Workshop
Discrete Systems and Calculus of Variations

Institute for Advanced Study, Technical University of Munich
Organized by Marco Cicalese, Gero Friesecke, Daniel Matthes
of the TUM Department of Mathematics & SFB TRR109

Invited Speakers:
Roberto Alicandro, Università di Cassino
David Bourne, Heriot-Watt University, Edinburgh
Martin Burger, Universität Erlangen-Nürnberg
Guillaume Carlier, Université Paris IX Dauphine
Anna Dall’Acqua, Universität Ulm
Lucia De Luca, CNR Rome
Manuel Friedrich, Universität Erlangen-Nürnberg
Phan Thành Nam, Ludwig-Maximilians-Universität Munich
Tim Laux, Universität Bonn
Mark Peletier, Eindhoven University of Technology
Alessandra Pluda, Università di Pisa
Marcello Ponsiglione, Università di Roma, Sapienza
Matthias Ruf, EPFL Lausanne
Filippo Santambrogio, Université Lyon
Lucia Scardia, Heriot-Watt University, Edinburgh
André Schlichting, Universität Münster
Bernhard Schmitzer, Universität Göttingen
Ulisse Stefanelli, Universität Wien
Florian Theil, University of Warwick
Oliver Tse, Eindhoven University of Technology
Oleksandr Vlasiuk, Vanderbilt University

Junior guest speakers:
Lea Boßmann, LMU München
Giacomo Greco, Eindhoven University of Technology
Anastasiia Hraivoronska, Eindhoven University of Technology
Josua Sassen, Universität Bonn
Manuel Seitz, Universität Wien
Andrew Warren, Université Paris-Saclay
Mark Peletier: How GENERIC arises from upscaling a Hamiltonian system

In this talk, on joint work with Alexander Mielke and Johannes Zimmer, I want to explain our recent insights in how irreversibility arises out of coarse-graining reversible systems. In this context, ‘irreversibility’ means a system in GENERIC form, and ‘reversible system’ is a Hamiltonian system. The big question is how and why entropy and the Onsager operator appear.

The mathematical version of this question consists of taking a Hamiltonian system, doing some ‘coarse-graining’ and then proving that, miraculously, the irreversible parts of GENERIC appear. We study a particular example, in which many calculations can be done by hand, and in which one can trace the origins of entropy and the Onsager operator back to the Hamiltonian system. This talk will be informal, because some of the steps have not been made rigorous yet, and there still is much to be learned. But I hope it will at least be interesting.

Florian Theil: Dislocation structures and the Read-Shockley law

An interesting question is how much crystalline order is destroyed by the presence of dislocations. Analysing the Ariza-Ortiz model we can demonstrate that it accounts for the presence of temperature and grain boundaries. For small angle grain boundaries, the Read-Shockley law emerges as an upper bound. We conjecture that the corresponding lower bound holds as well.

Roberto Alicandro: Topological singularities in periodic media

I will describe the emergence of topological singularities in periodic media within the Ginzburg-Landau model, the core-radius approach and a discrete model for screw dislocations. In particular I will investigate, through a multi-scale analysis, the interaction between the oscillation period of the composite and the length scale parameter of the Ginzburg-Landau functionals.

Matthias Ruf:
Stochastic homogenization of degenerate energies under optimal assumptions

We consider spatially degenerate gradient energies with weighted p-growth in the framework of stochastic homogenization. Under optimal moment conditions on the weights, we prove Gamma-convergence to a homogenized non-degenerate integral functional. If time permits, we also discuss properties of the homogenized integrand.
Monday, 7th November continued...

Guillaume Carlier: Hewitt and Savage for finite exchangeable laws with applications to optimal transport

In this talk, based on a joint work with Gero Friesecke and Daniela Vögler, I will describe a novel representation of finite exchangeable laws in the style of the De Finetti-Hewitt-Savage with universal correlated corrections. This sheds some light on the convex geometry of the set of finite exchangeable laws and their marginals and connections with some multi-marginals optimal transport problems will be discussed.

Tuesday, 8th November

Lea Boßmann: Edgeworth expansion for the weakly interacting Bose gas

We consider the ground state and the low-energy excited states of a system of weakly interacting bosons. We derive an Edgeworth expansion for the fluctuations of bounded one-body operators around the condensate, which yields corrections to a central limit theorem. Based on joint work with Sören Petrat.

Oliver Tse:
A gradient flow structure for nonlocal transport equations with nonlinear mobility.

In this talk, I will highlight the main ideas and strategy involved in giving a class of nonlocal transport equations with nonlinear mobility a rigorous gradient flow structure via the evolutionary Gamma-convergence of a family of discrete particle approximation.

