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Singularities in Discrete Systems

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Abstract. Discrete systems are ubiquitous in applications. Their analysis and simulation call for taming their inherent multiscale character, as microscopic dynamics lead to the emergence of structures across scales. This workshop brought together leading experts in the calculus of variations, discrete systems, and materials science to explore cutting-edge topics at the intersection of mathematics and physical modelling. Presentations spanned a variety of themes, including dislocation dynamics, crystallization, micromagnetics, fracture mechanics, and discrete-to-continuum transitions. Particular emphasis was placed on the rigorous analysis of singular structures, nonlocal interactions, and energy-driven pattern formation. Several talks also underscored emerging connections with data science.

Mathematics Subject Classification (2020): 35-XX, 49-XX, 74-XX.

Introduction by the Organizers

The workshop *Singularities in discrete systems* brought together 50 participants (45 on-site and 5 online) from a diverse range of countries, including Austria, France, Germany, Italy, Spain, the Netherlands, the UK, and the USA. Attendees came from various scientific backgrounds, spanning mechanics, mathematical analysis, and data science. Participants have been selected to ideally represent the breadth of current research directions in the field, ranging from purely atomistic models to computational approaches, from energy-driven pattern formation to aggregation phenomena emerging as long-time behaviour of aggregation-diffusion equations, and from defects in materials science to models of flocking and crowd dynamics. A significant number of young researchers joined the group.

The purpose of the workshop was to bring together leading scientists and early-career researchers working on various aspects of the mathematics of discrete systems. The organizers pursued a twofold goal: on the one hand, to provide a forum for exchange among the community's diverse research directions; on the other hand, to foster new approaches to open problems through cross-disciplinary dialogue.

The organizers believe these objectives were successfully achieved. The workshop featured a series of insightful talks showcasing the current state of research. These consistently sparked stimulating scientific discussions, many of which evolved and deepened over the course of the week and might well lead to new collaborations.

The talks covered a wide range of topics. The emergence and stability of ordered large-scale structures have been discussed in various settings: within lattices (Bétermin), in interaction with substrates (Kreutz), and in the context of objective structures (Schmidt) and metamaterials (Ortiz). A central theme of the workshop was the modelling and analysis of defects (Ariza, Briani, D'Elia, Garroni) and dislocations in solids (Acharya, Bach, Hudson), across multiple material systems and scales. Particle models and related methods were also covered (Bruna, Guo, Orlando, Wolfram), including applications to mean-field games and opinion formation. The interest in upscaled models of microscopic interactions was reflected in the high number and variety of nonlocal variational problems discussed in the meeting (Cristoferi, Daneri, Kreisbeck, Mora, Ponsiglione, Tolotti). Two application areas received particular attention: atomistic and discrete fracture mechanics (Braun, Buze, Kubin, Friedrich), and micromagnetism (Briani, D'Elia, Ginster, Giorgio, Happ). In addition, the workshop presented new results on learning algorithms (Bourdais, Bungert, Murray, Thorpe), image segmentation (Fischer), and discrete optimal transport (Quattrocchi). Finally, several talks focused on dissipative evolution, covering a wide spectrum of mechanical and aggregation-diffusion models (Chiesa, Fernandez Jimenez, Guo, Laux, Park, Sheldon).

The setting of the program was rather classical, featuring however a very well-received session of lightning talks delivered by young participants on Wednesday night. As organizers, we were very pleased with the high scientific level of the workshop, the quality and clarity of the talks, and the breadth of topics covered. This collection offers a snapshot of the field's current vitality and rapid development.

Workshop: Singularities in Discrete Systems

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Abstracts

Homogenization and continuum limit of mechanical metamaterials

Michael Ortiz
(joint work with J. Andrade, M. P. Ariza, S. Conti, J. Ulloa)

When used in bulk applications, mechanical metamaterials set forth a multiscale problem with many orders of magnitude in scale separation between the micro and macro scales. Direct numerical simulations of mechanical metamaterials are prohibitively expensive due to the separation of scales between the lattice and the macrostructural size. Hence, multiscale continuum analysis, specifically discrete-to-continuum methods, suggests itself as a means of characterizing the effective properties of metastructures at the macroscopic scale. However, mechanical metamaterials fall outside conventional homogenization theory on account of the flexural, or bending, response of their members, including torsion. Notwithstanding, we show [1] that homogenization theory based on calculus of variations and notions of Gamma-convergence can be extended to account for bending. The great advantage of these methods is that they determine, free of any *ansatz*, the functional form of the limiting continuum energy. In this manner, the homogenized metamaterials are shown to exhibit intrinsic generalized elasticity in the continuum limit. By exploiting the quadratic-form structure of the discrete energies, Gamma-convergence additionally supplies closed-form expressions for all effective properties. Examples of two and three-dimensional metamaterials, including honeycomb and octet-truss lattices, are presented in [1]. The convergence of the discrete energy to the continuum limit is illustrated in [3] by means of numerical examples.

To zeroth order, the continuum limit of metamaterials is micropolar, with both displacement and rotational degrees of freedom, but exhibits no size effect. To higher order, the overall energetics of the metastructure can be characterized explicitly in terms of the solution of the zeroth-order continuum problem by the method of Γ-expansion [2]. The analysis predicts that the discreteness of metamaterials effectively shields crack-tips, resulting in *lattice shielding*. The theory specifically predicts *anti-shielding*, i.e., *coarser is weaker*, in agreement with recent experimental observations.

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Parametrising dislocation dynamics with quantified uncertainties

Thomas Hudson
(joint work with Geraldine Anis, Peter Brommer)

Dislocations are line defects whose response to external forcing is critical for determining the strength of crystalline materials, and particularly those of metals. One class of alloys which are recognized for their strength even at high temperatures are Nickel–Aluminum alloys. These alloys have a complex microstructure, and in particular they separate into two phases, called the γ and γ' phases. It is believed that the interaction between dislocations and the precipitates is the mechanism behind the strength of these materials. In the work presented here [1], we interrogate this hypothesis using a reduced model, seeking to parametrise the model using data generated from atomistic simulations and retaining the uncertainty in these parameters so that such uncertainties can be propagated in models at larger length–scales.

Starting with atomistic simulations based on a potential fitted to capture the features of these alloys [2], we observe realizations of dislocation motion and extract time series data describing the motion of straight dislocation in the pure γ phase. The dislocation is created by removing a half-plane of atoms, and the cell is thermally equilibrated, after which the motion is driven by shear stresses induced by forces applied on atomic planes at some distance above and below the dislocation core. Snapshots of the atomistic configuration are stored and post-processed using the dislocation extraction algorithm [3].

The reduced model we propose is a second-order linear ordinary differential equation; by transforming the equation appropriately, we are able to formulate a Bayesian inverse problem to find appropriate parameters and sample the posterior using a Markov Chain Monte Carlo approach using the particular framework outlined in [4]. The resulting ensemble of models shows good agreement with the mean trajectory over around 10 dislocation trajectories obtained from atomistic simulation. This approach also allows us to capture correlated uncertainties in the parameters, information which is not captured by simpler fitting approaches. Moreover, we can use our approach to show that across a wide range of stress conditions, parameters in the model which are generally believed not to depend on the applied stress condition do not vary significantly.

While the approach discussed above gives excellent agreement with the mean trajectory over a number of realizations of the dynamics, there are fluctuations not accounted for by our simple deterministic model. In particular, the data indicates that in the low stress regime, thermal fluctuations may play a significant role in determining the motion, and I discuss ongoing work where we use stochastic forcing terms to account for these discrepancies, extending the deterministic approach.

Finally, to address the central challenge in determining the importance of precipitate interaction in the strength of the materials, I will present ongoing work where we formulate a model accounting for the interactions between dislocations and the different phases. Early indications suggest that our approach can indeed

be extended with success to this much more complex situation. Ultimately, the interpretable approach taken allows us to lay out the physical assumptions in the model, which we hope will allow us in future to translate these assumptions into Discrete Dislocation Dynamics models for the study of these materials at much larger length scales.

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On the minimization of nonlocal anisotropic interaction energies

Maria Giovanna Mora

(joint work with R. Frank, J. Mateu, L. Rondi, L. Scardia, J. Verdera)

Nonlocal interaction energies play a central role in describing the behaviour of large systems of particles in a wide range of applications. In this talk we focused on the minimization problem for an energy functional of the form

$$I(\mu) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} K(x-y)\, d\mu(x) d\mu(y), \qquad \mu \in \mathcal{P}(\mathbb{R}^N),$$

where the kernel $K : \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$ is even, lower semicontinuous, locally integrable, and bounded from below. Here $\mathcal{P}(\mathbb{R}^N)$ denotes the set of probability measures on $\mathbb{R}^N$.

We are interested in modelling interactions that are repulsive at short range and attractive at large distances. This behaviour corresponds to choosing K such that it diverges both at the origin and at infinity. A model example is the isotropic kernel

$$K_{\mathrm{iso}}(x) = \frac{1}{|x|^s} + |x|^\alpha \qquad \text{with } 0 < s < N,\ \alpha > 0. \tag{1}$$

After reviewing the main results on the existence and uniqueness of minimizers, we discussed their explicit characterization. In the isotropic case (1) with $\alpha = 2$ it is known that the unique minimizer (up to translations) is given by the measure

$$\mu_{s,\mathrm{iso}} = \begin{cases} c(r^2 - |x|^2)^{\frac{s-N+2}{2}} \chi_{B_r} & \text{for } N-4 < s < N, \\ c\mathcal{H}^{n-1} \llcorner \partial B_r & \text{for } 0 < s \le N-4, \end{cases}$$

where $c, r > 0$ are constants depending on s and N. As s decreases, the minimizer undergoes a transition: from a diffuse measure with bounded density (for $N-2 \le s < N$), to a diffuse measure with unbounded density (for $N-4 < s < N-2$),

and finally to a more singular measure supported on an $(N-1)$-dimensional set (for $0 < s \leq N-4$).

Now let $\Phi : \mathbb{S}^{N-1} \to \mathbb{R}$ be a smooth, even, strictly positive function, and consider the anisotropic Riesz kernel

$$W_s(x) = \frac{1}{|x|^s}\Phi\left(\frac{x}{|x|}\right) \qquad \text{with } 0 < s < N.$$

For the kernel $K(x) = W_s(x) + |x|^2$, with $s \in [N-3, N) \cap (0, 5]$, we proved that if the Fourier transform of W_s is strictly positive, then there exists an ellipsoid $E = RDB_1$, where R is a rotation and D is a positive definite diagonal matrix, such that the unique minimizer (up to translations) is the push-forward $f_\#(\mu_{s,\mathrm{iso}})$ of the measure $\mu_{s,\mathrm{iso}}$ by the map $f : x \mapsto RDx$.

It remains unclear whether the condition on s is purely technical or whether the result fails for s near $N-4$ or for s large. Our proof suggests that for $s \in (N-4, N-3)$ the support of minimizers may collapse onto a lower dimensional set. The upper bound on s is related to the integrability of the Fourier transform of $W_s * f_\#(\mu_{s,\mathrm{iso}})$, a property required to apply the Fourier inversion theorem and to express the potential $W_s * f_\#(\mu_{s,\mathrm{iso}})$ in a more convenient form.

Dynamics of screened particles towards equispaced ground states and applications to misfit dislocations

Marcello Ponsiglione
(joint work with Lucia De Luca, Michael Goldman)

We analyse the dynamics – driven by the gradient flow of negative fractional seminorms – of empirical measures towards equispaced ground states.

Specifically, we consider periodic empirical measures μ on the real line that are screened by the Lebesgue measure, i.e., with $\mu - dx$ having zero average; to each of these measures μ we associate a (periodic) function u satisfying $u' = dx - \mu$. For $s \in (0, \frac{1}{2})$ we introduce energy functionals

$$\mathcal{E}^s(\mu) := \frac{1}{2}\int_0^\Lambda dx \int_{\mathbb{R}} \frac{|u(x) - u(y)|^2}{|x-y|^{1+2s}}\, dy,$$

that can be understood as the density of the s-Gagliardo seminorm of u per unit length. For $s \in [\frac{1}{2}, 1)$ we define $\mathcal{E}^s_\varepsilon(\mu) := \mathcal{E}^s(\mu_\varepsilon)$, where μ_ε is obtained by mollifying μ on scale ε.

Particularly relevant is the critical case $s = \frac{1}{2}$, where the energy functional can be seen as a "positive ε" version of the renormalized energy considered in [5] for a (not necessarily periodic) distribution of screened charges lying on a straight line in the plane, once the infinite self energy of each particle is removed.

