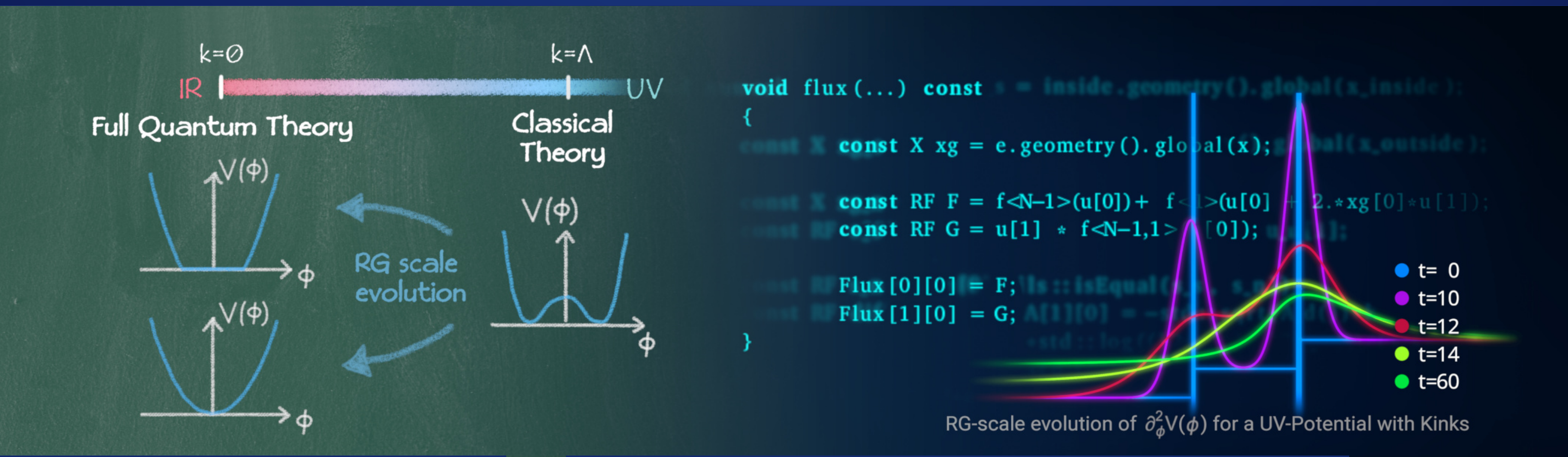
STRUCTURES | NEWS

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386



May 2024

LOCAL DISCONTINUOUS GALERKIN FOR THE FUNCTIONAL RENORMALIZATION GROUP ▸ Project Report on p.2

Contents

Upcoming

- **May 13:** RHIND Seminar on Physical Mathematics
- **May 15, 29:** CP 7 Lunch Seminar
- **May 21–24:** Chemical Compound Space Conference (CCSC2024)
- **May 22, 29:** CQD Colloquium
- **May 28:** Active Bystander Training

Connect with Us

Follow STRUCTURES on Social Media:

- @structures_hd
- @structures_heidelberg
- @STRUCTURES_HD

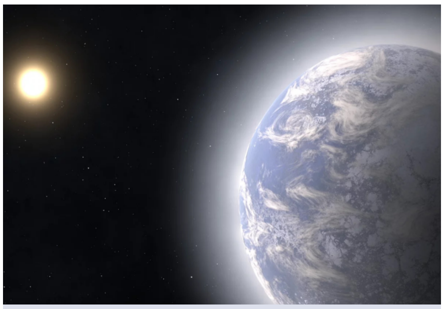
STRUCTURES BLOG:
www.structures.uni-heidelberg.de/blog

SHORT NEWS

Sub-Neptune Migration Solves Exoplanet Puzzle

A German-Swiss team of astronomers including STRUCTURES researchers Thomas Henning *(Director of Max Planck Institute for Astronomy, MPIA)* and Remo Burn *(Postdoc, MPIA)* has uncovered evidence for how the enigmatic gap in the size distribution of exoplanets at around two Earth radii emerges – a longstanding problem in exoplanetary research.

