Mathematical Analysis of Soft Matter

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July 1st-5th, 2024

1 Overview of the Field in the Context of the Meeting

Soft matter comprises a variety of physical systems that can be structurally altered by small stresses of the magnitude comparable to thermal fluctuations. They encompass a wide range of different substances, including liquids, colloids, polymers, foams, gels, liquid crystals and biological materials, that consequently require a large variety of mathematical tools for their modeling, analysis and simulation [1–3]. This workshop primarily focused on continuum models of liquid crystals, elastomers and gels that have attracted significant attention in the mathematical community throughout the last decade [4]. Even this, more narrow scope, covers a diverse set of topics, from modeling, variational methods and PDEs to algebra, topology, probability and scientific computation. The interest in liquid crystals stems not only form their significant role in technological applications, but also because they share common properties with other more exotic and harder to study materials and phenomena in basic science, such as biology, physics, and cosmology [5–8]. A liquid crystal is thus an ideal testbed to verify experimentally theoretical predictions, e.g., in cosmology. The recent advances in this area include rigorous characterization of topological singularities of minimizers of nonlinear variational problems for tensor-valued maps, proof of existence of solutions for systems of equations describing liquid crystal flow, investigation of pattern formation and control of thin elastic objects, among others [9]. The new frontier requires tackling problems associated with anisotropic elasticity, electrochemistry of liquid crystals, phase transitions, flow and modeling of newly discovered types of soft matter. All of these issues were addressed in the course of the workshop.

More precisely, the following set of themes were covered at the workshop:

1. The Landau-de Gennes [10] and Oseen-Frank models [11] were originally proposed to describe nematic liquid crystals within the framework of a variational theory. The distinction between these models is that they rely on different descriptors of the nematic state: vector- and tensor-valued in the Oseen-Frank and the Landau-de Gennes cases, respectively. The Landau-de Gennes theory originates from and is related to the Ginzburg-Landau theory of superconductivity with both of these theories being relaxations of an appropriate harmonic map problem. The Oseen-Frank model, on the other hand, is an anisotropic version of a harmonic map problem. The Ginzburg-Landau theory has been extensively studied in the last thirty years (Brezis, Béthuel, Hélein, Bauman, Phillips, Alama, Bronsard, Golovaty, Mironescu, Orlandi, Sandier, Shafrir, Sternberg, etc..) [12, 13], however, analysis of the Landau-de

Gennes variational problem is not a straightforward extension of these results due to higher dimensionality of both the ambient and the target spaces. The principal issue is to understand the structure of topological singular sets of minimizers of the Landau-de Gennes energy - their number, dimensionality, location, etc [14]. The singular solutions are of great interest to physicists/engineers as well as mathematicians, as the defects are visible under the microscope and are central to many potential applications of liquid crystal-colloid/liquid crystal-nanoparticle composites and liquid crystals in structured confinement [15]. Partial mathematical results in this direction have been obtained in the last ten years (Ball, Bauman, Canevari, Ignat, Lamy, Majumdar, Nguyen, Orlandi, Phillips, Rodiac, Slastikov, Sternberg, Zarnescu, etc.) [16, 17] but many issues still need to be understood, including homogenization in presence of singularities, interactions with colloidal particles, quantum effects (in particular related to quantum dots) and machine learning applications. One of the aims of the workshop was for the participants to present their recent results on analysis and simulations of the Landau-de Gennes model, to survey the current level of understanding of this model and to develop new directions of investigation. The Landau-de Gennes theory is, in fact, relatively new so that interesting issues exist not only in analysis but even at the level of modeling as there are surprising problems with certain regimes for the Landau-de Gennes model in a form that it is typically written. Some of the participants in this workshop have considered modifications to the standard model (Bauman, Phillips, Golovaty, Novack, Sternberg, Virga) [18] and the discussions regarding applicability of these changes will continue after the workshop.

2. The Ericksen-Leslie and Beris-Edwards models have been extensively used to study nematic flows, including in active media and extensive investigations of these systems are ongoing [19, 20]. Recent experiments (Lavrentovich, Ignés-Mulol, Sagués, Smalyukh) [21–23] on active matter have stimulated a significant new interest in modeling and simulations of these materials (Beller, Calderer, Ravnik, Virga) [24–28]. The studies of electrophoresis of colloidal particles in a nematic host (Calderer, Golovaty, Lavrentovich) [29] require similar machinery. On the analysis side, existence results for the Beris-Edwards model have been established by Zarnescu and collaborators [30]. The connection between modeling, analysis and simulations of nematic flows were discussed at this workshop and collaborative projects were identified. For example, one issue that was explored concerns mathematical origins of the phenomena when chiral distortions modes (twist) dominate over the achiral ones (splay and bend) in the active nematic steady state, even in simulations with isotropic elasticity [26, 31, 32].

3. The third thrust of the workshop, homogenization and topological singularities in colloidal systems, is another active topic of investigations that was addressed at the workshop [33, 34].

The talks related to these topics are discussed next.

2 Presentation Highlights and Description of the Talks

The workshop brought together senior and junior applied mathematicians and physicists working in various areas of mathematics and physics of soft matter, including analysis, numerical analysis and scientific computations, mathematical modeling and experiments. This broad range of scientific disciplines facilitated the interactions between applied mathematicians and physicists and fostered new interdisciplinary collaborations. Recent analysis results (Alama, Bronsard, Golovaty, Lamy) [35, 36] considered singularities of minimizers of the Landau-de Gennes energy of a nematic surrounding a single colloidal particle. However singularities associated with a collection of particles in a nematic host that have been observed both in experiments and simulations (Beller) [37] is a natural extension of these results that were discussed at the meeting. The talks by Stantejsky and Louizos were directly related to these topics. A related subject of interest that was explored is homogenization of nematic composites (Ceuca, Calderer, Canevari, Golovaty, Zarnescu) [33, 34]. Among the participants in the workshop are the leaders in continuum mechanics of liquid crystals (Virga) and experimental and theoretical physics (Kamien, Lavrentovich, Ravnik, Smalyukh) as well as leading analysts (Bauman, Canevari, DiPasquale, Lamy, Phillips, Sternberg, Stroffolini). Their participation provided for a high-level, well-rounded discussion of the topics outlined above. The most important role of this workshop was to bring together leading experts and young scientists to share their results and exchanging ideas while exploring new potential collaborations, and this was very successful. During the workshop the participants interacted and identified new problems that require innovative mathematical approaches. These discussions of future directions will have a significant impact on the future careers of students and postdocs attending the workshop, such as Doré, Garcia, Head, Klein, Kumari, Louizos, Severino, Schimming, and Stantejsky. The workshop also gave an opportunity for young scientists from North America to initiate international interactions and collaborations with participants from Europe and vice versa. The workshop allowed students, postdocs and early-career investigators to present their research to senior members of the applied mathematics community, and to have informal discussions with leading researchers in their discipline through scheduled discussions and informal meetings.

