SFB TRR109 – Discretization in Geometry and Dynamics
DGD Days 2023

18th – 22nd September 2023 in the Science and Study Center, Raitenhaslach

Talks and Abstracts

Tuesday, 19th September:

Jaume Alonso: Kahan-Hirota-Kimura discretisations and a 3D generalisation of QRT

The well-known QRT maps are a family of integrable birational maps in two dimensions that preserve a pencil of biquadratic curves. In this work we generalise them to three-dimensional maps preserving two pencils of quadrics. As in the original case, under the presence of a certain linear symmetry, we can define the so-called QRT roots, in this case of degree five. We also give certain geometric conditions under which they become of degree three. An application of this construction is the correction of Kahan-Hirota-Kimura discretisations of integrable continuous maps. These discretisations are also of degree three, but they do not always preserve the original number of conserved quantities, which in this case is two. An interesting example is the Zhukovski-Volterra gyrostat, whose KHK discretisation is integrable when two of the non-linear parameters are zero, but not when only one of them vanishes. Using our QRT root construction, we manage to correct the discretisation and make it integrable.
This is a joint work with Yuri Suris and Kangning Wei.

Felix Dellinger: Discrete Orthogonal Structures

In this talk we introduce a definition for orthogonal quadrilateral nets based on equal diagonal length in every quad. This definition can be motivated through Ivory's Theorem and rhombic bi-nets. We find that non-trivial orthogonal multi-nets exist, i.e. nets where the orthogonality condition holds for every combinatorial rectangle and present a method to construct them.
The orthogonality condition is well suited for numerical optimization. Since the definition does not depend on planar quadrilaterals it can be paired with common discretizations of conjugate nets, asymptotic nets, geodesic nets, Chebyshev nets or principal symmetric nets. This gives a way to numerically compute prinicipal nets, minimal surfaces, developable surfaces and cmc-surfaces

Daniel Cremers: Self-supervised Learning for 3D Shape Analysis

While neural networks have swept the field of computer vision and are replacing classical methods in many areas of image analysis and beyond, extending their power to the domain of 3D shape analysis remains an important open challenge. In my presentation, I will focus on the problems of shape matching, correspondence estimation and shape interpolation and develop suitable deep learning approaches to tackle these challenges. In particular, I will focus on the difficult problem of computing correspondence and interpolation for pairs of shapes from different classes -- say a human and a horse -- where traditional isometry assumptions no longer hold.
This work was done in collaboration with Marvin Eisenberger, Aysim Toker and Laura Leal-Taixé.

Tuesday continued…

Nina Smeenk: Discrete Constant Mean Curvature Surfaces in $\mathbb{R}^{2, 1}$ and Hyperbolic Orthogonal Ring Patterns

Smooth and discrete constant mean curvature surfaces and minimal surfaces have been extensively studied in various space forms. In $\mathbb{R}^3$ they are known to admit a geometrically nice discretization in terms of S-isothermic surfaces. Their discrete Gauss maps are closely related to spherical orthogonal ring and circle patterns respectively. In this talk we will consider the analogue discrete S-iosthmeric cmc surfaces in $\mathbb{R}^{2, 1}$ and their relation to hyperbolic orthogonal ring pattern. We will discuss the main similarities and differences to the Euclidean case and their effects on the construction of such surfaces.

Niklas Affolter: TCD maps

A TCD map is a map from a triple crossing diagram to projective space, satisfying an incidence requirement. We introduce projective invariants and dynamics TCD maps. The invariants allow for several existence and uniqueness theorems. We explain how the invariants relate to cluster algebras, and how dynamics relate to mutation in cluster algebra theory. Conveniently, TCD maps include as special cases a large number of known maps, including Q-nets, Line complexes, Darboux maps, Desargues maps, dSKP lattices, t-embeddings, T-graphs, the pentagram map, integrable cross-ratio systems and others. Additionally, via cluster algebra theory we obtain two subvarieties of the projective invariants: the resistor and the Ising subvariety. These two subvarieties allow a systematic explanation of the occurrences of dBKP and dCKP reductions in the literature.

Hector Andrade Loarca: PoissonNet: Resolution-Agnostic 3D Shape Reconstruction using Fourier Neural Operators

PoissonNet provides an innovative approach to 3D shape reconstruction from points. Unlike conventional neural networks that struggle with high-resolution 3D data, PoissonNet uses Fourier Neural Operators (FNOs) to transform point clouds into meshes. It trains effectively on low-resolution data, but shines in high-resolution scenarios, outperforming other models in quality. Our approach is further strengthened by a theoretical foundation on Poisson surface reconstruction using the Fourier Neural Operator.