Their computer simulations demonstrate that the migration of icy, so-called *sub-Neptunes* into the inner regions of their planetary systems could account for this phenomenon. Ordinarily, planets in evolved planetary systems, such as the Solar System, follow stable orbits around their central star. However, many indications suggest that some planets might depart from their birthplaces during their early evolution by migrating inward or outward. As they draw closer to the central star, evaporating water ice forms an atmosphere that makes the planets appear larger than in their frozen state. Simultaneously, smaller rocky planets gradually lose a portion of their original gaseous envelope, causing their measured radius to shrink over time. The authors reported their findings in Nature Astronomy.



Artistic representation of an exoplanet whose water ice is vaporizing and forming an atmosphere during its approach to a star. © Thomas Müller (MPIA)

EXPLORATORY PROJECTS

This research is partly funded by STRUCTURES' Exploratory Project EP 8.4: *"Planet Formation Retrieval using Invertible Neural Networks."*

Exploratory Projects (EPs) are a crucial element of innovation in the STRUCTURES cluster. They provide a flexible platform to propose and explore novel ideas & techniques, to foster new connections or even links to other areas of academia. With a biannual call for EPs, the cluster has funded over 60 projects to date, driving forward new directions in research.

Original Publication:

Burn, R., Mordasini, C., Mishra, L. *et al. Nat. Astron.* 8, 463–471 (2024). doi:10.1038/s41550-023-02183-7.

PROJECT REPORT

Local Discontinuous Galerkin for the Functional Renormalization Group

Invited summary by Friederike Ihssen (ITP; joint work with Jan M. Pawlowski, Franz Sattler and Nicolas Wink [1])

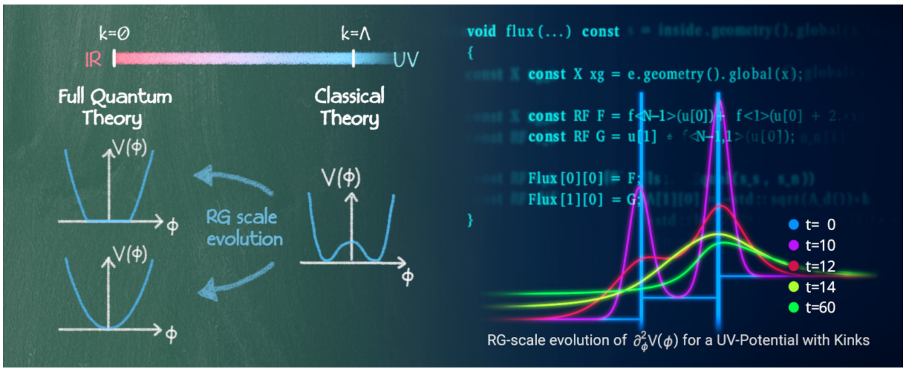
Renormalization Group (RG) methods [2] are a powerful tool to monitor the successive emergence of underlying physics and mechanisms in a given theory along a coarse-graining scale trajectory. The *functional Renormalization Group (fRG)* is a modern implementation thereof, which provides a quantitative approach to studying *phase structures* or *universal scaling properties*, i.e. the identical critical behaviour of different physical systems, in theories with *competing order effects*. However, the RG is by no means restricted to the physics of phase transitions, but by now is a fully developed non-perturbative tool for resolving all aspects of quantum field theories – from long-distance low-energy properties of *Quantum Chromodynamics* or Condensed Matter systems on one hand, and on the other, search for viable *ultraviolet completions* in *Quantum Gravity* or (beyond) *Standard Model* physics [3].

To better understand the work process of a fRG computation, we consider a theory of a single-component real scalar field $\phi \in \mathbb{R}$, drawing the analogy to the *Ising model* from statistical mechanics – a magnetic system of interacting spins arranged on a lattice. Our central quantity of interest is the *quantum effective action* $\Gamma[\phi]$, which can be thought of as the *Gibbs free energy* and used to obtain observables, such as the minimum ϕ_0 of the effective potential

$$V(\phi) = \frac{\Gamma[\phi]}{\mathcal{V}_d}, \quad \text{with} \quad \partial_\phi V(\phi)|_{\phi=\phi_0} = 0,$$

where $\mathcal{V}_d$ is the d-dimensional volume and $\phi(x) = \phi$ is some constant field configuration. The latter can be thought of as a mean field value over the entirety of spins. Then, the minimum ϕ_0 would be the expectation value of the mean magnetization $\langle M \rangle = \phi_0$.

