological constraints will be illustrated. A power law based on analytical models for predicting how the complexity of knots and catenanes formed by cyclic polymers scales with their lengths will be presented. Moreover, information from highly parallelized simulations about the phases, sizes and conformations of single knotted polymers in a solution will be provided.

Tba

M. Piatek[1]

[1] Nan, Nan, Nan

TBA

Bonded knotoids and linkoids

B. Gabrovšek[1]

[1] University of ljubljana, Ljubljana, Slovenia

The theory of knotoids has recently gained attention in the topological analysis of proteins as knotoids have been identified as objects that encode the topological structure (knotted type) of a protein backbone when projected to a plane. We will extend the theory on knotoids in two distinct ways. First, we will define multi-linkoids, where we consider several mutually entangled polypeptide chains. Second, we will consider bonded knotoids and linkoids, where we will integrate bonds into the knotted structure. In both cases we will present topological invariants to distinguish between these structures. The invariants will be based on the Jones polynomial and Kauffman's unplugging invariant. This is joint work with N. Gügümcü and L. Kauffman.

The statistical properties of entangled spatial graphs

P. Dabrowski-tumanski[1]

[1] Cardinal stefan wyszynski university, Warsaw, Poland

The random, volume-less polymers usually constitute a benchmark system for different experiments. In particular, it is known, how probable it is, that a (phantom) polymer with a given length gets knotted and what is the probability of each knot depending on the polymer length. However, the complex systems are rarely non-interacting, separated random loops. Usually, they form a large net with a lot of branching points. Therefore, in this work I will tackle the question of the statistics of graphs with branching points. I will show the classification of such graphs and present the first results showing, how probable it is to obtain a non-trivial random spatial graph with up to 4 branching points.

Closed polymer loops: simulated annealing of topology conserving planar crossing dynamics

K. Müller-nedebock[1]

[1] Stellenbosch university, Stellenbosch, South africa

In systems of closed polymer loops the statistical configurations available to the polymer chains are restricted to those that retain the nonlocal state of entanglement. One fruitful approach to dealing with entanglement constraints in the statistical physics of the chains is to restrict the summations over configurations of the loops through enforcing topological invariants. A quasi-dynamics of chain crossings in projection, cast as a reaction-diffusion system system inspired by the Reidemeister moves, which preserve the state of knottedness, can also be used to explore topological equivalence of knots [Rohwer, 2015]. We explore how stochastic simulation of such dynamics can test for knot equivalence and under simulated annealing.

A novel discrete algebra

T. Ioannidou[1]

[1] Aristotle university of thessaloniki, Thessaloniki, Greece

A novel discrete algebra is presented which follows by combining the SU(2) Lie-Poisson bracket with the discrete Frenet equation. Physically, the construction describes a discrete piecewise linear string in R3. The starting point of our derivation is the discrete Frenet frame assigned at each vertex of the string. Then the link vector that connect the neighbouring vertices assigns the SU(2) Lie-Poisson bracket. Moreover, the same bracket defines the transfer matrices of the discrete Frenet equation which relates two neighbouring frames along the string. The procedure extends in a self-similar manner to an infinite hierarchy of Poisson structures. As an example, the first descendant of the SU(2) Lie-Poisson structure is presented in detail. For this, the spinor representation of the discrete Frenet equation is employed, as it converts the brackets into a computationally more manageable form. The final result is a nonlinear, nontrivial and novel Poisson structure that engages four neighbouring vertices.

An Improved Approach to Coarse-Grained Modelling of Biological Polymers

M. Spinaci[1]

[1] Ca' Foscari University of Venice, Venice, Italy

Proteins are fundamental for many processes in living cells. Their biological function are de- termined by their overall folding pattern and the spatial arrangement of all atoms in a single polypeptide chain. Segments of the chain arrange into a local three-dimensional structure, i.e., the atoms are arranged in secondary structures such as alpha helices or beta sheets. The biological phenomena of interest span time and size scales that are difficult to achieve in fully atomistic Molecular Dynamics simulations. Therefore, several simplified Coarse Graining (CG) representation schemes have been developed for proteins to achieve these time and length scales. Although CG models have been successful, to our knowledge no model exists that can accurately reproduce within the same parametrization the geometric and thermodynamical properties of the two most common structural motifs, i.e., the alpha helices and the beta sheets. We are currently working on developing a new CG representation scheme for proteins to address this problem. This new model is implemented in a freely available simulation code [1, 2], which is a state-of-the-art software for simulations. Our model is based on recently developed model by Škrbić and coworkers [3, 4] to capture the structures of the building blocks of protein structures from first principles and with no adjustable parameters. Škrbić's model has provides significant insight, but it only deals with ground states and has a very crude representation of the three-dimensional properties of proteins. We have therefore kept the key features of the Škrbić model, and we are working on improving its predictions by introducing several new features. This model, once the parameters have been set, allows us to reproduce the main common structural motifs (i.e., alpha helices and beta sheets), and the competition between them, once the potential parameters have been set.

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[3] T. Skrbic, T. X. Hoang, A. Maritan, J. R. Banavar, A. Giacometti Proteins 2019, 87, 176. DOI:10.1002/prot.25619

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Tba

T. Skrbic[1]

[1] Nan, Nan, Nan

TBA

Recent developments and applications of the unicorn coarse-grained model of biological macromolecules

J. Liwo[1]

[1] University of gdansk, faculty of chemistry, Gdansk, Poland

Coarse-grained approaches are of growing importance in simulating complex systems, including biological macromolecules and their assemblies. These approaches enable us to extend the time- and size-scale of simulations by orders of magnitude. In this talk, the physics-based Unified Coarse Grained Model (UNICORN) (www.unres.pl) of biological macromolecules, which comprises polypeptide chains (UNRES, containing 2 sites per residue), nucleic acids (NARES-2P, 2 sites per residue), and polysaccharides (SUGRES-1P, 1 site per residue) will be discussed. Owing to the rigorous physics-based scale-consistent derivation of the energy function, which thus embeds the atomic details of the interacting sites in the effective potentials, the model performs well in the simulation of structure, dynamics, and thermodynamics of the systems under study despite aggressive coarse graining. In particular, the site-site interaction potentials have axial and not spherical symmetry and contain multibody terms that couple long-range interactions with local conformational states. The talk will address the theory of the model and recent theoretical developments, which include through-sequence multibody terms that correlate remote chain sections, torsional and other multibody potentials involving protein side chains that enable us to study amino-acid-residue racemization, the use of sparse data from nuclear magnetic resonance (NMR), chemical cross-link mass spectroscopy (XL-MS), and small-angle x-ray and neutron scattering (SAXS and SANS) experiments, as well as from bioinformatics, in simulations, and the relationship between the coarse-grained and all-atom/experimental time scales. Recent algorithmic developments of the UNICORN package, which include CPU- and memory-oriented code optimization and massive parallelization with MPI and OpenMP, which now enable us to study systems with 100,000+ residues, will also be addressed. Selected applications of the UNICORN package in protein- and DNA/RNA structure modeling, modeling protein-folding kinetics/pathways and free-energy landscapes, as well as in solving biological problems such as, e.g., effects of mutations on virus-capsid dynamics, will be discussed. Finally, the unres.pl web server for ab initio and data/bioinformatics-assisted modeling of protein structure and dynamics will be presented.

Alphafold predicts the most complex protein knot and composite protein knots

P. Virnau[1]

[1] Johannes gutenberg university, Mainz, Germany

The computer artificial intelligence system AlphaFold has recently predicted previously unknown three-dimensional structures of thousands of proteins. Focusing on the subset with high-confidence scores, we algorithmically analyze these predictions for cases where the protein backbone exhibits rare topological complexity, i.e. knotting. Amongst others, we discovered a 7_1-knot, the most topologically complex knot ever found in a protein, as well several 6-crossing composite knots comprised of two methyltransferase or carbonic anhydrase domains, each containing a simple trefoil knot. These deeply embedded composite knots occur evidently by gene duplication and interconnection of knotted dimers. Finally, we report two new five-crossing knots including the first 5_1-knot. Our list of analyzed structures forms the basis for future experimental studies to confirm these novel knotted topologies and to explore their complex folding mechanisms.

Mathematical analysis in characterization of carbon nanotubes (cnts)

B. Andonovikj[1]

[1] Faculty of technology and metallurgy, Skopje, North macedonia

This research discusses full molecular characterization of carbon nanotubes (CNTs) produced by electrolysis in molten salts. Each CNT has its own mathematical representation due to its hexagonal lattice structure. Multi-wall carbon nanotubes (MWCNTs) are considered and the focus is directed to determining their structural parameters: innermost and outermost diameters, chiral indices m and n, number of walls and their unit cell parameters. Corresponding frequency parts of Raman spectra of four experimentally produced CNTs are elaborated, as well as employment of Python programming and Mathematica for the most accurate (m,n) assignment. Determining the chirality of these samples enables calculation of other structural properties which are performed hereby, including their graph representation. The latter enables evaluation of different distance based topological indices (Wiener, Balaban, Sum-Balaban, Harary index, etc.) in order to predict some index-related properties of the molecules.