The workshop began on Monday with two tutorials: one by Dan Beller and one by Arghir Zarnescu. The aim of each tutorial was to introduce the physics behind liquid crystals in a manner accessible to mathematicians and the mathematics behind liquid crystals in a manner accessible to physicists. These presentations introduced a common language that facilitated exchange of ideas during the week. These tutorials were very well received and instrumental to the audience.

The following talks focused on mathematics of liquid crystals. The first talk by Giacomo Canevari described a free-discontinuity problem for smectic liquid crystals [38]. Giacomo presented results on a variational model for smectic A liquid crystals set in two dimensions among competitors in the space of special functions of bounded variation (SBV). He showed existence of minimizers as well as presented results on their defects. Mike Novack presented new powerful techniques to study a variational model for 3D soap films. This new approach allows to obtain mathematically the correct features of soap film by generalizing the homotopic spanning condition of Harrison-Pugh. This generalization promises to be very helpful in the understanding of soap films and other minimal surfaces problems.

Bianca Stroffolini presented interesting results on manifold-constrained free discontinuity problems and Sobolev approximation [39]. Such results promise to be very helpful to properly understand fracture defects in brittle structures. Patricia Bauman described new results on defect patterns of the Landau-de Gennes energy minimizers in three-dimensional slabs [40]. The slab is assumed to be smooth and simply connected while the competitors must be tangential to the top and bottom faces while being uniaxial on the lateral surfaces of the domain. Assuming the boundary conditions of a given degree on the lateral surface, the main result of the work is to obtain the precise locations and the number of defects.

Dominik Stantejsky talked about his recent results on the asymptotic limit of the Landau-de Gennes model for liquid crystals around an inclusion with an external magnetic field. Using very sophisticated geometric measure theoretical tools, he was able (jointly with F. Alouges and A. Chambolle) to obtain the Gamma-limit of the Landau-de Gennes functional in an appropriate regime and use it to describe the defects of minimizers [41]. These are shown to be lines or surfaces close to the colloid surface and are described by a generalized Plateau problem.

Xavier Lamy presented surprising and exciting results on the shape of entire vortex solutions of negative degree for the anisotropic Ginzburg-Landau system [42]. In particular, for small anisotropy, the existence of entire solutions with degree -1 at infinity is proven even though the problem cannot be reduced to a simpler one-dimensional radial equation, as in the isotropic case. Daniel Phillips presented new results on defects in planar nematic liquid crystal films. He studied the limit of the minimizers of the Ball-Majumdar energy for liquid crystal films as the nematic correlation length tends to zero and determined the defect structures and liquid crystalline patterns.

Peter Sternberg discussed minimizers of Ginzburg-Landau-type theories on surfaces, generalizing results by Ignat and Jerrard, whereby the vector field is replaced by a complex line bundle on a smooth manifold [43]. These results will prove useful in the study of the modeling of nematics deposited on surfaces. Dmitry Golovaty presented recent results on mathematical modeling of ferroelectric nematics, using a Ginzburg-Landau model with anisotropic elastic constants. He showed that the singular structures present in minimizers contain both point and line singularities [44].

Lorena Aguirre Salazar presented her recent results on an Ohta-Kawasaki model. She generalized results for the Thomas-Fermi-Dirac-von Weizsäcker and for the Ohta-Kawasaki models to a nonlocal diffuse interface energy with Coulomb repulsion in 3D. She showed the existence of minimizers for small masses and non existence for large masses and studied the limit as the mass goes to zero. These type of results are very important for the understanding of the model via existence of minimizers for nonlocal energy related to the liquid drop model or flocking phenomena. Dean Louizos talked about his new results on the Landau-de Gennes model with planar anchoring and a weak magnetic field. He studied defects of minimizers that occur on a colloid immersed in a nematic liquid crystal with an external magnetic field when strong planar anchoring on the surface is imposed. Using Γ convergence techniques, he was able to show that only point defects can occur in a particular small particle limit.

Finally, Federico Luigi Dipasquale presented impressive and technically advanced new results on biaxiality versus uniaxiality in Landau-de Gennes minimizers in 2D discs. He studied whether minimizers of the Landau-de Gennes energy are uniaxial or biaxial depending on a parameter in front of the potential. For large values, minimizers are uniaxial and for small values they are biaxial. The method is based on the study of an energy gap for the associated minimization problem for the Dirichlet integral and this method may prove useful in many problems related to harmonic maps and liquid crystals [45].

The physical perspective on soft matter, especially liquid crystals, was presented in talks that each focused primarily on one of the following five material categories: cholesteric (chiral nematic) liquid crystals, smectic liquid crystals, liquid crystal elastomers, ferroelectric materials, and active matter. Both experimental and theoretical/computational approaches were represented in each material category.