The fRG provides us with a tool to interpolate between a classical and a full quantum theory. Initially, we start with a classical action defined at a high energy scale Λ:



$$S[\phi] = \int d^d x \left[\tfrac{1}{2}(\partial_\mu \phi)^2 + V_{\text{cl}}(\phi)\right] + \Delta S_\Lambda,$$

with a classical potential V_{cl}. Quantum fluctuations are suppressed for momentum scales $|p| < k$, where k is the RG scale, by introducing an artificial mass term ΔS_Λ. During the interpolation process, the RG scale is successively lowered – going from the classical action, where quantum fluctuations below the initial scale Λ are suppressed, to the full quantum theory at $k = 0$, using an interpolant Γ_k.

This interpolation process is given by an exact equation for the scale-dependent effective action Γ_k [4]. Then, computing the phase structure of a given model is as easy as solving this evolution equation for a range of parameters in the initial classical potential. For example, we may start with a *Mexican hat*-type potential, which displays *spontaneous symmetry breaking* at the initial scale, i.e. has non-trivial classical minima $\phi_{0,\text{cl}} \neq 0$. Then, for some small values of this parameter, the quantum fluctuation will restore symmetry at $k = 0$ and we can determine the critical value of $\phi_{0,\text{cl}}$ for the quantum phase transition.

This is where partial differential equations (PDEs) arise in fRG: in fact, already in the simplest approximation, the RG time evolution of the effective potential is given by a highly nonlinear differential equation:

$$k\partial_k V_k(\phi) \propto \frac{k^{2+d}}{k^2 + \partial_\phi{}^2 V_k(\phi)},$$

where V_k is the now RG scale-dependent version of the effective potential V. If the (dimensionless) scale is identified as a 'time' variable $t = \log(k/\Lambda)$, and the uniform mean field value ϕ is identified as a spatial variable, then one can use conventional numerical methods to solve RG equations.

Our recent paper [1] applies numerical fluid dynamics techniques to solve convection-diffusion-type equations. Specifically, we evaluate the mean magnetization of a spin system using efficient open-source hydrodynamical libraries [5]. The quantum fluctuations enter the system trough an information flow, with wave-like propagation from high to low energies. Excitingly, in this picture, the creation of shock waves in the RG-scale evolution of the potential $V_k(\phi)$ is a mechanism for first-order phase transitions. However, the quantitative resolution of large gradients in a PDE requires the use of advanced numerical methods. One family of methods specialized for solving this type of PDEs are local *Discontinuous Galerkin methods*, which we have implemented for the first time in the fRG to solve Ising-type models. This marks an important step towards the qualitative and also quantitative resolution of first-order transitions, in particular in systems with competing order effects.

Literature

1. F. Ihssen, J.M. Pawlowski, F.R. Sattler, N. Wink. *Comput. Phys. Commun.* (300), 2024.
2. K.G. Wilson. *Phys.Rev.B* (4), 1971.
3. N. Dupuis, L. Canet, A. Eichhorn, W. Metzner, J.M. Pawlowski, *et al. Phys. Rept.* (910), 2021.
4. C. Wetterich. *Phys. Lett. B* (301), 1993.
5. M. Blatt, A. Burchardt, A. Dedner, C. Engwer, J. Fahlke, *et al. Archive of Numerical Software*, (4) No. 100, 2016.

AWARDS & HONORS

Dominika Wylezalek Receives Heinz Maier-Leibnitz Prize

Dr. Dominika Wylezalek
Emmy Noether Group Leader, ZAH

Dominika Wylezalek, an astrophysicist at the *Centre for Astronomy of Heidelberg University (ZAH)*, has been selected for the *Heinz Maier-Leibnitz Prize* by the German Research Foundation (DFG). This prize is the most important award for researchers in the early phases of their career in Germany. Endowed with 200,000 euros, it aims to support their research endeavours for up to three years.
The prize acknowledges Dominika Wylezalek's outstanding research on galaxy development, showing the pivotal role of *active galactic nuclei (AGN)* at the cores of massive galaxies. These regions, surrounding supermassive black holes, emit intense, highly energetic radiation and are believed to be the primary regulators of massive galaxy growth.
Since 2020, Dominika Wylezalek has been leading the Emmy Noether research group *"Galaxy Evolution and AGN (GALENA)"* at the *Astronomisches Rechen-Institut*, which is part of ZAH.