Wednesday, 20th September

Oliver Junge: Entropic transfer operators

We propose a new concept for the regularization and discretization of transfer operators in dynamical systems. Our approach is based on the entropically regularized optimal transport between two probability measures. In particular, we use optimal transport plans in order to construct a finite-dimensional approximation of some transfer operator which can be analysed computationally. We show that the spectrum of the discretized operator converges to the one of the regularized original operators. We analyse the relation between the discretized and the original peripheral spectrum for a rotation map on the n-torus. Finally, we report on corresponding numerical experiments, including one based on the raw trajectory data of a small biomolecule from which its dominant conformations are recovered.

Wednesday continued…

Viktoria Ehm: Geometrically Consistent Partial Shape Matching

Finding correspondences between 3D shapes is a crucial problem in computer vision and graphics, which is for example relevant for tasks like shape interpolation, pose transfer, or texture transfer. An often neglected but essential property of matchings is geometric consistency, which means that neighboring triangles in one shape are consistently matched to neighboring triangles in the other shape. Moreover, in practice one often has only access to partial observations of a 3D shape (e.g. due to occlusion, or scanning artifacts). In my presentation I show how to integrate state-of-the-art shape features into a novel integer linear programming partial shape matching formulation that ensures geometric consistency.

Jan Techter: Geometry and consistency of principal binets

In several classical examples discrete surfaces naturally arise as pairs consisting of combinatorially dual nets describing the "same" discrete surface. These examples include Koebe polyhedra, orthogonal circle patterns, orthogonal ring patterns, and discrete confocal quadrics. Motivated by this observation we introduce a discretization of parametrized surfaces via binets, which are maps from the vertices and faces of $\Z^2$ into $\R^3$. More specifically, we consider principal binets, which are binets with planar faces and orthogonal dual edges. They admit a natural discrete Gauss map and lifts to Möbius geometry, Laguerre geometry, and Lie geometry. For the multi-dimensional consistency, we consider binets on the vertices and faces of $\Z^N$, $N>2$.

David Hien: Topological Signatures for Analyzing Oscillations in Time Series

Nonlinear dynamical systems often exhibit rich and complicated recurrent dynamics. Understanding these dynamics is challenging, especially in higher dimensions where visualization is limited. Additionally, in many applications, time series data is all that is available. This motivates our TDA-based approach to study such systems. More precisely, we introduce the cycling signature which is constructed by taking persistent homology of time series segments in a suitable ambient space. Oscillations in a time series can then be identified by analyzing the cycling signatures of its segments. We demonstrate this through several examples. In particular, we identify and analyze 6 oscillations in a 4d system of ordinary differential equations.

Lukas Mayrhofer: Shape-driven simulation of protein self-assembly in 2D

Protein self-assembly is a large-scale process that cannot be replicated using all-atom molecular dynamics simulations. We develop a coarse-grained model with the goal of simulating this process for the tobacco mosaic virus, where the coat proteins self-assemble into a helical shell. In this talk, we provide a 2D proof-of-concept.

We base our approach on the premise that the geometric shape of the protein drives the solvation. Our model for the free solvation energy favors volume-minimizing structures while constraining the interpenetration of shapes. In particular, it allows for fast energy evaluation of large structures. A stochastic descent method drives the simulation by minimizing the energy (mainly using hybrid Monte Carlo). We simulate the dynamics of identical copies of an asymmetric 2D model shape, which robustly self-assemble into a unique final state. Our numerical experiments show that this self-assembly process is sensitive to parameters and shape modifications.

Wednesday continued…

Hana Dal Poz Kourimska: Homotopy reconstruction in the Euclidean space and Riemannian manifolds

Can we infer the topology of a set if we are only given a partial geometric information about it? Under which conditions is such inference possible? Niyogi, Smale, and Weinberger showed that, given a C^2 manifold of positive reach embedded in the Euclidean space and a sufficiently dense point sample on — or near — the manifold, the union of balls of certain radii centered on the point sample captures the homotopy type of the manifold. Their work has quickly gained recognition in the computational geometry society, since the homotopy groups of the aforementioned union of balls are easy to calculate.
We have expanded this seminal work in several directions. Instead of a C^2 manifold, we consider general closed sets of positive reach, and establish tight bounds on the quality of the sample, that guarantee a successful reconstruction. We achieve the same result for closed sets of positive reach embedded not only in the Euclidean space, but in any Riemannian manifold. In this case, we compare the manifold to spaces of constant curvature, and our bounds depend on the curvature of these spaces.

