Gero Friesecke: Crystallization and discrete differential geometry
Project: B08

Why do atoms typically self-assemble into crystalline order at low temperature? This deep question remains extremely poorly understood from a mathematical stand-point. Closely related, equally poorly understood, problems include:

- sphere packing (recent progress was made in dimensions 24 and 8, but not 3)
- the celebrated Abrikosov vortex lattice in Bose-Einstein condensates
- Wigner crystallization in the homogeneous electron gas
- self-assembly of viruses from their coat proteins.

My goal in this talk is two-fold: (1) to give a general introduction to crystallization problems, (2) to discuss recent progress for a basic model problem, minimization of the Heitmann-Radin energy in 2D. The ground state for any finite number of particles was shown by Heitmann and Radin to be a subset of the triangular lattice, via clever but very technical ad hoc arguments. Recently [1] this result was understood in a novel way via discrete differential geometry, by endowing the bond graph of general particle configurations with the ''right'' notion of discrete curvature and appealing to a recent discrete Gauss-Bonnet theorem by Knill which relates the sum/integral of curvature to defects and appears to be extremely promising for future work on understanding defects and their cores in crystals in a non-phenomenological way.

[1] L. De Luca, G. Friesecke, Crystallization in two dimensions and a discrete Gauss-Bonnet theorem, J Nonlinear Sci. 28, 69-90, 2018
[2] L. De Luca, G. Friesecke, Classification of Particle Numbers with Unique Heitmann-Radin Minimizer, J. Stat. Phys. 167, Issue 6, 1586–1592, 2017

Mats Vermeeren: Discretization of contact Hamiltonian systems using Herglotz' variational principle
Project: B02

Classical Hamiltonian mechanics can be generalized by building it on contact geometry instead of symplectic geometry. An important class of mechanical systems that have a contact structure are those with linear friction, but contact Hamiltonian systems have much wider applications, for example in thermodynamics and integrable systems. Just like their symplectic counterparts, contact Hamiltonian systems satisfy a variational principle, which was found by Gustav Herglotz. We use this variational principle to develop structure-preserving discretizations of contact Hamiltonian systems. This is joint work with Alessandro Bravetti (CIMAT, Mexico) and Marcello Seri (University of Groningen, Netherlands).

Olga Graf: Analog-to-digital conversion on a circle
Project: C02

Manifold models in data analysis and signal processing have become more prominent in recent years. In this talk, we will look at one of the main tasks of modern signal processing, namely, at analog-to-digital (A/D) conversion in connection with a simple manifold model (circle). We will focus on Sigma-Delta modulation which is a popular method for A/D conversion of bandlimited signals that employs coarse quantization coupled with oversampling. Classical Sigma-Delta schemes provide mismatches and large errors at the initialization point if the signal to be converted is defined on a closed manifold. Our results show how to design an update for the first and second order schemes on a circle based on the reconstruction error analysis such that for the updated scheme the reconstruction error is improved. An application of such A/D conversion schemes - digital halftoning on a closed surface - is discussed.

Ulrich Bauer & Oliver Junge: Identifying cycling motion using cohomology
Project presentation: B13

The aim of the new project B12 is to construct a coarse model of the global behaviour of a given dynamical system. This model will abstract from individual trajectories and rather provide coarse dynamical information in form of a directed graph or a Markov chain. In contrast to existing approaches, our model will incorporate information about cycling motion, generalizing the classic notion of periodic or quasiperiodic dynamics. The basic idea of our construction is to combine cohomological information about some invariant set with dynamical information either from an underlying model or from time series data.

Jan Techter: Incircular nets and mutually diagonal nets on quadrics
Project: A02

Incircular nets are defined as two sequences of lines in the plane with the combinatorics of the square grid such that each elementary quadrilateral admits an incircle. Incircular nets are closely related to systems of confocal conics as well as their discrete counterparts. We introduce several generalizations of these types of nets:

1. Canonical parametrizations of systems of confocal quadrics in space lead to non-planar analogs of incircular nets on individual quadrics together with a family of isometric deformations.
2. Octahedral grids of planes admitting touching cones at every vertex may be seen as spatial extensions as well as spatial generalization of incircular nets and are related to systems of confocal quadrics in Minkowski space.
3. Incircular nets in the hyperbolic and elliptic plane.