Optimal selection of parameters for production of multiwall carbon nanotubes (mwcnts) by electrolysis in molten salts using machine learning

V. Andonovikj[1]

[1] International Postgraduate School Josef Stefan, Ljubljana, Slovenia

The production and use of carbon nanotubes (CNTs) have become extremely widened within the last decade. Hence, the interest for producing non-expensive and quality CNTs is high and has motivated many research projects to date. This research considers design and development of new technology for production of MWCNTs by electrolysis in molten salts using non-stationary and stationary current regimes. The electrolysis is simple, ecological, economical, and flexible. It offers possibilities for accurate control of various parameters, such as applied voltage, current density, or temperature. We infer the underlying relationship between the parameters and the quality of the experimentally produced MWCNTs by making use of explainable tree-based Machine Learning (ML) models. We train several models in a supervised manner, where as model covariates we use the parameters of the MCWNTs, and as a target variable the quality of the produced MWCNT. All the experimental examples in our data set are labeled by domain experts. Controlling these parameters enables high-yield production, and particularly important, obtaining MWCNTs which are up to ten times cheaper compared to other existing technologies

Strength from defects: topological barriers to defect nucleation generate large mechanical forces in a liquid crystal

B. Zappone[1]

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Common fluids cannot sustain static mechanical stresses at the macroscopic scale because they lack molecular order. Conversely, crystalline solids exhibit long-range order and mechanical strength at the macroscopic scale. Combining the properties of fluids and solids, liquid crystal films respond to mechanical confinement by both flowing and generating static forces. The elastic response, however, is very weak for film thicknesses exceeding 10 nm. In this study, the mechanical strength of a fluid film was enhanced by introducing topological defects in a cholesteric liquid crystal, producing unique viscoelastic and optomechanical properties. Using a surface forces apparatus (SFA), the cholesteric was confined under strong planar anchoring conditions between two curved surfaces with sphere-sphere contact geometry, similar to that of colloidal particles, creating concentric dislocation loops. During surface retraction, the loops shrank and periodically disappeared at the surface contact point, where the cholesteric helix underwent discontinuous twist transitions, producing weak oscillatory surface forces. On the other hand, new loop nucleation was frustrated by a topological barrier during fluid compression, creating a metastable state. This generated exceptionally large forces with a range exceeding 100 nm, as well as extended blue-shifts of the photonic band-gap. The metastable cholesteric helix eventually collapsed under a high compressive load, triggering a stick-slip-like cascade of defect nucleation and twist reconstruction events. These findings were explained using a simple theoretical model and suggest a general approach to enhance the mechanical strength of 1d-periodic materials, particularly cholesteric-colloid mixtures.

Tuesday 6th

Topological control of colloids on magnetic patterns

T. Fischer[1]

[1] University of bayreuth, Bayreuth, Germany

Topology plays a crucial role in electronic systems protecting the transport of charge and spin against dissipative scattering, which in topologically trivial systems usually destroys the transport. In topologically nontrivial electronic systems a whole zoo of new kind of particles, originally postulated in high energy physics, with unusual transport properties could be found experimentally in medium energy solid state physics. The field is large enough to entertain the solid-state community for more than a decade. Here we show with experimental and theoretical examples [1-6] that similar, albeit not identical, behaviour can be found in soft matter systems, where driven magnetic colloids carrying a magnetic moment replace the electrons, and periodic magnetic patterns replace the background solid state.

References

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Topology and thermohydrodynamics in a ferroelectric nematic liquid crystal

P. Dr. salamon[1]

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The ferroelectric nematic is a novel liquid crystal phase that exhibits extraordinary properties such as huge permittivities, and spontaneous polarization while keeping fluidity [1]. We studied the texture and director structure including topological defects as a function of temperature in sessile droplets and discs of the liquid crystal RM734 that exhibits the ferroelectric nematic phase. We present an unexpected discovery of a thermal gradient-induced circular flow in the sessile drops, which appears only in the ferroelectric phase [2]. While the motion of small tracer particles clearly indicates the circular flow, the texture appears completely steady indicating laminar streams. We provide a simple model showing that the tangential arrangement of the ferroelectric polarization combined with the vertical thermal gradient and the pyroelectricity of the fluid drives the circular flow. These observations provide a fascinating example of the unique nature of fluid ferroelectric liquid crystals.

Breathing skyrmions in chiral magnets

S. Komineas[1]

[1] University of crete, Heraklion, Greece

Breathing oscillations of chiral skyrmions in magnets with the Dzyaloshinskii-Moriya interaction have been reported in many works. In an antiferromagnet, we employ an adiabatic approximation and derive a potential energy that directly implies breathing oscillations. The frequency of small amplitude breathing oscillations is determined. We further study the nonlinear regime and the features of larger amplitude oscillations. We show that there is a maximum amplitude supported by the potential energy. As a consequence, we predict theoretically and observe numerically skyrmion annihilation events, i.e., the collapse of the skyrmion configuration, due to the excitation of large amplitude breathing oscillations. The process is efficient when the skyrmion is only mildly excited so that its radius initially grows, while the annihilation event is eventually induced by the internal breathing dynamics. We reveal the counter-intuitive property that the skyrmion possesses a nonzero kinetic energy at the instance of its annihilation.

Topological defects at the colloidal scale: visualization, structure and role in chirality amplification

E. Grelet[1]

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Topological defects are ubiquitous in Nature, from condensed matter and geophysics to cosmology. In ordered systems, defects mediate phase transitions, and determine many distinctive features of materials, from crystal growth to mechanical properties in metals. However, despite theoretical predictions, the detailed structure of defects remains largely elusive, especially close to their core with the presence of a singularity. By using a model system of colloidal tip-labeled rod-shaped particles enabling improved resolution and contrast by optical microscopy, in situ visualization and quantitative characterization of elementary linear defects - dislocations - has been performed in lamellar structures [1]. The displacement field around dislocations as well as their local morphology (determination of the core size as well as their chiral handedness) will be presented. Finally, we will show the role of topological defects for driving chirality amplification to helical superstructures. We will discuss how dislocation defects not only promote the growth, but also control the chiral morphology and therefore the functionality of self-assemblies [2].

References

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Adhesion modulates cell migration and endothelial cell dynamics

R. Martins travasso[1]

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One of the most fundamental abilities required for the sustainability of complex life forms is active cell migration, being essential in diverse processes from morphogenesis to leukocyte chemotaxis in immune response. The movement of a cell is the result of intricate mechanisms, that involve the coordination between mechanical forces, biochemical regulatory pathways, and environmental cues. In this work we explore how mechanical interactions such as spatial restriction and adhesion affect migration of a self-propelled droplet in dense fibrous media. We perform a systematic analysis using a phase-field model and we propose a novel approach to simulate cell migration with dissipative particle dynamics modelling. With this purpose we have measured in our simulation the cell's velocity and quantified its morphology as a function of the fiber density and of its adhesiveness to the matrix fibers. We then use this model to explore polarization and dynamics of endothelial cells in a blood vessel. Specifically, we use this model to study two important processes related to endothelial cell organization and migration: endothelial cell polarization with flow in a blood vessel and sprouting angiogenesis. In the first scenario, we show that we can simulate the endothelial cell polarization and shape in a vessel by assuming that endothelial cells migrate in the blood flow direction with variable velocities. Their shape is strongly dependent on cell-cell and cell-matrix adhesion forces. We also show that when a single cell acquires the tip cell phenotype, it can prompt the growth of a sprout-like structure by recruiting its neighboring cells. This new sprout can be the start of a new blood vessel formed from the preexisting tube.

Active nematics: from cells to logical operations

T. Lopez-leon[1]

[1] Cnrs /espci, Paris, France

Active nematics are biomimetic liquid crystals in which a 2D network of microtubule filaments is set in motion by the action of molecular motors [1, 2]. They are model systems to describe a variety of processes in nature, including cytoplasmic streaming in cells, the collective behavior of bacterial colonies, or animal morphogenesis [3-5]. In their steady state, active nematics usually exhibit chaotic dynamics controlled by the motion of a large number of self-propelled topological defects [6]. Understanding the observed emergence of order in biological systems remains a challenge. In this talk, I will show how the chaotic motion of topological defects can be turned into an organized choreography using confinement and geometry [7, 8]. Directional motion arises spontaneously when the active nematic is confined to thin open channels, due to the interaction of the defects with the walls. Complex active flow networks can be built by connecting these channels together, imposing global topological constraints on the system that enable, for example, logical operations to be implemented. Finally, I will show that remarkable dynamic states arise when the active nematic is confined to the anisotropic surface of a micro-sized, ellipsoidal, smectic droplet.

