
Workshop on
“Current challenges in complex materials: modelling and analysis”

January 9 - 13, 2023

organized by

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Abstracts

Amit Acharya (Carnegie Mellon University)

Dynamics of line defects

Abstract: After briefly describing a ‘full’ continuum mechanical model for the dynamics of dislocations in a nonlinear elastic medium, a simple model for the dynamics of straight line-defects in an ‘elastic’ background will be discussed. With appropriate interpretation, the model can describe the dynamics of screw dislocations in solids, nematic wedge disclinations in liquid crystals, and fracture of solids. Interesting physical questions, e.g., existence of Peierls stress in a translationally invariant PDE model, will be described and motivated by numerically computed approximations, with particular focus on those that cannot be adequately settled on a computer.

Annika Bach (Sapienza University of Rome)

Emergence of topological singularities in the antiferromagnetic XY-model on the triangular lattice

Abstract: Antiferromagnetic spin systems are magnetic lattice systems in which the exchange interaction between two spins favors anti-alignment. Such systems are said to be geometrically frustrated, if due to the geometry of the lattice no spin configuration can simultaneously minimize all pairwise interactions. As a consequence of that, ground states of frustrated spin systems may exhibit nontrivial patterns and give rise to unconventional magnetic order. An example of such a system is the antiferromagnetic XY-model on the triangular lattice (AFX). Here the frustration leads to a concentration of energy at a surface scaling which can be tracked via the so-called chirality of the spin field. In this talk we are concerned with the discrete-to-continuum variational analysis of the AFX in an energetic regime where the system cannot overcome the energetic barrier of a chirality transition and instead finitely many vortex-type singularities emerge in the continuum limit.

This is joint work with M. Cicalese (TU Munich), L. Kreutz (CMU Pittsburgh), and G. Orlando (Politecnico Bari).

Anne Bernand-Mantel (LPCNO-INSA Toulouse)

Skyrmion theory in magnetic thin films: the role of non-local magnetic dipolar interaction

Abstract: Compact magnetic skyrmion are potential bit-encoding states for spintronic memory and logic applications that have been the subject of a rapidly growing number of studies in recent years. Nevertheless, despite numerous attempts, a satisfactory theoretical description of these objects is still lacking today due to the highly non-trivial character of the magnetostatic interaction that plays a major role in determining the nature of magnetization patterns in ferromagnetic materials. The orthodox theory of skyrmions in ultrathin ferromagnetic layers with interfacial DMI relies on a model that accounts for the dipolar interaction through an effective anisotropy term, neglecting long-range effects. At the same time, in single ferromagnetic layers with interfacial DMI, large chiral skyrmions, also called skyrmionic bubbles have been observed, suggesting a non-trivial interplay between DMI and long-range dipolar effects. We will present our recent work where we used rigorous mathematical analysis to develop a skyrmion theory that takes into account the full dipolar energy in the thin film regime and provides analytical formulas for compact skyrmion radius, rotation angle and energy [2,3]. Our theory predict the existence of a new regime at low DMI where skyrmions are stabilized by a combination of non-local dipolar interaction and a magnetic field applied parallel to their core. This predictions are confirmed by our numerical simulations.

Giacomo Canevari (Università di Verona)

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 along surfaces. In this talk, we discuss a free-discontinuity variational problem for smectic A liquid crystals in two dimensions. We focus on a specific form of the energy functional, which penalises dislocations of the layers along the defects and still retains some desirable mathematical properties, so as to guarantee 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 (Università Federico II, Napoli).

Xian Chen (Hong Kong University of Science and Technology)

Two tier compatibility conditions for phase transforming polycrystals

Abstract: For micro and nano-devices used for biomedical applications, e.g. neural stents and heart valves, both crystallographic compatibility and grain boundary engineering play profound role in their functionalities. But these two mechanisms are not well synergized. Here we theorize a two-tier compatibility criterion to *optimize the textures across the grain boundary*, to enhance the mechanical reversibility of transforming polycrystals under stress-induced phase transformation. In this talk, we will present an experimental demonstration that a micropillar fabricated at the grain boundary achieves a remarkable transformability under the demanding driving stress (600MPa) over 10,000 nanomechanical cycles without fulfilling the crystallographic compatibility condition by lattice parameters. The experiment provides an important insight to the design of low fatigue materials by considering the orientation dependent compatibility between grains. By modern nanotechnologies, it is possible to fabricate bi-crystal, tri-crystal and/or quart-crystal nano structures with designed textures, which underlies a new method for the smart materials and structures design.