We prove that the minimizers of $\mathcal{E}^s$ and $\mathcal{E}^s_\varepsilon$ are the equispaced configurations of particles with lattice spacing equal to one. Then, we prove the exponential convergence of the corresponding gradient flows to the equispaced steady states. Finally, although for $s \in [\frac{1}{2}, 1)$ the energy functionals $\mathcal{E}^s_\varepsilon$ blow up as $\varepsilon \to 0$, their gradients

are uniformly bounded (with respect to ε), so that the corresponding trajectories converge, as $\varepsilon \to 0$, to the gradient flow solution of a suitable renormalized energy.

The emergence of periodic structure as a result of minimization of convex functionals has been much investigated in the last decades; in [1] the minimization of the square of the L^2 norm has been considered, among functions having two opposite slopes. Such a result has been generalized in [2] to the case of two, possibly different, slopes. The case of fractional $\frac{1}{2}$-Gagliardo seminorm has been considered in [3], again for functions with equal opposite slope; their approach relies on a technique referred to as *reflection positivity* for which such a symmetry assumption is somehow required. In the aforementioned results, the functionals under minimization contains also a term penalizing the jumps of the slopes, which is multiplied by a certain (small) parameter that determines the periodicity scale.

In this paper we have adopted a more rigid approach: the slopes of the order parameter u are either 1 or $-\infty$ and, instead of a term penalizing the jumps of the slope, we have assumed that the region where the slope is $-\infty$ is quantized (the Dirac delta's have positive integer weights). Such a framework is very similar to that analysed in [4], in which the case of two generic different (in modulus) slopes has been treated with the aim of modelling misfit dislocations at semi-coherent interfaces [6]; the main novelty of our analysis with respect to the results in [4] is that here we also consider the dynamics of misfit dislocations driven by the gradient flow of the induced elastic energy.

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On crystallization in the plane for pair potentials with arbitrary norms

Laurent Bétermin

(joint work with Camille Furlanetto)

In this talk, we consider an interaction energy E defined on N-point configurations $X_N := (x_1, ..., x_N) \subset \mathbb{R}^2$ interacting through a potential $V : \mathbb{R}_+^* \to \mathbb{R}$ such that

$$\forall X_N := (x_1, ..., x_N) \in \mathbb{R}^2, \quad E(X_N) = \frac{1}{2} \sum_{i \neq j} V(\|x_i - x_j\|), \quad \|\cdot\| \text{ is a norm.}$$

Part I. Finite crystallization for the sticky disk. For fixed $N \geq 2$, we define $\mathcal{E}_{\|\cdot\|}(N) = \min_{X_N \subset \mathbb{R}^2} E(X_N)$, and for the Heitmann–Radin's sticky disk $V = V_{\rm HR}$ [5] defined as $V_{\rm HR}(r) = \begin{cases} +\infty & \text{if } r \in [0,1) \\ -1 & \text{if } r = 1 \\ 0 & \text{if } r > 1 \end{cases}$, two cases hold according to the shape of the unit sphere $S_{\|\cdot\|} = \{x \in \mathbb{R}^2 : \|x\| = 1\}$, where $\mathsf{A}_2 = \mathbb{Z}(1,0) \oplus \mathbb{Z}(\frac{1}{2}, \frac{\sqrt{3}}{2})$:

- if $S_{\|\cdot\|}$ is not a parallelogram, then $\mathcal{E}_{\|\cdot\|}(N) = -\lfloor 3N - \sqrt{12N-3} \rfloor$ achieved on a lattice being the image of the triangular lattice A_2 by a linear map;
- if $S_{\|\cdot\|}$ is a parallelogram, then $\mathcal{E}_{\|\cdot\|}(N) = -\lfloor 4N - \sqrt{28N-12} \rfloor$ achieved on a lattice being the image of the square lattice $\mathbb{Z}^2$ by a linear map.

The proof given in [1] is based on Brass' results [3] on the maximum number of minimal distances on 2d configurations, but also on Heitmann–Radin's crystallization's proof on A_2 for $\|\cdot\| = \|\cdot\|_2$ and De Luca–Del Nin [4] crystallization's proof on $\mathbb{Z}^2$ for $\|\cdot\| = \|\cdot\|_\infty$, the other cases following by a linear transform argument.

Part II. Lennard–Jones energy among lattices and p-norms Considering now only infinite lattice structures and $V(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$ the Lennard–Jones potential (for which no optimality result is known for $\mathcal{E}_{\|\cdot\|_2}$), one numerically observes the following phase transition for the minimizer once chosen $\|\cdot\| = \|\cdot\|_p$, $p \in [1,\infty]$:

$$\text{Square } (p=1) \to \text{Rhombic } (p \in (1,1.25)) \to \text{Triangular } (p \in (1.25,2]) \\ \to \text{asymmetric } (p \in (2,3.85)) \to \text{Square } (p > 3.85),$$

which seems very intriguing, where only the $p = 2$ case has been proven in [2].

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The Capacity of Data

Matthew Thorpe

(joint work with Jeff Calder, Dejan Slepčev, Adrien Weihs)

The *semi-supervised learning problem* is to find the missing labels from a partially labelled set of feature vectors, $\Omega_n = \{x_i\}_{i=1}^n$, with labels $\{\ell_i\}_{i \in \mathcal{I}_n}$. The set $\mathcal{I}_n \subseteq \{1,\dots,n\}$ indexes the labels, e.g. if $\mathcal{I}_n = \{1,\dots,n\}$ then every feature vector has a label. The objective is to estimate labels for $\{x_i\}_{i \in \{1,\dots,n\} \setminus \mathcal{I}_n}$.

The idea behind *Laplace Learning* is to assume similar feature vectors have similar labels. To define similarity between feature vectors we assume a graph structure where we have weights w_{ij} that represent how similar x_i is to x_j (the larger w_{ij} the more similar the feature vectors). This is represented as a variational problem corresponding to minimizing

$$\mathcal{E}_n^{(p)}(u_n) = \frac{1}{Z_n} \sum_{i,j=1}^{n} w_{ij} |u_n(x_i) - u_n(x_j)|^p$$

subject to $u_n(x_i) = \ell_i$ for all $i \in \mathcal{I}_n$ and where Z_n is a normalization constant.

This talk is about the asymptotics of the variational problem, i.e. what happens when $n \to \infty$. Motivated by computational efficiency and between-class resolution we scale the weights so that we get a local limit. In particular, assuming $x_i \in \mathbb{R}^d$, we define $w_{ij} = \frac{1}{\varepsilon^d} \eta\left(\frac{\|x_i - x_j\|}{\varepsilon}\right)$ and choose $\varepsilon = \varepsilon_n$. It's an easy calculation to show that, if $u \in \mathrm{C}^2(\mathbb{R}^d)$, $x_i \overset{\text{iid}}{\sim} \mu \in \mathcal{P}(\mathbb{R}^d)$ and $Z_n = \varepsilon_n^p n^2$ that (almost surely)

$$\mathcal{E}_n^{(p)}(u_n) \to \mathcal{E}_\infty^{(p)}(u) := \sigma_\eta \int_{\mathbb{R}^d} |\nabla u(x)|^p \rho^2(x) \, \mathrm{d}x$$

where ρ is the density of μ and $\sigma_\eta = \int_{\mathbb{R}^d} \eta(\|x\|)|x_1|^p \, \mathrm{d}x$ is a constant. For the variational problem we are interested in Γ-convergence, which was first done for $p = 1$ (but the proof essentially holds for all $p \geq 1$) in [1].

We see that, if we want to have pointwise constraints the problem: minimize $\mathcal{E}_\infty^{(p)}(u)$ subject to $u(x_i) = \ell(x_i)$ for all $i \in \{1, \dots, N\}$, that we need continuity. We therefore see that, since we work in the Sobolev Space $\mathrm{W}^{1,p}$ that we require $p > d$. However, this is not sufficient as one can show $\mathcal{E}_n^{(p)}(\delta_{x_1}) \sim \frac{1}{\varepsilon_n^p n}$ (approximately speaking the capacity of the point x_1) and therefore $u_n(x_i) = \ell_i$ for $i \in \{1, \dots, N\}$ and $u_n(x_i) = 0$ otherwise forms a sequence of approximate minimizers if $\varepsilon_n^p n \to \infty$. Following [2], we will show that the scaling rate $\varepsilon_n \sim n^{-p}$ is critical in the sense that $\varepsilon_n \gg n^{-p}$ leads to ill-posedness and $\varepsilon_n \ll n^{-p}$ leads to well-posedness (with a lower bound for graph connectivity). We show a similar result with the Fractional Laplacian [3]. Finally, we make a connection between solutions of the Laplace Learning problem and random walks on graphs to show that the problem, for $p = 2$, is asymptotically well-posed if $|\mathcal{I}_n| \gg n\varepsilon_n^2$ and asymptotically ill-posed if $|\mathcal{I}_n| \ll n\varepsilon_n^2$ [4].

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Stacking faults in the Γ-limit of a discrete model for partial edge dislocations

Annika Bach

(joint work with Marco Cicalese, Adriana Garroni, Gianluca Orlando)

The mechanical properties of crystalline materials is highly influenced by the presence and interaction of defects in their atomistic structure such as impurities, dislocations, stacking faults or grain boundaries. For example, dislocations have a crucial impact on the plastic deformation behaviour of crystals, as they allow atomic layers to slip past one another under stress. In this talk we are interested in investigating the interplay of those defects with so-called stacking faults, which typically appear in crystals with multiple stacking possibilities, in the passage from a simple atomistic to a continuum model. Specifically, we consider a two-dimensional discrete toy model introduced in [1] and we analyze its asymptotic behaviour as the lattice spacing vanishes in terms of Γ-convergence.

Under the assumption that only horizontal displacements are allowed, the discrete energies we consider are defined on scalar variables $u : \varepsilon\mathbb{Z}^2 \to \mathbb{R}$ (that can be interpreted as a horizontal displacement) and are obtained by summing up three key contributions: Elastic interactions between horizontal nearest neighbours of the form $(u(i+\varepsilon e_1) - u(i))^2$, 1/2-periodic interactions between vertical nearest neighbours of the form $\mathrm{dist}^2\big(u(i+\varepsilon e_2) - u(i); \frac{1}{2}\mathbb{Z}\big)$ and scaled 1-periodic interactions between second vertical neighbours of the form $\varepsilon\mathrm{dist}^2\big(u(i+\varepsilon e_2) - u(i); \mathbb{Z}\big)$. The elastic horizontal interactions correspond to the assumption that only horizontal displacements are allowed and hence no vertical slips are allowed, while the choice of the vertical nearest-neighbour interactions is inspired by [2] and allows for multiple stacking possibilities of atomic layers. Finally, the second-neighbour interactions penalize non-homogeneous stackings. After removing a logarithmic core contribution, we show that our discrete energies Γ-converge to a continuum energy consisting of three contributions: A core energy concentrated on limiting point singularities (corresponding to partial dislocations), a Coulomb-type interaction energy between those singularities, and a surface contribution. This last contribution corresponds to the minimal length of horizontal line segments joining the limiting point singularities and can be interpreted as the energetic contribution of the stacking faults that are required to resolve the dislocations tension.

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A new monotonicity formula and a sharp lower bound on the energy density for minimizers of the 2d Mumford–Shah functional

Julian Fischer

The minimization of the Mumfordi–Shah energy $E_{MS} : \mathrm{BV}(\Omega) \to \mathbb{R} \cup \{+\infty\}$,

$$E_{MS}[u] := \int_{\Omega \setminus S_u} |\nabla u|^2 \, dx + \mathcal{H}^{d-1}(S_u), \tag{1}$$

(where $\Omega \subset \mathbb{R}^d$ denotes a domain and where S_u denotes the singular set of u) is one of the most basic examples of a free discontinuity problem, a problem class in which the discontinuity set of the solution is itself subject to optimization. Proposed originally by Mumford and Shah [12] as a model for image segmentation, the Mumford–Shah energy may also serve as a model problem for Griffith-type energy functionals in fracture mechanics [11].

Existence of minimizers of the Mumford–Shah functional (1) was shown in [8, 4], while in [1] a partial regularity result for minimizers was proved: The singular set S_u of any minimizer is shown to be locally a $C^{1,\alpha}$ manifold, up to an exceptional set of vanishing $(d-1)$-dimensional Hausdorff measure. Higher integrability of the gradient ∇u of minimizers and improved dimension estimates on the exceptional set were established in [7, 9].

In the planar setting $d = 2$, in [10] we prove that any minimizer u of the Mumfordi–Shah functional (1) is subject to the energy density lower bound

$$\frac{1}{r}\bigg[\int_{B_r(x_0) \setminus S_u} |\nabla u|^2 \, dx + \mathcal{H}^{d-1}(S_u \cap B_r(x_0)) \bigg] \geq 2$$

around any point $x_0 \in S_u$ and for any $0 < r < \mathrm{dist}(x_0, \partial\Omega)$. Our result improves previous estimates by De Lellis and Focardi [6] and Bucur and Luckhaus [3], who achieved the lower bound ≥ 1 for the energy density. Our new lower bound is optimal, as examples of minimizers like the crack-tip [2] or a flat interface demonstrate.