Thursday, 21st September:

Ivan Spirandelli*:* Exotic self-assembly of hard spheres in a morphometric solvent

The self-assembly of spheres into geometric structures, under various theoretical conditions, offers valuable insights into complex self-assembly processes in soft systems. The morphometric approach to solvation free energy that we utilize here is a geometry-based theory that incorporates a weighted combination of geometric measures over the solvent accessible surface for solute configurations in a solvent. In this talk, I will demonstrate that employing the morphometric measure of solvation free energy in simulating the self-assembly of sphere clusters results, under most conditions, in maximum contact clusters. Under other conditions, it unveils an assortment of extraordinary sphere configurations, such as double helices and rhombohedra. This establishes a foundation for comprehending the diverse range of geometric forms in self-assembled structures, emphasizing the significance of the morphometric approach in this context.

Fabian Roll: Applied Topology: From Gromov Hyperbolicity to Algebraic Gradient Flows on Geometric Complexes

I will discuss some recent results on the interplay between discrete Morse theory and persistent homology, in the setting of geometric complexes. This concerns constructions like Rips, Čech, Delaunay, and Wrap complexes, which are fundamental constructions in topological data analysis. In particular, I will explain how a modification of a classical result by Rips and Gromov from geometric group theory helps to speed up the computation of the Rips persistent homology arising from viral evolution data. Moreover, I will explain how one can relate optimal representative cycles for persistent homology to the industry-tested Wrap surface reconstruction algorithm. Joint work with Ulrich Bauer (TUM).

Carl Lutz: Decorated Discrete Conformal Equivalence

We discuss a notion of discrete conformal equivalence for decorated piecewise euclidean surfaces (PE-surface), that is, PE-surfaces with a choice of circle about each vertex. It is closely related to inversive distance and hyperideal circle patterns. We present the corresponding discrete uniformization theorem.
This is joint work with A. Bobenko.

Thursday continued…

Camilla Brizzi: h-Wasserstein barycenter: some steps toward Monge's ansatz

During my talk I will briefly present the multi-marginal optimal transport problem, showing the connection, in case of Coulomb cost, with the Wigner crystallization conjecture, which can be thought as a Monge OT problem, and emphasizing the difficulties. I will then present the multi-marginal OT problem of the h-Wasserstein barycenter, as a generalization of the more known 2-Wasserstein barycenter. I will conclude mentioning the results toward the proof of Monge's ansatz, obtained together with G. Friesecke and T. Ried, providing some sketch of the proof.

Alessandro Lupoli: Quantization of Bandlimited Functions on the 2D-Torus

The study of quantization techniques for bandlimited functions has become increasingly important both for the results obtainable in some engineering applications (A/D converters, Digital Halftoning, Imaging), and for some Machine Learning and Deep Learning applications. The main issue is highlighted when trying to apply these algorithms to functions defined on closed manifolds, as cuts need to be introduced to apply them, and the schemes will typically not yield good reconstruction along the cuts.
This talk will explore the problem of quantization and reconstruction of a bandlimited signal on the 2D torus, highlighting how changing the sampling scheme can avoid the presence of artifacts generated by Sigma-Delta schemes. This is joint work with Professor Felix Krahmer.

Friday, 22nd September:

Andrea Kubin: On volume-preserving crystalline mean curvature flow in two dimension, discrete and continuous analysis

In this talk I will discuss some recent results on the crystalline area preserving mean curvature flow. In particular we will show that, under area constraint, the Algrem-Taylor-Wang scheme, starting from a given rectangle converges to a flat flow. We have analyzed these results in the Euclidean plane and in the square lattice. These results are in collaboration with M. Cicalese.

Kangning Wei: Computing Degree Growth of Birational Maps from Local Indices of Polynomials

One of the most important dynamical invariants associated to a birational map f is given by its dynamical degree, or equivalently, its algebraic entropy, which is defined via the rate of growth of the sequence $deg(f^n)$. More concretely, the degrees $deg(f^n)$. although not birationally invariant by themselves, are also of great interests in understanding the dynamics of the birational map. We propose a general method for computing the degrees $deg(f^n)$. More precisely, given a homogeneous polynomial P, we compute the iterated pullbacks of the polynomial by the map f. To do this, we perform a sequence of blowing ups and to each blowing up we associate a local index to a polynomial P. Together with the degree $deg(f^n)$, these local indices satisfy a recurrence relation which can be solved to obtain the degrees $deg(f^n)$. In two dimensional cases, we show that these indices are closely related to the intersection numbers. In principle however, this method is applicable to birational maps in any dimension.

Jannik Steinmeier: Discrete (constrained) elastic curves as invariants of Bäcklund transformations

Many flows of a discrete curve can be discretized by sequences of Bäcklund transformations. An example is the discrete smoke ring flow. We introduce an algorithm for the construction of discrete curves which stay rigid under such discrete flows. We take a closer look at the cases of two and three Bäcklund transformations which allow for the construction of elastic rods and planar constrained elastic curves respectively. We discuss their geometric properties and compare them to their smooth counterparts.