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2. M. Karami, K. Chu, Z. Zhu, Z. Wang, Q. P. Sun, M. Huang and X. Chen, Orientation- dependent superelasticity and fatigue of CuAlMn alloy under in situ micromechanical tensile characterization, *J. Mech. Phys. Solids*, 104787 (2022).

Răzvan Dumitru Ceucă (Basque Center for Applied Mathematics)

Cubic microlattices embedded in nematic liquid crystals: a Landau-de Gennes study

Abstract: We consider a Landau-de Gennes model for a connected cubic lattice scaffold in a nematic host, in a dilute regime. We analyse the homogenised limit for both cases in which the lattice of embedded particles presents or not cubic symmetry and then we compute the free effective energy of the composite material. In the cubic symmetry case, we impose different types of surface anchoring energy densities, such as quartic, Rapini-Papoular or more general versions, and, in this case, we show that we can tune any coefficient from the corresponding bulk potential, especially the phase transition temperature. In the case with loss of cubic symmetry, we prove similar results in which the effective free energy functional has now an additional term, which describes a change in the preferred alignment of the liquid crystal particles inside the domain. Moreover, we compute the rate of convergence for how fast the surface energies converge to the homogenised one

Giovanni Di Fratta (Università degli Studi di Napoli)

Curved thin-film limits of chiral Dirichlet energies

Abstract: We study the curved thin-film limit of a family of perturbed/chiral Dirichlet energies in the space of H^1 Sobolev maps defined in a tubular neighborhood of an $(n - 1)$ -dimensional submanifold N of $\mathbb{R}^n$ and with values in an $(m - 1)$ -dimensional submanifold M of $\mathbb{R}^m$. Under suitable regularity hypotheses on N , M , and of the perturbation, we show that the family of perturbed/chiral Dirichlet energies converges to an energy functional on N of an unexpected form, which is of particular interest in the theory of magnetic skyrmions. As a byproduct of our results, we get that in the curved thin-film limit, antisymmetric exchange interactions also manifest under an anisotropic term whose specific shape depends both on the curvature of the thin film and the curvature of the target manifold.

Likhith Ganedi (RWTH Aachen University)

Phase Separation in Heterogeneous Fluids

Abstract: Variants of the famous Modica-Mortola functional can be used to model phase separation in heterogeneous fluids by supposing a free energy of the fluid mixture to have periodic heterogeneities of the scale δ and the phase separation to happen on the scale of ε . While Γ -limits depend on the rate of convergence between δ and ε (and many of the regimes are still open-especially with inhomogeneous fluid phases), we will discuss recent results in the regime $\delta \ll \varepsilon$ and $\varepsilon \ll \delta$.

Adriana Garroni (Sapienza University of Rome)

Variational approach for grain boundaries

Abstract: The talk will focus on the role played by material defects in determination of the surface tension carried by grain boundaries in polycrystals. Defects induce elastic distortion in the bulk, therefore a variational model accounting for both, elastic energy and presence of defects, as the one proposed by Lauteri and Luckhaus, is the starting point for our analysis.

Zhiyuan Geng (Basque Center for Applied Mathematics)

Liquid crystal droplets and a nonlocal free boundary problem

Abstract: I will talk about a shape optimization problem which reduces to a nonlocal free boundary problem involving perimeter. This is a joint work with Fanghua Lin. The problem is motivated by a study of liquid crystal droplets with a tangential anchoring boundary condition and a volume constraint. We establish in 2D the existence of an optimal shape that has two cusps on the boundary. We also prove the boundary of the droplet is a chord-arc curve with its normal vector field in the VMO space, and its arc-length parametrization belongs to the Sobolev space $H^{3/2}$. In fact, the boundary curves of such droplets closely resemble the so-called Weil-Petersson class of planar curves. In addition, the asymptotic behavior of the optimal shape when the volume becomes extremely large or small is also studied.

