



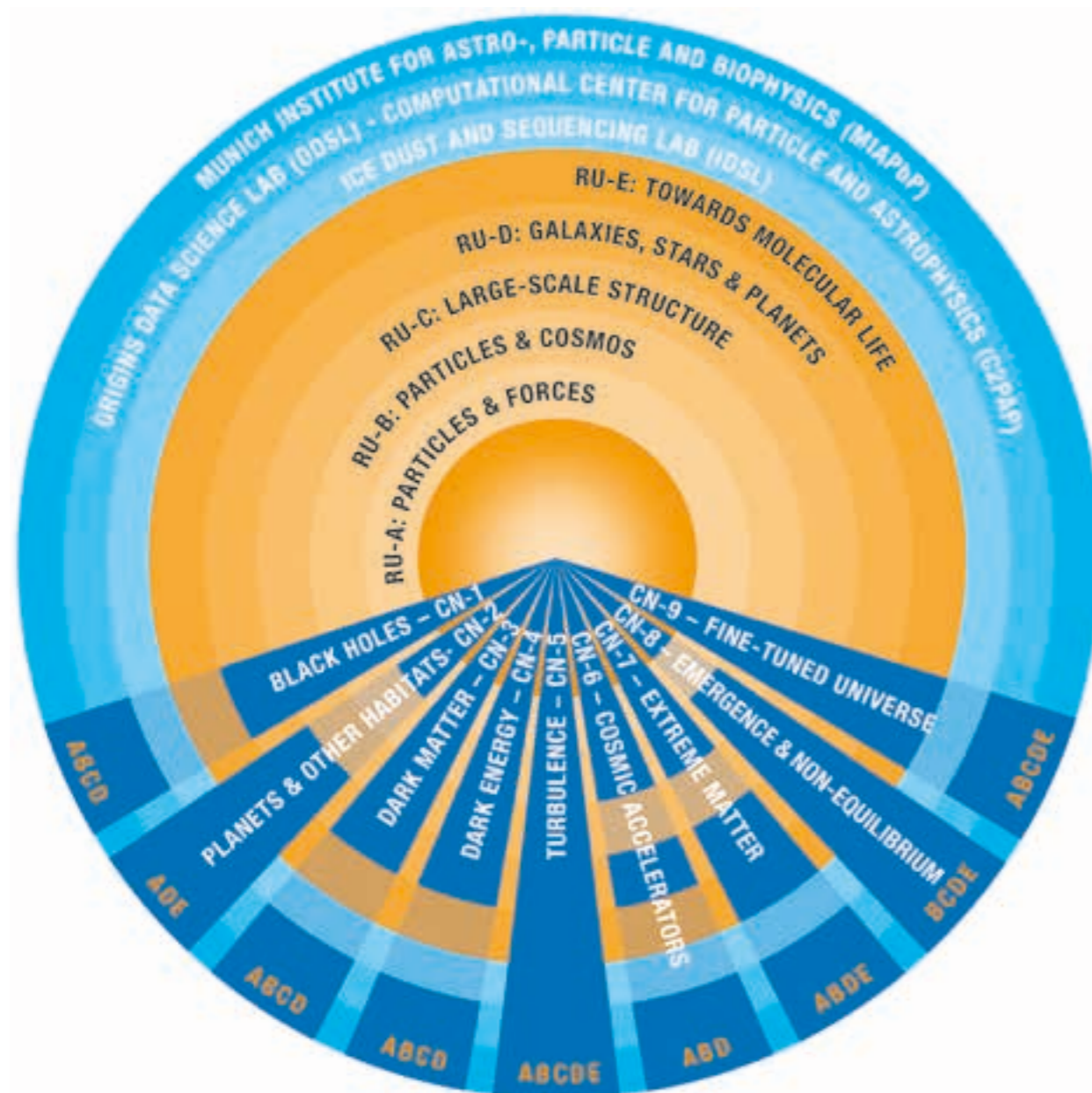
ORIGINS EXCELLENCE CLUSTER SCIENTIFIC HIGHLIGHTS

From the origin of the Universe to the first building blocks of life



CONTENT

| | |
|--|----|
| Foreword | 2 |
| Presence of liquid water during the evolution of exomoons orbiting ejected free-floating planets | 4 |
| First cosmological simulation of frequent dark matter self-interactions | 6 |
| Search for dark matter annihilation in space through detection of antimatter in cosmic rays | 8 |
| Ab-initio cosmological simulations | 10 |
| Using machine learning to detect shock surfaces in cosmological simulations | 12 |
| First neutrino image of an active galaxy | 14 |
| Constraining the equation of state of neutron stars via precision hadronic interaction measurements | 16 |
| Self-organisation and molecular transport in simple cell membranes | 18 |
| Classification of the exotic quarkonium state X(3915) at the Belle experiment | 20 |
| Cosmology beyond the 2-point function | 22 |
| Multi-Scale Star- and Planet Formation | 24 |
| Physical non-equilibria for prebiotic nucleic acid chemistry | 26 |



The Interconnected Universe of the ORIGINS Excellence Cluster.
The ORIGINS infrastructures MIAPbP, ODSL, C2PAP and IDSL (blue rings) are the global structures that facilitate workshops, interactions and support the realisation of projects in almost all of the different research units (RU-A,B,C,D, and E) and connectors (CN-1-9). © ORIGINS.

“It is only in interactions that nature draws the world.”