As a second main result and again in the planar setting $d = 2$, we establish a monotonicity formula for minimizers u of the Mumford–Shah energy (1): We prove that the *David–Léger entropy* [5]

$$F(r) := \frac{1}{r}\bigg[\int_{B_r(x_0) \setminus S_u} |\nabla u|^2 \, dx + \frac{1}{2}\mathcal{H}^{d-1}(S_u \cap B_r(x_0)) \bigg]$$

is subject to the monotonicity property

$$\min\{F(R), \tfrac{3}{2}\} \geq \min\{F(r), \tfrac{3}{2}\} + \int_r^R \tfrac{1}{\rho} D(\rho) \, d\rho$$

for any $x_0 \in \Omega$ and any $0 < r \leq R < \mathrm{dist}(x_0, \partial\Omega)$. Here, $D(\rho) \geq 0$ denotes a suitably defined dissipation functional.

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Formation of microstructure and occurrence of vortices in a frustrated spin system

Janusz Ginster

(joint work with Melanie Koser and Barbara Zwicknagl)

Given $\varepsilon, \alpha > 0$ and a spin field $u : \varepsilon\mathbb{Z}^2 \cap [0,1)^2 \to S^1$, we consider the following renormalized J_1-J_3 model:

$$I_\alpha(u) = -\alpha \sum_{|x-y|=\varepsilon} u(x) \cdot u(y) + \sum_{|x-y|=2\varepsilon} u(x) \cdot u(y).$$

As shown in [1], up to boundary effects, for $\alpha \in (0,4)$ the four ground states of I_α are helical spin configurations in which u rotates (clockwise or counterclockwise) with an optimal angle δ, depending on α, along the rows and columns.

The aim of this work is to investigate the emergence of patterns formed by different ground states due to incompatible boundary conditions. As a first step, it is shown in [3], by means of Γ-convergence, that after suitable renormalization the energies I_α converge as $\varepsilon, \delta \to 0$, with $\frac{\varepsilon}{\sqrt{2}\delta} \to \sigma \in (0,\infty)$, to the continuum energy

$$F_\sigma(\varphi) = \int_{(0,1)^2} \left(1 - (\partial_1\varphi)^2\right)^2 + \left(1 - (\partial_2\varphi)^2\right)^2 + \sigma^2(\partial_{11}\varphi)^2 + \sigma^2(\partial_{22}\varphi)^2 \, dx.$$

Here, $\nabla\varphi$ denotes the limit of the renormalized angular velocity fields associated with the spin configurations u.

Scaling laws for the minimal energy of functionals related to F_σ under incompatible boundary conditions (e.g., $\varphi(0,y) = (1-2\theta)y$ for $\theta \in (0,1/2)$) are proven in [2, 4, 5]. These results suggest that for small values of σ, patterns tend to form near the boundary segment $\{0\} \times (0,1)$.

The analytical techniques developed for the continuum setting can be adapted to the discrete model, leading to a partial scaling law result for $\inf_{u(0,\cdot)\equiv\text{const.}} I_\alpha$, see [3]. It is noteworthy that in the parameter regime leading to the limiting energy F_σ, so-called vortices – singularities of the discrete angular velocity field – are asymptotically excluded. In contrast, in [3] it is shown that in other parameter regimes for ε and α, minimizers of I_α under the boundary condition $u(0,\cdot) \equiv \text{const}$ necessarily develop such vortices.

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Atomistic-to-continuum convergence for quasi-static crack growth in brittle materials

Manuel Friedrich

(joint work with Joscha Seutter, Bernd Schmidt)

The passage from atomistic systems to continuum models in solid mechanics has been a thriving field of research in the last decades. The underlying idea is to bridge the microscopic description of matter with models on the continuum level by passing to the limit of vanishing interatomic distance, e.g., grounded on the variational tool of Γ-convergence. Among the vast body of literature, this approach has also been used to derive and validate continuum theories in brittle and cohesive fracture. Yet, most available results are restricted to static settings and the evolutionary nature of fracture processes has been largely neglected in this context.

The goal of the paper [3] is to study an atomistic-to-continuum limit for a model of a quasi-static crack evolution driven by time-dependent boundary conditions. We revisit a two-dimensional atomic mass spring system [4] of the form

$$E_\varepsilon(y) = \frac{\varepsilon}{2} \sum_{x,x' \in \mathrm{NN}_\varepsilon(\Omega)} W\Big(\frac{|y(x)-y(x')|}{\varepsilon}\Big),$$

where ε denotes the atomic distance, $\mathrm{NN}_\varepsilon(\Omega)$ denote the nearest-neighbour interactions in a portion of a triangle lattice contained in the reference domain Ω, and W is a classical interaction potential of Lennard–Jones-type. As shown in [4], the continuum Γ-limit is a Griffith-type functional of the form

$$E(u) = \int_\Omega \mathcal{Q}\big(\tfrac{1}{2}(\nabla u^T + \nabla u)\big)\,\mathrm{d}x + \int_{J_u} \phi(\nu_u)\,\mathrm{d}\mathcal{H}^1\,,$$

where $\mathcal{Q}$ denotes a quadratic form and ϕ is an anisotropic density depending on the normal ν_u at the jump set J_u. We consider time-dependent boundary conditions and supplement the atomistic model with a suitable irreversibility condition accounting for the breaking of atomic bonding. In a simultaneous limit of vanishing interatomic distance and discretized time step, we identify a continuum model of quasi-static crack growth in brittle fracture, in the spirit of the seminal work by Francfort and Marigo [2]. In particular, we identify a limiting pair $t \to (u(t), \Gamma(t))$, associating to each time t a displacement $u(t)$ of the reference configuration and a crack set $\Gamma(t)$, satisfying

- (a) irreversibility: $\Gamma(s)$ is contained in $\Gamma(t)$ for $0 \le s < t$.
- (b) static equilibrium: for every t the pair $(u(t), \Gamma(t))$ minimizes the energy E at time t among all admissible competitors.
- (c) nondissipativity: the derivative of the internal energy equals the power of the applied forces.

The proof of the unilateral static equilibrium relies on a careful adaptation of the jump-transfer argument by Francfort and Larsen [1] to the atomistic setting.

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Continuous symmetry breaking: a rigorous approach

Sara Daneri

(joint work with Eris Runa)

We introduce a rigorous approach to the study of the symmetry breaking and pattern formation phenomenon for isotropic functionals with local/nonlocal interactions in competition.

We consider a general class of nonlocal variational problems in general dimension in which an isotropic surface term favouring pure phases competes with an

isotropic nonlocal term with power law kernel favouring alternation between different phases.

More precisely, for $d \geq 1$, $J > 0$, $L > 0$ and $E \subset R^d$ $[0, L)^d$-periodic, let

$$\tilde{F}_{J,p,d}(E, [0, L)^d) = \frac{1}{L^d} J\mathrm{Per}(E; [0, L)^d) - \frac{1}{L^d} \int_{[0,L)^d} \int_{R^d} \Big|\chi_E(x + \zeta) - \chi_E(x)\Big| K(\zeta)\, dx\, d\zeta,$$

where $\mathrm{Per}(\cdot, [0, L)^d)$ is the classical isotropic perimeter functional relative to $[0, L)^d$ and K is an isotropic integrable kernel with p-power law decay at infinity.

If the kernel decays at infinity like a power $p > d+1$, there is a critical constant $J_c > 0$ such that for $J > J_c$, $\tilde{F}_{J,p,d} \geq 0$ and it is minimized by the trivial sets $\emptyset, R^d$, while for $J < J_c$ the trivial sets are not minimizers. The critical constant J_c is given by

$$J_c = \int_{R^d} |\zeta_1| K(\zeta)\, d\zeta, \quad \zeta_1 = \langle \zeta, e_1 \rangle.$$

Symmetry breaking and striped pattern formation was conjectured to hold for $J < J_c$, $|J - J_c| \ll 1$.

Our main result (see [1]) consists in proving such a conjecture when $p \geq d + 3$.

Close to the critical regime in which the two terms are of the same order, we give a rigorous proof of the conjectured structure of global minimizers, in the shape of domains with flat boundary (e.g. stripes or lamellae).

The natural framework in which our approach is set and developed is the one of calculus of variations and geometric measure theory.

Among others, we identify a nonlocal curvature-type quantity which is controlled by the energy functional and whose finiteness implies flatness for sufficiently regular boundaries.

The power of decay of the considered kernels at infinity, i.e. $p \geq d+3$, is related to pattern formation in synthetic antiferromagnets.

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Finite crystallization via stratification

Leonard Kreutz
(joint work with Manuel Friedrich, Ulisse Stefanelli)

We present a new technique for proving two-dimensional crystallization results in the square lattice for finite particle systems. We begin by introducing the finite crystallization problem [1] and briefly reviewing relevant results from the literature. We then describe the model under consideration, featuring configurational energies with two-body short-range interactions and three-body angular potentials that favor square-lattice bond angles. A short overview of the bond-layer

induction method – originally used to prove crystallization for the sticky-disc potential [6] – is given before presenting our new approach. In this new method, each configuration is associated with a bond graph, which is then modified by identifying chains of successive atoms. This technique, called stratification, reduces the crystallization problem to a minimization task, corresponding to a slicing proof of the isoperimetric inequality. Our approach recovers the classical crystallization result on the square lattice from the literature [4, 7] and yields a new relative crystallization result [5]. We then discuss the non-uniqueness of minimizers for these edge-isoperimetric problems and provide optimal fluctuation estimates [2] for the relative case. Depending on the interaction strength β between substrate and crystal, we either recover the classical $N^{3/4}$-law when $\beta \in \mathbb{Q}$ – which bounds the difference between minimizers by $N^{3/4}$ particles and is known from other edge-isoperimetric problems (see e.g. [3, 8]) – or, when $\beta \in \mathbb{R} \setminus \mathbb{Q}$ is algebraic, we show that minimizers differ by at most $N^{1/3}$ atoms.

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Discrete-to-continuum convergence rates for graph-based learning with singular PDEs

Leon Bungert

(joint work with Jeff Calder, Tim Roith)

In this talk we are considering the problem of semi-supervised learning using graphs. The problem can be formulated easily: Given a large but finite set of data points $\Omega_n = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$, and a small subset of labeled points $\mathcal{O} \subset \Omega_n$ with labels $g : \mathcal{O} \to \mathbb{R}$, the task is to find a function $u_n : \Omega_n \to \mathbb{R}$ which extends the labels, i.e., $u = g$ on $\mathcal{O}$. To select a reasonably "smooth" extension u_n, a common approach consists in converting the data set into a weighted graph $G_n = (\Omega_n, \omega_n)$ and defining u_n to be the solution of a (nonlinear) mean value property on $\Omega_n \setminus \mathcal{O}$ subject to the labeling condition $u = g$ in $\mathcal{O}$. Here we are considering the graph

infinity Laplace equation $\Delta_\infty^n u_n = 0$ in $\Omega_n \setminus \mathcal{O}$, where the graph infinity Laplace operator arises as singular limit of p-Laplace operators as $p \to \infty$ and is given by

$$\Delta_\infty^n u_n(x) := \max_{y \in \Omega_n} \omega_n(x,y)\,(u(y) - u(x)) + \min_{y \in \Omega_n} \omega_n(x,y)\,(u(y) - u(x))\,.$$

To understand and quantify the behavior of solutions to this semi-supervised learning model in the large data limit $n \to \infty$, we investigate its continuum limit which is the partial differential equation (PDE) $\Delta_\infty u = 0$ in $\Omega \setminus \mathcal{O}$ subject to $u = g$ in $\mathcal{O}$ and Neumann boundary conditions on $\partial\Omega \setminus \mathcal{O}$. Here Ω is an open subset of $\mathbb{R}^d$ and for the purpose of this talk we imagine Ω as being convex. Solutions have to be understood in the viscosity sense, where the so-called infinity Laplacian of a smooth function u is defined as $\Delta_\infty u(x) := \langle \nabla u(x), D^2 u(x) \nabla u(x) \rangle$.