The first talk on cholesteric liquid crystals was given by Ivan Smalyukh, who described experimental findings alongside numerical modeling regarding knotted configurations of confined cholesterics. The topological stability enjoyed by knotted vortex lines allows these knots to be viewed mesoscopically as quasiparticles. Analogous phenomena were revealed in chiral magnetic solids and in magnetic colloidal systems with biaxial symmetry. Techniques were presented by which these quasiparticles can be transformed and assembled by application of external magnetic or electric fields. Randall Kamien spoke about his theoretical work with experimentalist collaborators to understand the geometry of focal conic domain packings in a sessile cholesteric droplet [46]. While focal conic domains follow similar packing laws in smectic liquid crystals, the cholesteric fluid in this work permitted unprecedented three-dimensional resolution of the confocal conic section defect lines. Extensions to classical rules of focal conic domain packings were shown to explain the observed behaviors. Lisa Tran spoke about experimental work on cholesteric droplets with time-varying anchoring conditions (surface tension anisotropy): an emergent stripe lengthscale at twice the size of the cholesteric pitch was shown to result from a type of Helrich-Hurault instability [47]. Recent work on cellulose nanocrystal films was presented as a potential route to ecologically responsible green paints by means of the structural coloration properties of the cholesteric phase. Tran also briefly mentioned work to understand defects and effective anchoring in strongly confined nematic or smectic systems of colloidal rods.

Liquid crystal elastomers (LCEs) were discussed by Vianney Gimenez-Pinto, who presented finite element simulations (in conjunction with collaborators' experiments) of shape morphing actuation modes in response to light [48]. The LCEs' in-surface director field was patterned with topological defects, and modeling revealed how three-dimensional nematic deformation modes relaxed the strain imposed by these defects through the finite thickness of the material. Inspired by the Japanese art of kirigami, Gimenez-Pinto demonstrated how to use defined cuts and creases in the un-actuated, planar LCE to obtain desired three-dimensional geometries in the actuated state.

The talks of Oleg Lavrentovich, Maxim Lavrentovich, and graduate studeent Priyanka Kumari covered ferroelectric materials, especially the recently discovered ferroelectric nematic phase [49,50] formed by certain achiral molecules with large dipole moments. Kumari and O. Lavrentovich explained the spontaneous emergence of chiral twisted domains in (intrinsically achiral) ferroelectric nematics as resulting from a tradeoff between nematic elasticity and the electrostatic energy of the polarization field aligned with the nematic director [51]. Complex three-dimensional structures are obtained upon application of an external electric field. Observations of domain walls in the shapes of conic sections were explained as satisfying the physical boundary conditions for a polarization field that remains approximately divergence-free away from the domain walls [52]. Similarities and differences between such "soft ferroelectrics" and more broadly studied solid-state ferroelectric materials were elucided by the talk of M. Lavrentovich, who described the nature of domain walls in each system and models of these walls' motions.

Active nematics were studied in talks by Francesc Sagués and Jordi Ignés-Mullol, postdoctoral scholars Cody Schimming and Louise Head, and graduate students Claire Doré and Brandon Klein. Sagués and Ignés-Mullol presented experimental progress in controlling a model system of active nematics comprising aqueuous suspensions of microtubules with kinesin motor proteins. By using two types of kinesin that dimerize under application of blue light, or by mixing the active nematic with a light-polymerizable protein, the new techniques allow for precise spatiotemporal control over activity. Extended illumination was shown to cause collapse of the active nematic into a biphasic active fluid, with the interface stabilized by the illumination against the bend instability characteristic of extensile active nematics. Modeling by collaborators posits a higher-order active term in the hydrodynamic theory that produces hierarchical buckling like that seen in experiments. Sophisticated control over activity and boundary conditions allows for advances such as rectified flows and cantilever "pillars" as force tracers for precise, independent measurements of material properties [53]. Doré presented progress on controlling active nematic flows in microfluidic networks, toward functional logic gates for microfluidic circuits. Her talk elucidated the bifurcations associated with defect motions subject to the constraint of topological charge conservation. Klein presented computational results that demonstrate new ways in which confinement can replace the bulk chaotic flows of active nematics with periodic orbits [25], including a rationalization and generalization for the influence of cusps on defect braiding motions as demonstrated in recent experimental work [54]. Schimming presented a new theoretical approach to active nematics modeling through a coarse-grained approach that views that defect as active quasiparticles, with the bulk fluid effectively integrated out. Head revealed a constraint followed by both simulated and experimental active nematics, whereby $+1/2$ defects are confined to lines of balancing vorticity and shear magnitudes in the flow field [55]; preliminary computational results were also presented to extend this flow-defect coupling to more complicated three-dimensional active nematics. Sussman's talk covered theoretical approaches to a different, although related, class of active fluids: flows and flocking in microscopically polar (rather than nematic) systems such as in swarming behavior of living organisms. He argued for the need for a deeper understanding of how non-reciprocal (momentum non-conserving) interactions between active agents affect the emergent phenomenology at the material scale [56].

Graduate students Paul Severino and Jane B.D.M. Garcia gave talks on smectic liquid crystals. Severino discussed the constraints that smectic order imposes on knots in topological defect lines; specifically, certain classes of knot configurations require additional point defects. Connections were drawn between these structures and focal conic domains, as well as Morse-theoretic approaches in which the point defects appear as critical points in a hypersurface [57]. Garcia's talk described computational modeling of the smectic-to-nematic phase transition for a liquid crystal in geometrically structured confinement. Her iterated application of Landau-de Gennes numerical relaxation demonstrated correlations of nematic-phase topological defects with smectic-phase focal conic domains, as well as with Gaussian curvature in the boundary [58].

3 Panels

Two panels and one informational session were held during the workshop: (1) Panel on underrepresented minorities in STEM fields; (2) Panel on interdisciplinary research and professional networks; and (3) Informational session on obtaining external funding in the United States.

3.1 Panel on Underrepresented Minorities in STEM Fields

The organizer Carme Calderer led the discussion on the status of underrepresented minorities in STEM fields, addressing issues of academic climate, noticing a lack of balance of resources across the North-American geography. It was acknowledged that good progress has been made overall in increasing the number of women in academic positions, especially in mathematics. It was mentioned that some institutions have increased the number of women faculty members by changing the algorithm of hiring, for example, by abandoning the practice to hire faculty by fields of research. It was also mentioned that an improvement on departmental climate has taken place in the recent years, mostly due to the inflow of young faculty members who are less influenced by the established toxic patterns in departmental life, although some issues still remain. In particular, the number of women in academic positions still seems to dip in the later stages of their career.

It was also noted, that in physics the number of women faculty has not experienced significant growth and that most departments in the United States still critically lag behind in incorporating members of underrepresented groups.