Dmitry Golovaty (University of Akron)

Tetrahedral frame fields via constrained third order symmetric tensors

Abstract: Tetrahedral frame fields can be used to describe certain phases in bent-core nematic liquid crystals. I will describe the problem of constructing a tetrahedral frame field in three dimensional domains in which the boundary normal vector is included in the frame on the boundary. This involves identifying an isomorphism between a given tetrahedral frame and a symmetric, traceless third order tensor under a particular nonlinear constraint. This constraint can be relaxed by postulating an appropriate Ginzburg-Landau-type functional. Using gradient descent, one retrieves a globally defined limiting tensor outside of a singular set. The tetrahedral frame can then be recovered from this tensor by a determinant maximization method, developed in this work. The resulting numerically generated frame fields are smooth outside of one dimensional filaments that join together at triple junctions. This is a joint work with Matthias Kurzke, Alberto Montero and Dan Spirn.

Davit Harutyunyan (University of California at Santa Barbara)

On the extreme rays of the cone of 3 times 3 quasiconvex quadratic forms

Abstract: This talk is concerned with the study of the extreme rays (strong extremals) of the convex cone of 3 times 3 quasiconvex quadratic forms. Those are interesting from both quasiconvex analysis and theory of composites perspective. We characterize the forms, the acoustic tensor of which is an extremal polynomial, proving that the extremality of the determinant implies either strong extremality or polyconvexity of the form. By providing counterexamples, we show that similar results do not hold in higher dimensions. These results improve the ones on weak extremals previously obtained by the first author and G. Milton.

This is joint work with N. Hovsepian (Rutgers University).

Radu Ignat (Université Paul Sabatier, Toulouse)

Separation and interaction energy between domain walls in a nonlocal model coming from micromagnetics

Abstract: We analyse a nonconvex variational model from micromagnetics with a nonlocal energy functional, depending on a small parameter $\epsilon > 0$.

The model gives rise to transition layers, called Néel walls, and we study their behaviour in the limit $\epsilon \rightarrow 0$. The analysis has some similarity to the theory of Ginzburg-Landau vortices. In particular, it gives rise to a renormalised energy that determines the interaction (attraction or repulsion) between Néel walls to leading order. But while Ginzburg-Landau vortices show attraction for winding numbers of the same sign and repulsion for those of opposite signs, the pattern is reversed in this model.

First, we show that the Néel walls stay separated from each other and second, we determine the interaction energy between them.

The theory gives rise to an effective variational problem for the positions of the walls, encapsulated in a Gamma-convergence result. This is a joint work with R. Moser (Univ. of Bath).

Xavier Lamy (Université Paul Sabatier, Toulouse)

Generation of vortices in the Ginzburg Landau heat flow

Abstract: In the two-dimensional Ginzburg-Landau heat flow, a configuration with a logarithmic energy bound has well-formed vortices and their motion is well-understood. For an initial condition with a finite number of nondegenerate zeros, but possibly very high energy, we show that the initial zeros are conserved and the flow rapidly enters the logarithmic energy regime. This is joint work with M.Kowalczyk.

Marta Lewicka (University of Pittsburgh)

The Monge-Ampere system: convex integration in arbitrary dimension and codimension

Abstract: In this talk, we will be concerned with flexibility of weak solutions to the Monge-Ampere system via convex integration. This system is a natural extension of the Monge-Ampere equation $\det \nabla^2 v = f$, in the contexts of: (i) isometric immersions and (ii) nonlinear elasticity.

The main technical ingredient consists of the “stage” construction, in which we achieve the Holder regularity $\mathcal{C}^{1,\alpha}$ of the approximating fields, for all $\alpha < \frac{1}{1+d(d+1)/k}$ where d is an arbitrary dimension and $k \geq 1$ is an arbitrary codimension.