For studying the continuum limit we first need to assume that the data set Ω_n approximates some continuum domain Ω as $n \to \infty$ and we measure the approximation quality by the Hausdorff distance $\delta_n := d_H(\Omega_n, \Omega)$. An important example is data generated as i.i.d. samples from some probability distribution supported in $\overline{\Omega}$ with positive density with respect to the Lebesgue measure in which case $\delta_n \sim \left(n^{-1} \log n\right)^{\frac{1}{d}}$ with very high probability. Another essential ingredient for the continuum limit is the construction of the edge weights ω_n where we assume that $\omega_n(x,y) = \eta\left(\varepsilon_n^{-1}|x-y|\right)$ for some non-increasing function $\eta : [0,\infty) \to [0,\infty)$ with support in $[0,1]$ and some scaling parameters $(\varepsilon_n)_{n\in\mathbb{N}}$. In this scenario we prove in [1] that without further assumptions on Ω_n and for every $\tau > 0$ we have

$$\max_{\Omega_n} |u_n - u| \leq C(\Omega, \eta, u) \left(\tau + \sqrt[3]{\frac{\delta_n}{\varepsilon_n \tau} + \frac{\varepsilon_n}{\tau^2}} \right).$$

By optimizing over τ this allows us to derive an explicit convergence rate of the solution of the graph problem to that of the continuum PDE, for all graph scalings which satisfy $\delta_n \ll \varepsilon_n \ll 1$. Even more, under the condition that the data set Ω_n is a uniform i.i.d. sequence or a Poisson point process with intensity n and for graph scalings just above the critical percolation threshold, meaning $\varepsilon_n = C(d)\left(n^{-1}\log n\right)^{\frac{1}{d}} \sim \delta_n$ with a large enough constant $C(d) > 0$ for the graph to be connected, in [2] we improve these results to

$$\max_{\Omega_n} |u_n - u| \leq C(\Omega, \eta, u) \left(\tau + \sqrt[3]{\log n \frac{\delta_n}{\sqrt{\varepsilon_n \tau^3}} + \frac{\varepsilon_n}{\tau^2}} \right).$$

Optimizing over τ again produces a rate which (up to log factors) scales like $\delta_n^{\frac{1}{9}}$. For both results the critical ingredient is to use suitable comparison principles to reduce the problem to the study of ratios of graph distance functions.

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On the Stability of Objective Structures

Bernd Schmidt
(joint work with Martin Steinbach, Augsburg)

Objective structures, introduced by James in [2], form a far reaching generalization of crystal lattices. They are given as the orbit $\mathcal{G} \cdot x_0$ of a single point $x_0 \in \mathbb{R}^n$ under the action of a discrete group $\mathcal{G}$ of isometries on $\mathbb{R}^n$. If particles are assumed to interact via suitable pair potentials, such systems model a variety of interesting systems including general crystals and lower dimensional structures such as nanotubes.

Our goal is to provide a stability analysis for these structures. While the special case of lattices has been analyzed (see, in particular, [1]), in our general case two main difficulties arise:

(A) $\mathcal{G}$ may be non-abelian,
(B) $\mathcal{G} \cdot x_0$ may not invade all of $\mathbb{R}^n$.

This is in sharp contrast to the case of lattices, where $\mathcal{G}$ is group of translations spanning all of $\mathbb{R}^n$.

In view of (A), our first result is an efficient description of the dual space $\hat{\mathcal{G}}$ which allows us to apply Fourier analysis methods. We achieve this in [3] by showing that representations of $\mathcal{G}$ can be characterized by finitely many 'wave vector domains'.

The difficulty that results from (B) is that our structures can be asymptotically of lower dimension. In particular, a full stability result is not to be expected as buckling in response to compressive loads may occur. We approach this problem by carefully choosing seminorms that measure the deviations of deformations to rigid motions, some of them only within the extended dimensions of the structure itself.

A main step of our analysis is to establish Korn type inequalities with respect to these seminorms, cf. [4]. Our main stability result in [5] then provides a characterization of the stability constants in terms of the representations of $\mathcal{G}$. We formulate it in such a way that it directly lends itself to an efficient numerical algorithm for checking stability in terms of the underlying structure and interaction potentials. We complement this by providing matching upper bounds for the energy. This, in particular, also justifies our choice of seminorms.

Finally, we apply our analysis to a carbon nanotube with non-trivial chirality. We prove stability (in a strong sense) within the tensile regime and (in a weaker sense) even at equilibrium, cf. [5].

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Nonlocal gradients in variational problems: Heterogeneous horizons and local boundary conditions

Carolin Kreisbeck
(joint work with Hidde Schönberger)

Nonlocal models offer advantages over classical ones, as they are often more accurate, more general, and require less regularity. In continuum mechanics, peridynamics is a nonlocal framework well-suited for modeling discontinuous and singular effects, such as fractures. Our focus here lies on new models of hyperelasticity, where the classical deformation gradient is replaced by a nonlocal analogue, an averaged linear approximation that accounts for interactions within a finite range called the horizon. A common issue with nonlocal models, however, is that they usually require more computational resources and present difficulties in handling boundary conditions accurately. To address this, local-to-nonlocal coupling combines both modeling approaches, often by shrinking the horizon near the boundary to ensure a seamless transition to a local description.

Following the set-up of the work in progress [2], we consider as a key object the heterogeneous nonlocal gradient of a function $u : \Omega \to \mathbb{R}^m$ with $\Omega \subset \mathbb{R}^n$ a bounded Lipschitz domain given by

$$D_{\rho(\cdot)}u(x) = \delta(x)^{-n} \int_\Omega \frac{u(y)-u(x)}{|y-x|} \otimes \frac{y-x}{|y-x|} \rho\Big(\frac{y-x}{\delta(x)}\Big)\, dy \quad \text{for } x \in \Omega;$$

here $\delta : \Omega \to (0,\infty)$ describes a space-dependent horizon with $\delta(x) \le \operatorname{dist}(x, \partial\Omega)$ and $\rho : \mathbb{R}^n \setminus \{0\} \to [0,\infty]$ is a radially symmetric kernel with constant horizon, supported in the unit ball of $\mathbb{R}^n$ and satisfying the properties of the general setting in [1]. Particularly relevant examples of such homogeneous kernels include the Riesz fractional gradient and its finite-horizon version obtained via truncation. An important observation in handling $D_{\rho(\cdot)}$ is that it corresponds to a restricted pseudo-differential operator with Hörmander symbol, which allows the use of analytical tools such as mapping properties and parametrices as almost inverses. In particular, this enables to prove a powerful translation mechanism linking heterogeneous nonlocal gradients to classical ones, see [2]. Unlike in the constant horizon case, this relation holds only up to controllable lower-order operators.

Our refined approach to nonlocal hyperelasticity gives rise to vectorial variational problems with energy functionals of the form

$$\mathcal{F}_{\rho(\cdot)}(u) = \int_\Omega f(x, D_{\rho(\cdot)}u)\, dx \qquad \text{for } u \in H_g^{\rho(\cdot),p}(\Omega;\mathbb{R}^m),$$

where $p \in (1,\infty)$ and $f : \Omega \times \mathbb{R}^n \to [0,\infty]$ is a Carathéodory function with standard growth and coercivity behavior. The naturally associated function spaces are

the heterogeneous nonlocal Sobolev spaces $H^{\rho(\cdot),p}(\Omega;\mathbb{R}^m)$, for which we develop a comprehensive theory in [2]. Besides embedding and regularity results, this includes a trace theorem showing that $H^{\rho(\cdot),p}(\Omega;\mathbb{R}^m)$ has the same traces as the standard Sobolev space $W^{1,p}(\Omega;\mathbb{R}^m)$. Thus, although nonlocal in nature, these spaces admit classical traces, allowing to prescribe Dirichlet boundary data g in the usual Sobolev trace space, i.e., $g \in W^{1-1/p,p}(\partial\Omega;\mathbb{R}^m)$. Another essential tool in this framework is a Poincaré inequality, which is also established in [2].

The existence of minimizers for variational problems involving $\mathcal{F}_{\rho(\cdot)}$ in the case of quasiconvex or polyconvex integrands f can then be obtained in view of the weak lower semicontinuity of these functionals, the proof of which exploits the aforementioned translation mechanism.

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Hidden Convexity of continuum theories of dislocations and plasticity

Amit Acharya

(joint work with Jacobo Bielak, Janusz Ginster, Udit Kouskiya, Robert Pego, Siddharth Singh, Noel Walkington, Xiaohan Zhang)

We describe a dissipative dynamical theory of dislocations leading to plasticity called Field Dislocation Mechanics. Some physical outcomes of the theory are demonstrated for a 'small deformation' ansatz within the theory. These are the potential existence of a stress threshold to the motion of a single dislocation in a translationally invariant PDE model, the existence of stacking faults, and the existence of supersonic dislocation motion in prestrained elastic strips consistent with molecular dynamics simulations [1].

We then briefly discuss a technique for constructing dual convex variational principles corresponding to general systems of physical governing equations, like Field Dislocation Mechanics [2, 3, 4]. We illustrate the scheme by computing results for the inviscid Burgers equation as a degenerate elliptic problem in space-time domains [5], traveling wave solutions like solitons, dispersive solitons, and disintegrated solitons, of a semi discrete Burgers equation [7], and elastodynamic solutions for an elastic model with a double well nonconvex elastic energy [6]. In [6], the existence of variational dual solutions to the elastostatic PDE corresponding to the Euler–Lagrange equations of the non-quasiconvex energy functional for the St.-Venant Kirchhoff material is rigorously shown.

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Replicator dynamics as the limit of Moran processes

Gianluca Orlando

(joint work with Marco Morandotti)

The *replicator equation* is the dynamical system

$$\dot{\lambda}_i = b_i(\lambda) := \lambda_i\big((A\lambda)_i - \lambda^\top A\lambda\big)\,, \quad i = 1, \dots, M\,, \quad \text{(with initial data)}, \tag{1}$$

in the unknown $\lambda\colon [0,T] \to \mathbb{R}^M$, where $A \in \mathbb{R}^{M\times M}$ is a fixed matrix of coefficients. After noticing that the $(M-1)$-simplex $\Delta^{M-1} \subset \mathbb{R}^M$ is invariant under the action of the dynamical system, one interprets (1) as a model that describes, in an averaged fashion, the typical evolution of proportions of strategies in a population. Specifically, λ_i represents the proportion of agents in a population that choose to adopt a given strategy u_i from a set of possible strategies $\mathcal{U} = \{u_1, \dots, u_M\}$. The right-hand side in the equation favours the spread of strategies that outperform the average, when expected payoffs are measured in terms of A.

In [5], we derive (1) as the large-population limit of a finite-population Markov chain that describes the choice of strategies from the point of view of individuals. This is the so-called *Moran process* [4], a discrete-time (with time step τ_k) birth-death process in a population of N_k individuals. At each time step: 1) An individual is sampled in the population to reproduce with probability proportional to the fitness of the strategy $f_i = (1 - w_k) + w_k\pi_i$, where $w_k \in (0,1)$, and π_i is the expected payoff (computed in terms of A) for adopting strategy u_i when interacting with an individual met randomly in the population; 2) An individual is sampled randomly uniformly to abandon its strategy. To derive the limit of the resulting piecewise affine random paths $t \mapsto \lambda^k(t) \in \Delta^{M-1}$ describing the proportions of strategies in the finite population, we resort to an Eulerian formulation of the process that describes the evolution of the law of the random proportions

$\Lambda_t^k = \lambda^k(t)_{\#}\mathbb{P} \in \mathcal{P}(\Delta^{M-1})$. This solves, in the distributional sense, a discrete continuity equation

$$\partial_t \Lambda_t^k + \mathrm{div}(b\Lambda_t^k) = \mathrm{error}(k)\,, \tag{2}$$

where $\mathrm{error}(k) \to 0$ as $\tau_k \to 0$ (continuous-time limit), $N_k \to +\infty$ (large-population limit), $w_k \to 0$ (weak selection regime), under a precise assumption on the relation between these three parameters. In the limit, (2) becomes precisely the Eulerian version of (1). We mention [2, 3, 1] for strictly related results.

A crucial technical step in the result concerns compactness of the paths $t \mapsto \Lambda_t^k \in \mathcal{P}(\Delta^{M-1})$ with respect to the 1-Wasserstein distance $\mathcal{W}_1$. Straightforward estimates on the discrete stochastic process do not guarantee automatically equi-continuity properties for these paths. Compactness has to be proven directly with more refined estimates that rely on the PDE (2) and following the lines of the original Arzelà–Ascoli Theorem.

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Axial symmetry of DMI-stabilized Skyrmions on the disk

Leon Happ

(joint work with Giovanni Di Fratta, Valeriy V. Slastikov)

In mathematical terms, magnetic Skyrmions (an eponym in tribute to theoretical physicist Tony Skyrme) can be viewed as local minimizers of the micromagnetic energy functional with a non-trivial topological degree (Skyrmion number)

$$\mathcal{Q}(m) := \frac{1}{4\pi}\int_D m \cdot (\partial_1 m \times \partial_2 m)\,\mathrm{d}x \in \mathbb{Z}.$$

First observed experimentally in 2009 at TU Munich [1], such structures have by now been extensively studied. It is believed that due to their size – in certain materials, Skyrmions have diameters in the nanometer-scale regime –, their topological stability, and the ability to move, create and annihilate them, they hold the key for a revolution in data storage devices, a research direction commonly referred to as spintronics (cf. [2]). In recent years, similar vortex structures have

also been detected in chiral liquid crystals, ferroelectrics and the polarization of light, making a thorough mathematical understanding of such configurations even more relevant (cf. [3], [4] and [5]).