André Schlichting: Multiscale limits in gradient systems: Effective capacities emerging in two-terminal networks

Many gradient systems are tilt-independent, meaning that a change in the driving functional does not lead to a change in the dissipation potential. Such tilt independence separates the driving functional from the dissipation potential, guarantees a clear model interpretation, and leads to strong convergence concepts of gradient systems. However, many discrete and nonlocal functions are tilt dependent. We illustrate a lack of tilt-independence in a discrete setting. For a class of ‘two-terminal’ fast subnetworks, we give a complete characterization of the dependence on the tilting, which strongly resembles the classical theory of equivalent electrical networks. Joint work with Mark Peletier (TU Eindhoven).

Lucia De Luca: A variational approach to edge dislocations in the triangular lattice

We discuss discrete and continuous models for edge dislocations in the framework of plane elasticity. We focus, in particular, on the elastic energy induced by a family of edge dislocations in the triangular lattice and we study, within the rigorous formalism of Gamma-convergence, its asymptotic behaviour as the lattice spacing vanishes.
Tuesday, 8th November continued…

Giacomo Greco: Small-time limit of the Schrödinger problem: convergence of the gradients of potentials to the Brenier map

The Schrödinger problem consists in finding the most likely evolution of a system of independent particles conditionally on the observation of their initial and final configurations and it is equivalent (via Large Deviation theory) to an entropy minimization problem. After a brief introduction, we are going to show the convergence of the gradients of the Schrödinger potentials to the Brenier map in the small-time limit. The proof will rely on gradient estimates of the potentials that we establish under very mild general assumptions. Based on joint work with A. Chiarini, G. Conforti and L. Tamanini.

Oleksandr Vlasiuk: Asymptotics of optimal covering and other short-range interactions on sets of low smoothness

We first discuss a general framework for studying asymptotic properties of point configurations optimizing short-range interactions. A collection of conditions for existence of such asymptotics is introduced, involving no smoothness assumptions on the underlying set. We then focus on the best covering and maximal polarization, originating in the notion of Kolmogorov’s metric entropy. Existence of asymptotics for these functionals is derived for d-rectifiable sets and self-similar fractals. This resolves a conjecture by Graf and Luschgy, and strengthens the classical results of Kolmogorov and Tikhomirov.

Wednesday, 9th November

Tim Laux: The large-data limit of the MBO scheme for data clustering

The MBO scheme is an efficient algorithm for data clustering, the task of partitioning a given dataset into several meaningful clusters. In this talk, I will present the first rigorous analysis of this scheme in the large-data limit.

The starting point for the first part of the talk is that each iteration of the MBO scheme corresponds to one step of implicit gradient descent for the thresholding energy on the similarity graph of the dataset. It is then natural to think that outcomes of the MBO scheme are (local) minimizers of this energy. We prove that the algorithm is consistent, in the sense that these (local) minimizers converge to (local) minimizers of a suitably weighted optimal partition problem.

To study the dynamics of the scheme, we use the theory of viscosity solutions. The main ingredients are (i) a new abstract convergence result based on quantitative estimates for heat operators and (ii) the derivation of these estimates in the setting of random geometric graphs. To implement the scheme in practice, two important parameters are the number of eigenvalues for computing the heat operator and the step size of the scheme. Our results give a theoretical justification for the choice of these parameters in relation to sample size and interaction width. This is joint work with Jona Lelmi (U Bonn).
Wednesday, 9th November continued…

Andrew Warren: Basic properties of some nonlocal Wasserstein-type distances

The seminal result of Benamou and Brenier provides a characterization of the Wasserstein distance as the path of the minimal action in the space of probability measures, where paths are solutions of the continuity equation and the action is the kinetic energy. Here we consider a fundamental modification of the framework where the paths are solutions of nonlocal (jump) continuity equations and the action is a nonlocal kinetic energy. The resulting nonlocal Wasserstein distances are relevant to fractional diffusions and Wasserstein distances on graphs. We characterize the basic properties of the distance and obtain sharp conditions on the (jump) kernel specifying the nonlocal transport that determine whether the topology metrized is the weak or the strong topology. A key result of the paper are the quantitative comparisons between the nonlocal and local Wasserstein distances.

Manuel Friedrich: Finite crystallization via stratification

In this talk, I present a new technique to prove two-dimensional crystallization results in the square lattice for finite particle systems. We consider configurational energies featuring two-body short-ranged particle interactions and three-body angular potentials favoring bond-angles of the square lattice. To each configuration, we associate its bond graph which is then suitably modified by identifying chains of successive atoms. This method, called stratification, reduces the crystallization problem to a simple minimization that corresponds to a proof via slicing of the isoperimetric inequality in $l_1$. Based on joint work with Leonard Kreutz.