When $d = 2$ and $k = 1$, we recover the previous result by Lewicka-Pakzad for the Monge-Ampere equation. Our construction can be translated to the isometric immersion problem, where for $k = 1$ we recover the result by Conti-Delellis-Szekelyhidi, and for large k we quantify the result by Kallen.

Massimiliano Morini (Università di Parma)

Capillary surfaces and a model of nanowire growth

Abstract: After recalling the classical variational formulation of the capillarity problem and some related results, we consider a model for vapor-liquid-solid growth of nanowires proposed in the physical literature.

In this model, liquid drops are described as local or global volume-constrained minimizers of the capillarity energy outside a semi-infinite convex obstacle modeling the nanowire.

We first address the existence of global minimizers and then, in the case of rotationally symmetric nanowires, we investigate how the presence of a sharp edge affects the shape of local minimizers and the validity of Young's law.

Finally, we study the regularity of the contact line between the drop and the nanowire near the sharp edge.

Cyrill Muratov (Università di Pisa)

Magnetic skyrmions under confinement

Abstract: We present a variational treatment of confined magnetic skyrmions in a minimal micromagnetic model of ultrathin ferromagnetic films with interfacial Dzyaloshinskii-Moriya interaction (DMI) in competition with the exchange energy. Under Dirichlet boundary conditions, we prove existence of topologically non-trivial energy minimizers that concentrate on points in the domain as the DMI strength parameter tends to zero. Furthermore, we derive the leading order non-trivial term in the Γ -expansion of the energy in the limit of vanishing DMI strength that allows us to completely characterize the limiting magnetization profiles and interpret them as particle-like states whose radius and position are determined by minimizing a renormalized energy functional. In particular, we show that in our setting the skyrmions are strongly repelled from the domain boundaries, which imparts them with stability that is highly desirable for applications.

Felix Otto (Max Planck, Leipzig)

Bias in the Representative Volume Element method: periodize the ensemble instead of its realizations

Abstract: We study the Representative Volume Element (RVE) method, which is a method to approximately infer the effective behavior a_{hom} of a stationary random medium, described by a coefficient field $a(x)$ and the corresponding linear elliptic operator $-\nabla \cdot a \nabla$. In line with the theory of homogenization, the method proceeds by computing $d = 3$ (d denoting the space dimension) correctors, however on a “representative” volume element, i. e. box with, say, periodic boundary conditions. The main message of this article is: Periodize the ensemble instead of its realizations.

By this we mean that it is better to sample from a suitably periodized ensemble, e. g. by conditioning on periodicity, than to periodically extend the restriction of a realization $a(x)$ from the whole-space ensemble $\langle \cdot \rangle$. We make this point by investigating the bias (or systematic error), i. e. the difference between a_{hom} and the expected value of the RVE method, in terms of its scaling w. r. t. the lateral size L of the box. In case of periodizing $a(x)$, we heuristically argue that this error is generically $O(L^{-1})$. In case of a suitable periodization of $\langle \cdot \rangle$, we rigorously show that it is $O(L^{-d})$. In fact, we give a characterization of the leading-order error term for both strategies.

We carry out the rigorous analysis in the convenient setting of ensembles $\langle \cdot \rangle$ of Gaussian type, which allow for a straightforward periodization, passing via the (integrable) covariance function. This setting has also the advantage of making Malliavin calculus available for optimal stochastic estimates of correctors. We actually need control of second-order correctors to capture the leading-order error term in the presence of cancellations due to point symmetry. This is joint work with Nicolas Clozeau, Marc Josien, and Qiang Xu.