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Topological assignment of dna knots and catenanes by high resolution atomic force microscopy

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The topology of DNA is tightly regulated due to its profound effect upon DNA replication, transcription, and recombination. DNA topology describes how the two strands of the double helix intertwine intramolecularly, and how intermolecular relationships between multiple molecules occur. Topologically complex DNA conformations can be formed accidentally or intentionally through DNA-protein transactions, such as accidentally during the strand-exchange action of type-II topoisomerases, or intentionally by the reactions of site-specific recombinases. Despite the long history of DNA topology as a field of study, it remains difficult to determine the exact topology of complex DNA molecules, such as knots and catenanes (links). In recent years Atomic Force Microscopy (AFM) imaging has matured into a powerful technique for the investigation of DNA structure. In this work we utilised an E. coli DNA recombination system for the generation of topologically complex knotted or catenated DNA circles. While these DNA recombination products had been investigated using biochemical techniques, they had not yet been verified on a single-molecule level using microscopy. We used high resolution AFM to investigate the topological assignment of these DNA molecules in comparison to our models and the previous biochemical evidence.

Dna fluctuations reveal the size of topological domains

E. Skoruppa[1]

[1] Kuleuven, Leuven, Belgium

DNA plectonemes are ubiquitous in genomic DNA and represent a key regulatory mechanism orchestrating DNA readout, recombination, and genome maintenance. Magnetic tweezers have been used extensively to explore the behavior of supercoiled linear DNA molecules and to characterize its interaction with various classes of DNA-binding proteins. The readout in these experiments is usually based on protein induced changes in endpoint extension, where thermal fluctuations constitute a limiting factor for e.g. time-resolution. Au contraire, in this work we show that fluctuations can be leveraged to detect protein binding modes that are undetectable via the first moment. Using a combination of high-speed magnetic tweezers experiments, Monte Carlo simulations, and analytical theory based on a two phase model, we map out the dependence of DNA extension fluctuations as a function of supercoiling density and external force. We find that in the plectonemic regime the extension variance increases linearly with increasing supercoiling density and trace its principle origin to phase-exchange fluctuations. Based on this observation we show that association of DNA-bridging proteins elicits a change in the extension variance which allows us to predict the size of the generated topological domain. In addition, transient (partial) dissociation of DNA bridging proteins is demonstrated to result in dynamic sampling of different topological states, allowing us to deduce the torsional stiffness of the plectonemic state and the kinetics of protein-plectoneme interactions.

Nonequilibrium thermodynamics of dna nanopore unzipping

A. Suma[1]

[1] Università degli studi di bari, Bari, Italy

Using theory and simulations, we carried out a first systematic characterization of DNA un- zipping via nanopore translocation. Starting from partially unzipped states, we found three dynamical regimes depending on the applied force, f : (i) heterogeneous DNA retraction and rezipping (f < 17pN), (ii) normal (17pN < f < 70pN) and (iii) anomalous (f > 70pN) drift-diffusive behaviour. We show that the normal drift-diffusive regime can be effectively modelled as a one-dimensional stochastic process in a tilted periodic potential. We derive the effective potential from a suitable theoretical analysis of the non-equilibrium unzipping trajectories and demonstrate that it corresponds to the free-energy landscape of the unzipping process. Importantly, this novel approach for solving the inverse problem offers new strategies for inferring DNA-unzipping potentials of mean force from translocation experiments, paving the way for broader applications in periodic systems with drift-diffusion.

Role of dna sequence and topology in regulating nucleoprotein complexes

A. Japaridze[1]

[1] Delft university of technology, Delft, Netherlands

The interplay between DNA sequence and topology for protein recruitment and genome organization remains poorly understood. In the first half of my talk I will focus on the role protein binding site location along the DNA plays in organizing nucleoprotein complexes [1]. Here, we use atomic force microscopy and solid-state nanopores to investigate long-range nucleoprotein structures formed by the binding of FIS and H-NS proteins, to DNA molecules with distinct binding-site arrangements. We find that linear arrangement of otherwise identical protein binding sites can govern the higher-order architecture of the nucleoprotein complexes. Based on linear sequence arrangement the protein-DNA complexes differed in shape, stiffness and compaction, as well as the extent of DNA accessibility to protein binding. In the second half of my talk I will discuss how human centromeric regions are organized and folded [2]. Centromeres are essential regions of chromosomes acting as platforms for kinetochore assembly and microtubule attachment to guide proper genome segregation. Most centromeres, across multiple species are enriched with particular AT-rich DNA sequences, though their structural and regulatory roles are not well understood. We provide direct evidence that human centromeric DNA self-organizes into non-B-form secondary DNA structures. It forms well defined nanometer-sized hairpins, that form non-randomly across the centromeres that help recruit proteins that compact and reshape centromeres.

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Nanomechanical crowding at the interface between rna and soft surfaces

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[1] Jozef stefan institute and universidad autonoma de madrid, Mainz, Germany

Nanomechanical crowding remains theoretically unexplored at the interface of RNA molecules and soft surfaces. Existing RNA molecular models tend to reach very complex ensembles on themselves to be combined to e.g. external mechanical interactions with soft surfaces. Here, we introduce a multiscale approach which couples a tractable RNA coarse-grained model1,2 with an elastic energy component3. Within this approach, we study the specific role of RNA's secondary structure patterns on the deformation of soft surfaces by characterizing representative motifs of an RNA virus2. We also vary the length of the investigated molecules and discuss scaling trends for longer RNAs. Under controlled molecular crowding conditions we analyze the effects of conformational entropy and the interplay between surface energy per monomer and deformation lengths. Our findings add a novel way to address the mechanisms of response of encapsulated RNA inside crowded macromolecular environments, like the ones faced during RNA delivery.

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Statistical mechanics of rna as a branched polymer

A. Rosa[1]

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The statistical physics of branched polymers is surprisingly rich and its applications range from polymer physics to chromosome folding in eukaryotes to RNA conformations. In this talk, I will discuss some preliminary work focusing on the branching properties of generic and viral RNA chain molecules.

Tba

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TBA

Wednesday 7th

Channels with helical modulation display stereospecific sensitivity for chiral superstructures

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[1] Polymer institute, slovak academy of sciences, Bratislava 45, Slovakia

By means of coarse-grained molecular dynamics simulations, we explore chiral sensitivity of confining spaces modelled as helical channels to chiral superstructures represented by polymer knots. The simulations show that helical channels exhibit stereosensitivity to chiral knots localized on linear chains by effect of external pulling force and also to knots embedded on circular chains. The magnitude of the stereoselective effect is stronger for torus knots, the effect is weaker in the case of twist knots, and amphichiral knots do exhibit no chiral effects. The magnitude of the effect can be tuned by the so-far investigated radius of the helix, the pitch of the helix and the strength of the pulling force. The model is aimed to simulate and address a range of practical situations that may occur in experimental settings such as designing of nanotechnological devices for the detection of topological state of molecules, preparation of new gels with tailor made stereoselective properties, or diffusion of knotted DNA in biological conditions.

Pressure of semi-flexible linear and ring polymers inside a spherical cavity

P. Cifra[1]

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Peter Cifra and Tomáš Bleha Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 845 41 Bratislava 45, Slovakia, cifra@savba.sk The main emphasis in this research is on the computation of the pressure p a polymer exerts on internal surface of a spherical cavity of the size D. The dependence of various polymer properties on pressure at confinement is presented. The simulations are primarily aimed on comprehensive comparison of the pressure in polymers differing by the chain topology (linear/ring) and by the chain stiffness (flexible/semi-flexible). While semi-flexible chain show invariably higher pressure than flexible, interestingly, in context of chain topology effects, for both flexible and semi-flexible chains only minor effect of the chain topology on the pressure is found. It was confirmed that the scaling relations assuming a semidilute solution in a sphere deduced for linear flexible chain are also applicable to the ring analogues. However, the original scaling relations for flexible chains had to be modified including chain persistence length P. We quantified the enhanced free energy penalty upon compression of semi-flexible chain by two integration methods. Segment density profiles expressed salient features due to the difference in chain stiffness and topology. Accordingly, the bond orientation functions and scattering functions for ring and linear chain provides info on the variations in the structural ordering and formation of toroid in the sphere. The energy changes due to the chain bending energy were identified as a major source of the enhanced pressure in the confined semi-flexible relative to flexible chain.

