STRUCTURES | NEWS

STRUCTURES
CLUSTER OF
EXCELLENCE

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

Adapted from NASA/JPL-Caltech. Network overlay: Sebastian Stapelberg

July 2023

Contents

Upcoming

- **Akademische Mittagspause**
  Mo-Fr 1pm, Peterskirche, until Jul 19
- **Jul 19-23**: Roadshow “Universe on Tour – Licht aus! Sterne an!”
- **Jul 20, 21**: STRUCTURES Days
- **Aug 22-25**: Schöntal Discussion Workshop: Turbulence & Chaos
- **Oct 4,5**: Workshop HI meets AI

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STRUCTURES COMMUNITY

New STRUCTURES Professors

The STRUCTURES Cluster of Excellence welcomes two new professors:

Prof. Michela Mapelli leads the new research group *Gravitational-Wave Astrophysics* at ZAH/ITA. A leading expert on binary black hole formation, she investigates the formation of compact object binaries and plays an active role in planning the next-generation gravitational wave detector, *Einstein Telescope*. Her expertise will be valuable to the STRUCTURES cluster, where she aims to pursue new research lines and start collaborations across multiple disciplines.

Prof. Tristan Bereau is a computational physicist at ITP. Having a strong background in the development and application of molecular simulation methods, his research focuses on the intersection of machine learning and multiscale modelling. Some of the specific areas he investigates include chemical-space exploration, physics-inspired machine learning, deep backmapping and the kinetic properties of coarse-grained models, aligning perfectly with the objectives of STRUCTURES. *We wish both new members a good start and look forward to many joint projects!*

STRUCTURES ACTIVITIES

Workshop: Human Intelligence Meets Artificial Intelligence

How can Artificial Intelligence (AI) help to better understand Human Intelligence (HI)? How can we leverage deep learning models to explain HI's neural mechanisms and how can HI inspire the development of AI? The workshop *Human Intelligence Meets Artificial Intelligence*, jointly organized by *Field of Focus 4* and the *STRUCTURES Cluster of Excellence*, will bring together experts on HI and AI to discuss recent progress in these areas and stimulate novel ideas bridging both fields.

Oct 4-5, Marsilius Kolleg
Register by Sep 15

Register now! The workshop will take place from **Oct 4-5**. **Registration is open until Sep 15**. Please find more details at *structures.uni-heidelberg.de/workshop_HI_meets_AI*.

PROJECT REPORT

CP 2: The Challenge of Understanding Planet Formation

Invited article by Cornelis Dullemond (ZAH/ITA), Hubert Klahr (MPIA), Robert Strzodka (ZITI), and Matthias Bartelmann (ITP):

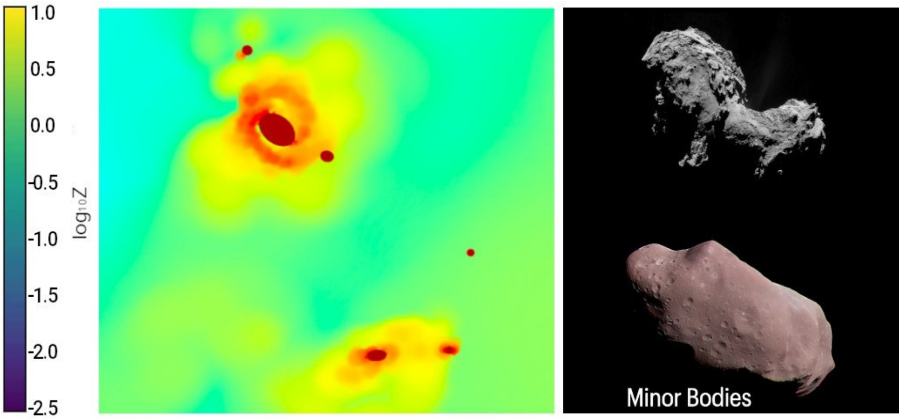

Fig 1: Synthetic planetesimals from our numerical simulations of pebble cloud collapse *(Polak and Klahr 2023)* next to examples of planetesimals known from the Solar System: comet 67P/Churyumov-Gerasimenko (*top, image credit: ESA/Rosetta/NAVCAM, CC BY-SA IGO 3.0*) and asteroid (243) Ida (*bottom, image credit: NASA/JPL*). Once these 10-100 km sized objects were abundant in the solar nebula and started the planet formation process.