(C. ROVELLI, THE JOURNEY TO QUANTUM GRAVITY, 2017)

FOREWORD

It is all connected: the intricate filaments of the cosmic large-scale structure with the innate properties of the fundamental forces and their associated fields and particles, the rise and evolution of stars and galaxies with the local chemical landscape. It all leads to the most complex and fascinating form of thermodynamic non-equilibrium we know of – Life. The ORIGINS Excellence Cluster explores how the origin of the Universe is connected to the emergence of life from differing and sometimes unexpected perspectives.

This report presents a first collection of research highlights from novel co-operations within ORIGINS that reflects the way our cluster works and how it will thrive: interactions among scientists from seemingly unrelated fields of research with distinct methods and languages and collaborations across our partner institutes. As further ongoing joint projects bear fruit, we will print the next collection of ORIGINS research highlights.

The presented research highlights would not have been possible without the

ORIGINS infrastructures: the Computational Centre for Particle and Astrophysics (C2PAP), where the next generation numerical codes are developed and most of the simulations and computationally heavy calculations happen, the ORIGINS Data Science Lab (ODSL) which specialises in developing advanced techniques for pattern recognition, statistical analyses of complex multi-connected data and machine learning to deal with noisy and large data sets, the Lab for Rapid Space Missions (LRSM) which just launched a nano-satellite payload onto the ISS, the Ice, Dust and Sequencing Lab (IDSL) that provides the setup for biophysical experiments in search for the initial conditions of life, and last but not least the Munich Institute for Astro-, Particle and Biophysics (MIAPbP). MIAPbP is our centre for scientific exchange that hosts local and international guests. Project reports from our infrastructures are subject to a forthcoming brochure.

We collected this first set of highlights with the kind help of our RU-managers Steffen Hagstotz (RU-C) and Alex Ruf (RU-E), ORIGINS Fellow Alexandre

Barreira (RU-C), and Thomas Kuhr (RU-A coordinator), our CN managers Henrique Rubira (CN-3), Angelo Caravano (CN-4), Ludwig Böss (CN-5), Artem Bohdan (CN-6), Raffaele del Grande (CN-7) and George Dadunashvili (CN-8) and Mathias Garny (CN-3 coordinator). Thank you very much for taking the time to summarise scientific highlights from your research units and connectors.

We thank Halina Abramowicz (SAC Chair) for the inspiring discussions during her visit to the Cluster in October of 2022 for the Council Meeting and especially for motivating us to start this collection and to demonstrate our progress on the interconnected Universe.

June 2023

Andreas Burkert and Stephan Paul
(Spokespersons)

Alice Smith-Gicklhorn
(Science Manager)

Odele Straub
(Science Communication)



Artistic view of an exomoon with liquid water generated by the authors using MidJourney.

Presence of liquid water during the evolution of exomoons orbiting ejected free-floating planets

SUMMARY

Liquid water is one of the most important ingredients for the emergence of life as we know it on Earth. Researchers of the ORIGINS Cluster from the fields of astrophysics, astrochemistry and biochemistry have now determined in a novel, interdisciplinary collaboration the necessary properties that allow moons around free-floating planets to retain liquid water for a sufficiently long time and thus enable life.

THE STORY

For the emergence of life on Earth, liquid water is a crucial component. Since only one planet is known so far to have given rise to life, the scientists assume that also elsewhere the presence of liquid water plays a pivotal role in the chemical evolution that can lead to the emergence of life. In and outside our solar system, the habitable zone defines an annular region around the central star in which planets are neither too hot nor too cold for liquid water. Moons can also be habitable – even if they belong to planets beyond the habitable zone. In that case, however, they must have a heat source other than stellar heat, such as changing tidal forces. Indeed, Saturn's moon Enceladus has an ocean of liquid water hidden beneath its ice crust thanks to tidal heating.

The discovery of dozens of free-floating planets (FFPs) in our galaxy has changed our understanding of the early evolution of planetary systems and theories of planet formation. These lonely wanderers were probably ejected from their planetary systems by dynamic instabilities and thus no longer have a

parent star. However, if they have moons in tight orbits, they can gravitationally bind them. This works best for Jupiter-like planets with Earth-sized moons. In this way, new, unexpected places emerge where life could form.

In a previous study of liquid water on moons of starless planets, researchers from the ORIGINS cluster demonstrated that Earth-sized moons around Jupiter-like planets may indeed have liquid water. Their results suggested that the amount of water possible on the lunar surfaces is only a fraction of the total volume of all terrestrial oceans, which is still a hundred times the water content of Earth's atmosphere. This amount is already enough to enable the chemical processes that can lead to life. Local wet-dry cycles (evaporation and condensation), as recently shown in a study of the first stages in the evolution lead by Alan Ianeselli (at the time ORIGINS PhD student, won ORIGINS PhD Award 2022), provide the necessary chemical complexity that could promote the accumulation of molecules and the polymerization of RNA.