Translocation kinetics of vesicles through narrow pores

A. Milchev[1]

[1] Bulgarian academy of sciences, institute of physical chemistry, Sofia, Bulgaria

We use extensive Molecular Dynamics (MD) simulations to study the osmotically induced translocation of partially filled vesicles through narrow pores. The dependence of the average translocation time, τ_{tr}, on vesicle size M, pore radius R_p, and strength of the driving force, ΔP, are examined for vesicles in a broad interval of sizes M. The time τ_{tr} is found to grow with decreasing pore size by an universal scaling law, $\tau_{tr} \propto (R_p - R_{cr})^{-2/3}$, where $R_{cr}(M, \Delta P)$ denotes the critical pore radius when the vesicle gets stuck in the pore. With regard to applied pressure, P, we find a power law relationship, $\tau_{tr} \propto \Delta P^{-\omega}$, where $\Delta P = P - P_{cr}$ with P_{cr} being the least pressure that can still drive the vesicle through a pore of size R_p. The exponent ω varies with R_p and tends to unity as the pore size narrows, $R_p \to R_{cr}(M, \Delta P)$. In addition, τ_{tr} is found to attain a minimum for an optimal value of the membrane bending rigidity. The variation of vesicle shape, surface area, volume and translocated fraction of the vesicle with time elapsed since the onset of the process is shown to change qualitatively with varying pore size.

Defect structures in cholesterics with extremely short pitch and in the twist-grain boundary (tgb) phases characterized by various experimental technique.

V. Novotna[1]

[1] Institute of physics ascr, Prague, Czech republic

The cholesteric phase represents a twisted structure driven by the molecular chirality. Periodicity of the helical structure (pitch) is often in the range of the visible-light wavelength up to several microns. During our research of lactic acid derivatives, we found a series of cholesterics which exhibits extremely short pitch length, 150-300 nm. A finger-print textures reflect the periodicity of studied compounds and can be detected by AFM technique. In a particular example we proved the pitch length by resonant X-ray technique. Another example of liquid crystalline mesophases with a regular array of defects is a twist grain boundary (TGB) phase. We studied compounds with TGB phases which exists at the room temperature, and we pursued their structure by various experimental techniques. We observed the surface of the smectic film by AFM microscope and detected a periodic relief. We found that the displacement amplitude is in the scale of few nanometres, with the periodicity of about 500 nm. Such periodicity is in accordance with the periodicity of the TGBC blocks' rotation estimated by polarizing microscopy. A simplified model interpreting the observed smectic surface displacement as the consequence of rotating TGBC blocks inside the sample is proposed. The AFM data were fitted to the theoretical formula describing such model of the surface displacement.

Spontaneous twisting of hard rod nematics

A. Ferrarini[1]

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Nematic liquid crystals are characterized by uniaxial orientational order and a uniform director field as a ground state. However, it is well known that molecular chirality can lead to the formation of chiral structures, e.g., in cholesteric and blue-phases or in half-skyrmion configurations. Here, using an extension of Onsager-Straley theory, we show that nematic order of hard rods entails an intrinsic tendency to twist. The anisotropic hard-core potential is arguably the simplest form of pair potential able to originate spontaneous breaking of mirror symmetry in a 3D fluid. The underlying physical mechanism, based on an elastic instability, is distinct from the common mechanism for the formation of chiral structures in microscopically chiral systems. The theoretical results will be discussed in relation to the recent discovery of a double twisted ground state in lyotropic chromonic liquid crystals.

Topology of equilibrium and flowing nematics

S. Čopar[1]

[1] Faculty of mathematics and physics, university of ljubljana, Ljubljana, Slovenia

Liquid crystals and topological defects are entangled at their core, and studying nematic textures and patterns ultimately reduces to seeing the manifestation of topological rules under a geometric constraint and elasticity minimization specific to the studied phenomenon. The point defects and line defects, seen in simple geometries, give rise to entangled and knotted line defects, when colloidal inclusions and twist are introduced. Textures substrates, inclusions set out in a lattice, and different shapes of inclusions, as well as external fields, can act as the providers of geometric context to the otherwise geometry-agnostic topological formalism. When intrinsic chirality is present, it stabilizes different three-dimensional solitons and gives rise to interesting interactions between them. Another layer of complexity is brought along when the nematic is subjected to shear flow. Even in a steady-state flow, nontrivial structure can be achieved in a system that is completely uniform in the absence of flow. I will walk through the ever growing tangle of related nematic and cholesteric systems that each exposes a different aspect of the underlying topology. I will discuss the intricacies that arise when chirality and flow are involved, and the role of topology in applications.

Probabilistic and topological approaches to potential z-dna genomic sequences

J. Bozeman jr[1]

[1] American university of malta, Bormla, Malta

It is well known what sequences of bases in DNA are likely to be in left-handed form, i.e. the Z-DNA conformation. We look at stochastic profiles of such sequences in the fasta format to determine the probability of these occurring. These genomic sequences have been found in rodent parvoviruses, salmonella and some carcinogens, for instance. It is thought that these orderings can cause the deleterious effects due to the different binding properties of Z-DNA as compared to the right-handed B-DNA, e.g. with certain proteins. We also examine the effect on the 3-dimensional conformation of the molecule when those orderings are in the left-handed version. Portions of DNA in this conformation can lower the stress on the molecule.

Reorganizing the somatic genome with sperm proteins

N. Kaplan[1]

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During spermatogenesis, chromatin organization undergoes major changes. Small basic proteins called protamines replace the majority of histones in mature sperm cells, allowing extreme chromatin condensation. Due to the complexity of the sperm maturation process, a model for studying the sperm DNA packaging and its ramifications has yet to be established. To study in detail the effects of protamine on chromatin packaging, we expressed protamine in human somatic cell lines. We combined confocal microscopy and Hi-C to observe changes in genome organization both at the level of single-cell dynamics and bulk population in detail. Interestingly, microscopy shows dramatic changes in genome organization driven by protamine expression, but these are not reflected by dramatic changes in the Hi-C.

Tba

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[1] Nan, Nan, Nan

TBA

Structure and dynamics of eukaryotic chromosomes

M. di Stefano[1]

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Chromosome organization and dynamics regulate many fundamental processes in the cell nucleus, including DNA transcription, replication, and repair. Experiments unveiled that chromosome spatial organization is hierarchical from large chromosome territories to local domains or TADs. Likewise, chromosome dynamics is heterogeneous and can be liquid-like or gel-like, depending on the cell condition. Here, I will present recent applications of biophysical modeling to study the principles regulating the structure and dynamics of chromosomes. First, we used modeling to suggest that epigenomics-driven interactions contribute to shaping the chromosome spatial organization of the plant A. thaliana. Second, our simulations unveiled that the mechanisms leading to TADs formation may cause the heterogeneous dynamic behaviors of chromosomes observed experimentally. These projects showcase that biophysical models can help explain how experimentally observed structures fold and, ultimately, unravel potential factors and molecular mechanisms regulating chromosome structure and dynamics.

Thursday 8th

Active semiflexible polymer under shear flow

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The dynamic behavior of a self-propelled semiflexible filament of length L is considered under the action of a linear shear flow. The system is studied by using Brownian multi-particle collision dynamics. The system can be characterized in terms of the persistence length Lp of the chain, of the Peclet number, and of the Weissenberg number. The quantity Lp/L measures the bending rigidity of the polymer, the Peclet number Pe is the ratio of active force times L to thermal energy, and the Weissenberg number Wi characterizes the flow strength over thermal effects. In this presentation we will focus our attention to intermediate values of Pe corresponding to the weak spiral regime when no external flow is applied. The numerical results allow us to outline the main features of the physics underlying the considered system:

- At low values of Wi, polymer is stretched by activity and aligned by shear along the flow direction. This effect is more marked in the case of more flexible chains.

- At the intermediate values of Wi, polymer is prone to tumble due to shear and this promotes a contraction of the chain.

- At very high values of Wi, activity sums up to shear enhancing polymer stretching and deformation.

Interplay between topology and confinement in active polymers

E. Locatelli[1]

[1] Department of physics and astronomy, university of Padova, Padova, Italy

Active systems, due to the local breaking of equilibrium, allow for phenomena that their equilibrium counterparts cannot attain. This correspondence between microscopic local equilibrium breaking and the meso/macroscopic structure formation is a general feature that have been observed in diverse systems including bacteria and synthetic swimmers. A similar behaviour can be observed also in the case of polar active polymers, i.e. polymers made of active monomers whose activity is directed as the local tangent to the polymer backbone. For example, a coil-to-globule-like transition takes place for isolated active chains in three dimension, highlighted by a marked change of the scaling exponent of the gyration radius[1]. Driven by the relevance of confinement and topology on the structural and dynamical properties of passive systems, we investigate the interplay between these latter and activity for tangentially active polymers. We explore the dynamics of active polymers in corrugated channels, highlighting the differences with respect to the passive case[2]. n the bulk, isolated rings display two different regimes at high enough activity: short rings tend to become "stiffer" and to assume a disk-like conformation, whereas long rings collapse, forming tight structures that show the hallmarks of dynamical arrest[3]. Finally, when placed under confinement, suspensions of short active rings assemble in ordered phases [4]. References:

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Crowding-enhanced diffusion for highly entangled self-propelled stiff filaments

S. Mandal[1]

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We study a strongly interacting crowded system of self-propelled stiff filaments by event-driven Brownian dynamics simulations and an analytical theory to elucidate the intricate interplay of crowding and self-propulsion. We find a remarkable increase of the effective diffusivity upon increasing the filament number density by more than one order of magnitude. This counterintuitive "crowded is faster" behavior can be rationalized by extending the concept of a confining tube pioneered by Doi and Edwards for highly entangled, crowded, passive to active systems [1]. We predict a scaling theory for the effective diffusivity as a function of the Péclet number and the filament number density. Subsequently, we show that an exact expression derived for a single self-propelled filament with motility parameters as input can predict the nontrivial spatiotemporal dynamics over the entire range of length and timescales. In particular, our theory captures short-time diffusion, directed swimming motion at intermediate times, and the transition to complete orientational relaxation at long times.