We live on a rocky planet called Earth. Everything we do, all of our lives, all of our experiences take place on this planet, all within a tenuous veneer of air on its surface. It is very natural to ask: *"Why is the Earth here? How did it form?"*

Since almost 30 years, we know that the Universe is teeming with planets, both rocky and gaseous. Statistically, every star has one or more such companions. Planets are so common that one would expect their formation to be a straightforward process. In reality, however, planet formation is one of the most elusive puzzles in astronomy. We have a better understanding of how strange objects such as neutron stars are born than how an ordinary planet is formed. This has several reasons: our own Solar System is old, 4.567 billion years to be precise, and it is hard to reconstruct the very beginnings of it. Other stars, in particular young stars which are still surrounded by their *protoplanetary disk*, are very far away, so that it is hard to observe planet formation processes in these disks even if they happen right now.

But perhaps the biggest difficulty is the physics of the planet formation process itself: it starts from tiny cosmic dust particles, smaller than a micrometre, that stick together to form ever bigger dust aggregates, and ends with full-grown rocky planets of many thousands of kilometres in radius. This process covers 40 orders of magnitude in mass and involves complicated details such as the gravitational mutual interaction of billions of so-called *planetesimals* (several-kilometre-size bodies, somewhat like asteroids), the frictional mutual interaction of the gas with massive clouds of gazillions of *pebbles* (centimetre-size dust “bunnies”) – allowing for such clouds to collapse and form planetesimals – as well as the accretion of pebbles onto so-called *planetary embryos* (not-yet-fully grown planets). The overwhelmingly large number of particles involved, and their non-equilibrium dynamics, makes this a very tough problem to solve. Even though the first theories were developed in the 1950s, only in the last two decades computers and modeling codes became powerful enough to scratch the surface of this problem.

From Dust to Planets: Understanding How Complex Structures Arise

Comprehensive Project (CP) 2 aims at developing new methods, both numerical/computational and analytical, to deal with this challenge. In one sub-project, the interaction of clouds of *pebbles* with a turbulent flow is addressed using a method called *Kinetic Field Theory* (KFT), which applies techniques from theoretical physics to particle dynamics (Shi et al. 2023, in prep.) KFT, originally developed to study solids is now being successfully applied to cosmic structure formation. It provides a general theoretical framework for studying the non-equilibrium evolution of large numbers of classical particles interacting with each other. The main advantage of analytic methods like this is that limitations in particle number and spatial resolution do not apply, and that the emergence of structures can be traced back to fundamental physical processes. Applying KFT to planet formation, it has recently been possible to prove that structures will form inevitably in *protoplanetary disks* beginning on small scales and progressing to larger scales with time, whose overall properties are independent of scale. Furthermore, it was possible to show that an optimal particle size exists for which structure formation is most efficient.

The dynamics of these *pebble clouds* after the onset of cloud gravitational collapse are followed with novel computational approaches. The modified *Lagrangian gas dynamics* code *GIZMO* simulates collapsing pebble clouds until planetesimals have formed, including the phase transition from a disperse state of pebbles embedded in gas to the solid phase of comet or asteroid

COMPREHENSIVE PROJECTS

Comprehensive projects (CP) define the main research lines of STRUCTURES. They have a broad scope and address our key questions combining methods from different disciplines.

(Polak & Klahr 2023). For asteroids we found that the observed size distribution of primordial asteroids can be explained by the stochasticity of the collapse process without invoking a mass distribution for the gravitationally unstable pebble cloud. This strengthens our concept of a *Jeans mass* for planetesimal formation (Klahr & Schreiber 2020, 21). In that concept, turbulence defines a minimum mass needed for self-gravity among the pebbles to overcome turbulent diffusion.

We also found that quite often, binaries, and even *contact binaries*, are formed, similar to what is known to be common in the outer parts of the Solar System: the Kuiper belt. A famous *contact binary* in the Kuiper belt is *486958 Arrokoth*, recently visited by the *New Horizons* space mission.