The orbit of exomoons around FFPs becomes less eccentric and thus more circular over time. This reduces the tidal forces and thus the heating efficiency. In a unique collaboration, PhD student Giulia Rocchetti (ESO, previously a Master's student at LMU), under the guidance of ORIGINS scientists, Barbara Ercolano (LMU, Astrophysics), Karan Molaverdikhani (LMU), Tommaso Grassi (MPE, Astrochemistry) and Dieter Braun (LMU, Biophysics), developed a new, realistic model that can calculate the evolution of lunar orbits over long timescales. These are timescales of several billion years, as required for the evolution of life. They found that exomoons with small orbital radii not only have the best chance of surviving their planet's ejection from its planetary system, but also remain eccentric for the longest period of time and thus can optimally produce tidal heat. In addition, dense atmospheres favour the preservation of liquid water. In summary, Earth-sized moons with Venus-like atmospheres in close-in orbits around their orphan planets are interesting new candidates for habitable worlds.



PUBLICATIONS

- * G. Rocchetti, T. Grassi, B. Ercolano, K. Molaverdikhani, A. Crida, D. Braun, A. Chiavassa (2023), *Int. J. of Astrobio.* 1-30
- * A. Ianeselli, M. Atienza, P. Kudella, C. Mast, U. Gerland, D. Braun (2022), *Nat. Phys.* 18, 579–585



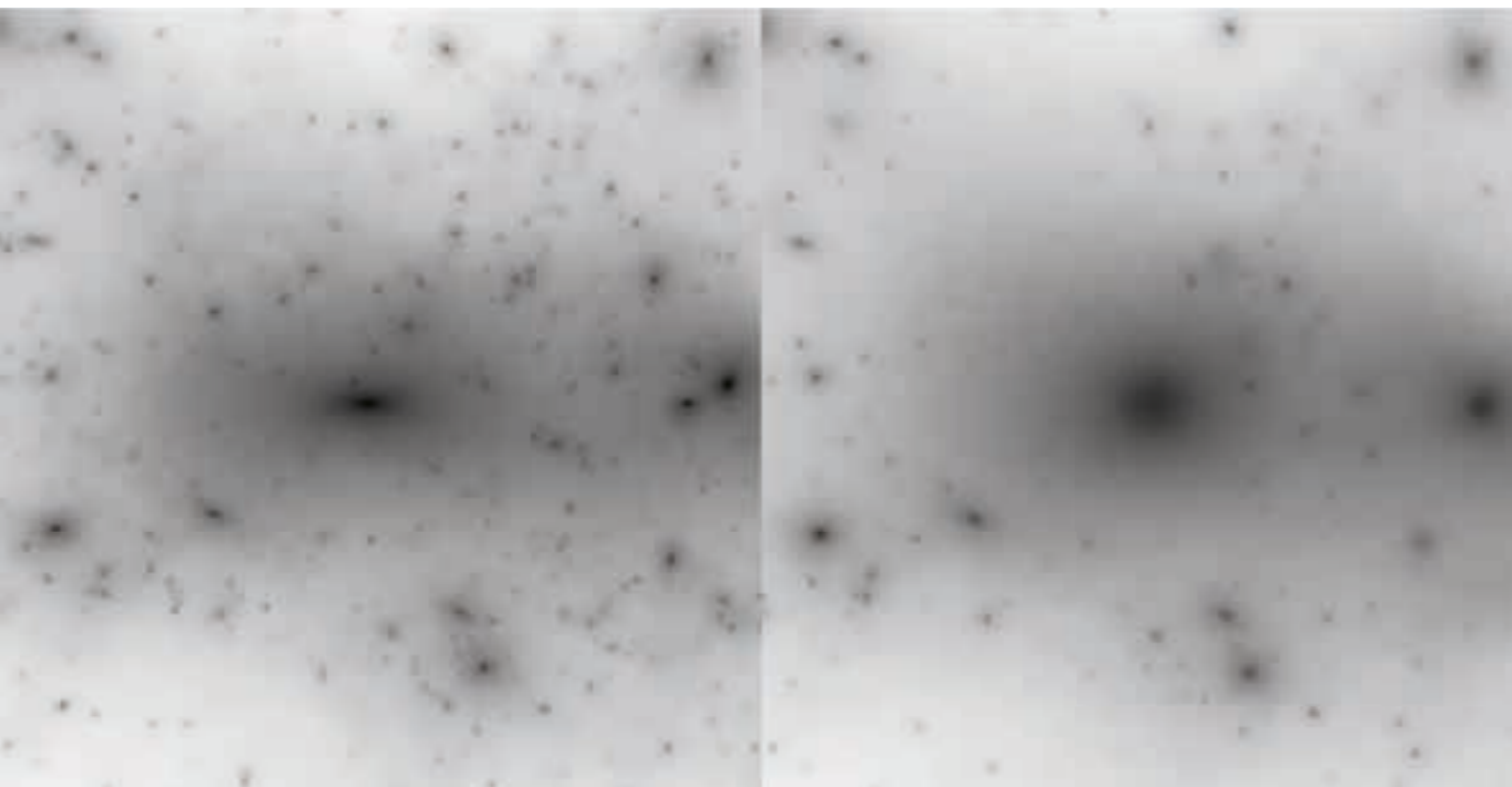
FUNDING INFORMATION

- * Alan Ianeselli had an ORIGINS funded PhD position in the Braun Lab
- * Andrea Chiavassa was funded through the ORIGINS guest program from January – April 2022.

