STRUCTURES | NEWS

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

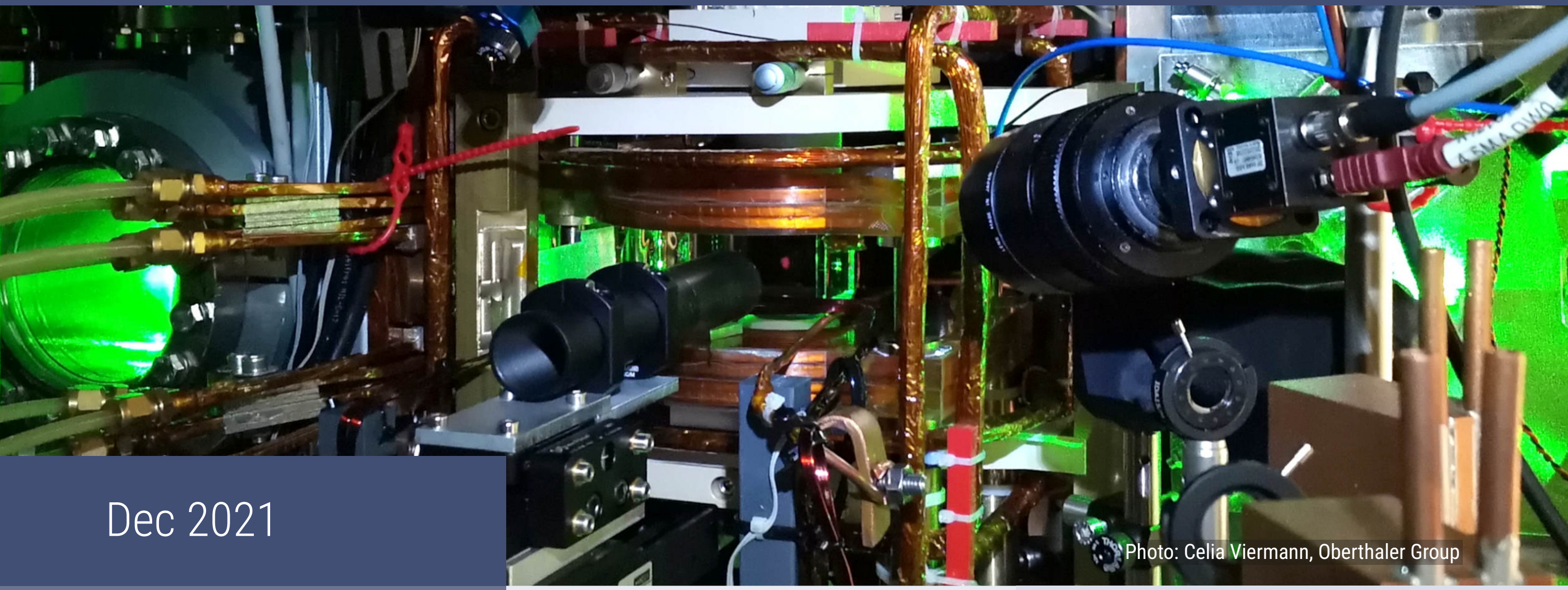
Photo: Celia Viermann, Oberthaler Group

Dec 2021

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Upcoming

Jour Fixe:
- Jan 21: Anna Erzberger, EMBL
- Jan 28: Fabian Hahner, MI

Public Talks & Workshops:
- TBA: Herlinde Koelbl: Postponed to 2022.
- Dec & Jan: Eva Wolfangel (Nature Marsilius Visiting Professorship): Science Communication Workshops

General Assembly:
Feb 04: Next General Assembly

More Information can be found on the STRUCTURES website.

Happy Holidays!

Dear members,

At the end of the year, we would like to thank all of you for the good and fruitful cooperation. It is great to see the commitment and enthusiam of our long term members and our new STRUCTURES professors and scientists. We have been very happy to welcome them in Heidelberg, and they have started their collaboration with us at full speed. Next year, we will be welcoming our External Advisory Board Members in Heidelberg on June 21st. We are looking forward to discuss research results and future directions with them.

🎄 **Top image:** The Christmas colors green and red can also be found in this ultra-cold atom experiment (BECK machine, Oberthaler group). It creates a two-dimensional Bose-Einstein condensate of potassium-39 at temperatures of 100nK, one of the coldest known spots in the universe. Spot the cloud!

Many thanks to all of you who contribute to STRUCTURES in many different ways! May you and your loved ones stay healthy and have a good start into the new year 2022. We wish you a Merry Christmas and for the new year health, happiness and success to everyone!