The organizer Daniel Beller recalls the specific discussion that took place in the panel:

At least one attendee questioned how widespread is the progress in gender balance of mathematics faculty, how widely used are the beneficial hiring practices that were mentioned, and whether improvements in departmental climate are truly being felt across a large number of departments. I think it is great to focus on certain departments as success stories in improving gender balance, but I suggest being cautious in extrapolating to field-wide trends without examining survey data carefully.

To this end, the Pew Research Center notes that *"STEM Jobs See Uneven Progress in Increasing Gender, Racial and Ethnic Diversity. Higher education pipeline suggests long path ahead for increasing diversity, especially in fields like computing and engineering"* [59].

The following points were made by attendees as possible positive steps towards improving minority inclusiveness in academics:

1. The panel discussed persistence of a big gap in educational resources between the North of the US and California, and the deep South. The North, interior and coastal areas, are also those with the most presence of NSF mathematical institutes.

   A possible first step to help remedy such a situation would be establishing mathematical institutes or branches of existing ones in the deep South. Outreach programs from such institutes could have very positive and enriching roles in such communities.

   One idea explored by the panel was to suggest opening a BIRS-affiliated research center in the south of the United States.

   One graduate student attendee mentioned graduate school application fees as an issue negatively impacting participation of students from the Global South, including many from groups underrepresented in science globally, regarding their participation in scientific research and advanced education. This comment triggered considerable discussion about how to make academia more globally inclusive, including through conference locations and outreach.

2. Available data from the American Mathematical Society indicates that small colleges (referring to those with enrollments a lot smaller than typical state universities) often lack the variety of course offerings to competitively prepare students for graduate school. The panel encouraged members of the mathematical community to be proactive in helping bridge such a course gap, by enrolling in the National Alliance for Doctoral Studies in the Mathematical Sciences (*Math Alliance*)—a community of math sciences faculty and students. Among this organization's goals is an increase the number of doctoral degrees in the quantitative sciences among groups that have been traditionally underrepresented in those fields.

3. A participating postdoc from an underrepresented minority group also brought up a difficulty that often affects students in the low income bracket: coming up with the necessary funds to cover the graduate school application fee. This restricts the number of institutions where a student can apply to. For instance, it was mentioned that often students cannot apply to both, their *dream* and *safety* programs. One suggestion that was voiced was to establish a small grants program, possibly administered by the undergraduate office in the department, to help students meet the application needs.

3.2 Panel on Strategies and Career Opportunities in the Mathematical and Physical Sciences

One of the organizers, M. Carme Calderer, led the discussion on career opportunities. It was noted that graduate students and postdocs will very likely be in the market in academia, government, industry or healthcare. In addition to jobs requiring data science, in the next few years, there will be a sharp increase of academic and industry positions involving AI and targeting Ph.D's in STEM. Academic mentors should be aware of such opportunities, e.g., students seeking industry jobs could be advised to complete a summer school or bootcamp in one of area of data science or take an appropriate university course. The panelists also noted that network building is essential to foster job mobility and growth in industrial settings and that undergraduate or graduate students who are focused towards academic jobs would highly benefit from holding industrial internships.

3.3 Informational Session on Obtaining External Funding in the United States

Dmitry Golovaty presented an overview of funding programs at the Division of Mathematical Sciences of the US National Science Foundation and answered questions from the audience consisting primarily of beginning investigators.

4 Outcomes of the Meeting

The exceptional feature of this workshop was its strong interdisciplinary flavor and the eagerness of the participants to make connections and exchange ideas across disciplines. Many of the participants were meeting for the first time, and this provided a unique fertile environment for discovery and the creation of new networks and collaborations. Much of this interaction was due to the schedule mixing talks by physicists and by mathematicians, and the pleasant environment of the coffee breaks provided by BIRS throughout the meeting, where participants could discuss informally in small groups. The feedback which we have received has been uniformly positive, with many expressing satisfaction with the diversity of methods and viewpoints, and the openness of attendees to discussion and collaboration across disciplines, which one rarely experiences in conferences. We hope and expect that these contacts begun at the workshop will grow into working collaborations between researchers, yielding new insights and scientific breakthroughs in the near future. In particular, the participants expressed very clearly that they would like a similar workshop to take place in two years time so that the new directions and results can be shared and further developed.

5 Titles and Abstracts of the Talks

Daniel Beller: Tutorial: Liquid crystals in models and in reality

Abstract: I will give an overview of some commonly used physical models of liquid crystals and their defects, alongside example experimental systems that these models are used to describe. I will especially emphasize the assumptions and approximations made by these models, the cases and scales at which they are expected to break down, and how successful they have been in describing the experiments. I will close with a perspective on a few selected modeling challenges that remain important open questions.

Arghir Zarnescu: Introduction into mathematics of soft matter

Abstract: We will present some basic models and problems concerning a representative soft matter system, the nematic liquid crystals. We will aim to present and motivate in simple terms mathematical issues that the models generate and how mathematicians approach them, focusing on the possible relevance of these studies from a physics perspective.

Ivan Smalyukh: Knotted Chiral Meta Matter

Abstract Knots of vortex lines within physical fields were postulated to behave like particles already starting from Gauss and Kelvin, and recently topological order and phases represent an exciting inter-disciplinary research frontier [60]. I will describe knotted vortices that emerge in the physical order parameter fields of chiral liquid crystals. A combination of numerical modeling and nonlinear optical imaging uncovers the internal structure and topology of individual vortex knots and the various hierarchical organizations that they form via different reconnections. I will discuss their stability in molecular and colloidal liquid crystals of different symmetries and will show how low-voltage electric fields can switch between different types of behavior. Finally, I will discuss how this emergent paradigm of dynamic knotted meta matter could allow for imparting new designable material properties and physical behavior [61–63].

Randall Kamien: A Bouquet for Apollonius

Abstract Focal conic domains, are defects characteristic of layered liquid crystal phases. Their association can built flowers where petals are the ellipses of the Dupin cyclides involved in these defect. We report here the observation of focal conic flowers in cholesteric droplets sessile on a glass surface and surrounded by glycerol. The observation of the droplets in different directions helps to solve the 3D architecture of the flower. The effects of the droplet size and of the pitch value are also reported.