Interestingly, there seems to be the conviction among physicists that magnetic Skyrmions are always axially symmetric, i.e., they are determined by a radial profile function, from which the whole Skyrmion can be recovered by rotating it about a perpendicular axis. For example, in [2] one reads that Skyrmions are "axisymmetric two-dimensional solitons" and "localized axisymmetric configurations of a magnetization vector". However, form a mathematical point of view, these statements have the character of a conjecture; while all components of the micromagnetic energy (see below) are axial symmetric, *a priori*, this does not exclude the possibility of symmetry breaking.

In my talk I present a recent unfinished joint work with Giovanni Di Fratta and Valeriy Slastikov that supports the abovementioned hypothesis in the sense that we prove the existence of axially symmetric local minimizers with topological degree one in the small parameter regime. To be precise, on the disk $D := B_1(0) \subset \mathbb{R}^2$ we study the energy (where $m_\perp := (m_1, m_2)$ in Cartesian coordinates)

$$\mathcal{E}(m) := \frac{1}{2}\int_D \Big\{|\nabla m|^2 - 2\kappa m_\perp \cdot \nabla m_3 + (Q-1)|m_\perp|^2\Big\}\,\mathrm{d}x,$$

with $\kappa > 0$, $Q \geq 1$, over the class $\mathcal{A} := \{m \in H^1(D;\mathbb{S}) : m = -\hat{e}_3 \text{ on } \partial D\}$, where we combine (from left to right) exchange energy with surface Dzyaloshinskii–Moriya interaction (DMI) (going back to [6, 7]) and perpendicular anisotropy. The second contribution, incorporating antisymmetric exchange effects due to spin-orbit coupling and emerging in crystalline structures lacking inversion symmetry, plays a pivotal role in the stabilization of magnetic Skyrmions (cf. [8], [2]). For want of general techniques to deduce axial symmetry of minimizers, we make the *ad hoc* axially symmetric ansatz (in polar coordinates)

$$m_0(r,\varphi) := -\sin(\theta(r))\hat{e}_r - \cos(\theta(r))\hat{e}_3$$

for an optimal profile function $\theta : [0,1] \to [0,\pi]$ with $\theta(0) = \pi, \theta(1) = 0$ uniquely determined through the corresponding Euler–Lagrange equation, and prove that this indeed constitutes a stable local minimizer of our energy functional. It is easily validated that $\mathcal{Q}(m_0) = 1$, i.e., m_0 represents a (Néel type) Skyrmion. Our main result reads as follows.

Theorem. *For $\kappa > 0$ and $Q - 1 \geq 0$ sufficiently small there exists some constant $C > 0$ and some $\varepsilon > 0$ such that for $m \in \mathcal{A}$ with $\|m - m_0\|_{H^1} < \varepsilon$ there holds*

$$\mathcal{E}(m) - \mathcal{E}(m_0) \geq C\|m - m_0\|_{H^1}^2.$$

Our findings complement a work of Li and Melcher [9], where the authors demonstrate a related statement for the whole space $\mathbb{R}^2$. Our proof relies on a Fourier decomposition of the Hessian of the energy and a fine analysis of the monotonicity of the optimal profile function, motivated by [9] and using ideas from [10] and [11].

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Dissipative Hamiltonian structure of the kinetic Fokker–Planck equation

Sangmin Park

The short talk, based on the preprint [1], concerns the kinetic Fokker–Planck equation (KFP) with the confinement potential $U : \mathbb{R}^d_x \to \mathbb{R}$ and friction $\alpha > 0$

$$\partial_t \mu_t + v \cdot \nabla_x \mu_t - \nabla_x U \cdot \nabla_v \mu_t - \alpha(\nabla_v \cdot (v\mu_t) + \Delta_v \mu_t) = 0. \tag{1}$$

The equation takes place in the phase space $\mathbb{R}^{2d} = \mathbb{R}^d_x \times \mathbb{R}^d_v$.

Let $(\mathcal{P}_2(\mathbb{R}^{2d}), W_2)$ be the 2-Wasserstein space on $\mathbb{R}^{2d}$ and let $\mathcal{H} : \mathcal{P}_2(\mathbb{R}^{2d}) \to (-\infty, +\infty]$ be the relative entropy functional with respect to the probability measure $\mu_\infty(dxdv) \propto e^{-U(x)-|v|^2/2}\, dxdv$, which is the invariant measure of (1). Then KFP (1) can be formulated as the dissipative Hamiltonian flow of $\mathcal{H}$ in the Wasserstein space in the following way:

$$\partial_t \mu_t + \nabla \cdot (\mu_t (J + S) \mathrm{grad}\mathcal{H}(\mu_t)) = 0, \text{ where } J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, S = \begin{pmatrix} 0 & 0 \\ 0 & -\alpha \end{pmatrix}. \tag{2}$$

Here, $\mathrm{grad}\mathcal{H}(\mu) \in L^2(\mu; \mathbb{R}^{2d})$ is the Wasserstein gradient of the functional $\mathcal{H}$ at $\mu \in \mathcal{P}_2(\mathbb{R}^{2d})$. Ambrosio and Gangbo [2] first rigorously studied Hamiltonian ODEs in the Wasserstein space, corresponding to $\alpha = 0$.

Motivated by the minimizing movements scheme and the symplectic Euler scheme for Hamiltonian flows in $\mathbb{R}^{2d}$, we propose the following variational scheme

for KFP: Given an initial datum $\mu_0 \in \mathcal{P}_2(\mathbb{R}^{2d})$, a time step $h > 0$, and the number of iterations $N \in \mathbb{N}$, iteratively define the discrete solutions $(\mu_{ih}^N)_{i=0}^N$ by

$$\begin{aligned} \bar{\mu}_{(i+1)h}^N &\in \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^{2d})} \frac{W_{2,v}^2(\mu_{ih}^N, \nu)}{2h} + \int_{\mathbb{R}^{2d}} \nabla U(x) \cdot v \, d\nu(x,v) + \alpha \mathcal{H}(\nu) \\ \mu_{(i+1)h}^N &\in \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^{2d})} \frac{W_{2,x}^2(\bar{\mu}_{(i+1)h}^N, \nu)}{2h} - \int_{\mathbb{R}^{2d}} v \cdot x \, d\nu(x,v). \end{aligned} \tag{3}$$

The metric $W_{2,v}$ (resp. $W_{2,x}$) is the geodesic distance induced by W_2 on the linear subspace of $\mathcal{P}_2(\mathbb{R}^d_x \times \mathbb{R}^d_v)$ with fixed x-(resp. v-)marginals (cf. Pezek and Poyato [3]); by convention $W_{2,v}(\mu,\nu) = +\infty$ when their x-marginals do not coincide.

The energy functionals in each step of the algorithm are convex along geodesics (and generalized geodesics) in the relevant metric; to our knowledge the variational scheme is the first algorithm for KFP (and more generally, the Vlasov–Fokker–Planck equation) with such geodesic-convexity properties.

A straightforward analysis using the convexity of (3) and the Euler–Lagrange equation yields the following.

Theorem (Park, '24 [1]). *Let $\nabla_x U$ be Lipschitz and $\mathcal{H}(\mu_0) < +\infty$. Then the piecewise-constant interpolation between discrete solutions $\mu_t^N = \mu_{ih_N}^N$ for $t \in [ih_N, (i+1)h_N)$ converges pointwise narrowly to the distributional solution of KFP on the time interval $[0,T]$ as $h_N = T/N \to 0$.*

The above theorem recovers the existence of a distributional solution of KFP without relying on any known results; only the uniqueness of solutions is used to obtain the convergence of the full sequence.

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Explicit minimizers of the anisotropic Riesz potential

Edoardo Giovanni Tolotti

(joint work with Maria Giovanna Mora, Luca Rondi, Lucia Scardia)

We consider the following interaction energy defined on probability measures

$$I_s^\Phi(\mu) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} \underbrace{\frac{1}{|x-y|^s} \Phi\left(\frac{x-y}{|x-y|}\right)}_{W_s(x-y)} d\mu(x)\, d\mu(y), \qquad \mu \in \mathcal{P}(\overline{E}),\ s \in (0,d).$$

Here, $\overline{E}$ is the closure of a non-degenerate ellipsoid, while $\Phi : \mathbb{S}^{d-1} \to \mathbb{R}$ is an even, positive, and continuous function describing the anisotropy of the interactions. Such functionals are the Γ-limit of the natural rescaling of discrete pairwise interaction energies. In particular, they arise in the discrete-to-continuum limit of dislocation models. We recall that a similar problem is considered in [1], where the minimization is taken over probability measures over $\mathbb{R}^d$ and a quadratic confinement term ensures compactness of their support.

The existence of minimizers is classical. Moreover, when $\Phi \equiv 1$ (namely, there is no anisotropy), and E is a ball, the minimizer is unique and it is explicitly known since the 30s (see [3]).

For a general anisotropy profile, a sufficient condition for uniqueness is that $\widehat{W}_s \geq 0$. In this case, being a minimizer is equivalent to solve the Euler–Lagrange equations associated to the problem.

The objective of the talk is to show that it is possible to characterize the unique minimizer for a broad class of anisotropies and Riesz exponents. Indeed, we show that, for any Φ such that $\widehat{W}_s \geq 0$ and $s \in [d-2, d)$, the unique minimizer of I_s^Φ is the pushforward onto E of the isotropic minimizer. In particular, the minimizer of I_s^Φ and I_s^1 coincide. This result is obtained showing that the candidate minimizer solves the Euler–Lagrange equations.

The range $s \in (0, d-2)$ behaves differently. In this case, we do not have a characterization but we show that the minimizer depends on the anisotropy. Indeed, we prove that for any exponent in this range there is an anisotropy Φ for which the minimizer of I_s^1 case does not minimize I_s^Φ.

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Competting effects in fourth-order aggregation-diffusion equations. A gradient flow perspective

Alejandro Fernández-Jiménez

(joint work with José A. Carrillo, Antonio Esposito, Carles Falcó)

We are interested into understanding cell-cell adhesion, a phenomenon responsible for tissue growth and patterning formation. The process combines the diffusion of cells with aggregation due to chemical or physical pressure (e.g. protein binding) to produce tissues. In [2], Falcó, Baker and Carrillo introduce the system

$$\begin{aligned} \partial_t \rho &= -\operatorname{div}\left(\rho \nabla \left(\kappa \Delta \rho + \alpha \Delta \eta + \beta \rho + \omega \eta\right)\right), \\ \partial_t \eta &= -\operatorname{div}\left(\eta \nabla \left(\alpha \Delta \rho + \Delta \eta + \omega \rho + \eta\right)\right) \end{aligned} \tag{1}$$

in order to understand this cell-sorting phenomena through a PDE model. The work in [2] provides the modelling perspective. Afterwards, to improve our understanding of the model we study existence in [1]. As a first step, we consider the corresponding one-species equation (with a more general local pressure) given by

$$\partial_t \rho = -\mathrm{div}(\rho \nabla(\Delta \rho)) - \chi \Delta \rho^m, \quad \text{in } (0,\infty) \times \mathbb{R}^d \tag{2}$$

where $m \geq 1$ and $\chi > 0$. We realise that (2) is the 2-Wasserstein gradient flow of

$$\mathcal{F}_m = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla \rho(x)|^2 \, \mathrm{d}x - \chi \mathcal{E}_m[\rho]$$

where $\mathcal{E}_m[\rho] = \frac{1}{m-1} \int_{\mathbb{R}^d} \rho^m$ if $m > 1$ or $\mathcal{E}_m[\rho] = \int_{\mathbb{R}^d} \rho \log \rho$ if $m = 1$. Thereby, using the Gagliardo–Nirenberg inequality we find that there exists a critical exponent $m_c := 2 + \frac{2}{d}$ governing the behaviour of (2). If $1 \leq m < m_c$ (*subcritical regime*), the free energy is bounded from below and we also have H^1 compactness in space. If $m > m_c$ (*supercritical regime*), the free energy is unbounded. If $m = m_c$ we are on the *critical regime*. In this case, there exists a parameter χ_c such that for $0 < \chi \leq \chi_c$ the free energy is bounded from below in the set of probability measures and if $0 < \chi < \chi_c$ we also have H^1 compactness. However, if $\chi > \chi_c$ the free energy is unbounded. The critical parameter χ_c is identified by the sharp constant of a suitable inequality [3]. Then, for the subcritical regime and critical regime with $0 < \chi < \chi_c$ we show existence of weak solutions via the JKO scheme.