CN-2

PLANETS AND OTHER HABITATS

First cosmological simulation of frequent dark matter self-interactions



The dark matter of a galaxy cluster from a cosmological simulation. Left: the system is displayed when simulated with collisionless dark matter. Right: the same system evolved with frequent dark matter self-interactions. Typical effects of self-interactions are visible. These manifest in a lower density of the central halo, its rounder shape and suppression of the substructure, i.e. the cluster has fewer satellites. © Moritz Fischer



PUBLICATIONS

- * M. Fischer, M. Brüggen, K. Schmidt-Hoberg, K. Dolag, A. Ragagnin, A. Robertson (2021), *MNRAS*, 510, 4080
- * M. Fischer, M. Brüggen, K. Schmidt-Hoberg, K. Dolag, F. Kahlhoefer, A. Ragagnin, A. Robertson (2021), *MNRAS*, 505, 851
- * M. Fischer, M. Brüggen, K. Schmidt-Hoberg, K. Dolag, F. Kahlhoefer, A. Ragagnin, A. Robertson (2022), *MNRAS* 516, 2, 1923-1940
- * M. Fischer, N.-H. Durke, K. Hollingshausen, C. Hammer, M. Brüggen, K. Dolag (2023), *arXiv:2302.07882*
- * H. Rubira, A. Mazoun, M. Garny, *JCAP* 01 (2023) 034



FUNDING INFORMATION

- * Moritz Fischer and Henrique Rubira are ORIGINS funded postdocs
- * Lorenzo de Ros and Asmaa Mazoun are ORIGINS funded PhD students

SUMMARY

Despite its success over the past decades, the cosmological concordance model Λ CDM provides an unsatisfactory description of our Universe. The nature of its major components, namely dark matter and dark energy, is unknown. Diverse efforts are undertaken to shed light on the physical properties of dark matter. Among the most promising candidates are particles which are subject to self-interactions beyond gravity. They have the potential to explain the cracks in our Λ CDM description, such as the core/cusp and related problems as well as the so-called H_0 and S_8 tension on larger scales.

THE STORY

Dark matter, whose existence can explain numerous cosmological and astrophysical observations, is usually assumed to be collisionless. While dark matter plays a decisive role in shaping the structure of the observed Universe, the dominant components of visible matter interact among themselves and are largely responsible for the complexity of astrophysical processes. To what extent interactions of dark matter particles with themselves can impact the structure formation of the Universe is a long-standing puzzle. Addressing it requires insights from particle physics, as well as dedicated numerical N-body and hydrodynamical simulations that span from galactic to cosmological scales.

Klaus Dolag (LMU, Coordinator CN-3, CN-5, and C2PAP) and ORIGINS funded postdoc Moritz Fischer (LMU) are tackling the question how the presence of dark matter could affect structure formation with N-body simulations of a particular type of self-interacting dark matter. To that end, Moritz Fischer has developed a code to simulate the impact of dark matter self-interactions using a novel approach that captures various types of interactions that are known to be relevant also for visible matter. Together with his collaborators

he developed a formalism that takes into account the impact of very frequent self-scattering with small scattering angles. This occurs for example when the self-interaction is mediated by a very light exchange particle, i.e. a long-range Yukawa-type interaction potential. Moritz Fischer investigated in detail the differences between these and elastic, isotropic self-scatterings by simulating for instance galaxy cluster mergers or their formation in the cosmological context.

Any realistic particle physics model predicts that both small- and large-angle scatterings are present to a certain degree. Therefore, in a next step, the numerical implementation will be adapted such that it takes into account the angle- and velocity-dependence of the cross section as predicted in a particular particle physics model. The favourable properties of providing a more plausible description of the dark matter distribution on small scales with self-interactions (angle and velocity dependence of cross section) obtained from the simulation setup hint at a specific particle physics framework. Lorenzo de Ros, a joint ORIGINS PhD student in the groups of Martin Beneke (TUM, Coordinator RU-A) and Mathias Garny (TUM, Coordinator CN-3), has the task

to work out how a microscopic model of dark matter links to a simulation of galaxy cluster mergers.

In a related project, ORIGINS PhD Asmaa Mazoun and ORIGINS PD Henrique Rubira investigate the impact of long-range dark matter interactions on cosmological scales, combining cosmic microwave and large-scale structure observations. Asmaa Mazoun is jointly supervised by astroparticle theorist Mathias Garny (TUM, coordinator CN-3) and observational cosmologist Joe Mohr (LMU).

A close connection of particle theory and cosmological simulation and observation groups has been established to tackle the challenge of bridging about thirty orders of magnitude in length scale between the interactions of dark matter particles and their implications on cosmological scales. The projects of Moritz Fischer, Lorenzo de Ros, Asmaa Mazoun and Henrique Rubira would not have taken place without the stimulus and support from CN-3. They directly follow the ORIGINS milestones CN-3.1, CN-3.2 and CN-3.4. Moritz Fischer has given three talks on his research during ORIGINS events, and Henrique Rubira two.