Giacomo Canevari: A free-discontinuity problem for smectic liquid crystals

Abstract Smectic liquid crystals are a phase of matter in which the constituent molecules tend to align locally parallel to one another and to arrange themselves in layers. Experimental evidence shows that the configuration of the layers in smectic films may be rather complex, possibly with defects - that is, localised regions of sharp change in the orientation of the layers. Defects may occur at isolated points, along lines or surfaces. In this talk, we discuss a free-discontinuity variational problem for smectic A liquid crystals in two dimensions, set in the space SBV. We focus on a specific form of the energy functional, which penalises dislocations of the layers along the defects and is lower semicontinuous, so that minimisers exist. The talk is based on joint work with John M. Ball (Heriot-Watt University, Edinburgh and Hong Kong Institute of Advanced Studies) and Bianca Stroffolini (Universit Federico II, Napoli).

Michael Novack: A variational model for 3D features in films/foams

Abstract Area minimization among a suitable class of 2D surfaces is the basic variational model describing the interfaces in films/foams. In this talk we will discuss a modification of this paradigm in which surfaces are replaced with regions of small but positive volume. The model captures features of real films/foams, such as Plateau borders, that cannot be described by zero volume objects. We will also discuss the PDE approximation of this problem via the Allen-Cahn equation and its relation to Plateau's laws, which govern the possible singularities.

Vianney Gimenez-Pinto: Modeling the actuation of liquid crystal elastomer kirigami imprinted with topological defects

Abstract Liquid crystal elastomers (LCE) are soft materials that combine the elasticity of rubber and the ordering of liquid crystals. Under external stimuli, they exhibit complex morphing including out of plane actuation: twisting, bending, folding, etc. Via numerical experiments implementing finite element elastodynamics, we study the stimulus-responsive shape morphing of these materials. In the spirit of kirigami (the Japanese art of cutting and folding paper), we investigate the light-driven actuation of samples custom-cut to specific geometries. The microstructure in our LCE kirigami include in-plane liquid crystal defects with a preset topological charge coexisting with splay or twist in the liquid crystal director along sample thickness. We demonstrate the actuation of a variety of samples, including the fluttering of a bio-mimetic elastomer butterfly. Our numerical studies are in remarkable agreement with experimental results and demonstrate a fascinating actuation behavior arising from the interplay between microstructural topology, macroscopic geometry, and stimulus-response.

Oleg Lavrentovich: Patterns of spontaneous polarization in ferroelectric nematic liquid crystals

Abstract A ferroelectric nematic liquid crystal is formed by achiral molecules with large dipole moments. Its orientational order is universally described as unidirectionally polar, which raises the question of how the structure avoids a strong depolarization field and splay deformations which bring about a bound charge. We demonstrate a rich plethora of polarization patterns [51, 52, 64] that form in confined ferroelectric nematics not constrained by crystallographic axes. Domain walls adopt the shapes of conic sections, separating domains with uniform and circular polarization [52]. When a flat ferroelectric nematic slab is anchored only at one bounding plate, its ground state is optically active, with left- and right-hand twists of polarization [51]. Although the helicoidal deformations and defect walls separating domains of opposite handedness increase the elastic energy, the twists reduce the electrostatic energy and weaken when the material is doped with ions. An externally applied electric field unwinds the helices and produces complex three-dimensional structures. The study shows that the polar orientational order of molecules could trigger chirality in the soft matter with no chemically induced chiral centers.

Bianca Stroffolini: Manifold-constrained free discontinuity problems and Sobolev approximation

Abstract We discuss a recent result, obtained in collaboration with Federico Luigi Dipasquale, on the regularity of local minimisers of a prototypical free-discontinuity problem involving both a manifold-valued constraint on the maps and a variable-exponent growth in the energy functional. To be more precise, we work in 2D domains, with sphere-valued special functions with bounded variation, and the energy functional we consider is the sum of the integral of the p()-power of their approximate gradient and of the H^1- measure of their jump set. The approach we follow is remiscent of the one devised by Conti, Focardi, and Iurlano to prove existence of strong minimisers for the Griffith energy and it is divided in two steps. As a first step, we extend to this setting the Sobolev approximation results for special functions with bounded deformation and small jump set originally proven by Conti, Focardi, and Iurlano. In second place, we use this extension and a suitable adaptation of the classical blow-up technique due to De Giorgi, Carriero and Leaci to prove the announced partial regularity theorem, avoiding truncation techniques.

Maxim Lavrentovich: Domain walls in hard and soft ferroelectrics

Abstract Ferroelectric materials are utilized in various applications such as sensors, actuators, optical devices, and memory storage. The functionality of these materials hinges upon transitions between different polarization states. These transitions are mediated by the motion of domain walls. We develop the theoretical approaches needed to understand the structure and motion of ferroelectric domain walls in two distinct scenarios: crystalline materials, where such walls are Ising-like with atomic-scale widths, and in the recently discovered ferroelectric liquid crystal materials, where the domain walls have a continuously-varying polarization and the associated splay, twist, and bend elastic deformations. For solid state materials, noise plays a critical role in the microscopic dynamics and can be included within the Landau-Ginzburg-Devonshire modelling framework. On the other hand, in soft materials, the elastic and electrostatic energies compete to create large, stable solitonic structures.

Patricia Bauman: Defect Patterns of Landau-de Gennes Energy Minimizers in Three- Dimensional Slabs

Abstract We investigate minimizers of the Landau-de Gennes energy for liquid crystals in a three-dimensional slab, Ω x $(-\delta, \delta)$, where the cross section Ω is a simply connected smooth domain in the $\mathbb{R}^2$. The minimizers are required to be tangential on the top and bottom faces and to satisfy prescribed uniaxial boundary conditions on the lateral surface of degree $d/2$ where $d \in \mathbb{N}$. We analyze the patterns of these minimizers, including estimates on the nature, number, and location of their defects; and how they depend on the degree of their boundary conditions, the Landau-de Gennes parameter $\epsilon > 0$, and the slab thickness 2δ. In particular, assuming that $\delta = \epsilon^\alpha$, we show that in the thin slab case $1/2 < \alpha < 1$, energy minimizers have d defects each of degree $1/2$ for epsilon sufficiently small. But in the thick case $0 < \alpha < 1/2$, they have $d/2$ defects of degree 1 if d is even; whereas if d is odd, they have (d-1)/2 defects of degree 1 and one defect of degree $1/2$. This is joint work with Daniel Phillips.