We can extend these techniques in order to cover (1) as well. System (1) is the 2-Wasserstein gradient flow of the free energy

$$\boldsymbol{\mathcal{F}}[\rho, \eta] = \int \frac{\kappa}{2} |\nabla \rho|^2 + \frac{1}{2} |\nabla \eta|^2 + \alpha \nabla \rho \cdot \nabla \eta - \frac{\beta}{2} \rho^2 - \frac{1}{2} \eta^2 - \omega \rho \eta.$$

If $\kappa > \alpha^2$ we can prove that $\boldsymbol{\mathcal{F}}[\rho, \eta] \geq C_\rho \mathcal{F}_2[\rho] + C_\eta \mathcal{F}_2[\eta]$. Hence, we can work analogously to the one-species case. We recover that the free energy is bounded from below and we have H^1 compactness in space for ρ and η. Thus, we are able to show existence of weak solutions for (1) using the JKO scheme.

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Nonlocal analysis of energies in Micromagnetics

Rossella Giorgio
(joint work with Elisa Davoli, Giovanni Di Fratta, and Luca Lombardini)

Considering the micromagnetic energy functional

$$\int_\Omega |\nabla m|^2\,dx + \int_\Omega \mathrm{curl} m \cdot m\,dx + \int_{\mathbf{R}^3} |h_{\mathtt{d}}[m\chi_\Omega]|^2\,dx, \tag{1}$$

defined for $m \in H^1(\Omega;\mathbf{S}^2)$, where $\Omega \subset \mathbf{R}^3$ is a bounded Lipschitz domain, we study conditions under which a nonlocal analysis of micromagnetic energies can be formally justified. The energy (1) comprises the classical Dirichlet energy, an antisymmetric exchange term and the magnetostatic-self energy which is a *nonlocal* contribution determined by $h_d[m] \in L^2(\mathbf{R}^3;\mathbf{R}^3)$ such that

$$\mathrm{div}(m\chi_\Omega + h_d[m]) = 0, \quad \mathrm{curl}\, h_d[m] = 0 \text{ in } \mathbf{R}^3. \tag{2}$$

First, relying on [1], we consider a nonlocal-to-local approximation of the two exchange energy functionals

$$\int_\Omega |\nabla m|^2\,dx + \int_\Omega \mathrm{curl} m \cdot m\,dx$$

using nonlocal functionals of the form

$$\iint_{\Omega\times\Omega} \Big(\rho_\varepsilon(x-y)\frac{|m(x)-m(y)|^2}{|x-y|^2} + \frac{\nu_\varepsilon(x-y)}{|x-y|}\cdot\big(m(x)\times m(y)\big)\Big)dx\,dy,$$

with $(\rho_\varepsilon)_\varepsilon$ and $(\nu_\varepsilon)_\varepsilon$ suitable families of localizing kernels. The key points are a pointwise convergence result and a Γ-convergence argument.

After the nonlocal approximation, we neglect the antisymmetric contribution and study the existence and qualitative properties of minimizers for the simplified *nonlocal* energy

$$\iint_{\Omega\times\Omega} j(x-y)|m(x)-m(y)|^2 dx\,dy + \int_{\mathbf{R}^3} |h_{\mathtt{d}}[m\chi_\Omega]|^2 dx, \tag{3}$$

defined for $m \in L^2(\Omega;\mathbf{S}^2)$. This energy functional combines a more general nonlocal symmetric interaction with the magnetostatic self-energy satisfying (2). To obtain strong compactness, we require that j is symmetric, Lévy-integrable, and singular at the origin. Furthermore, for spherical domains, we generalize [2] by identifying critical radii R^* and R^{**} delineating distinct regimes of minimizers: for $R \le R^*$ uniform configurations are energetically preferable (*small-body regime*), while for $R \ge R^{**}$, non-uniform magnetizations become dominant (*large-body regime*). These transitions are analyzed through a nonlocal Poincaré-type inequality and explicit energy comparisons between uniform and vortex-like states.

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Viscoelasticity and Growth

Andrea Chiesa
(joint work with Ulisse Stefanelli)

We present a model for the evolution of a viscoelastic compressible solid undergoing phase change [1]. We assume that the material presents two phases, of which one grows at the expense of the other by *accretion*. In particular, the phase-transition front evolves in a *normal* direction to the accreting phase, with a growth rate depending on the deformation. This behavior may be observed in swelling in polymer gels, where the swollen phase accretes in the dry one and cause a volume increase, and in some solidification processes. The focus of the modelization is on describing the interplay between mechanical deformation and accretion. On the one hand, the two phases are assumed to have a different mechanical response, having an effect on the viscoelastic evolution of the medium. On the other hand, the time-dependent mechanical deformation is assumed to influence the growth process. The mechanical and phase evolutions are thus fully coupled.

The state of the system is described by the pair $(y,\theta):[0,T]\times U\to\mathbb{R}^d\times[0,\infty)$, where $T>0$ is some final time and $U\subset\mathbb{R}^d$ $(d\geq 2)$ is the reference configuration of the body. Here, y is the deformation of the medium while θ determines its phase. More precisely, for all $t\in[0,T]$ the *accreting (growing) phase* is identified as the sublevel $\Omega(t):=\{x\in U\mid\theta(x)<t\}$, whereas the *receding phase* corresponds to $U\setminus\overline{\Omega(t)}$. The deformation y satisfies the viscoelastic evolution equations

$$-\operatorname{div}\big(\partial_F W^a(\nabla y)+\partial_{\dot F}R^a(\nabla y,\nabla\dot y)-\operatorname{div}\mathrm{D}H(\nabla^2 y)\big)=f\quad\text{in}\quad\bigcup_{t\in[0,T]}\{t\}\times\Omega(t)$$

$$-\operatorname{div}\big(\partial_F W^r(\nabla y)+\partial_{\dot F}R^r(\nabla y,\nabla\dot y)-\operatorname{div}\mathrm{D}H(\nabla^2 y)\big)=f\quad\text{in}\quad\bigcup_{t\in[0,T]}\{t\}\times(U\setminus\overline{\Omega(t)})$$

and θ solves the generalized eikonal equation

$$\gamma\big(y(\theta(x),x),\nabla y(\theta(x),x)\big)|\nabla\theta(x)|=1\ \text{ in } U\setminus\overline{\Omega_0}$$

and $\theta=0$ on $\Omega(0)\subset\subset U$. We show that the coupled system above admits a weak/viscosity solution, where the viscoelastic evolution is solved weakly, whereas the growth dynamics equation in the viscosity sense. We moreover prove that solutions fulfill the energy equality, where the energetic contribution of the phase transition is characterized.

Despite the vast engineering literature on growth mechanics (see in particular [3]), to the best of our knowledge, no existence result for finite-strain accretive-growth is currently available. In the linearized case, an existence result for the model [3] has been obtained in [2].

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Propagation of chaos for multi-species moderately interacting particle systems with attractive Coulomb potentials

Shuchen Guo

(joint work with José Antonio Carrillo, Alexandra Holzinger)

We consider a class of multi-species aggregation-diffusion systems on $\mathbb{R}^d$ ($d \geq 3$):

$$\partial_t \bar{f}_\alpha = \sum_{\beta=1}^{n} \operatorname{div}(\bar{f}_\alpha \nabla V_{\alpha\beta} * \bar{f}_\beta) + \sigma_\alpha \Delta \bar{f}_\alpha, \tag{1}$$

for fixed number of species $n \in \mathbb{N}$, and for indexes of species $\alpha, \beta = 1, 2, \dots, n$, with $\bar{f}_\alpha(0) = \bar{f}_\alpha^0 \in L^1 \cap L^\infty(\mathbb{R}^d)$. The interaction potential is given by $V_{\alpha\beta} = a_{\alpha\beta} V$ with the following assumptions:

(i) the constants $a_{\alpha\beta} \in \mathbb{R}$, especially $a_{\alpha\beta} > 0$ and $a_{\alpha\beta} < 0$ corresponding to repulsive and attractive regimes between α-th and β-th species;
(ii) the potential $V(x) = 1/|x|^s$ and $0 < s \leq d-2$, which covers sub-Coulomb and Coulomb interactions.

Under the smallness condition on the initial data, we prove the global well-posedness result of (1) in the space $\bar{f}_\alpha \in L^\infty(0, T; L^1 \cap L^\infty) \cap L^2(0, T; H^1)$, $\alpha = 1, 2, \dots, n$.

The another object is the generalised moderately interacting particle dynamics:

$$\mathrm{d}X^\varepsilon_{\alpha,i}(t) = -\frac{1}{N} \sum_{\beta=1}^{n} \sum_{j=1}^{N} \nabla V^\varepsilon_{\alpha\beta}(X^\varepsilon_{\alpha,i}(t) - X^\varepsilon_{\beta,j}(t))\, \mathrm{d}t + \sqrt{2\sigma_\alpha}\, \mathrm{d}B_{\alpha,i}(t), \tag{2}$$

where the potential $V^\varepsilon_{\alpha\beta} = a_{\alpha\beta} V * \chi^\varepsilon$ with mollifier $\chi^\varepsilon(x) = \varepsilon^{-d} \chi(\varepsilon^{-1} x)$ and radially symmetric $\chi \in C_c^\infty(\mathbb{R}^d)$. There is an algebraic connection between ε and N such as $\varepsilon = N^{-\ell}$. The distribution of the particles can be described by the Liouville equation on $\mathbb{R}^{Nnd}$:

$$\partial_t f_{N,\varepsilon} = \sum_{\alpha,\beta=1}^{n} \sum_{i=1}^{N} \operatorname{div}_{x_{\alpha,i}} \Big(f_{N,\varepsilon} \frac{1}{N} \sum_{j=1}^{N} \nabla V^\varepsilon_{\alpha\beta}(x_{\alpha,i} - x_{\beta,j}) \Big) + \sum_{\alpha=1}^{n} \sum_{i=1}^{N} \sigma_\alpha \Delta_{x_{\alpha,i}} f_{N,\varepsilon}. \tag{3}$$

Our main result is to derive the aggregation-diffusion systems (1) from the stochastic interacting particle systems (2) via relative entropy method with quantitative bounds. More specifically, we show an algebraic L^1-convergence between the joint distribution (3) and the limiting PDE (1). For any n-tuples $\mathbf{K} = (K_1, \dots, K_n)$, it holds for some suitable ζ that

$$\sup_{t \in [0,T]} \big\| f^{(\mathbf{K})}_{N,\varepsilon} - \prod_{\alpha=1}^{n} \bar{f}_\alpha^{\otimes K_\alpha} \big\|_{L^1} \leq \frac{C(T)}{N^\zeta}, \quad \alpha = 1, 2, \dots, n. \tag{4}$$

In the proof, the first step is to make use of the relative entropy between the joint distribution (3) and an approximated limiting aggregation-diffusion system. A crucial argument is to show convergence in probability by a stopping time argument which is developed in [2]. To overcome the difficulty of the attractive Coulomb

case, an auxiliary function constructed in [3] has been used. The second step is to obtain a quantitative convergence rate to the limiting aggregation-diffusion system (1) from the approximated PDE system in the first step. This is shown by evaluating a combination of relative entropy and L^2-distance.

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Discrete-to-continuum limits of optimal transport with linear growth on periodic graphs

Filippo Quattrocchi

(joint work with Lorenzo Portinale)

As discovered by Jordan, Kinderlehrer, and Otto [5], one remarkable property of Wasserstein distances is that they induce geometries on spaces of measures under which some common PDEs – such as the heat equation – can be seen as *gradient flows*. To deal with evolution equations in *discrete* settings, dynamical transportation functionals [2, 6, 7] have been introduced by adapting the Benamou–Brenier formulation of Wasserstein distances [1].

Let $G = (\mathcal{X}, \mathcal{E})$ be a graph. Given a curve of measures $(m_t)_{t\in(0,1)}$ on the vertices $\mathcal{X}$, discrete vector fields $(J_t)_{t\in(0,1)} \subseteq \mathbb{R}^{\mathcal{E}}$, and a cost function F, we define the *action* $\mathcal{A}\big((m_t, J_t)_t\big) := \int_0^1 F(m_t, J_t)\,\mathrm{d}t$. The analogue of Wasserstein distances is the dynamical transportation *minimal action* functional [4]

$$\mathcal{MA}(m_0, m_1) := \inf_{(m_t,J_t)_t \in \mathcal{CE}(m_0,m_1)} \mathcal{A}\big((m_t, J_t)_t\big)\,, \qquad m_0, m_1 \in \mathcal{M}_+(\mathcal{X})\,, \tag{1}$$

where the infimum is taken among all solutions to a suitably defined *discrete continuity equation*, with $(m_t)_{t\in(0,1)}$ connecting m_0 and m_1.