Marcello Ponsiglione: Crystallization and coarse graining of particles governed by pairwise interactions

In this talk I will briefly introduce the classical problem of crystallization for systems of particles governed by short range repulsive/long range attractive potentials. Then, I will focus on systems governed by power law type potentials, discussing the role played by the tail of such potentials. Finally, I will describe new crystallization problems for oriented particles, with possible applications to collective behavior.

Anastasiia Hraivoronska: A variational approach to discrete-to-continuum convergence of evolutionary equations

I will present a discrete-to-continuum limit of reversible random walks on tessellations via a variational approach. The approach relies on the so-called ‘cosh’ generalized-gradient-flow formulation of the corresponding forward Kolmogorov equation. We establish sufficient conditions on sequences of tessellations and jump intensities under which a sequence of random walks converges to a diffusion process with a possibly spatially-dependent diffusion tensor. I will also comment on applying this result to a variational convergence of a numerical approximation to the aggregation-diffusion equation.
Wednesday, 9th November continued…

David Bourne: Optimal transport and non-optimal weather

I will present an application of optimal transport theory to simplified models of large-scale rotational flows (weather). The semi-geostrophic equation is used by researchers at the UK Met Office to diagnose problems in simulations of more complicated weather models. It has also attracted a lot of attention in the applied analysis community, e.g., Alessio Figalli’s work on the semi-geostrophic equation is listed in his Fields Medal citation. In this talk I will discuss the semi-geostrophic equation in geostrophic coordinates (SG), which is a nonlocal transport equation, where the transport velocity is defined via an optimal transport problem. Using recent results from semi-discrete optimal transport theory, we give a new proof of the existence of weak solutions of the SG equations. The proof is constructive and leads to an efficient numerical method. I will conclude talk by showing some simulations of weather fronts.

This is joint work with Charlie Egan, Théo Lavier and Beatrice Pelloni (Heriot-Watt University and the Maxwell Institute for Mathematical Sciences), Mark Wilkinson (Nottingham Trent University), Steven Roper (University of Glasgow), Colin Cotter (Imperial College London) and Mike Cullen (Met Office - retired).

Thursday, 10th November

Filippo Santambrogio: Critical points in uniform quantization

I will consider the problem of approximating a given diffuse measure on a domain of $\mathbb{R}^d$ with an atomic one, with fixed number $N$ of atoms. Two variants of this problem are studied, when the masses of the atoms are free (which consists in finding an optimal Voronoi tessellation) or when they are prescribed to be equal to $1/N$ (where, instead, Laguerre cells pop up). Both problems can be attacked via an iterated algorithm originally due to Lloyd, where atoms are moved at each step to the barycenters of the corresponding cell. Despite the underlying optimization problem being non-convex, this converges in practice to reasonable solutions.

The goal of the talk is to suggest some reasons why this happens, studying properties of critical points and of stable critical points in the case of the uniform weights $1/N$. The results that I will present are obtained in various works in collaboration with Q. Mérigot, with our former student C. Sarrazin, and with A. Figalli.

Lucia Scardia: Minimisers of anisotropic Coulomb energies in 3d

Nonlocal energies are continuum models for large systems of particles with long-range interactions. Under the assumption that the interaction potential is radially symmetric, several authors have investigated qualitative properties of energy minimisers. But what can be said in the case of anisotropic kernels?

I will present some results and partial answers in this direction obtained in a long-standing collaboration with Maria Giovanna Mora and Luca Rondi, and with Jose’ Antonio Carrillo, Joan Mateu and Joan Verdera.
Bernhard Schmitzer: 
**Entropic transfer operators for data-driven analysis of dynamical systems**

The transfer operator is an elegant way to capture the behavior of a (stochastic) dynamical system as a linear operator. Spectral analysis can then in principle reveal (almost) invariant measures, cyclical behavior, as well as separation of the dynamics into different time scales. In practice this analysis can rarely be done analytically, due to the complexity of the operator or since it may not be known in closed form. A central objective is therefore to numerically approximate this operator (or its ajoint: the Koopman operator) or to estimate it from data. In this talk we introduce a new estimation method based on entropic optimal transport and show convergence to a smoothed version of the original operator as more data becomes available. This involves an interplay between three different length scales: the discretization scale given by the data, the blur scale introduced by entropic transport, and the spatial scale of eigenfunctions of the operator.