CN-3

PROPERTIES OF DARK MATTER



Schematic representation of antihelium annihilation in the material of the ALICE detector at CERN as well as in the Universe.
© ORIGINS/S. Kwauka; NASA/ESA/CXC/SSC/STScI and CERN

Search for dark matter annihilation in space through detection of antimatter in cosmic rays



PUBLICATIONS

- * ALICE Collaboration (2023), *Nat. Phys.* 19, 61-71
- * L. Šerkšnytė, S. Königstorfer, P. von Doetinchem, L. Fabbietti, D. Gomez-Coral, J. Herms, A. Ibarra, T. Pöschl, A. Shukla, A. Strong, I. Vorobyev (2021), *Phys. Rev. D* 105, 083021
- * P. von Doetinchem et al. (2020), *JCAP* 08 035 (white paper)



FUNDING INFORMATION

- * LRSM and MIAPbP are ORIGINS Infrastructures
- * PhD student Pöschl funded by LRSM/ORIGINS
- * PhD student Königstorfer funded by ORIGINS
- * The AMBER experiment is supported by ORIGINS

SUMMARY

Cosmic-ray antiparticles like antideuterons (a positron and an antineutron) could hold the key to uncover exotic phenomena in our Galaxy, such as dark-matter decay or annihilation and primordial black hole evaporation. In a cooperation of ORIGINS researchers at ALICE/CERN and LRSM/ORIGINS the joint experimental research and theoretical modelling lead to the most up-to-date calculation of the antideuteron fluxes from cosmic-ray collisions with the interstellar medium and from exotic processes.

THE STORY

The mystery of dark matter (DM) is addressed through simulations, observations, direct searches and theoretical investigations. Most direct searches for DM are ground-based and assume that DM winds interact with sensitive detectors and leave, depending on the assumed nature of hypothesized DM particles, a signal through particle recoil or electromagnetic signatures. For many years, cosmic-ray experiments like Pamela, AMS-2 and its precursors have measured the flux of antiparticles (positrons and antiprotons) in an attempt to interpret the observed γ -ray excess in the Galactic Center as DM annihilation. Dark matter is assumed to be electrically neutral, flavourless, not carrying baryon number and to annihilate into fermion-antifermion pairs. This would produce a possibly localized source of antimatter particles within a small range of energies. However, this scenario is plagued by large uncertainties regarding a background of particles that originates from collisions of “standard” cosmic rays with the interstellar medium (ISM). Thus, this method has almost been discarded owing to large systematics. However, most such backgrounds are found at energies above 1-10 GeV. And this is where ORIGINS entered the game.

Originally, the experimental particle physics group of Stephan Paul (TUM) established first contacts with theorist Alexandre Ibarra (TUM), both part of ORIGINS, to pursue the idea of a new scientific payload on a micro-satellite mission to detect very-low-energy anti

protons. Ibarra proposed to use antimatter particles in cosmic rays as signs for annihilation of dark matter particles in our galaxy, thereby extending the scope from antiprotons to antideuterons. This led to a cooperation with an American group and the launch of GAPS, a balloon mission to search for low-energy antimatter in Earth’s upper atmosphere. In parallel, Laura Fabbietti’s (TUM) group who works with the ALICE experiment at CERN analysed and modelled the production of antinuclei in high-energy heavy-ion collisions (PhD project of Laura Šerkšnytė – ALICE/Fabbietti) and measured the absorption cross-section for antinuclei with matter (PhD project of Stefan Königstorfer – ALICE/Fabbietti). Both measurements made key contributions to model the generation and propagation of antinuclei in our galaxy and to estimate the background rate stemming from ordinary secondary production by ordinary matter. The results suggest that antiparticles generated from DM annihilation should have low energies and that only few “conventional” processes would populate this energy regime.

Conventional background production of antimatter has to be well understood and new measurements particularly aim towards antimatter energies relevant for background generation to a possible DM annihilation signal. The various experiments cover different kinematics in terms of centre of mass energies of collisions as well as final state anti-matter energies and also collision partners (e.g. p-p, p-He, Pb-p,

Pb-Pb). All fundamental cross section measurements must be accompanied by simulations of cosmic ray propagation in our galaxy (PhD thesis of Thomas Pöschl – TUM/Paul).

These challenges were recently addressed at a MIAPbP workshop. Specialists in the fields of cosmic rays, antimatter detection and propagation modelling met up with experts in particle physicists who aim to precisely determine the production rate of antiprotons and very light antinuclei at CERN with the experiments AMBER, LHCb and ALICE.

Fabbietti continues her work with ALICE and foresees a long-term involvement in a big-science project dubbed AMS-100, a large-scale antimatter detector at the Lagrange point. Paul with the LRSM team pursues a small-scale detector (AFIS) in space and at AMBER (Spokesperson Jan Friedrich – ORIGINS) antiproton (antideuteron) production.

The search for antiparticles in cosmic rays as sign for dark matter annihilation has become an established research line of the ORIGINS cluster through the cooperation of Fabbietti, Ibarra and Paul. The collaboration resulted already in two publications that included also Andrew Strong (MPE) as well as several PhD students of Fabbietti, Ibarra and Paul. CN-3 now acts as incubator for new coherent research projects of ORIGINS that have the potential to open new doorways to unravel the mystery of dark matter.

CN-3

PROPERTIES OF DARK MATTER

Ab-initio cosmological simulations

SUMMARY

During his ORIGINS funded PhD project, Angelo Caravano (LMU) developed the first simulation of the inflationary epoch of the Universe. An interdisciplinary collaboration within the ORIGINS Cluster is now exploiting this simulation to develop a new kind of cosmological simulations, with the aim of testing particle physics models of the early-Universe against observations of the cosmic large-scale structure.