STRUCTURES COMMUNITY

Young Researchers Convent Elects New Representatives

The STRUCTURES Young Researchers Convent (YRC) has elected Freya Elisabeth Jensen, Marvin Sipp and Ricardo Waibel as their new speakers. The YRC speakers take care of the YRC and represent it in the Steering Board. We congratulate and wish the new speaker team a successful start!
The new team follows the previous speaker duo, Ricardo Waibel and David Maibach. We thank all previous and new speakers for their great and valuable commitment!
In order to introduce the new speakers, we interviewed them briefly, asking three questions. Below are their short interviews:

ℹ The YRC is a subgroup of STRUCTURES that brings together, represents and gives early-career scientists the necessary support to realize their own projects. Learn more at: *www.structures.uni-heidelberg.de/YRC.php*

Interview with Freya Jensen:

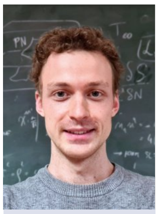
Freya Jensen
PhD student, AG Kanschat, IWR

What are you working on? I am working in the field of topological data analysis. My main focus lies on persistent homology computation for big data sets.

What fascinates you about being a scientist? First, I really enjoy using my knowledge in a field of pure mathematics like algebraic topology to gain insights into "real world problems." And additionally, solving the problems I come across in my project can be a lot of fun, like solving a very big puzzle.

Why did you apply to be YRC speaker?
The YRC offers young scientists many opportunities, such as travelling to conferences or workshops, the Schöntal Workshop, and inviting scientists themselves. As I was already involved a little in the organisational side of the YRC and enjoyed working with the team of speakers and other people involved, I wanted to continue.

Interview with Marvin Sipp:



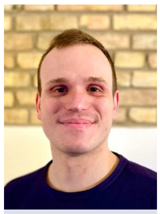
Marvin Sipp
PhD student, AG Bartelmann, ITP

What are you working on? My main research interests are in cosmology, field theory, and gravity. I currently try to understand the formation and evolution of cosmic structure by using methods from non-equilibrium statistical field theory.

What fascinates you about being a scientist? Thinking hard about difficult problems in order to learn more about how nature works is just an immense pleasure. For me, the scientific knowledge of humankind is one of the greatest cultural treasures.

Why did you apply to be YRC speaker?
The YRC offers great opportunities, like workshops and travel grants, from which I have been benefiting a lot. I had already co-organized a YRC Schöntal workshop, and being a speaker is another way for me to give something back and continue the great work of my predecessors.

Interview with Ricardo Waibel:



Ricardo Waibel
PhD student, AG Heisenberg, ITP

What are you working on? I work in the field of cosmology and gravity. Mainly, this focuses on gravitational waves on cosmological backgrounds and specifics of how to measure gravitational waves with the new space-based detector called LISA (launch in 2035).

What fascinates you about being a scientist? I think we enjoy lots of freedom in our research, and it fascinates me how individuals use this to come up with beautiful explanations for previously poorly understood questions.

Why did you apply to be YRC speaker?
I was already a speaker in the previous period and really enjoyed the work. It was great organizing several things from funding calls to events, and representing the early-career researchers within the cluster.