Dominik Stantejsky: Asymptotic Limit of the Landau-de Gennes Model for Liquid Crystals Around an Inclusion

Abstract After a general introduction about liquid crystals and their singularities, I present a variational convergence result based on the Landau-de Gennes model describing the Saturn ring effect around an immersed particle with homeotropic and an external magnetic field. We will see how the energy concentrates on lines and surfaces close to, or on the particle surface, leading to a generalized Plateau problem. Some properties of the limit functional will be given and I discuss examples of minimizers for some chosen particle shapes.

Xavier Lamy: Entire vortex solutions of negative degree for the anisotropic Ginzburg-Landau system

Abstract The anisotropic Ginzburg-Landau system

$$\Delta u + \delta\nabla(\mathrm{div}u) + \delta\mathrm{curl}^*(\mathrm{curl}u) = (|u|^2 - 1)u,$$

for $u\colon \mathbb{R}^2 \to \mathbb{R}^2$ and $\delta \in (-1, 1)$, models the formation of vortices in liquid crystals. We prove the existence of entire solutions such that $|u(x)| \to 1$ and u has a prescribed topological degree $d \leq -1$ as $|x| \to \infty$, for small values of the anisotropy parameter $|\delta| < \delta_0(d)$. Unlike the isotropic case $\delta = 0$, this cannot be reduced to a one-dimensional radial equation. We obtain these solutions by minimizing the anisotropic Ginzburg-Landau energy in an appropriate class of equivariant maps, with respect to a finite symmetry subgroup. This is joint work with M.Kowalczyk and P.Smyrnelis.

Daniel Phillips: Defects in Planar Nematic Liquid Crystal Films

Abstract We examine minimizers for the Ball-Majumdar energy modeling a liquid crystal film defined on a bounded simply connected domain in . The minimizers satisfy boundary conditions on the lateral edge that induce defects (disclinations) within the film. We determine the defect structures, liquid crystal patterns and estimates on the energies for minimizers as the elasticity parameter tends to zero. In particular, we show that away from the defect sites, the limit pattern is a local minimizer for a planar Frank energy. This is joint work with Patti Bauman.

Epifanio Virga: From minimal surfaces to a variational theory of soft shells

Abstract Minimal surfaces are ubiquitous in nature. Here they are considered as geometric objects that bear a deformation content. By refining the resolution of the surface deformation gradient afforded by the polar decomposition theorem, we identify a bending content and a class of deformations that leave it unchanged. These are the bending-neutral deformations, fully characterized by an integrability condition. We prove that (1) every minimal surface is transformed into a minimal surface by a bending-neutral deformation and (2) given two minimal surfaces, there is a bending-neutral deformation that maps one into the other. Thus, all minimal surfaces have indeed a universal bending content. The lecture will show how these kinematic concepts pave the way to a natural, variational theory of soft shells.

Peter Sternberg: Two generalizations of Ginzburg-Landau theory on surfaces

Abstract In recent years, the analysis of Ginzburg-Landau type energy functionals has been successfully extended by Ignat and Jerrard to the setting of tangent vector fields defined on a smooth closed surface. Here we discuss two extensions of these results. With an eye towards the modeling of nematics deposited on a surface, the first generalization entails replacing the vector field by a complex line bundle, a setting that includes Q- tensors, The second project involves a tangent vector field sitting on a surface with a singularity, namely a cone. This is joint work with Christian Cofoid, Dmitry Golovaty, Alberto Montero and Etienne Sandier (in various combinations).

Dmitry Golovaty: Mathematical modeling of ferroelectric nematics

Abstract I will present recent results on modeling of ferroelectric nematics using a Ginzburg- Landau-type model with anisotropic elastic constants. We show that the singular structures exhibited by the minimizers of this energy contain both point and line singularities and describe these structures for particular examples of domains/boundary conditions. This is a joint work with Priyanka Kumari, Oleg Lavrentovich and Peter Sternberg.

Claire Doré: The key role of geometry in active nematic flow networks

Abstract Like many other active fluids, the dynamics of active nematics is bistable when confined to narrow channels: they flow spontaneously at a preferred speed in one randomly selected direction. But how do active nematic flows self-organize in microfluidic networks? In this talk, we shed light on this uncharted territory

by reporting recent experiments with the microtubule-based active nematic (AN). We focus on small-sized open networks with inputs and outputs connected to the external, unconfined AN film that acts as a thermal reservoir. Following a bottom-up approach, we first examine the behavior in open individual channels and characterize how channel geometry specifically length, width, and wall patterning controls the flow rate. Next, we study bifurcation networks, where the topology creates a conflict between mass conservation and the bistability of active flows: the three channels cannot sustain flow at the preferred speed simultaneously. For symmetric geometries, we find that, contrary to theoretical conjectures and recent experiments with polar fluids, the flow splits at the junction. However, we demonstrate that it is possible to direct the flow along a particular path by introducing geometrical asymmetries in the bifurcation network. Finally, we show how the design rules derived from the observation of bifurcations can be applied to create a functional logical gate circuit.

Jordi Ignes-Mulol: Coupling across the active/passive liquid crystal interface: flow control and emergent phenomena.