The subject of this talk is the discrete-to-continuum limit of dynamical transportation functionals. One of the main results in this regard, due to Gladbach, Kopfer, Maas, and Portinale [4] establishes the Γ-convergence in the large-scale limit for periodic graphs embedded in $\mathbb{R}^d$, under an assumption of *superlinearity* for the cost function. While such an assumption includes many interesting cases, it excludes, e.g., discrete counterparts of the 1-Wasserstein distance. In a joint work with Portinale [8], we extend the aforementioned result to the case where the cost function is *asymptotically linear*.

Theorem ([8])**.** *Let $G_\epsilon = \epsilon G$ be the rescaling of a $\mathbb{Z}^d$-periodic graph G in $\mathbb{R}^d$, and let F_ϵ be an appropriate rescaling of a convex, lower semicontinuous, and* asymptotically linear *function F. Then, as $\epsilon \to 0$, the corresponding rescaled*

action functionals $\mathcal{A}_\epsilon$ Γ-converge to a functional $\mathbb{A}_{\rm hom}$ which can be expressed through a cell formula in terms of F, and $\mathcal{MA}_\epsilon$ Γ-converge to the minimal $\mathbb{A}_{\rm hom}$-action $\mathbb{MA}_{\rm hom}$ (i.e., the continuous counterpart of (1) *holds in the limit).*

Another natural question is whether the classical p-Wasserstein distances can be recovered as limits of their discrete counterparts. For $p = 2$, the answer is conditional on a geometric property of the periodic graph, cf. [3, 4]. In [8], we instead answer negatively for $p = 1$ in dimension ≥ 2. In this case, although the limit is a 1-Wasserstein distance constructed from some underlying norm on $\mathbb{R}^d$, such a norm – which depends on the graph – has a polytope as unit ball, and therefore cannot be the Euclidean norm (if $d \geq 2$).

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Finite-difference approximation of Griffith energy

Anna Kubin

(joint work with Stefano Almi, Elisa Davoli, Emanuele Tasso)

We consider a *continuous finite difference approximation* of the linearized Griffith energy. Our aim is to extend the results obtained in [3] for the Mumford–Shah functional to the vectorial framework.

Following the approach of [3], we analyze the sequence of functionals

$$\mathcal{F}_\varepsilon(u,\Omega) := \frac{1}{\varepsilon}\int_{\frac{\Omega-\Omega}{\varepsilon}} \left(\int_{\Omega\cap(\Omega-\varepsilon\xi)} \arctan\left(\frac{((u(x+\varepsilon\xi)-u(x))\cdot\xi)^2}{\varepsilon}\right) \mathrm{d}x \right) e^{-|\xi|^2} \mathrm{d}\xi \tag{1}$$

defined for measurable functions $u \in L^0(\Omega;\mathbb{R}^n)$. We prove that this sequence Γ-converges in $L^0(\Omega;\mathbb{R}^n)$ to the Griffith functional

$$\mathcal{G}(u,\Omega) = \frac{\pi^{\frac{n}{2}}}{2}\int_\Omega \left(|e(u)|^2 + \frac{1}{2}\mathrm{div}(u)^2\right)\mathrm{d}x + \frac{\pi^{\frac{n+1}{2}}}{2}\mathcal{H}^{n-1}(J_u).$$

The main challenge in analyzing (1) lies in establishing compactness for sequences u_ε with equibounded energy $\mathcal{F}_\varepsilon(u_\varepsilon)$. Compactness results in GSBD are not applicable here, as the functionals $\mathcal{F}_\varepsilon$ are defined on the space of measurable maps, without assuming any differential structure or a priori integrability. Remarkably, compactness can still be recovered via the Fréchet–Kolmogorov theorem, which reduces to proving the equicontinuity of translations. This technical step shares common ideas with [1], where the compactness result of [2] was revisited, avoiding the use of Korn- or Korn–Poincaré-type inequalities. However, due to the lack of a symmetric gradient and the additional integration over directions $\xi \in \mathbb{R}^n$ in the structure of (1), we cannot select a preferred basis to control translations, as done in [1]. Nevertheless, the fine properties of the functionals $\mathcal{F}_\varepsilon$ allow us to control translations and apply the Fréchet–Kolmogorov theorem.

The final step in the proof of compactness consists in showing that the limit function u belongs to $\mathrm{GSBD}(\Omega)$, thereby identifying the domain of the Γ-limit of $\mathcal{F}_\varepsilon$. Broadly speaking, the additional integration over directions $\xi \in \mathbb{R}^n$ in (1) leads to a limiting function space consisting of measurable vector fields that exhibit generalized bounded deformation in a "L^1-sense". Our arguments consist in deriving fine properties of the limiting space and then proving that it coincides with GSBD via an integral-geometric argument.

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Discreteness makes you think

Riccardo Cristoferi

(joint work with Marco Bonacini, Ihsan Topaloglu)

What is the effect of taking a discrete group of symmetries in a minimization problem over sets?

We consider three prototypical examples where, on the one hand, discreteness makes us re-think about tools and strategies at our disposal, and on the other hand, it shakes classical beliefs that arose when considering all possible symmetries.

The first case is that of a Riesz type of non-local energy. When maximizing it over the class of measurable sets having a fixed volume, spherical rearrangements give us that the unique (up to rigid motions) solution is given by the ball. Namely, the most symmetric object in the class of admissible competitors. Is the same true even if we restrict our attention to polygons in two dimensions? Namely, is the regular polygon the unique solution? By using a sequence of Steiner symmetrizations, in [1] we prove this claim for the case of three and four sides.

What happens when we investigate the critical points? By using a suitable class of variations, in [1] we show that, as for the continuum case, only the regular tri and four-gons are the only critical points.

How to generalize those techniques for a larger number of sides? Moreover, what happens when we move to three dimensions, where, in general, a regular polytope does not exist? What is the correct notion of 'most symmetric object' in such a case?

Finally, we consider the problem of minimizing the sum of an anisotropic perimeter and the Riesz non-local energy over sets with a fixed mass. In the case of the isotropic perimeter, for small masses, the unique minimizer is given by the ball, namely, by the Wulff shape of the perimeter term. Is it then true that the Wulff shape is the minimizer for small masses? Surprisingly, this turns out to be false for any non-constant smooth anisotropy, but true for a large class of crystalline anisotropies. This is achieved in [2] by proving a quadratic control of the non-local term with respect to the natural distance between sets.

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Upscaling an atomistic model of anti-plane near-crack-tip plasticity

Maciej Buze

(joint work with Patrick van Meurs)

In a cracked crystalline solid, near-crack-tip plasticity refers to the rearrangement of atoms in the vicinity of the crack tip due to stress concentration [1]. This process is primarily governed by the nucleation and motion of dislocations – topological defects that carry irreversible (plastic) deformation [2]. As such plasticity can inhibit further crack growth [3, 4], a precise mathematical understanding of the underlying mechanisms is essential for assessing material structural integrity.

In our work [5, 6], we formulate and study a minimal anti-plane atomistic bond-energy model that is sufficiently rich to capture interaction between a Mode III crack opening and screw dislocations.

We show that the model is well defined over a suitable class of atomistic displacements. We establish existence and non-existence results for optimal configurations accommodating dislocations at prescribed locations. We prove discrete regularity results quantifying how fast atomistic effects decay compared to the far-field leading order contributions from continuum linearised elasticity. To achieve our results, we introduce a novel geometric and functional framework of the lattice

manifold complex, in which a cracked crystal is described by a CW complex structure defined on the Riemann surface $\mathcal{S} = \{(z, w) \in \mathcal{C}^2 \mid w^2 = z\}$, thus extending the celebrated Ariza–Ortiz model [7] to a spatially inhomogeneous discrete domain.

The above results about the atomistic model allow us to we further establish a rigorous atomistic-to-continuum limit in which jointly the lattice spacing vanishes and the number of dislocations grows unboundedly. The limiting continuum interaction energy aligns with known linearised elasticity models for Mode III crack and screw dislocations interaction [4]. Finally, in the upscaled description we study the notion of the energetically optimal density of dislocations. We prove that there exists a critical value of the stress intensity factor, which is a measure of how "wide" a crack opening is, beyond which the optimal density has support bounded away from the crack, thus pointing to the formation of the so-called plastic-free zone ahead of the crack, which was reported in several TEM experiments [8, 9].

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Stochastic homogenization in micromagnetics

Lorenza D'Elia

(joint work with Elisa Davoli, Jonas Ingmanns)

Magnetic skyrmions, a small swirling vortex-like topological defects in the magnetization texture [3], have recently attracted extensive attention in many fields of research due to their potential as carriers of information for future storage devices.

In this talk, we present effective theories for composite chiral magnetic materials with a microstructure encompassing random effects. Extending [2] in stochastic framework, under the assumptions of stationarity and ergodicity, we carry out a variational analysis of a micromagnetic energy functional defined on magnetizations taking value in the unit sphere, and including both symmetric and antisymmetric exchange contributions. The latter determines the specific chirality of magnetic skyrmions.

Using the notion of quenched stochastic two-scale convergence [1, 4], we fully characterize the Gamma-limit of the micromagnetic energies. Moreover, we provide explicit formulas for the effective magnetic properties of the composite material in terms of homogenization correctors.

Eventually, we specify our analysis to the case in which the micromagnetic specimen is a multilayer with random microstructure. In particular, in this case, we present an explicit characterization of minimizers of the effective symmetric and antisymmetric exchanges. Such a characterization shows the emergence of chiral structures, providing quantitative evidence of Dzyaloshinskii's predictions on the emergence of helical structures in composite ferromagnetic materials with stochastic microstructure.

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Graphene: from point defects to tunable twins

Pilar Ariza
(joint work with F. Arca, J.P. Mendez, M. Ortiz)

Graphene has been widely investigated as a basis for post-silicon generation nanoelectronics, owing to its outstanding mechanical and electronic properties. We present an application of the theory of discrete dislocations of [1] to the analysis of topological defects in graphene [2]. We present numerical evidence that twinning operates as an accommodation and relaxation mechanism in graphene [3]. We show that twins may arise spontaneously in graphene layers containing arrays of dislocations and that twinning results in a significant reduction in energy.

Material engineering techniques such as coupling graphene layers to a hexagonal boron nitride substrate, introducing doping elements, or cutting graphene layers into narrow nanoribbons, can induce from small to medium transport gaps (0.1-0.6 eV) required for nanoelectronic applications. In addition, techniques that combine different graphene domains with varying electronic structures can open higher transport gaps. For instance, asymmetric grain boundaries and twin structures can induce transport gaps as large as 1.54 eV and 1.15 eV [4], respectively.

We show, through the use of the Landauer–Büttiker (LB) formalism and a tight-binding (TB) model, that the transport gap of twinned graphene can be tuned through the application of an uniaxial strain in the direction normal to the

twin band [5]. Remarkably, we find that the transport gap E_{gap} bears a square-root dependence on the control parameter $\epsilon_x - \epsilon_c$, where ϵ_x is the applied uniaxial strain and $\epsilon_c \sim 19\%$ is a critical strain. We interpret this dependence as evidence of criticality underlying a continuous phase transition, with $\epsilon_x - \epsilon_c$ playing the role of control parameter and the transport gap E_{gap} playing the role of order parameter.

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Macroscopic limits of systems with excluded-volume interactions

Maria Bruna

I discussed macroscopic limits of strongly interacting particles, which diverge significantly from those of weak (mean-field) or moderately interacting particles, especially in scenarios involving multiple species. These models are important for understanding many-particle systems in applications where strong excluded-volume effects and confinement are dominant. A simple model for diffusive pairwise-interacting particles at positions $X_1, \dots, X_N \in \mathbb{R}^d$, $d \geq 2$, is:

$$\mathrm{d}X_i = \sqrt{2}\,\mathrm{d}W_i - \chi_N \sum_{\substack{j=1 \\ j\neq i}}^{N} \nabla u\left(\frac{X_i - X_j}{\ell_N}\right)\mathrm{d}t$$

where W_i are N-independent Brownian motions in $\mathbb{R}^d$, $u : \mathbb{R}^d \to \mathbb{R}$ is a repulsive interaction potential, and $\chi_N, \ell_N > 0$ are the strength and range of the interaction, respectively. The mean-field scaling is $\chi_N = 1/N$ and $\ell_N = \mathcal{O}(1)$, while the strong scaling corresponds to $\chi_N = \mathcal{O}(1)$ and $\ell_N \ll 1$.