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Tba

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TBA

Ph-antenna residues trigger large-scale conformational change in proteins

I. Coluzza[1]

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CD81 is a human receptor that clusters into microdomains to mediate cell signalling processes. Previous structural studies on the α-helical CD81 large-extracellular-loop domain (CD81LEL) have shown that it can adopt different conformations (from closed to open), depending on the environmental pH conditions. However, the precise mechanism governing the CD81LEL plasticity has remained elusive so far. Here, by combining molecular dynamics simulations and experiments on wild type CD81LEL we show a novel mechanism connecting pH changes to a modulation of the solvation shell by "antenna" residues that in turns induces CD81LEL to open. The antenna residues are D139 and E188. At acidic conditions, such residues generate a cascade signal propagating through CD81 changing the local solvation , and in turns trigger the closed-to-open conformational change on CD81LEL. We further proved the key role of D139 and E188 by introducing mutations that switch off their sensitivity to pH. As expected, the mutations stabilize the closed conformation. This new signal transduction mechanism might play a role in other cellular receptors that function along the endosomal pathway.

Alphaknot - efficient distributed knot detection for alphafold-solved protein models

P. Rubach[1]

[1] Warsaw school of economics, Warsaw, Poland

AlphaKnot is a server that measures entanglement in AlphaFold-solved protein models while considering pLDDT confidence values. AlphaKnot has two main functions: 1) providing researchers with a webserver for analyzing knotting in their own AlphaFold predictions and 2) providing a database of knotting in AlphaFold predictions from the 21 proteomes for which models have been published. The knotting is defined in a probabilistic fashion. The knotting complexity of proteins is presented in the form of a matrix diagram which shows users the knot type for the entire polypeptide chain and for each of its subchains. The dominant knot types as well as the computed locations of the knot cores (i.e. minimal portions of protein backbones that form a given knot type) are shown for each protein structure. Based mainly on the pLDDT confidence values, entanglements are classified as Knots, Unsure, and Artifacts. The database portion of the server can be used, for example, to examine protein geometry and entanglement-function correlations, as a reference set for protein modeling, and for facilitating evolutional studies. The knot detection requires significant computational power, therefore, to analyze the data contained in the AlphaKnot database a specialized tool was developed the kafka-slurm-agent that enabled to run the knot identification on 3 clusters simultaneously. The same software is used to manage AlphaKnot server jobs. The AlphaKnot can be found at https://alphaknot.cent.uw.edu.pl/

"new knots in human proteome!"

W. Niemyska[1]

[1] University of warsaw, Warsaw, Poland

The fact that proteins can have their chain formed in a knot is known for almost 30 years. However, as they are not common, only a fraction of such proteins is available in the PDB databases. It was not possible to assess their importance and versatility up until now because we did not have access to the whole proteome of an organism, let alone a human one. The arrival of efficient machine learning methods for protein structure prediction, such as AlphaFold and RoseTTaFold, changed that. We analyzed all proteins from human proteome (over 20 000) in search for knots and found them in less than 2% of the structures. Using a variety of methods, including homolog search, clustering, quality assessment and visual inspection, we determine the nature of each of the knotted structures and classify it as either knotted, potentially knotted or an artifact and deposited in a database available at: https://knotprot.cent.uw.edu.pl/alphafold. It came out that over 75% of knots in human proteins may be artifacts. This information may be helpful for AlphaFold improvement. Among potential knots we found knot 6_3 which would be the first knot in proteins with unknotting number higher than one! In the talk I want to concentrate on that knot.

A new therapeutic strategy from protein folding simulations

P. Faccioli[1]

[1] University of trento, Trento, Italy

In this talk, I will first discuss how the development of path integral based algorithms introduced in our group has made it possible predict the folding pathways of many biologically relevant proteins, using realistic all-atom force fields in explicit solvent[1-3]. Based on this technological advancement, we proposed an entirely new paradigm for drug discovery named Pharmacological Protein Inactivation by Folding Intermediate Targeting (PPI-FIT), based on finding small molecules that can hinder the protein folding process. Using the PPI-FIT paradigm, we have discovered a molecule that can selectively modulate the cellular expression of the human prion protein, which is involved in several fatal neurodegenerative diseases and for which conventional methods have been largely ineffective [4]. This technology was later applied to a number of protein targets and led to founding Sibylla Biotech, which has recently signed a series A investment for 23 Million Eur. Sibylla has further developed the computational technology, now allowing for all-atom explicit solvent simulations of co-translational folding. An experiment is planned for January 2023 in the International Space Station, to exploit microgravity conditions to attempt the crystallization of partially folded PrP proteins in complex with one of the small molecules discovered using PPI-FIT. Enlarging the range of applicablity of our simulation schemes to a larger class of biomolecular transitions is not trivial, especially when it is not possible to rely on experiments to obtain atomistic structural information about the energetically stable conformation. In the last part of this talk, we report on our recent attempts to overcome this limitation based on integrating path integral methods with machine learning and quantum computations [5-7].

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How entangled proteins can be? Prediction and in vitro verification.

J. Sulkowska[1]

[1] University of Warsaw, Warsaw, Poland

The presence of knots in protein 3D structures is well established[1]. However, as they are not common[2], only a fraction of such proteins is available in the PDB database. It was not possible to assess their importance and versatility up until now because we did not have access to the whole proteome of an organism. The development of efficient machine learning methods for protein structure prediction, such as AlphaFold and RoseTTaFold, changed that [3]. First, we analyzed all proteins from human proteome (over 20 000) in search for knots and found them in less than 2% of the structures. Using a variety of methods, including homolog search, clustering, quality assessment and visual inspection, we determined the nature of each of the knotted structures and classifed it as either knotted, potentially knotted or an artifact and de-posited in a database available at: https://knotprot.cent.uw.edu.pl/alphafold. It turns out that over 75% of knots in human proteins may be artifacts. However, among potential knots we found knot 6_3 which would be the first knot in proteins with unknotting number higher than one[4]. Second, we focused on proteins which can be even more complex and possess two knots on a single chain (up to now, only single knots were found). For the first time, we searched different databases for double knotted proteins. Using AlphaFold we predicted a few families of doubly knotted proteins and studied in detail their structure and function. Using experimental approach, we showed that such proteins can fold and perform their intended function 3, Fig. **??**. Finally, we established AlphaKnot[4], the first server to assess entanglement of AlphaFold-solved protein models with regard to thier pLDDT data. The server has two main functionalities. One is a database of structures from all of 21 full proteomes solved by AlphaFold which have been published up to 2022. Second is a user-friendly web server for researchers to analyze their own AlphaFold predictions. By using pLDDT confidence score, we classified predictions into categories which allow for detailed analysis, whether the protein model is correctly solved. This allowed us to discover new types of knot in the human proteome[4]. By cross-validating AlphaFold predictions with our server and RoseTTa predictions, we showed that AlphaFold, while overall a great tool, can have problems with correctly modeling knot topology of proteins. We show examples of AlphaFold models with wrongly predicted topology as well as give possible explanations of such occurrences.

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Regulatory effects of proline isomerization on the phase behavior of intrinsically disordered proteins

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Responsiveness of polypeptides and polymers in aqueous solution plays an important role in biomedical applications and in designing advanced functional materials. Elastin-like polypeptides (ELPs) are a well-known class of synthetic intrinsically disordered proteins (IDPs), which exhibit a lower critical solution temperature (LCST) in aqueous solutions. Here, we compare the influence of cis/trans proline isomerization on the phase behavior of single ELPs in water and aqueous binary mixtures. Our results reveal that proline isomerization can be used to regulate the solvation behavior of ELPs and the effects are solution dependent. In pure water, proline isomerization tunes the conformational behavior of ELPs while keeping the transition temperature unchanged. Yet, in water-ethanol mixtures, the cis chain re-opens again as ethanol concentration increases. Our study opens a novel direction of regulating the solvation behavior of ELPs for their future applications.