Albert Chern: Reflectionless Boundary Condition with Discrete Complex Analysis
Project: A5, C7

Seeking reflectionless boundary conditions for wave equations has been a non-trivial problem in numerical PDEs. The method of perfectly matched layer (PML) is regarded as the state-of-the-art approach. A PML is a wave-absorbing layer attached to the boundary designed so ideally that the interface produces no reflection wave. Mathematically, PML equations are viewed as alternate realizations of the analytic continuation of the wave equation. However, it had been believed that numerical reflections are inevitable in discretized PML equations due to discretization error. In this work we adopt the linear discrete complex analysis and replicate the PML theory in the discrete setup. The discovered discrete PML becomes the first truly reflectionless boundary treatment for the discrete wave equation.

Arseniy Tsiypenyuk: Variational Approach to Fourier Phase Retrieval
Project: B08

We introduce a space-and-time continuous gradient flow for phase retrieval whose time discretization yields the celebrated error reduction (ER) algorithm [J.R.Fienup, Phase retrieval algorithms: a comparison, Appl. Opt. 21, 2758-2769,1982]. We prove global existence of weak solutions to this flow, and show that a single explicit Euler timestep of size \Delta t = 1 recovers precisely the ER algorithm. Moreover, we give numerical examples of stationary points of the flow which fail to be fixed points of the ER algorithm, and show that the fixed points of ER correspond to stationary points of the flow satisfying certain extra conditions. A related interpretation of the more complicated hybrid-input-output (HIO) algorithm is indicated on a formal level.
Joint work with Gero Friesecke.

Hana Kourimska: A new discrete Gaussian curvature and discrete uniformization theorem
Project: A01

The uniformisation theorem states that any closed oriented Riemannian surface is conformally equivalent to one with constant Gaussian curvature. In my talk I introduce a discretisation of this theorem for polyhedral surfaces. The key contribution is the introduction of a new formula for discrete Gaussian curvature.

Michael Strobel: Non-Standard Analysis in Dynamic Projective Geometry
Project: Z02

In the talk we demonstrate the integration of non-standard analysis into projective geometry. Especially, we will analyze the properties of a projective space over a non-Archimedean field. One major application of the developed theory is the automatic removal of singularities in dynamic geometric constructions. Furthermore, we will give fast (infinitesimal) discretization methods that allow the removal of such singularities in real time.

Marco Cicalese & Barbara Zwicknagl:

Project presentation: B11

Abhishek Rathod: Fast and simple algorithms for minimum cycle basis and minimum homology basis.

Project: C04

We study the problem of finding a minimum homology basis, that is, a shortest set of cycles that generates the 1-dimensional homology classes with Z_2 coefficients in a given simplicial complex K. This problem has been extensively studied in the last few years. For general complexes, the current best deterministic algorithm, by Dey et al., runs in O(N^\omega + N^2 g) time, where N denotes the number of simplices in K, g denotes the rank of the 1 homology group of K, and \omega denotes the exponent of matrix multiplication. Dey et al. also designed a randomized 2-approximation algorithm for the same problem that runs in O(N^\omega \sqrt{N \log N}) expected time. In this paper, we present two simple randomized algorithms that computes the minimum homology basis of a general simplicial complex K. The first algorithm runs in \tilde{O (m^\omega) time, where m denotes the number of edges in K, whereas the second algorithm runs in O(N m^{\omega-1}) time.
We also study the problem of finding a minimum cycle bases in an undirected graph G with n vertices and m edges. The best known algorithm for this problem runs in O(m^\omega) time. Our algorithm, which is much simpler, but slightly more expensive, runs in \tilde{O}(m^\omega) time.

Ulrich Pinkall: Discretizing fluids into filaments and sheets

Project presentation: C07

Project C07 is about generating high-level ("discretized") descriptions of velocity fields as a collection of vortex rings. C07 is not a new project but its orientation has broadened and will now include reconstruction of vortex rings from video capture (using deep learning techniques) and applications to simulating the Magnetohydrodynamics of solar flares.

Carsten Lange: Presentation A03