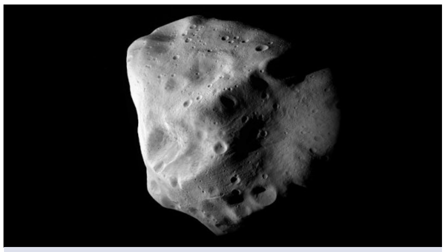
AWARDS & HONORS

Hubert Klahr Receives ERC Grant to Probe Origins of Solar System's Minor Bodies

Hubert Klahr
Professor at MPIA

Hubert Klahr, head of the theory group at the *Max Planck's Institute's (MPIA) Planet & Star Formation* department, and a principal investigator of the STRUCTURES Cluster, has secured one of the prestigious *European Research Council*'s *Advanced Grants*. The prize, endowed with 2.49 million euros of funding over the next five years, will support his pioneering project *"Turbulence, Pebbles, and Planetesimals: Origin of Minor Bodies in the Solar System (TiPPi)."*

The *TiPPi* project will focus on understanding the origins of minor celestial bodies like asteroids and comets in our solar system. Innovative numerical and machine learning methods will be used for a combined study of three phases of planetesimal formation, including the effects of turbulence, pebble sizes and dust opacities, and the elasticity and porosity evolution of the forming planetesimals. The project will not only promote insights into the early history of our solar system but also provide connections to the diversity of exoplanetary systems. The techniques developed will be beneficial to the broader scientific community.



Main belt asteroid 21 Lutetia (© ESA 2010 MPS for OSIRIS Team MPS/UPD/LAM/IAA/RSSD/INTA/UPM/DASP/IDA)

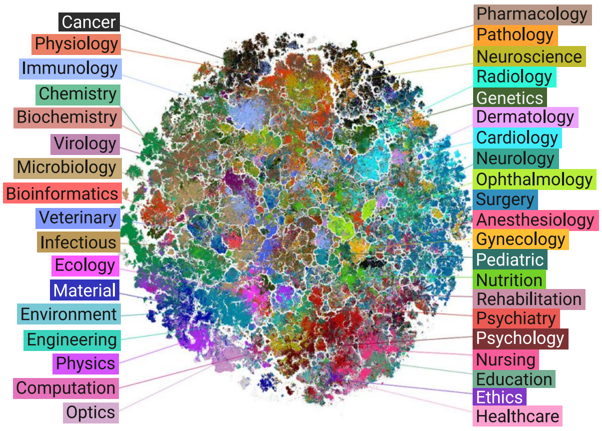
The ERC Advanced Grant recognizes exceptional senior researchers, with only 255 recipients selected from 1829 applications across Europe.

SHORT NEWS

Innovative Visualization Unveils Biomedical Research Landscape

Biomedicine and the life sciences are a rapidly growing field. With more than 1.5 million scientific articles published every year, it is challenging to track the evolution of biomedicine in time.

An international team of researchers including Dmitry Kobak, who has been a visiting professor for machine learning at STRUCTURES from Oct. 23 to Mar. 24, has now created an unprecedented visualization of the biomedical and life science literature, offering insights into the fields' evolution and social disparities within academia. Using the abstract texts from 21 million English articles in the *PubMed* database, the team developed a two-dimensional atlas showing global research trends and their evolution in time. The atlas, created with the help of *Large Language Models* (LLMs), surpasses previous visualizations both in scope and detail.



Visualization of medical literature: embedding of the PubMed Dataset (Text labels enlarged, reproduced from González-Márquez et al., CC BY)

This visualization enables exploration of diverse topics, such as the emergence of COVID-19 literature, shifts in neuroscience research focus, adoption of machine learning methods, gender imbalances in authorship, and identification of retracted fraudulent papers.

Through an interactive website, https://static.nomic.ai/pubmed.html, users can navigate the atlas, zoom in on specific areas, and search for articles. The study highlights the power of advanced language models for innovative visualizations of vast text corpora, offering researchers new tools for tracking the progress of science.

Original Publication:

R. González-Márquez, L. Schmidt, B.M. Schmidt, P. Berens, D. Kobak, 2024, Patterns (100968), doi: 10.1016/j.patter.2024.100968.

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

- @structures_hd
- @structures_heidelberg
- @STRUCTURES_HD

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).

IMPRESSUM & CONTACT

Exzellenzcluster STRUCTURES
Universität Heidelberg
Philosophenweg 12 & Berliner Straße 47
D-69120 Heidelberg
office@structures.uni-heidelberg.de

Text, Editing & Layout:
Sebastian Stapelberg / STRUCTURES Office, Editorial Board, Guest Authors and Speakers.