With Season's greetings,

Anna Wienhard, Manfred Salmhofer and Markus Oberthaler

New STRUCTURES Speaker: Markus Oberthaler


Markus Oberthaler(KIP)

The General Assembly has elected Markus Oberthaler (KIP) as new spokesperson of STRUCTURES. He follows Ralf Klessen (ITA / ZAH), who decided to resign as spokesperson and steering board member due to personal reasons. We thank Ralf Klessen for years of dedication and efforts for STRUCTURES, and we are happy to keep Ralf as an active member and speaker of CP1. We wish Markus, to whom STRUCTURES has always been a matter to the heart, all the best in his new position and are looking forward to further great years with him, Manfred and Anna as spokespersons.


Ralf Klessen (ITA / ZAH)

In the steering board, Cornelis Dullemond (ITA / ZAH) will take over the freed position. We are happy to welcome him as a new board member and wish him all the best for his new position!

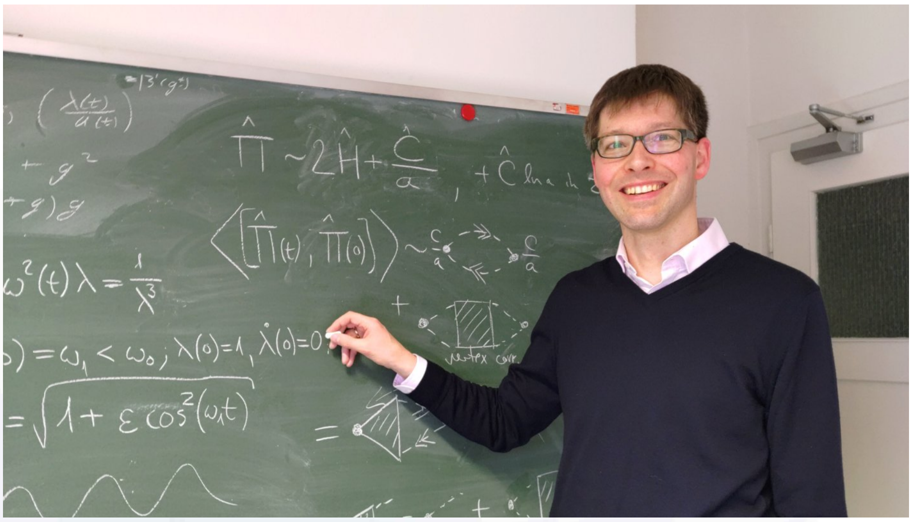

Cornelis Dullemond (ITA / ZAH)

MEMBER INTERVIEWS

STRUCTURES Asks: Tilman Enss

In our newsletters, we regularly present interviews with the faculty members of STRUCTURES to give you the opportunity to get to know them a little better. For this edition, we interviewed Tilman Enss. He is Professor for Theoretical Physics, and his office is located at the top of the Philosophenweg.

Tilman Enss is member of CP4 “Quantum Structure and Dynamics” and actively engaged in three exploratory projects: EP 2.3 “Universality on Network Structures from Quantum Dynamics to Big Data”, EP 5.2 “Structure formation in driven Bose-Fermi mixtures” and EP 5.5 “Critical behaviour of epidemic models on distinct network topologies and applications to the study of brain disease”.



Tilman Enss is professor for Theoretical Physics at ITP. (Photo: Sara Konrad / STRUCTURES Office)

What are you working on? My group focuses on many-body theory, dynamics and transport in strongly correlated quantum systems, and our research ranges from ultracold atomic gases to superconductors and quantum wires. We are interested in the collective behaviour of strongly correlated quantum particles. This topic builds on a range of attractive theories and offers a multitude of versatile research directions.

Is there a central equation of your scientific career or an equation of the week? The equations of the functional renormalisation group (fRG) have been part of my work for many years now. Recently, I was intrigued by the Ermakov equation:

$$\frac{d^2x}{dt^2} + \omega^2(t)x = \frac{1}{x^3}.$$

This nonlinear differential equation describes the expansion of a scale invariant fluid. If the curvature of the confining potential changes in time as $\omega^2(t)$, the solution $x(t)$ predicts the size of the fluid. In a cold atom experiment in Selim Jochim’s group we found deviations from this prediction and thus observed a quantum scale anomaly [PA Murthy et al., Science 365, 268 (2019)].

What do you like best about your job? My job offers the opportunity to set my own priorities and to follow what I am interested in with a flexible work schedule. I like working on my own as well as doing research in collaboration with colleagues from different scientific fields. In addition, it is wonderfully appealing to be in contact with young scientists during the lectures and within my group. It is very fascinating to see their fresh ideas and technical sophistication. Being located at “Philosophenweg” gives me ample opportunities to exchange with theoretical physicists. Students, Postdocs, Professors and Emeriti – we all enjoy the historical research flair combined with top-notch science on “our” hill.