Abstract Liquid crystals combine fluidity with long range orientational order. Their anisotropic physical properties are at the origin of technological applications, and result in fascinating problems when energy minimization conflicts with topological constraints due to boundary conditions, often involving the formation of topological defects. Liquid crystals can be easily driven away from equilibrium with electric, magnetic or flow fields. Recently, active liquid crystals have been discovered and characterized. They are intrinsically out of equilibrium, with constituents that transform chemical energy into flows and mechanical work. Examples are often found in nature, such as bacteria colonies or eukaryotic cell epithelia, and, recently, in artificial preparations, such as in-vitro reconstitutions of cytoskeletal proteins. In this presentation, I will focus on our experiments with the active material forms through the combination of microtubules and dimerized kinesin molecular motors. With the assistance of a depleting agent, microtubules and motors associate, forming thick elongated fibers that, in the presence of adenosine triphosphate, become extensible and prone to buckling instabilities. In the presence of a water/oil interface, the fibers condense in a quasi-two-dimensional layer where long-range orientational order emerges. This results in a two-dimensional active nematic, with the proliferation of self-propelling +1/2 defects and passively-advected -1/2 defects, in a seemingly disordered regime that has been called active turbulence [65]. We take advantage of the influence exerted by the oil rheology on the structure and dynamics of the active nematic to replace the usual isotropic oil with a thermotropic liquid crystal. The anisotropy of the passive liquid crystal provides us with a handle to control active flows using an external magnetic field coupled to the passive mesogen. When the latter is in the lamellar smectic-A phase, and under a homogeneous in-plane magnetic field, oil viscosity is orders of magnitude higher along the magnetic field that perpendicular to it. This results in an alignment transition of the active nematic along the easy flow direction, and turbulent active flows become quasi-laminar, with a well-defined spatial arrangement [66, 67]. Since aligned extensile fibers are prone to bend distortions, accumulated active stress is frequently released through sudden, localized outburst of transversal distortions and flows, which quickly dissipate. Interestingly, when the active nematic layer is laterally confined inside narrow channels, transversal instabilities are prevalent and encompass the whole system. Although the active turbulence regime seems to have been reestablished, a steady state flow pattern emerges in the form of a lattice of antiparallel vortices that originate in the self-propelled defect motion. Moreover, the spatial distribution of active filaments has developed a density pattern complementary to the vortex lattice. On the other hand, the hydrodynamic coupling leads to the formation of new patterns in the passive mesogen due to local flow alignment following drag exerted by the active layer. We have explored this response for dierent passive mesophases: nematic, cholesteric, and smectic A. The spatiotemporal patterns are essentially defect-free, which opens the perspective of studying a defect-free active turbulent system.

Cody Schimming: Analytical Model for the Velocity of Defects in Two-Dimensional Active Nematics

Abstract The behavior of topological defects in active nematics are intrinsically coupled to their macroscopic flows. Therefore, a better understanding of the complicated interactions between defects in these systems is essential to realizing their potential applications. In this talk, using a recently developed approximation scheme for the kinematics of nematic defects [68] and recent calculations for the flow field generated by defects in active nematics [69], I will present an approximate, analytical expression for the velocity of a topological defect in the presence of other defects in two-dimensional active nematics. The velocity may be

decomposed into contributions from the coulomb interaction between defects, advection from flows generated by active stress, and the deflection of defects in shear flow. Focusing on the interaction between just two defects yields insights into phenomena observed in continuum numerical simulations and experiments. Finally, I will discuss our current efforts to numerically simulate a particle model for an active nematic using the expression for defect velocities.

Lorena Aguirre Salazar: On an Ohta-Kawasaki Model set on the space

Abstract We examine a non-local diffuse interface energy with Coulomb repulsion in three dimensions inspired by the Thomas-Fermi-Dirac-von Weizsäcker, and the Ohta- Kawasaki models. We consider the corresponding mass-constrained variational problem and show the existence of minimizers for small masses, and the absence of minimizers for large masses. Finally, we explore the asymptotic behaviour of the energy as the mass goes to zero. This is joint work with Profs. Xin Yang Lu and Jun-Cheng Wei.

Brandon Klein: Topological Entropy Production in Confined Active Nematics

Abstract In active nematic liquid crystals, topological defects drive chaotic flows in the bulk, yielding a positive Lyapunov exponent. While confined geometries of active nematics have been shown to be able to produce ordered flows, little is known about the types of periodic motion these flows permit for topological defects. To explore different active steady states, we simulate an active nematic system using active Beris-Edwards nematodynamics with curved boundary walls and a tunable winding number around the boundary to fix the net topological charge. We find that there are several ordered flows attainable that produce periodic motion of topological defects. Using tools from braid theory, we show connections between these defect motions andthe production of topological entropy, and specifically, that these ordered defect motions produce more chaotic mixing than the well-known topological chaos. We provide an analytical and numerical understanding of the emergence of these ordered flows and discuss their stability for higher net topological charges. Our findings suggest routes to controllable bulk active flows and stable self-mixing patterns realizable in future experiments.

Paul Severino: The Topological Structure of Knotted Smectic Defects

Abstract Defects in smectic liquid crystals, owing to the breaking of translational symmetry, exhibit intricate topological behavior compared to their nematic counterparts. Using tools from knot theory, we study the ability of screw dislocations, edge dislocations, and smectic disclinations to form knots and links. Remarkably, we find that it is not always possible to knot smectic defects without introducing other defects into the system. We provide a lower bound on the number of point defects required to form a smectic dislocation or disclination of any given knot type. These extra point defects can be interpreted as focal conic-like structures, where the knot and point defects play the role of the ellipse and hyperbola, respectively. Our work uncovers a deep connection between smectic liquid crystals and modern topics in Morse-Novikov/knot theory.

Dean Louizos: On the Landau-de Gennes model with planar anchoring and a weak magnetic field

Abstract In this talk I will discuss the 3D Landau-de Gennes model for nematic liquid crystal with an external magnetic field around an immersed particle. I will show that if we impose strong planar anchoring on the surface, then in the large particle limit, and assuming a weak magnetic field, we can characterize the defects that occur. We will see that only point defects can occur for minimizers in this regime.