A Unified Multi-Scale Description

An important focus of CP2 lies in the unification of all scales (from dust to planets) into a single modeling treatment. N-body dynamics are employed for large objects, while small dust particles are treated statistically using a Monte Carlo approach. The challenge lies in smoothly transitioning between these methods, but we have successfully overcome it, proving that our new modeling method adheres to the laws of physics even under extreme conditions (Beutel & Dullemond 2023). Furthermore, in striving for an improved computational efficiency of the method, we made advances in a small subfield of mathematics called “interval arithmetics” (Beutel & Strzodka 2023).

Original Publications:

- Polak, B. & Klahr, H. 2023. *The Astrophysical Journal*, 943(2),125. doi:10.3847/1538-4357/aca58f.
- Shi, J., Bartelmann, M., Dullemond, C. P., & Klahr, H. 2023 *in prep*.
- Klahr, H., & Schreiber, A. 2020. *The Astrophysical Journal*, 901(1), 54. doi:10.3847/1538-4357/abac58
- Klahr, H., & Schreiber, A. 2021. *The Astrophysical Journal*, 911(1), 9. doi:10.3847/1538-4357/abca9b.
- Beutel, M., & Dullemond, C. P. 2023. *Astronomy & Astrophysics*, 670, A134. doi:10.1051/0004-6361/202244955.
- Beutel, M., & Strzodka, R. 2023. *Next Generation Arithmetic*, 38–60. Springer Nature Switzerland. doi: 10.1007/978-3-031-32180-1_3.

STRUCTURES COMMUNITY

We Are STRUCTURES

In each newsletter, we introduce members of the Young Researchers Convent (YRC). For this issue, we interviewed:

Interview with Sarah Lisa Görlitz:

Sarah Lisa Görlitz
Master student, AG Tilman Enss, ITP

What are you working on?
One focus of our research is studying pattern formation in Bose-Einstein Condensates (BECs). We collaborate with the Oberthaler group to better understand real and momentum space patterns in time-periodically driven 2D BECs. I currently apply numerical methods and Floquet theory to coupled driven BECs to see if similar localization occurs there.

What are you an expert for?
I am working on becoming an expert in many-body theory, especially in the context of cold atoms. I am also working on my coding skills in Python and Mathematica.

What is your connection to STRUCTURES?
As a member of Prof Enss group, I am also part of STRUCTURES. I really enjoy the talks organized by STRUCTURES, like the CQD-Colloquium and the Jour Fixe, which give me the opportunity to learn about exciting research within and outside of my field.

What has been your greatest scientific success up to now?
Completing my BSc thesis (with Prof Masciocchi) on the initial stage of a heavy-ion collision and its impact on predicted particle yields. In October it will hopefully be my MSc thesis on pattern formation in BECs.

How does one recognize you?
If you see a physicist at Philweg 19 with reddish hair, freckles and a coffee in her hand, chances are high that it's me :).

Interview with Denis Brazke:

Denis Brazke
PhD student, AG Knüpfer / Marciniak-Czochra, IMa

What are you working on?
I primarily analyze models that describe pattern formation in biomembranes. My research explores their asymptotic and effective behaviour, as well as parameter estimation. Often, the models involve competing local and nonlocal quantities, requiring intricate analysis.

What are you an expert for?
While I wouldn't call myself an expert, I'm becoming more proficient in non-local isoperimetric problems and harmonic analysis.

What is your connection to STRUCTURES?
My PhD work aligns with CP3 and I'm part of *STRUCTURES' Outreach Committee*. In addition, I actively organize and participate in various STRUCTURES events.

What has been your greatest scientific success up to now?
Mathematically, I believe my contributions to understanding the asymptotic behaviour of a specific non-local isoperimetric problem have been significant. My PhD advisors and I quantified asymptotic behaviour even when the non-locality is not purely repulsive. I also consider my impact on students a measure of success. I take pride in communicating complex concepts easily and effectively.

How does one recognize you?
I'm quite tall, tend to talk a lot, and I'm one of the few people who doesn't drink coffee. Additionally, I have a tendency to exceed time limits when teaching (a lot).