We are interested in the limit behavior as $N \to \infty$. For indistinguishable particles, the weak scaling results in the McKean–Vlasov PDE in the limit. Localizing the interaction leads to an equation

$$\partial_t \rho = \nabla \cdot [\nabla \rho + \rho \nabla \rho],$$

which coincides (up to constants) with the limit equation having taken the moderate scaling, $\chi_N = N^{\beta-1}$, $\ell_N = N^{-\beta/d}$ with $\beta \in (0, \frac{d}{d+2})$ studied in [1], or the strong scaling [2]. However, this commutativity of the limits breaks down for

multi-species or anisotropic interactions. I explore a possible connection with exclusion processes in lattice gases, where this commutability "breakdown" is better understood in the context of *non-gradient type* systems [3].

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On models for opinion formation

Marie-Therese Wolfram

(joint work with Andrew Nugent and Susana Gomes)

The development and analysis of opinion formation models has become a very active area of research in the last year with contributions from mathematics, physics, sociology, and computer science. An important class of models are agent-based models in which individuals update their opinions via binary interactions. In particular, 'bounded confidence' interactions, which were first proposed by Hegselmann and Krause in [1], capture how agents interact only with others whose opinions lie within a given confidence threshold. These type of models exhibit rich emergent behaviors including consensus and cluster formation.

This talk focuses on the development and analysis of models for opinion formation in static and dynamic (social) networks, see [2]. I will start with the classic bounded confidence models and discuss how one can include underlying network structures. Furthermore, I will touch on the respective mean-field limits – nonlinear partial differential equations, which often have a gradient flow structure.

A central theme of the presentation will be on opinion control: how can one modify the underlying network structure to steer the collective opinion towards a desired outcome or prevent consensus, see [3]. I will present controllability results and discuss various control strategies. The analytical insights will be complemented by numerical simulations that illustrate the practical implications and limitations of different control mechanisms.

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Surface tension for grain boundaries

Adriana Garroni
(joint work with Sergio Conti, Vito Crismale, Martino Fortuna, Annalisa Malusa, Emanuele Spadaro)

A sharp interface model for grain boundaries should incorporate two important features. It should be well posed in the space of configurations that represent the polycristals and should account for the lattice invariance.

A typical polycristal configuration is indeed described by an order parameter which is (essentially) piecewise constant taking values in the set of rotations (representing the orientation of the single grain). Precisely, it should be a field in $\mathrm{SBV}(\Omega;\mathrm{SO}(d))$, with gradient equal to zero.

The well posedness in this space is guaranteed by an energy of the form

$$\int_{J_A} \varphi(A^+, A^-, \nu)\, \mathcal{H}^{d-1}, \quad A \in \mathrm{SBV}(\Omega, \mathrm{SO}(d))$$

where φ is super-quadratic if $|A^+ - A^-| \sim 0$. A second feature is to require invariance under the group $\mathcal{G}$ of the symmetries of the underlying lattice. In a paper in collaboration with Fortuna and Spadaro [2], we obtain such a model in dimension 2, as the asymptotic limit of the Lauteri–Luckhaus model [1]. The result is a surface tension which satisfies the Read and Schockley law for small angle grain boundaries. Nevertheless, this derivation does not incorporate lattice invariance.

A second approximation of the Ambrosio–Tortorelli type, with a phase-field model which is defined on Sobolev fields with values in ${}^{M^{d\times d}}\!/_{\mathcal{G}}$ is obtained in collaboration with Conti, Crismale, and Malusa. This result produces a sharp interface model with the required features and find application to the image segmentation of policrystals.

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Energy concentration in a two-dimensional magnetic skyrmion model: variational analysis of lattice and continuum theories

Luca Briani
(joint work with Marco Cicalese, Leonard Kreutz)

In this talk, I am interested in models for the appearance of Skyrmions in magnetic thin films stabilised by Dzyaloshinskii–Moriya (DMI) interactions. In these models, the leading energy is as follows:

$$F_{h,\kappa}(u) = \int_{\mathbb{R}^2} |\nabla u|^p \, dx + h \int_{\mathbb{R}^2} |u - \mathbf{e}_3|^2 \, dx + \kappa \int_{\mathbb{R}^2} u \cdot \nabla \times u \, dx,$$

where the vector field $u : \mathbb{R}^2 \to \mathbb{S}^2$ represents the density of dipole moments in the material and the energy $F_{h,\kappa}$ is the energy per film thickness. The first two terms of the energy, known as Exchange interactions and the Zeeman term favor the alignment of the vector field u to a preferred background state while the third term, representing the DMI interaction, plays the role of an anti-symmetric exchange term that disfavors aligned configurations. Mathematically, a Skyrmion can be viewed as a spin configuration that locally minimizes the energy $F_{h,\kappa}$ among configurations with a fixed topological degree. Such a topological constraint introduces significant technical difficulty to the variational problem. The problem of existence of Skyrmion in a DMI-driven models was first addressed in by C. Melcher in [2].

Our analysis concerns the diverging anisotropy regime ($h \to \infty$) of the energy $F_{h,\kappa}$. We show a weak compactness result, in terms of the topological charge density of the vector field u, defined by the measure $q(u) := u \cdot (\partial_x u \times \partial_y u) \, d\mathcal{L}^n$. In particular, we characterize the structure of the weak* limit of the measures $q(u_n)$ for a sequence of energetically bounded vector fields u_n as an atomic measure with quantized coefficients. We also determine the Γ-limit of the energies in terms of the total variation of such a limit measure. Additionally, we present a lattice-type analogue of $F_{h,\kappa}$ and we define a notion of discrete topological charge for an $\mathbb{S}^2$-valued map defined on a lattice. This allows us to bridge the discrete and continuum theories. The results presented are based on the preprint [1].

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Incompleteness of the Sinclair expansion for the elastic field around the crack tip in atomistic fracture models

Julian Braun
(joint work with Maciej Buze)

The elastic field around a crack opening is known to be described by continuum linearised elasticity in leading order. In this talk, I will present the next term in a rigorous atomistic asymptotic expansion in the case of a Mode III crack in anti-plane geometry. The aim of such an expansion is twofold. First, it shows that the well-known flexible boundary condition expansion due to Sinclair is incomplete, meaning that, in principle, employing it in atomistic fracture simulations is no better than using boundary conditions from continuum linearised elasticity. And secondly, the higher order far-field expansion can be employed as a boundary condition for high-accuracy atomistic simulations. To obtain the results, I will show an asymptotic expansion of the associated lattice Green's function. In an interesting departure from the recently developed theory for spatially homogeneous cases, this includes a novel notion of a discrete geometry predictor, which accounts for the peculiar discrete geometry near the crack tip.

More explicitly, in polar coordinates the linear elastic prediction has the form

$$u_0 = Kr^{1/2}\sin(\tfrac{\theta}{2}),$$

where $K \geq 0$ is the stress intensity factor. We then prove that the next order is given by

$$u_1 = C_1(K)r^{-1/2}\sin(-\tfrac{\theta}{2}) + \frac{C_2K^3}{64}r^{-1/2}\Big(\log r \sin\tfrac{\theta}{2} + \frac{1}{6}\sin\tfrac{5\theta}{2}\Big),$$

where $C_1(K)$ is a real constant depending on K and C_2 is a real constant depending on the interatomic potential both with characterizing formulas. The first term is a Sinclair type term though classically there is no characterization of the constant C_1. However, the second term is quite different. It comes from the nonlinearity of the problem and shows the incompleteness of the Sinclair expansion.

This expansion is rigorous as we prove that for large r

$$D\bar{u} = Du_0 + Du_1 + O(r^{2-\delta})$$

for any $\delta > 0$. Here D denotes a local finite difference stencil and $\bar{u}$ is the solution of the full nonlinear, atomistic problem.

Geometric variational problems from dimension reduction algorithms in data science

Ryan Murray
(joint work with Adam Pickarski)

Dimension reduction algorithms, such as principal component analysis (PCA), multidimensional scaling (MDS), and stochastic neighbor embeddings (SNE and tSNE), are a widely used tool for data exploration, visualization, and subgroup

identification. These algorithms are typically posed as an optimization problem over a finite family of particles involving attraction and repulsion energies. While these algorithms see broad application across many scientific fields, our theoretical understanding of non-linear dimension reduction algorithms remains limited.

This talk describes recent work which builds theoretical foundations for these algorithms. In particular, we consider energies of the form

$$J(T) := \iint c(x, x', T(x), T(x'))d\mu(x)d\mu(x'),$$

where $T : \mathbb{R}^d \to \mathbb{R}^m$ with $m \ll d$. The costs we consider are of the form $c(\langle x, x'\rangle, \langle T(x), T(x')\rangle)$ or $c(\|x - x'\|^2, \|T(x) - T(x')\|^2)$, and which are convex in their second argument. Such energies cover a wide range of algorithms, such as multi-dimensional scaling and Sammon mappings, and have also been previously identified [1] in the computer science literature as a scaling limit for SNE.

This talk discusses three main results [2] pertaining to these energies: 1) The existence of relaxed minimizers, in the sense of measures on the product space as in optimal transportation; 2) First-order necessary conditions associated with any minimizer to the relaxed energy, which take the form of a parametrized, finite-dimensional optimization problem; 3) The fact that relaxed minimizers must actually be supported on the graph of a function using second-order variations. In some cases such solutions can also be demonstrated to be finitely parametrizable, and in some cases to be necessarily discontinuous on a finite number of surfaces.

We illustrate examples of numerical solutions to these problems obtained by standard libraries do not satisfy such necessary conditions, which calls for the development of new algorithms which can leverage these necessary conditions. Similar analysis in the context of the tSNE [3] and the Gromov–Wasserstein distance (in progress) is also discussed.

References

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The gradient-flow structure of the Verigin problem and its natural time discretization

Tim Laux
(joint work with Anna Kubin and Alice Marveggio)

The Verigin problem models the flow of two immiscible, compressible fluids through a porous medium. We define weak solutions described by a (mass) density ρ and a phase indicator function χ satisfying the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho u) = 0 \quad \text{in the sense of distributions,} \tag{1}$$

encoding conservation of mass, and the Gibbs–Thomson law

$$\rho u = H\nabla\chi - \nabla(\rho - c\chi) \quad \text{in the sense of distributions,} \tag{2}$$

encoding both the balance of forces on the free boundary as well as Darcy's law in the bulk. Here H denotes the mean curvature of $\partial\{\chi = 1\}$ and u the fluid velocity.

The total free energy of the system is given by $E(\rho,\chi) = \int \psi(\rho,\chi)\,d\rho + \int |\nabla\chi|$, where $\psi(\rho,\chi) = \log\rho + \frac{\chi}{\rho}(\rho - c)$. Our first observation is that (1)–(2) is the Wasserstein gradient flow of E, as suggested by the free energy dissipation

$$\frac{d}{dt}E(\rho,\chi) \le -\int |u|^2\,d\rho. \tag{3}$$

Starting from arbitrary initial conditions with finite free energy, our main result establishes the existence of distributional solutions (ρ, u) satisfying (1)–(3) and

$$\chi \in \{0,1\} \quad \rho\text{-a.e. in space-time.} \tag{4}$$

This result is obtained by the JKO scheme [1] that builds time-discrete approximations (ρ_h, χ_h) with time step size $h > 0$. Note that our problem is quasi-static in χ; *i.e.*, the metric is completely degenerate in χ-direction. This has two consequences: *(i)* Unlike in many other free boundary problems, we *unconditionally* obtain sets of finite perimeter in the limit $h \to 0$. Inspired by [3], we show that the phase boundary is an almost minimizer of the area functional and $|\nabla\chi_h| \overset{*}{\rightharpoonup} |\nabla\chi|$ as measures on space-time. Reshetnyak's continuity theorem then allows us to pass to the limit in the Euler–Lagrange equation and obtain (2). *(ii)* While it follows from a version of the Aubin–Lions lemma that ρ_h converges strongly in L^1, the compactness in time of χ_h is challenging. Nevertheless, the Kantorovich potential ϕ_h (transporting a time step to the previous one) allows us to transfer time-compactness from ρ_h to χ_h via

$$\log\rho_h - \chi_h - \phi_h = \text{const.} \quad \rho_h\text{-a.e.,} \tag{5}$$

which in turn implies (4). Indeed, we show that the nonlinear splitting $\rho \mapsto (\phi,\chi)$ into a smooth ($H^1(\rho)$) function ϕ and a pure jump function χ according to (5) is unique and stable: For any two such splittings, we show (with $p = \frac{d}{2(d-1)}$)

$$\int |\chi - \tilde\chi|\min\{\rho,\tilde\rho\} \le C\int |\rho - \tilde\rho| + C\Big(\int |\rho - \tilde\rho|\Big)^p \Big(\int |\nabla\phi|^2\,d\rho + \int |\nabla\tilde\phi|^2\,d\tilde\rho\Big)^p.$$

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