THE STORY

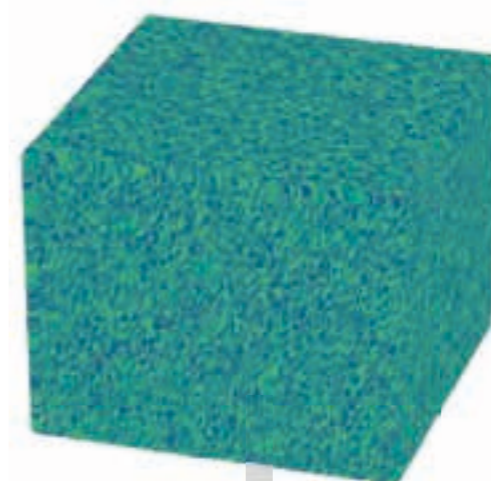
The large-scale structure of the cosmos can be traced back to a phase of accelerated expansion of the early Universe known as inflation. This early expansion, which shares important properties with today's accelerated expansion, stretched the microscopic quantum fluctuations to large cosmological scales and acted as an initial trigger for the formation of the large-scale structure. To study this mechanism, Angelo Caravano, at the time an ORIGINS funded PhD student of Jochen Weller (LMU) and Eiichiro Komatsu (MPA), developed in a collaboration with Kaloian Lozanov (MPA) the first cosmological simulation of the inflationary epoch of the Universe.

These simulations offer a new and unique way to study the observational signatures of the physics at play during inflation, namely to directly connect

early and late-time cosmology. Specifically, the simulation gives for the first time the full density perturbation predicted by inflation. This in turn can be used as realistic initial condition for cosmological N-body simulations for structure formation, as it allows simulations that start deep in the inflationary epoch and end in the present-day matter distribution of the Universe.

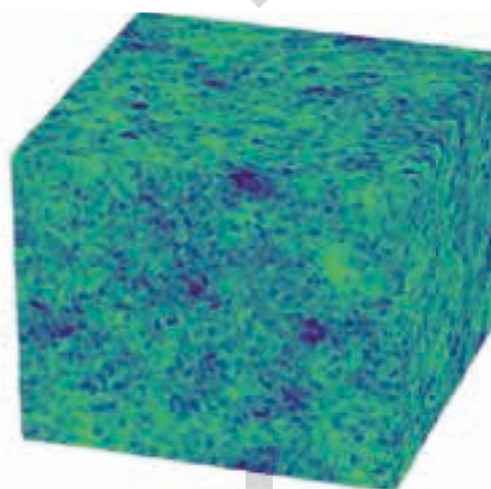
The approach can be used to better understand the effects of inflation on the properties of cosmic large-scale structure. Angelo Caravano is currently collaborating with experts in cosmological simulations and large-scale structure, Drew Jamieson (MPA), Fabian Schmidt (MPA) and Eiichiro Komatsu (MPA) to develop and use these new ab initio cosmological simulations. This opens a new avenue for cosmological simulations: the direct comparison of different models for the early Universe with observations.

An important application is the search for cosmological parity violation, i.e. the possibility that the statistical properties of the Universe are not invariant under mirror reflection. Recently, Jiamin Hou et al. (2022) detected a signal for parity violation in the large-scale structure distribution of galaxies. Angelo Caravano is now working with Hou, an ORIGINS-funded visitor mentored by Ariel Sanchez (MPE), to understand the origin of this signal in the early Universe. To address this question, they analyse the results of Angelo Caravano's simulations using the same tools that Jiamin Hou uses for observational data. These simulations are based on an inflation model that is expected to lead to parity-violating physics known as axion inflation.



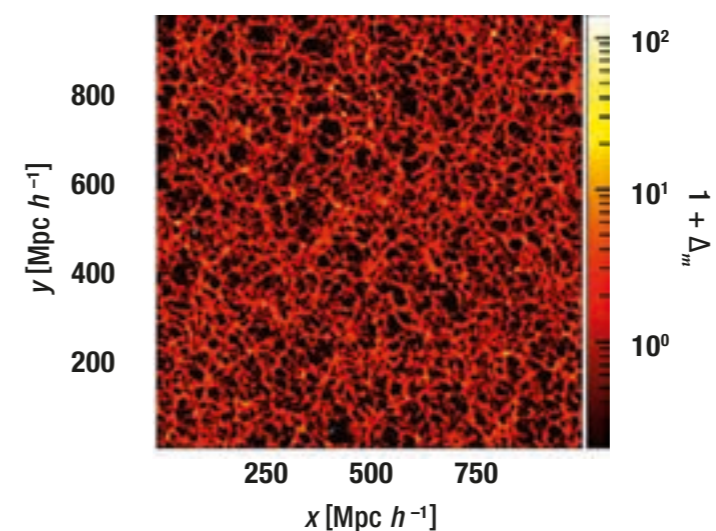
Initial quantum fluctuations
(just after the Big Bang)

EARLY-UNIVERSE LATTICE SIMULATION



Primordial density field
(end of inflation)

COSMOLOGICAL N-BODY SIMULATION



Cosmic large-scale
structure (today)

An illustration of the ab initio cosmological simulation, starting from Big Bang quantum fluctuations (top) and ending in the large-scale distribution of matter in the Universe today (bottom). © A. Caravano



PUBLICATIONS

- * A. Caravano, E. Komatsu, K. Lozanov & J. Weller (2021) JCAP, 12(12):010
- * A. Caravano, E. Komatsu, K. Lozanov & J. Weller (2022), Phys. Rev. D, 105:123530
- * A. Caravano, Dissertation (2022), LMU München, arXiv:2209.13616
- * A. Caravano, E. Komatsu, K. Lozanov & J. Weller, arXiv:2204.12874



FUNDING INFORMATION

- * PhD student Angelo Caravano funded by ORIGINS
- * ORIGINS funded visiting researcher Jiamin Hou

CN-4

PROPERTIES OF DARK ENERGY

Using machine learning to detect shock surfaces in cosmological simulations

SUMMARY

As galaxy clusters form, they dissipate a large fraction of their potential energy in the form of shocks in the intra-cluster medium. This process accelerates cosmic ray electrons in arc-like structures with sizes of up to several Mpc, which are observed by radio telescopes as so-called radio relics. ORIGINS scientists cooperated in developing a state-of-the-art machine learning algorithm to detect coherent shock surfaces in the highest resolution simulations of galaxy clusters to date.