Miha Ravnik (University of Ljubljana)

Ionically Charged Topological Defects in Nematic Fluids

Abstract: Controlling the electric charge in liquid electrolytes is of prime importance in a range of applications such as supercapacitors, or the self-assembly of particles in colloidal or biological settings. However, realizing localised charge profiles in the bulk of such electrolytes generally requires the presence of surfaces which poses a fundamental constraint on the material design. Here, we show using numerical modelling that nematic topological defects in nematic electrolytes can perform as regions for local charge separation, forming charged defect cores and, in some geometries, even electric multilayers, analogous to electric double layers found in isotropic electrolytes. Specifically, we show that flexoelectricity and ion solvability perform as the main mechanisms for the effective charging of the nematic. Different bulk and surface geometries will be discussed, including flat interfaces and colloids. More generally, the relevance of this work is for possible applications where topological defects act as diffuse ionic capacitors or as ionic charge carriers.

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[2] J. C. Everts, B. Senyuk, H. Mundoor, M. Ravnik and I.I. Smalyukh, Sci. Adv. 7, eabd0662 (2021).

[3] J. C. Everts and M. Ravnik, Phys. Rev. X 11, 011054 (2021).

Tobias Ried (Max Planck, Leipzig)

The Mathematics of the Magnetisation Ripple-Variational Methods for a Singular SPDE

Abstract: The magnetisation ripple is a microstructure formed in thin ferromagnetic films. It can be described by minimisers of a non-convex energy functional leading to a nonlocal and nonlinear elliptic SPDE in two dimensions driven by white noise, which is singular. In this talk I will describe how the universal character of the magnetisation ripple can be addressed using variational methods based on Γ -convergence. (Joint work with R. Ignat, F. Otto, and P. Tsatsoulis)

Michele Ruggeri (University of Strathclyde)

Numerical methods for antiferromagnetic and ferrimagnetic materials

Abstract: Antiferromagnetic and ferrimagnetic materials are seen as the future of spintronic devices. In this talk, we discuss the numerical approximation of a continuum model for these types of material. The model is an extension of the classical micromagnetic model for ferromagnets: the magnetic state of the material is described by two unit-length vector fields, representing the magnetization of two sublattices, which are coupled to each other by means of a suitable expression of the exchange energy. We present a finite element discretization of the model, considering both the stationary case (energy minimization) and the dynamic case (a system of two exchange-coupled Landau-Lifshitz-Gilbert equations)

Theresa Simon (WWU Münster)

The elastica functional as the critical Gamma-limit of the screened Gamow model

Abstract: I will consider the large mass limit of a nonlocal isoperimetric problem in two dimensions with screened Coulomb repulsion. In this regime, the competition between perimeter and the repulsion simplifies to leading order by the nonlocal interaction localizing on the boundary of the sets. For an appropriate choice of screening constant, the surface area is exactly cancelled, requiring an analysis

of the next order contribution. It turns out that then the nature of the problem changes from length minimization to curvature minimization: I will prove that the Gamma limit is given by (the relaxation of) the elastica functional, i.e., the integral over the squared curvature over the boundary. This is joint work with Cyrill Muratov and Matteo Novaga.

Ivan Smalyukh (University of Colorado Boulder)

Knotted Solitonic Matter

Abstract: Topological order and phases represent an exciting research frontier [1], but knots in fields were postulated to behave like particles already starting from Gauss and Kelvin. Experimentally they were found only as transient features and could not self-assemble into three-dimensional crystals. I will describe energetically stable solitonic knots that emerge in the physical fields of chiral liquid crystals and magnets [2,3]. While spatially localized and freely diffusing in all directions, they behave like colloidal particles and atoms, self-assembling into crystalline lattices with open and closed structures, as well as forming low-symmetry mesophases and gas- or liquid-like states [2,3]. A combination of energy-minimizing numerical modeling and nonlinear optical imaging uncovers the internal structure and topology of individual solitonic knots and the various hierarchical crystalline and other organizations that they form. These solitonic knots are robust [1-4] and topologically distinct from the host medium, though they can be morphed and reconfigured by weak stimuli like electric or magnetic fields. I will discuss their stability in molecular and colloidal liquid crystals of different symmetries [5-7] and will show how low-voltage electric fields can switch between the heliknoton [2,3] and hopfion [4] embodiments of such knot solitons while preserving their topology. Finally, I will discuss how this emergent paradigm of knotted solitonic matter could allow for imparting new designable material properties and for realizing phases of matter that so far could not be found in naturally occurring materials.