Do you have any advice for young researchers on choosing their career path? I am sure that there are many different ways to find one's own career path and even diverse advice may be supportive. For me, it was central to decide on the basis of my personal interest in specific topics. That has always given me the strength and motivation I needed until my question of interest was solved. This career path is not without risk but you should never forget that you can make it.

Coffee or tea? White- or Blackboard? Mac, Linux or Windows? I choose coffee or tea depending on the occasion, I am absolutely in favour of a blackboard, and fairly relaxed in switching between different types of computers.

You have been involved in STRUCTURES from early on. What is so fascinating for you? I am impressed by the way in which STRUCTURES supports scientific dialogue and manages to act as a think tank for innovative research questions. The exploratory projects are very attractive elements for scientific interaction among scientists of different age, experience and background. In addition, the exploratory projects make it easy to invite our new STRUCTURES colleagues to participate and join our research activities. I do not want to miss the EPs.

The weekly Jour Fixe with its talks and time for discussion offers accessible introductions to new topics and methods beyond my field. I always underline the event in my calendar.

CP REPORT

From CP 6: The Role of a Coupling Block in Invertible Neural Networks

Invited guest article by Felix Draxler

Original Publication: *Felix Draxler, Jonathan Schwarz, Christoph Schnörr, Ullrich Köthe: "Characterizing The Role of A Single Coupling Layer in Affine Normalizing Flows", awarded Honorable Mention at the German Conference on Pattern Recognition (DAGM GCPR) 2020.*

Deep Affine Normalizing Flows are efficient and powerful models for high-dimensional density estimation from data and the generation of new samples [DSDB16]. They approximate an arbitrary data distribution $p(x)$ by learning an invertible mapping $T(x)$ such that given samples are mapped to normally distributed latent codes $z := T(x)$. In other words, they reshape the data density $p(x)$ to form a normal distribution $z \sim \mathcal{N}$. Upon convergence, samples from the normal distribution can be mapped to samples from the target distribution:

$$T^{-1}(z) \sim p(x).$$

While being simple to implement and fast to evaluate, affine flows appear not very expressive at first glance. They consist of invertible layers called coupling blocks. Each block leaves half of the input's dimensions untouched and subjects the other half to just parameterized translations and scalings. In practice however, coupling blocks achieve top perfomance in several challenging applications such as solving inverse problems [AKRK18], sampling from Boltzmann distributions [NOKW19] and generative classification [AMRK20].

In our work, we take a step towards closing the gap between theory and applications by dismantling the affine flow. More precisely, we analyze a single affine coupling block rigorously.

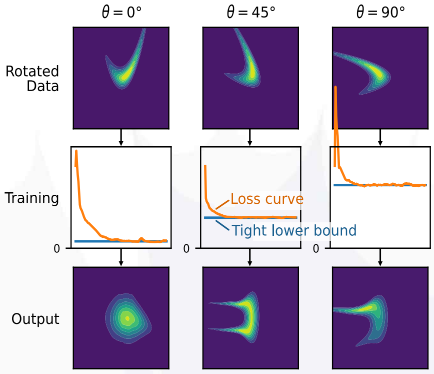


Fig. 1: An affine coupling layer pushes the input density towards standard normal. Its success depends on the rotation of the input (*top row*). We derive a lower bound for the error that is actually attained empirically (*center row, blue and orange curves*). The solution with lowest error is clearly closest to standard normal (*bottom row, left*).

We show that when trained with the maximum likelihood (ML) method, the typical information-theoretic loss for density estimation, this block learns first- and second-order moments of the conditional distribution of the changed dimensions given the unchanged dimensions.

From this insight, we derive a tight lower bound on how much a single block can reduce the loss for a given rotation of the data. This is visualized in Fig. 1 where the bound is evaluated for different rotations of the data. The lower bound allows the formulation of a layer-wise training algorithm that chooses an optimal rotation in each step. Traditionally, the rotations are drawn randomly irrespective of the data at hand.

We confirm and visualize our findings on toy datasets. Our experiments show that the rotations determined from our bound improve the speed and quality of training compared to layer-wise training with random rotations.

In the future, we hope to explain how several blocks work together when successfully approximating complicated data distributions $p(x)$.

About the Author:
Felix Draxler is a PhD Student in the Visual Learning Lab at the Heidelberg Collaboratory for Image Processing (HCI).