RESEARCH SPOTLIGHT

From Space to Earth: *Uncovering the Potential Role of Meteorites in Kick-Starting Life*

An international team of researchers from *Heidelberg Initiative for the Origins of Life (HIFOL)* has made a significant breakthrough in extending our understanding of the origins of life on Earth. Their joint collaborative research between *McMaster University (Hamilton, Canada), LMU Munich* and *Heidelberg University*, under participation of *STRUCTURES* scientists, has focused on the building blocks of life known as prebiotic molecules. By studying carbonaceous chondrites – a class of meteorites – they have discovered prebiotic molecules that could have played a vital role in the formation of RNA, a critical step in the emergence of living systems.

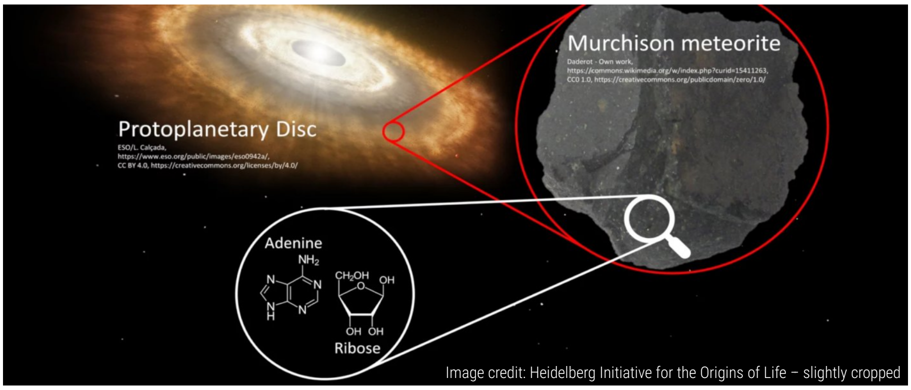

Image credit: Heidelberg Initiative for the Origins of Life – slightly cropped

The findings suggest that meteorites may have delivered these life-building blocks to our planet, bridging the gap between non-living matter and life itself. The research sheds light on the potential role of meteorite impacts as a catalyst for the emergence of life, not only on Earth but potentially beyond. The search for the origins of life on Earth is ongoing, and these new findings provide valuable insights into this ongoing scientific exploration.

RESEARCH SPOTLIGHT

Fast Exoplanet Detection with Conditional Invertible Neural Networks (cINNs)

An interdisciplinary team of scientists from STRUCTURES and University of Bern has achieved a breakthrough in characterizing the interior of exoplanets. By utilizing conditional invertible neural networks (cINNs), the team has developed a significantly faster method for inferring interior properties of exoplanets. The current approach to characterizing exoplanets relies on time-consuming Markov Chain Monte Carlo (MCMC) sampling. The novel cINN method, developed by researchers from Center of Astronomy (ZAH) in collaboration with the Interdisciplinary Center for Scientific Computing (IWR) has allowed significant speed-ups. To this aim, the researchers trained a neural network on 5.6 million internal structure models. This allowed to accurately map internal structure parameters of exoplanet K2-111b to observable features such as planetary mass, radius, and host star composition. The introduction of cINNs as an alternative to MCMC sampling presents a major advancement in exoplanet research, enabling orders of magnitude faster inference of an exoplanet's composition – driving the exploration of distant worlds further.

Original Publication:

Haldemann J., Ksoll V., Walter D., Alibert Y., Klessen R.S., Benz W., Koethe U., Ardizzone L., Rother C. 2023. *Astronomy & Astrophysics*, 672, A180. doi:10.1051/0004-6361/202243230.

ℹ CONDITIONAL INVERTIBLE NEURAL NETWORKS

Conditional invertible neural networks (cINNs) are a novel architecture developed at Heidelberg's Visual Learning Lab. They combine the benefits of invertible neural networks (INNs), which excel in solving inverse problems, with conditioning inputs. Inverse problems involve determining hidden parameters of a system from a set of measurements. In many tasks, this reverse mapping is ambiguous and challenging.

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The production of this newsletter is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy EXC 2181/1 - 390900948 (the Heidelberg STRUCTURES Excellence Cluster).

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