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2. J.-S. B. Tai and I. I. Smalyukh. Science 365, 1449 (2019).
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7. H. Mundoor, J.-S. Wu, H. Wensink and I.I. Smalyukh. Nature 590, 268 (2021).

Bianca Stroffolini (University of Naples Federico II)

A 2D model for ferronematics with weak coupling

Abstract: Nematic liquid crystals (NLC) present an intermediate phase between liquid and solids, indeed they combine fluidity with the directionality of solids.

The NLC exhibit long-range orientational order with special directions of averaged molecular alignment, referred to as **directors** in the literature and the directional nature of NLCs make them susceptible to external electric and magnetic fields, incident light and temperature. However, due to small values of magnetic susceptibility, large magnetic fields are required for the magneto-nematic response. In 1970 Brochard and de Gennes suggested to introduce magnetic nanoparticles (nanoparticles with magnetic moments) in order to enhance the magneto-nematic coupling, thereby allowing novel magneto-optic responses in addition to the conventional electro-optic responses. In this way, one can control the nematic directors, denoted by $\mathbf{n}$, by the surface-induced mechanical coupling between NLCs and MNPs and equally, control the magnetization profiles by the nematic anisotropy through the MNP-NLC interactions.

We work with dilute ferronematic suspensions relevant for a uniform suspension of MNPs in a nematic medium, such that the distance between pairs of MNPs is much larger than the individual MNP sizes

and the volume fraction of the MNPs is small. In these dilute systems, the MNP-MNP interactions and the MNP-NLC interactions are absorbed by an empirical magneto-nematic coupling energy. Let $\Omega \subset \mathbb{R}^2$ be an open set (simply connected) in the plane and $\mathbf{Q}: \Omega \rightarrow \mathcal{S}_0^{2 \times 2}$ is a $\mathbf{Q}$ tensor and $\mathbf{M}: \Omega \rightarrow \mathbb{R}^2$ is the magnetic field. Our energy has three components : a reduced LdG free energy for NLCs, a Ginzburg-Landau free energy for the magnetization and a homogenised magneto-nematic coupling term:

$$\mathcal{F}_\epsilon(\mathbf{Q}, \mathbf{M}) := \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{\xi}{2} |\nabla \mathbf{M}|^2 + \frac{1}{\epsilon^2} f(\mathbf{Q}, \mathbf{M}) \right) dx \quad (1)$$

In two dimensions, we have

$$f(\mathbf{Q}, \mathbf{M}) := \frac{1}{4} (|\mathbf{Q}|^2 - 1)^2 + \frac{\xi}{4} (|\mathbf{M}|^2 - 1)^2 - c_0 \mathbf{Q} \mathbf{M} \cdot \mathbf{M}, \quad c_0 > 0.$$

We study a special limit of the effective free energy in (1), for which both ξ and c_0 are proportional to ϵ and we study the profile of the corresponding energy minimizers in the $\epsilon \rightarrow 0$ limit, subject to Dirichlet boundary conditions for $\mathbf{Q}$ and $\mathbf{M}$. This can be interpreted as a "super-dilute" limit of the ferronematic free energy for which the magnetic energy is substantially weaker than the NLC energy, and the magneto-nematic coupling is weak.

Caterina Zeppieri (WWU Münster)

Gamma-convergence and homogenisation of phase-field functionals

Abstract: In this talk we analyse the limit behaviour of general elliptic, phase-field functionals of Ambrosio-Tortorelli type. Under mild assumptions on the regularised volume and surface terms, we show that if the volume integrand grows superlinearly in the gradient-variable, then the functionals converge to a brittle energy-functional; i.e., to a free-discontinuity functional whose surface integrand does not depend on the jump-amplitude of the limit variable. This result is achieved by showing that volume and surface terms always decouple in the limit. As an application of the abstract convergence result as above, the case of homogenisation of gradient damage models will be also discussed.