References:

1 [AKRK18] Lynton Ardizzone, Jakob Kruse, Carsten Rother, and Ullrich Köthe. Analyzing Inverse Problems with Invertible Neural Networks. In International Conference on Learning Representations, 2018.
2 [AMRK20] Lynton Ardizzone, Radek Mackowiak, Carsten Rother, and Ullrich Köthe. Training Normalizing Flows with the Information Bottleneck for Competitive Generative Classification. Advances in Neural Information Processing Systems, 33, 2020. arXiv: 2001.06448.
3 [DSDB16] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real nvp. arXiv preprint arXiv:1605.08803, 2016.
4 [NOKW19] Frank Noé, Simon Olsson, Jonas Köhler, and Hao Wu. Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. Science, 365(6457):eaaw1147, 2019. Publisher: American Association for the Advancement of Science.

CP6: NETWORKS & MACHINE LEARNING: MATHEMATICAL STRUCTURES

Machine learning has become a spectacularly successful tool. Its product, the 'learned machine', is an emergent structure, which is not completely understood. Research in CP6 addresses questions both of fundamental and of practical importance: How can we characterize the underlying structure of most natural data that makes their mathematical representation occupy only a tiny part of the potentially available space? How can we improve training and representation to optimize detection of structure in data on a large scale? Our research brings together expertise in network theory, image recognition, and topology, as well as input from statistical mechanics.

STRUCTURES COMMUNITY

We Are STRUCTURES

In each newsletter, we introduce three members of our Young Researchers Convent (YRC) to you via short interviews:

Louise Kluge
MSc Student, AG Kanschat, IWR; member of the E-MOSAICS Collaboration

What are you working on? In my most recent project, I worked on characterising the large-scale distribution of globular clusters in a simulation of a large cosmological volume by means of correlation functions. Globular clusters are very bright, dense star clusters which serve as our main probes of star formation in far-away galaxies.

What are you an expert for? Through my past internships, I gained expertise in working with data from radio interferometers, such as the ALMA telescope, which I used to characterise substructure in giant molecular clouds and examine the [CII] luminosity-star formation rate relation in high-redshift galaxies. With my most recent work exploring structure formation in a large-volume cosmological simulation, I am working on becoming an expert in characterising and quantifying structure of astrophysical systems and the mathematical methods behind it.

What was your greatest scientific success up to now? When working on large-scale cosmological simulations from the E-MOSAICS project, I calculated, for the first time, the two-point correlation function of globular clusters over a wide range of length scales, which is a very exciting result. With the upcoming EUCLID survey, this will actually become observable and it will be very intriguing to see how well my prediction holds.

What is your connection to STRUCTURES? Since I am a student in mathematics but also very active in astrophysics, I appreciate the interdiscplinary environment of STRUCTURES. I am most interested in the connections between structure formation on a small scale (CP2) and large-scale cosmological structures (CP1) via multiscale processes and I enjoy learning how we can study them by means of astrophysical observations, cosmological simulations and innovative methods such as topological data analysis.

Colin Davalo
PhD Student, AG Pozzetti, MI

What are you working on? I am working on deformations of discrete groups into Lie groups, and on the geometry of symmetric spaces.

What are you an expert for? I have some knowledge about some topics in geometric group theory. I am quite curious about applications that these topics could have in other fields.

How does one recognize you? I am often smiling (below the mask unfortunately), and you can often find me walking around Heidelberg on weekends.

What is your connection to STRUCTURES? Some of the geometric objects that I am interested in have a physical interpretation in the theory of supersymmetry. Another thing that I find interesting is the idea that symmetric spaces can be used to represent data efficiently.

What are you working on? I study Billiards for Sub-Riemannian manifolds. Currently I focus on the Reeb setting, where the high-momentum Sub-Riemannian flow approximates the Reeb flow, so the study of the Reeb flow reflects back to the Sub-Riemannian geodesic flow.

Lucas Dahinden
Postdoc, AG Albers, MI

What are you an expert for? In symplectic / contact geometry there is great interest in Reeb orbits on a hypersurface of contact type. My speciality, Rabinowitz-Floer homology, is a homological invariant designed to encode these orbits the same way Morse homology encodes critical points of a function.

What was your greatest scientific success up to now? I proved that bounds on topological entropy that arise from growth of Rabinowitz-Floer homology also hold for non-autonomous Reeb flows. Technically, I proved for non-autonomous Rabinowitz-Floer homology that monotone continuation morphisms are consistent with the action filtration.

How does one recognize you? If you hear whistling in the hallways of the Mathematikon, chances are it is me.

STRUCTURES ON THE WEB
https://structures.uni-heidelberg.de

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Each person depicted in the images has provided consent to the use of their pictures.

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