Jane Bernadette Denise Garcia: Influence of confining surface Gaussian curvature on the winding character of nematic disclination lines

Abstract On curved surfaces, liquid crystal topological point-defects are attracted to Gaussian curvature of the same sign. We show that this coupling extends to the endpoints of disclination lines of 3D nematic liquid crystals arising in a hybrid-aligned system with a double-undulated boundary with homeotropic anchoring and an opposite flat boundary with degenerate planar anchoring. We explore the properties of the multistable disclination lines exhibited by this system. Using Landau-de Gennes numerical modeling, we investigate how the Gaussian curvature of the boundary surface influences the winding character of the disclination lines in the liquid crystal bulk. The winding characters of the disclination lines have been observed to vary rapidly along the defect contours. We calculate the rotation vector to describe local defect winding, and use energetic

arguments to understand the heterogeneity of the multistable disclination landscape. This is joint work with Mohamed Amine Gharbi and Daniel A. Beller.

Priyanka Kumari: Chiral ground states of ferroelectric liquid crystals

Abstract Ferroelectric nematic liquid crystals are formed by achiral molecules with large dipole moments. Their three-dimensional orientational order is described as unidirectionally polar. We demonstrate that the ground state of a flat slab of a ferroelectric nematic unconstrained by externally imposed alignment directions is chiral, with left- and right-handed twists of polarization. Although the helicoidal deformations and defect walls that separate domains of opposite handedness increase the elastic energy, the twists reduce the electrostatic energy and become weaker when the material is doped with ions. This work shows that the polar orientational order of molecules could trigger chirality in soft matter with no chemically induced chiral centers.

Daniel Sussman: Flows, flocking, and unusual hydrodynamics in active and living soft matter

Abstract How is the emergent behavior of non-equilibrium systems different from equilibrium ones, what new collective motion and pattern formation can be found in living as opposed to simply active systems? This talk will combine large scale simulations of a variety of flocking models and a theoretical framework – Toner-Tu hydrodynamics – meant to describe flocking organisms as a type of active polar aligning matter. I will first argue that in a standard numerical model of flocking particles the aligning interactions of coarse grained representations of flocking agents correspond to nonreciprocal forces, i.e., forces that violate Newtons third law. These forces lead to novel terms in the hydrodynamic description of these simulations, and I will discuss how these novel terms lead to new collective dynamics at large scales. Finally, I will connect these ideas to both long-standing puzzles in the field and speculations about actual flocking and schooling behaviors observed in nature.

Francesc Sagues: New theoretical insights and rheological measurements from modified formulations of the AN microtubule/kinesin system

Abstract A couple of modified preparations of the usual AN microtubule/kinesin system will be presented, and their potentialities explored. First, a photosensitive version of the active nematic will be briefly described that enables to study the response of the system to different patterns of distributed activity. In the second formulation, presented in more detail, we report on our recent work with a hybrid version of the AN system after mixing the proteinic material with a light-polymerizable component. Two different scenarios will be commented. First, we report how a spatially extended illumination collapses the nematic order through substrate friction and leads to a biphasic active fluid. Second, by employing specifically illuminated motifs, we are able to estimate for the first time rheological parameters of the active nematic material.

Lisa Tran: Controlling the assembly of molecular and colloidal liquid crystals

Abstract Liquid crystals are the basis of the modern display industry because of their unique properties. Yet, liquid crystalline ordering occurs in systems beyond displays and across length scales: from molecular to colloidal assemblies. Controlling the structuring of liquid crystals across these length scales remains an open challenge. Geometrical constraints can generate patterns and defects localized, melted regions of disorder that can minimize the total elastic distortion in the system. In this talk, I will present the formation of defects within molecular and colloidal liquid crystals that are induced through geometrical frustration. I will begin by presenting work on a molecular, chiral liquid crystal confined to a spherical shell, with the use of microfluidics. I will then present experiments where surface-active colloids are patterned at the liquid crystal-water interface. I will then end by surveying ongoing experiments in my group that probe the role of confinement for structuring larger-scaled, colloidal liquid crystals, such as cellulose nanocrystals and silica nanorods. These organizing principles provide insight on pattern formation in anisotropic elastic materials, across length scales, the mechanisms of which can be leveraged for designing new materials.

Louise Head: Interplay of active nematic defects and flow structures

Abstract Active nematics are a class of liquid crystals driven out-of-equilibrium by the intrinsic activity of their rod-like constituents. In bulk, global nematic order is destabilised by the coupled feedback between

nematic deformations and active flows, resulting in a steady-state population of half-integer nematic topological defects. This talk will demonstrate that despite turbulent-like flows, there exists a strong cross-field constraint between motile +1/2 topological defects and viscometric surfaces, which are contours of the flow where vorticity and strain-rate balance. Through experiments of microtubule-kinesin based active nematics and nematohydrodynamic simulations, we establish the importance of these contours as paths for +1/2 defect dynamics, which determine the handedness of defect trajectories and the sites of defect pair creation and annihilation. We show through a series of models that the constraint is maintained through an interdependence of viscometric surfaces, +1/2 defects, and line-like structures of nematic bend deformation. These results identify that active nematic defects should not be viewed as solitary points but are one component of mesoscale nematic structures, which suggests potential new avenues for exploring topological dynamics.

Federico Luigi Dipasquale: Biaxiality vs uniaxiality in Landau-de Gennes minimisers in 2D discs

Abstract We consider the problem of minimising the (simplest) Landau-de Gennes (LdG) energy in two-dimensional discs, under axial symmetry, a physically relevant pointwise norm- constraint in the interior, and radial anchoring on the boundary. The goal is to study the uniaxial or biaxial character of minimisers. We show that the latter depends crucially on the value of a parameter appearing in front of the potential and penalising biaxiality. For large, minimisers are uniaxial. As decreases, biaxiality is less penalised and a threshold is met at which uniaxial and biaxial minimisers coexist. Below , all minimisers are biaxial. For all biaxial minimisers, *complete biaxial escape* occurs. The cornerstone of the argument consists in an *energy gap* between *small* and *large* maps in the associated minimisation problem for the Dirichlet integral. Here, a map is called *small* if it does not escape the spherical cap containing the image of the boundary data, and *large* otherwise. The energy gap is made fully explicit by describing the set of optimal maps in both the small and the large case. A major difficulty in the analysis lies in dealing with a possible lack of compactness in minimising sequences. This problem arose in a natural way in the framework of a broader investigation, carried out in a joint work with Vincent Millot and Adriano Pisante, of qualitative properties of LdG minimisers in 3D cylinders.

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