Mechanism study of radical homopolymerization of multivinyl monomers: applicability of flory-stockmayer theory

J. Lyu[1]

[1] University college dublin, Dublin, Ireland

Flory and Stockmayer (F-S theory) defined that the polymerization of multivinyl monomers (MVMs) inevitably leads to gelation even at low monomer conversion based on two assumptions: (1) independent and equivalent vinyl groups, (2) no intramolecular cyclization. However, it is still debatable whether it is applicability to the conventional free radical polymerization (FRP) and reversible deactivation radical polymerization (RDRP) (such as atom transfer radical polymerization (ATRP)) is controversial, especially regarding the prediction of gel point and the extent of intramolecular cyclization. In this work, Monte Carlo simulations were used to study FRP and ATRP of divinyl monomers using two kinetic models: with cyclization (w.c.) and without cyclization (wo.c. – corresponding to F-S theory) models. In terms of the applicability of F-S theory to FRP of MVMs, the results of the Monte Carlo simulations of FRP/FRcP of divinyl monomers were compared with the calculated gel points based on F-S theory and the experimental data. It is found that the F-S theory can successfully predict the gel points of FRP of MVMs, moreover, the intramolecular cyclization has a negligible impact on the polymerization process and the gel point before gelation. Thus F-S theory is suitable for the prediction of FRP of MVMs. Regarding its applicability to ATRP of divinyl monomers, the simulated gel points of ATRP of divinyl monomers using w.c./wo.c. model were compared with those obtained from simulations using dynamic lattice liquid (DLL) model, from ATRP experiments and from calculation using F-S theory. The results show that the gel points obtained from both models are lower than the values from DLL model and experiments. This indicates that F-S theory is not sufficient for predicting polymerization of MVMs via ATRP. And this inapplicability is not only due to neglecting intramolecular cyclization, but also due to spatial restrictions which cause the reactivity and accessibility of vinyl groups becoming non-equivalent in ATRP of MVMs. The new insights provided by this work will rectify the traditional impression in the field of polymer science on the applicability of F-S theory to different polymerization systems, and inspire new thinking on the intermolecular and intramolecular topology control.

Friday 9th

Programmable degradation of dna hydrogels

Y. Gutierrez fosado[1]

[1] University of edinburgh, Edinburgh, United kingdom

DNA nanostar (DNAns) hydrogels are well studied examples of equilibrium gels, yet their functionalization via proteins remains poorly investigated. In this talk, I will report on the design of DNAns hydrogels with time-varying programmable degradation by restriction enzymes. By encoding a different number of restriction sites on each of the DNAns arms, we observe that it is possible to precisely modulate the viscoelastic properties of these gels and control their degradation rate. We further characterise our non-equilibrium systems using multi-scale Molecular Dynamics simulations, which uncover the relationship between the geometry of DNAns building blocks and the gel viscoelasticity. Our results are promising in the design of the next generation of DNA gels with time-varying and programmable material properties that may be employed in drug delivery and tissue regeneration.

A single-chain model for the linear viscoelasticity of unentangled melts of associating polymers

H. Liu[1]

[1] Université paris cité, Paris, France

Existing single-chain models for unentangled associating polymers account for the association by assigning the sticky junctions a large value of the monomeric friction coefficient, which prevents them to move in space unless stickers effectively dissociate. With such assumption comparison of model predictions with linear viscoelastic data is not fully successful in the intermediate range of frequency. In this work we improve agreement with data by developing a single-chain model where sticky junctions are allowed to quickly move in space without dissociating. We also account for a random distribution of the stickers, but differently from the recent model by Jiang et al. [1]. Predictions of the model are successfully compared with unentangled melt data for two different copolymer chemistries, and different sticker concentrations. Particularly significant are the data by Cui et al. [2] of melts of polymers with only 2 stickers per chain, revealing that sticky junctions are in fact also endowed with a fast mobility.

Introducing a variable entanglement density constitutive rheological model based on principles of non-equilibrium thermodynamics

P. Stefanou[1]

[1] Cyprus university of technology, Limassol, Cyprus

Chain uncrossability leads to the development of topological interactions in high molecular weight polymer melts and concentrated polymer solutions known as entanglements. According to the tube model of de Gennes, [1] and Doi and Edwards [2], the polymer motion due to entanglements is confined within a tube-like region whose axis coincides with the primitive path of the chain and its diameter provides a measure of the strength of topological interactions. Under flow, chains are deformed and oriented, meaning that certain entanglements are expected, on average, to be lost. Detailed nonequilibrium molecular dynamics (NEMD) simulations [3] have shown that the net effect is a strong reduction in the average number of entanglements per chain, a mechanism known as convective constraint release (CCR) [4]. However, these models failed to consider that the entanglement density should be a decreasing function of the shear rate. More recently, these models have been modified to accommodate for this failure [5]. However, these models have not been shown to be thermodynamically admissible. In this work, a variable-entanglement density constitutive model is developed for the description of the rheological properties of entangled polymer melts and concentrated polymer solutions by combining ideas from nonequilibrium thermodynamics [6] and network theory. It proposes two differential equations: one for the average number of entanglements per chain and one for the conformation of entanglement strands. Direct comparison with nonequilibrium molecular dynamics simulation data shows that the model can accurately describe the loss of entanglements due to the applied flow. Additional comparison confirms the capability of the new model to describe the viscometric functions in shear using a realistic value of the CCR parameter.

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Computer simulations of melts of ring polymers with non-conserved topology

M. Ubertini[1]

[1] Sissa, Trieste, Italy

In this talk I will present computer simulations of a dynamic Monte Carlo algorithm for polymer chains on the FCC lattice which takes explicitly into account the possibility to overcome topological constraints by controlling the rate at which nearby polymer strands may cross through each other. By applying the method to systems of interacting ring polymers at melt conditions, we characterize their structure and dynamics by measuring, in particular, the amounts of knots and links which are formed during the relaxation process. In comparison to standard melts of unknotted and unconcatenated rings, our simulations demonstrate that the mechanism of strand crossing makes polymer dynamics faster provided the characteristic time scale of the process is smaller than the typical time scale for chain relaxation in the unperturbed state, in agreement with recent experiments employing solutions of DNA rings in the presence of the type II topoisomerase enzyme. In the opposite case of slow rates the melt is shown to become slower, and this prediction may be easily validated experimentally.

Hypergraph and hypermatrix models for higher-order connectivity

C. Zapata carratala[1]

[1] Society for multidisciplinary and fundamental research / wolfram research, Alicante, Spain

In this talk I will present the approach of Arity Science (https://arity.science/) to model higher-order connectivity via hypergraphs. Beyond the conceptual clarity and data faithfulness that hypergraphs provide, I will show how they suggest novel mathematical formalisms that generalize the basic ways in which we analyse data: linear algebra is generalized into a manner of linear hyperalgebra involving irreducible higher-arity operations. In particular, this approach suggests new computational and modelling approaches to loop networks (such as kinetoplast DNA) that involve links of various kinds and arities (Hopf, Whitehead, Borromean, Brunnian, etc.).

Orderly Molecular Entanglements

D. Leigh[1]

[1] University of Manchester, Manchester, United kingdom

Knots are important structural features in DNA and some proteins, and play a significant role in the physical properties of both natural and synthetic polymers[1]. Although billions of prime knots are known to mathematics, few have been achieved through chemical synthesis[2].Here we will discuss the latest progress from our laboratory, including the synthesis of some of the most complex molecular knots and links (catenanes) to date[3-9] and the introduction of 2D molecular weaving[10]

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Cooperative motions and topology-driven dynamical arrest in prime knots

A. Lappala[1]

[1] Nan, Nan, Nan

Knots are entangled structures that cannot be untangled without a cut. Topological stability of knots is one of the many examples of their important properties that can be used in information storage and transfer. Knot dynamics is important for understanding general principles of entanglement as knots provide an isolated system where tangles are highly controlled and easily manipulated. To unravel the dynamics of these entangled topological objects, the first step is to identify the dominant motions that are uniquely guided by knot structure and its complexity. We identify and classify motions into three main groups— orthogonal, aligned, and mixed motions, which often act in unison, orchestrating the complex dynamics of knots. The balance between these motions is what creates an identifiable signature for every knot. As knot complexity increases, the carefully orchestrated dynamics is gradually silenced, eventually reaching a state of topologically driven dynamical arrest. Depending on their complexity, knots undergo a transition from nearly stochastic motions to either non-random or even quasiperiodic dynamics before culminating in dynamical arrest. Here, we show for the first time that connectivity alone can lead to a topology-driven dynamical arrest in knots of high complexity. Unexpectedly, we noticed that some knots undergo cooperative motions as they reach higher complexity, uniquely modulating conformational patterns of a given knot. Together, these findings demonstrate a link between topology and dynamics, presenting applications to nanoscale materials.