Alessandra Pluda: **Steiner problem, global and local minimizers of the length functional**

The Steiner problem, in its classical formulation, is to find the 1-dimensional connected set in the plane with minimal length that contains a finite collection of points. Although existence and regularity of minimizers is well known, in general finding explicitly a solution is extremely challenging, even numerically. A possible tool to validate the minimality of a certain candidate is the notion of calibrations.

In this talk I will introduce the different definitions of calibrations for the Steiner problem available in the literature, I will give examples of existence and non-existence of calibrations and I will show how one can easily get information on both global and local minimizers.

Manuel Seitz: 
**Discrete-to-continuum linearization of gradient flows in atomistic systems.**

Although there is a vast literature on static discrete-to-continuum results in various flavors, the evolutive case is fairly underexplored. In this talk we take a step towards a dynamic theory by considering atomistic-to-continuum linearization of gradient flows. This can be viewed as the evolutive counterpart to the discrete-to-continuum linearization result of Schmidt [Netw. Heterog. Media, 4 (2009), no. 4].

More precisely, we show that solutions of the $L^2$-gradient flow problem with respect to the atomistic energy converge to the $L^2$-gradient flow of the linear elastic energy as the interatomic distance tends to zero. The proof is based on a variational evolution approach, inspired by Sandier and Serfaty [Comm. Pure Appl. Math. 57 (2004), no. 12]. Here, the main difficulty is to prove lower-semicontinuity of the norm of the $L^2$-gradients.

This is a joint work with Manuel Friedrich (FAU Erlangen) and Ulisse Stefanelli (U. Vienna).
Thursday, 10th November continued...

Anna Dall’Acqua: Elastic Flow with modulated Stiffness

On planar closed curves with fixed prescribed length, we consider a bending energy that depends on an additional density variable. The aim is to study the associated $L^2$-gradient flow. Using the fact that we are in the plane, we can use the tangent angle to reconstruct the curve. By this approach the flow equation is a parabolic system of second order with suitable Lagrange multipliers. These are needed to impose, on one side, the condition that the curves remain closed during the evolution, and, on the other, that the length as well as the total mass are kept fixed along the flow.

We discuss global existence of solutions, qualitative properties and asymptotic behavior. This is joint work with Gaspard Jankowiak, Leonie Langer and Fabian Rupp.

Friday, 11th November

Ulisse Stefanelli: Angle-rigid configurations in $\mathbb{Z}^2$

Assessing the stability of discrete structures calls for investigating the strict minimality of point sets with respect to configurational energies. We focus on two- and three-body interactions and characterize stable configurations as those which cannot be deformed without changing distances between first neighbors or angles formed by pairs of first neighbors. Such configurations are called angle-rigid.

After recalling some related concepts in graph theory, we tackle the case of finite configurations in $\mathbb{Z}^2$, seen as planar three-dimensional point sets. A sufficient condition preventing angle-rigidity is presented. This condition is also proved to be necessary when restricted to specific subclasses of configurations.


Josua Sassen: A Stochastic Bilevel Problem for Elastic Shape Optimization

In this talk, we will translate a bilevel stochastic optimization approach, as used in economy-driven decision-making, to a mechanical shape optimization problem. In this mechanical setting, the leader decides on an optimal material distribution on a thin elastic object to minimize a tracking-type cost functional, while the follower chooses forces from an admissible set to maximize a compliance objective. The material distribution is stochastically perturbed in a construction phase between the two decisions.

To model this, we consider pessimistic bilevel stochastic programs in which the follower maximizes over a compact convex set a strictly convex quadratic function, whose Hessian stems from linearized elasticity and depends on the leader’s decision. The resulting random variable is evaluated by a convex risk measure, which is minimized in the final stochastic bilevel problem. Through extensive computational results, we will illustrate the bilevel optimization concept and demonstrate the effect of the interplay of follower and leader in shape design. Furthermore, we will discuss some theoretical results on the existence of optimal solutions under various assumptions on the model.
Friday, 11\textsuperscript{th} November continued….

**Phan Thành Nam: Correlation energy of electrons in mean-field regime**

The correlation energy of high-density Jellium is expected to be given by the Gell-Mann–Brueckner formula $c_1 \rho \log(\rho)+c_2 \rho$. We will discuss an analogue of this formula in the mean-field regime and derive a rigorous upper bound by variational method. The talk is based on joint work with Martin Ravn Christiansen and Christian Hainzl.

**Martin Burger: Kinetic Models for Processes on Dynamic Networks**

In this talk we discuss the derivation of kinetic and subsequent macroscopic equations for processes related to processes on dynamic networks. We consider in particular the case when networks are co-evolving during other processes and discuss suitable descriptions as well as issues to derive simple closure relations. We further discuss the variational implications of certain closure relations for gradient flows.