THE STORY

Cosmic rays in the form of relativistic electrons provide powerful insights into the origin and history of large-scale structure formation. The most prominent of these observations are the previously mentioned radio relics, where shocks expand into the turbulent, magnetized plasma of the intra-cluster medium (ICM) and accelerate electrons to relativistic velocities on the scale of several Mpc. In contrast, the zones where this acceleration happens are only of the scale of the electron cyclotron radius, which in these cases is of the order of a few AU. The acceleration zones can be viewed as quasi-2D surfaces moving through the ICM.

Recent high-resolution radio observations show complex surface structures of radio relics. These are believed to be originating from variations in local sound speed and plasma turbulence in and behind the shock surface, leading to variations of the sonic Mach number across the shock surface. Modern small-scale plasma simulations indicate that the efficiency with which electrons and protons are accelerated at shocks strongly depends on the sonic Mach number at the shock surface. Cosmological simulations of galaxy clusters only very recently reached resolutions where the complex interplay of shocks and their surfaces can be studied. High resolution naturally leads to vast amounts of data, which makes identifying regions of interest in these simulations a significant computational challenge.

Inspired by discussions at the ORIGINS PhD days 2021, an annual event for scientific exchange between early-career scientists organised by the ORIGINS PhD representatives Elena Hoemann, Martin Ha-Minh, and Philip Lügghausen, the PhD students Max Lamparth (TUM) and Ludwig Böss (LMU) started a collaboration to combine their expertise on machine learning and cosmological simulations.

They aimed to develop an algorithm scalable to state-of-the-art-sized data sets while maintaining physical motivation to study complex shock surfaces in cosmological simulations. This was inspired by the idea of Klaus Dolag (LMU, CN-5 and C2PAP Coordinator) who suggested to implement shock surface detection into the classical on-the-fly structure finder SUBFIND which was written by Volker Springel (MPA, RU-D Coordinator) in 2001. However this kind of classification problem also lends itself well to Machine Learning algorithms.

The resulting algorithm, VIRGO, combines different statistical machine learning and deep learning methods to solve the outlined unsupervised classification problem of separating cosmic shock wave surfaces from non-shock wave particles while labelling each shock wave.

They successfully tested the extent of VIRGO's performance on multiple high-resolution simulations under different

circumstances and on a large-scale cosmological simulation with several shock wave centres.

VIRGO can now be used to identify large-scale shocks in simulations and find coherent shock surfaces, providing a powerful tool to study particle acceleration in simulations of cosmological structure formation. VIRGO is public and open source and its input parameters can be easily extended to work with multiple simulation codes, making it available for the broad scientific community in- and outside of ORIGINS.

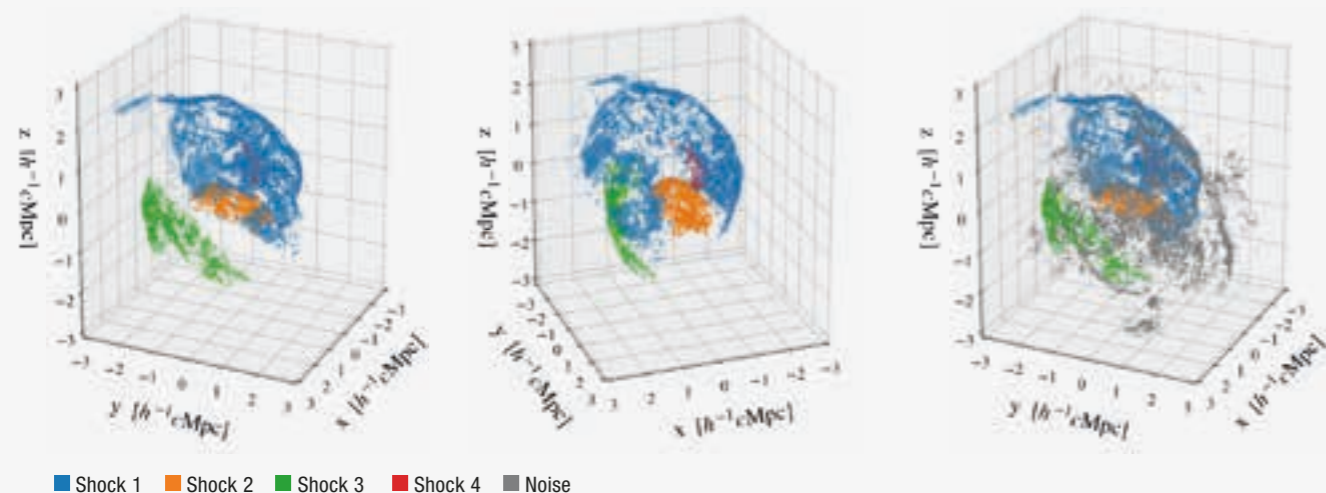
Post-processing of the high-resolution simulation was performed on the ORIGINS compute cluster infrastructure C2PAP. The algorithm was accepted as an extended abstract to the Machine Learning and the Physical Sciences workshop at the NeurIPS 2022, one of the largest ML conferences. The paper was submitted to MNRAS, currently undergoing the last steps of the referee process.