Knots and ai – learning to unknot

P. Sulkowski[1]

[1] University of warsaw, Warsaw, Poland

Abstract: I will discuss various features of knot theory that make it a particularly interesting playground from the viewpoint of machine learning. In particular, I will focus on the unknot recognition problem, and show how successfully it can be solved combining techniques from machine learning and natural language processing. The methods developed in this program can be also used in the analysis of entangled biomolecules.

List of Posters

Wednesday Session

Thermal properties of knotted block copolymers using the Wang-Landau algorithm

N. Abbasi taklimi[1]

[1] University of Szczecin, Szczecin, Poland

An extensive study of single knotted copolymers containing two kinds of monomers A and B is presented. Using the Monte Carlo Wang-Landau algorithm, the thermal properties of coarse grained knotted polymers on a simple cubic lattice fluctuating in a solution are investigated. Two different setups are considered: charged block copolymers in a ion solution and the case in which the solvent is good for the A monomers and bad for the B monomers. The structural changes in the conformations of the knots at different temperatures are visible in the plots of the gyration radius and the specific heat capacity. When attractive interactions are present, it is found that with increasing polymer lengths new peaks appear in the specific heat capacity. This implies that knots formed by copolymers have a more complex phase diagram than homopolymers, including the possible presence of metastable states. A precise interpretation of the peaks is provided. In certain diblock copolymers, in which one type of monomers is much more abundant than the other, it is possible to distinguish three different states, one compact and two swollen states with different sizes. In view of possible applications in medicine and the construction of intelligent materials, it is also shown that the behavior of copolymer knots can be tuned by changing both the monomer configuration and the topology. We find that the strongest electrostatic bonds between the monomers are formed by charged copolymers in which short segments with A monomers are alternated by short segments with B monomers. Such knots undergo a very fast and abrupt swelling after the breaking of these bonds by thermal fluctuations. The effects of topology allow to tune the knot size and to increase or decrease the temperatures at which the observed phase transitions or rearrangements of the system occur. While we observe a general fading out of the influence of topology in longer polymers, our simulations have captured a few exceptions to this rule.

Interplay between cellulose nanocrystals and a copolymacrolactone system with potential for hosting hydrophobic structures

A. Chiriac [1]

[1] Petru poni institute of macromolecular chemistry, Iasi, Romania

Cellulose nanocrystals (CNC) as biodegradable and renewable in nature are well known structures used like sustainable and environmentally friendly materials in multiple applications from drug delivery, environmental remediation, up to energy storage. The hydrophilic nature of CNC can be covalent or noncovalent chemical modified using the hydroxyl groups from surface. We recently synthesised poly(ethylene brassylate-co-squaric acid) (PEBSA) a new copolymacrolactone system prepared by ring-opening of ethylene brassylate (a macrocyclic lactone obtained from natural sources) condensed with squaric acid in the presence of 1-hexanol as initiator. The performed studies evidenced the ability of PEBSA for hydrophobic compounds encapsulation. The present study is dedicated to the investigation of the compatibility between CNF and PEBSA in order to obtain a new self-assembled network with special properties. Moreover, we expect that the non-covalent bonds created between CNF and PEBSA will not affect the properties of the two polymer structures involved in the formation of the interpenetrated system.

Influence of two novel mutations in mlasa disease on yars2 - trna complex

M. Fortunka[1]

[1] Centre of new technologies university of Warsaw, Warsaw, Poland

Recently found two novel mutations of YARS2 protein cause severe symptoms of rare genetic disease MLASA. The idea of the research was to explain the connection between two indirect mutations and the enzymatic reaction stop. YARS2 complex with tRNA was built using homology modelling of lacking tRNA binding sites and tRNA rigid docking. Then there were performed molecular dynamics simulations of mutated and non-mutated versions of the complex. The last step was analysing the data by the dynamical network analysis, which led me to propose mechanism of mutation influence on the catalysis.

Varying the grafting position on a cyclotide scaffolding: a computational study on the induced dynamical implications

N. Ilieva[1]

[1] Institute of information and communication technologies, bulgarian academy of sciences, Sofia, Bulgaria

Cyclotides are special knotted proteins, 28-37 amino acid residues long, stabilized by three pairs of disulfide bonds - the cyclic cystine knot (CCK) motif. They exhibit a wide range of biological activities - antimicrobial, insecticidal, antitumor, and anti-HIV, to mention some. Their size, conformational stability, temperature resistance, and resistance to proteolytic degradation make them a perfect stabilizing skeletal construct for grafting other biologically active epitopes, with some specific conformations and new functions emerging as a result of this grafting. However, the dynamic consequences of the grafting procedure remain to be understood. In the present computational study, we take a systematic approach in analyzing the implications on the geometry and dynamics of topologically non-trivial biomolecules undergoing a grafting procedure by engineering virtual mimics, inspired by the prospective Parkinson inhibitor MCoCP4. We observe substantial differences in the volatility and conformational plasticity of different parts of the engineered mimics depending on the grafting position, charge distribution, and initial conformation specifics that provide a rigorous basis for objective criteria meant to be used as guidelines in the design of grafted molecules with predefined therapeutic properties.

Second order lagrangians for (2+1)-dimensional generalized boussinesq equations and an extension of the krupka-betounes equivalent

M. Palese[1]

[1] University of torino, italy, Torino, Italy

In his 1872 seminal paper Boussinesq provided a mathematical description of solitary waves as travelling wave solutions of a nonlinear dispersive equation, which describes physical phenomena in diverse fields of sciences, biology, condensed matter physics, plasma physics, plasma waves, and fluid mechanics. It finds applications in a wide range of real world phenomena which mimic, with suitable variants, the motion of long dispersive shallow water waves, from physiology (e.g. cilia-assisted transport of a biofluid, natural convection in the human eye), to dynamics of soils, from oceanography to fundamental forces of nature. In particular, (2+1)-dimensional models also encompass vortex-like phenomena. We determine second order Lagrangians for (2+1)-dimensional generalized Boussinesq equations and we discuss some aspects concerning conservation laws associated with invariance properties of the associated extension of the Krupka-Betounes equivalents. Such equivalents are constructed by means of a recursive formula involving geometric integration by parts formulae.

Biocompatible electrospun nanofibers based on indigenous proteins and biodegradable polymers for potential wound dressings

M. Rapa[1]

[1] University politehnica of Bucharest, Bucuresti, Romania

Traditional wound management includes main materials such as cotton gauze dressings, hydrogels and foams, more detailed in form of bandages, cohesive wraps, composite dressings, non-adherent dressings, body netting, impregnated gauze, or natural materials like leaves, cobwebs, and honey. This approach is not able to facilitate the better wound healing so the investigation for new materials that lead to moist dressing have been under investigation among researchers. Modern wound dressings are multifunctional and improve the wound healing rate by accelerating the healing process, providing physical protection and maintaining the moisture content of the wound microenvironment. In this paper, the dual layers based on biodegradable matrices such as poly(lactic acid) (PLA), poly(ethylene oxide) (PEO) and poly(vinyl pyrrolidone) (PVP) loaded with keratin and bovine collagen glue fabricated by using mono and coaxial electrospinning technology for potential wound dressings were created. The advantages of these nanofibers consist in that there is not necessary to remove the dressing during healing period, the mechanical strength of dressings is assured and the encapsulated proteins are controlled released. Polyethylene oxide (PEO) was used to enhance the encapsulation efficiency and accelerate the release rate of keratin. Keratins are used in wound dressing materials because they are responsible for the organized proliferation of the keratinocytes and maintaining their integrity in the epithelium. Collagen it is well known to accelerate fibroblasts' formation and the closure of the wound. The morphology and the biocompatibility of the electrospun nanofibers were investigated. The results showed a nanofibrous structure of each layer and the assembled product proved in vitro and in vivo biocompatibility as compared with control.

List of Participants

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Müller-Nedebock Kristian	South Africa
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Zapata Carratala Carlos	Spain
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Useful Information

Venue

The Venue is located at the first floor of the **Polo Ferrari 1, via Sommarive 5, Trento**. Room A106 is located to the left of the main entrance.

Talks will be held in room **A106** of Polo Ferrari 1 (Povo 1) building.

Coffee breaks and lunches will be offered in the room **acquario** at the Povo 1 building.

The **poster session** will be held on Wednesday and Thursday afternoon in the **atrium** of the Povo 1 building.

Wi-Fi will be available during the conference using Eduroam.

The use of FFP2 masks is not mandatory on the University premises, but is recommended while inside the lecture room.

Talks and posters

The timings are as follows.

- 12 minutes + 5 minutes for questions for short talks
- 25 minutes + 10 minutes for questions for keynote talks.

To save time, we will keep a computer connected to the projector in the room. We ask you to prepare your presentation in either .pdf, .ppt, or .key format and

provide it to us before your session. We will provide more information later on about this. Since a few people can not attend the conference due to health reasons or last-minute commitments, we will have a few online talks, and will broadcast the talks in Trento over zoom, if not otherwise requested by the speaker.

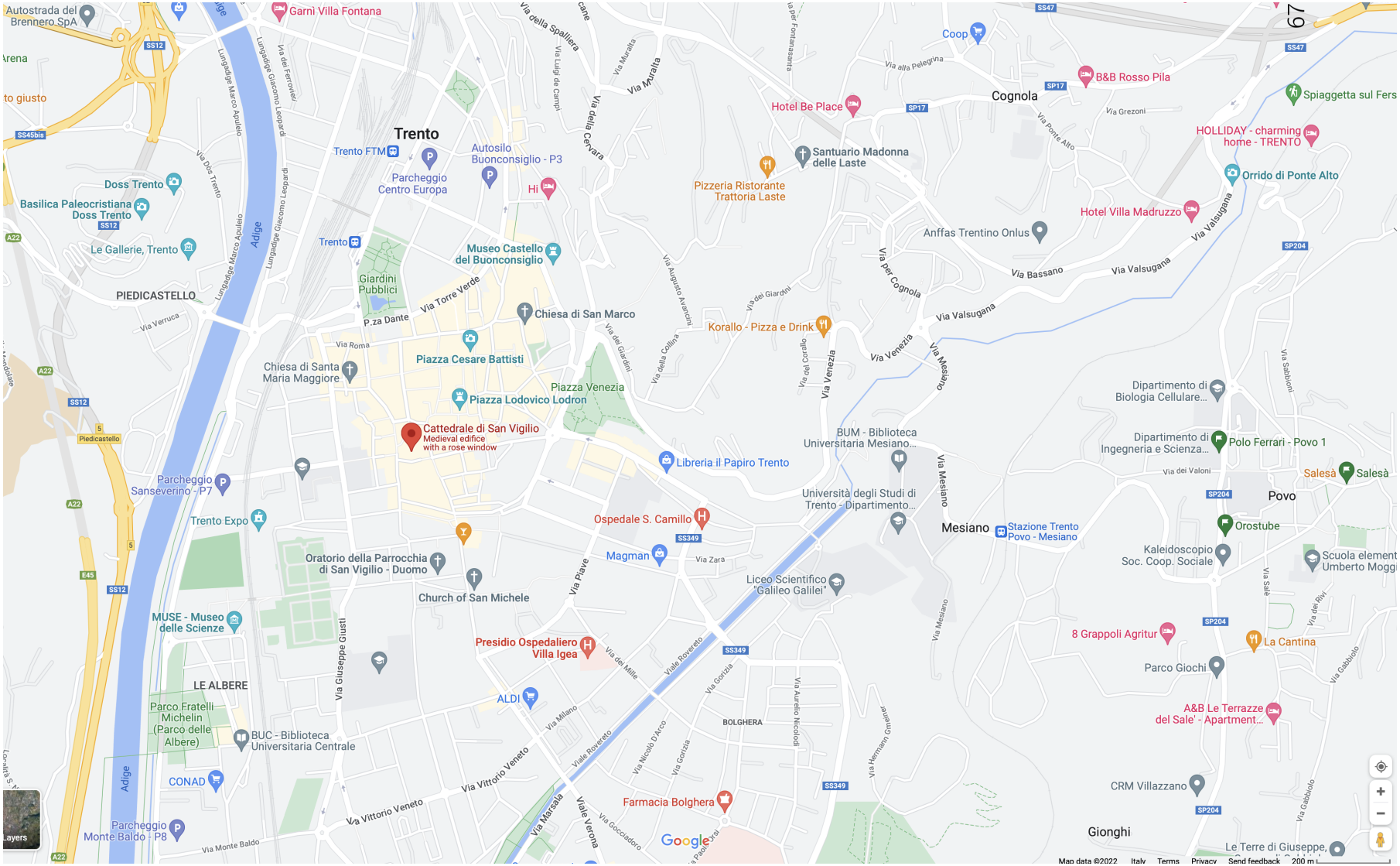
How to get to the Polo Ferrari 1?

The building is part of the "Polo Collina" of the university of Trento and is located in Via Sommarive 5 (see map).

- **Bus:** line 5, 5] from the city center and railway station, line 13 from the southern part of Trento. See Trentino trasporti webpage
- **Train:** From Trento main station, Trento S. Chiara, ..., Pergine, there is a train line stopping in Mesiano. See
- **On foot:** It is possible to reach the location on foot, but it takes about 40 minutes from the city center, as Polo Collina is situated about 200 m above the city.

Covid-related measures in Italy and on University premises

It is mandatory to wear an FFP2 mask when on public transportation, in hospital, and in pharmacies. We **strongly** recommend wearing a mask while attending the conference.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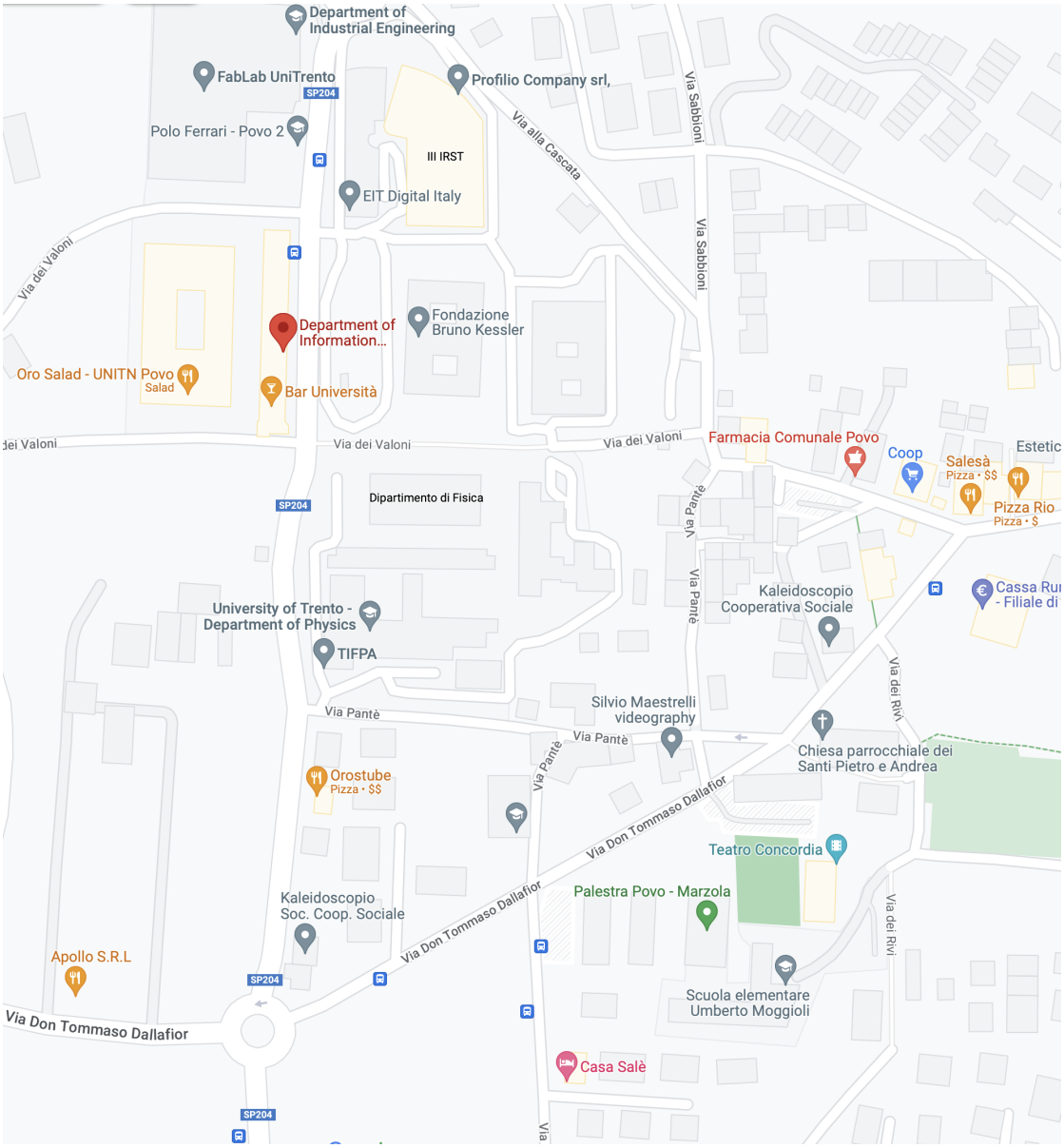
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