The open exchange between early career scientists from the diverse scientific backgrounds within the cluster at the ORIGINS PhD days provided a fertile ground to start collaborations with original research ideas, at all stages of a PhD.



The high-resolution simulation of the COMPASS set, which was used as the main dataset for VIRGO.

Rainbow colours indicate sonic Mach number and show the soap-bubble like surface of highly resolved shocks in galaxy clusters. © COMPASS/K.Dolag



Classification of coherent shock surfaces. Colours show the individual shock surfaces, gray points in the right-most plot indicate shocked tracer particles which are classified as noise surrounding the surfaces. © Lamparth et al. 2022



PUBLICATIONS

- * M. Lamparth, L. Böss, U. Steinwandel, K. Dolag (2022), NeuRIPS 2022, ML4PS Workshop, https://ml4physicalsciences.github.io/2022/files/NeurIPS_ML4PS_2022_186.pdf
- * M. Lamparth, L. Böss, U. Steinwandel, K. Dolag (2023), arXiv:2208.06859
- * VIRGO Code, publicly available: <https://github.com/maxlampe/virgo>



FUNDING INFORMATION

- * PhD student Lamparth is partially funded by ORIGINS
- * PhD student Böss is partially funded by ORIGINS
- * The ORIGINS PhD days are funded by ORIGINS and planning is supported by cluster management
- * C2PAP is an ORIGINS infrastructure

CN-5

TURBULENCE IN THE UNIVERSE

SUMMARY

Cosmic accelerators are believed to be present in various astrophysical environments, including supernova remnants, active galactic nuclei, blazars, and gamma-ray bursts. They produce various high-energy particles, such as protons, electrons, gamma rays and neutrinos up to energies far beyond what the LHC at CERN can achieve. However, despite years of research, detailed physics of cosmic accelerators remains largely unknown. Now, the first neutrino image of an active galaxy starts to shed light on this question.

THE STORY

Neutrinos are produced in the trillions in the Universe in a variety of high-energy events. They are accelerated by processes that are still unknown in the most dramatic processes in the Universe: exploding stars, gamma-ray bursts and cataclysmic events involving black holes and neutron stars. They are the most abundant massive elementary particles, however, they have hardly any mass and are electrically neutral. This allows them to travel through space almost entirely unhindered, but it also makes them notoriously difficult to detect.

Huge telescopes are needed to decipher the messages of cosmic neutrinos: volumes of several cubic kilometres of ice or water, instrumented with thousands of light sensors. The sensors capture the light trail created by the collision of a neutrino with a water molecule. To determine the energy and direction of the original particle, the path of the neutrino is reconstructed using detailed simulations.

Theo Glauch who received the ORIGINS PhD Award 2021, developed in his thesis in the group of Elisa Resconi (TUM, Coordinator of CN-6) an application based on artificial neural networks that reconstructs and classifies

data from high-energy neutrinos from the IceCube detector at the South Pole. His improved selection procedure has already led to new discoveries: in a collaboration with ORIGINS PI Paolo Padovani (ESO) they found that some of the neutrino measurements could be associated with active galactic nuclei, including the blazars 3HSP J095507.9+355101 and TXS 0506+056.

A recent breakthrough has changed the landscape of CN-6. More than 80 neutrinos detected by the IceCube neutrino observatory were associated with NGC1068, an active galaxy with a highly obscured central region. The association of these high-energy neutrinos with NGC1068 suggests that they originate from the centre of the galaxy and are the result of extreme acceleration of matter in the vicinity of the black hole. This remarkable discovery was recently published in *Science* by the IceCube collaboration, in which Elisa Resconi and ORIGINS funded postdoc Christian Haack (TUM) played a major role.

They organised a workshop “NGC 1068 as a Cosmic Laboratory” at MIAPbP, dedicated to the study of NGC1068 as a cosmic accelerator (March 6 to 9, 2023).

For four days, astronomers, astrophysicists, and plasma physicists discussed various components of NGC 1068, namely the star-forming region, outflow, jet, and black hole environment, and their possible relevance to the IceCube neutrino association. The workshop was multidisciplinary and a resounding success. The main results will be presented soon in a review paper in *Nature Astronomy*.

Elisa Resconi recently launched an initiative to develop a new observatory for cosmic neutrinos in the Pacific Ocean, the Pacific Ocean Neutrino Experiment (P-ONE). Christian Spannfellner (TUM), an ORIGINS PhD student in the Resconi group, is involved in the development of P-ONE’s optical modules. The prototype of a 1000-meter-long measuring line attached to the seafloor with 20 optical elements is currently being developed at the Technical University of Munich with the leading support of ORIGINS. In a next step, as part of the ERC project NEUTRINOSHOT, the first detector segment with three of these measuring ropes will be set up off the Canadian coast at a sea depth of 2.6 km. It will demonstrate the functionality of P-ONE and measure the first neutrinos.



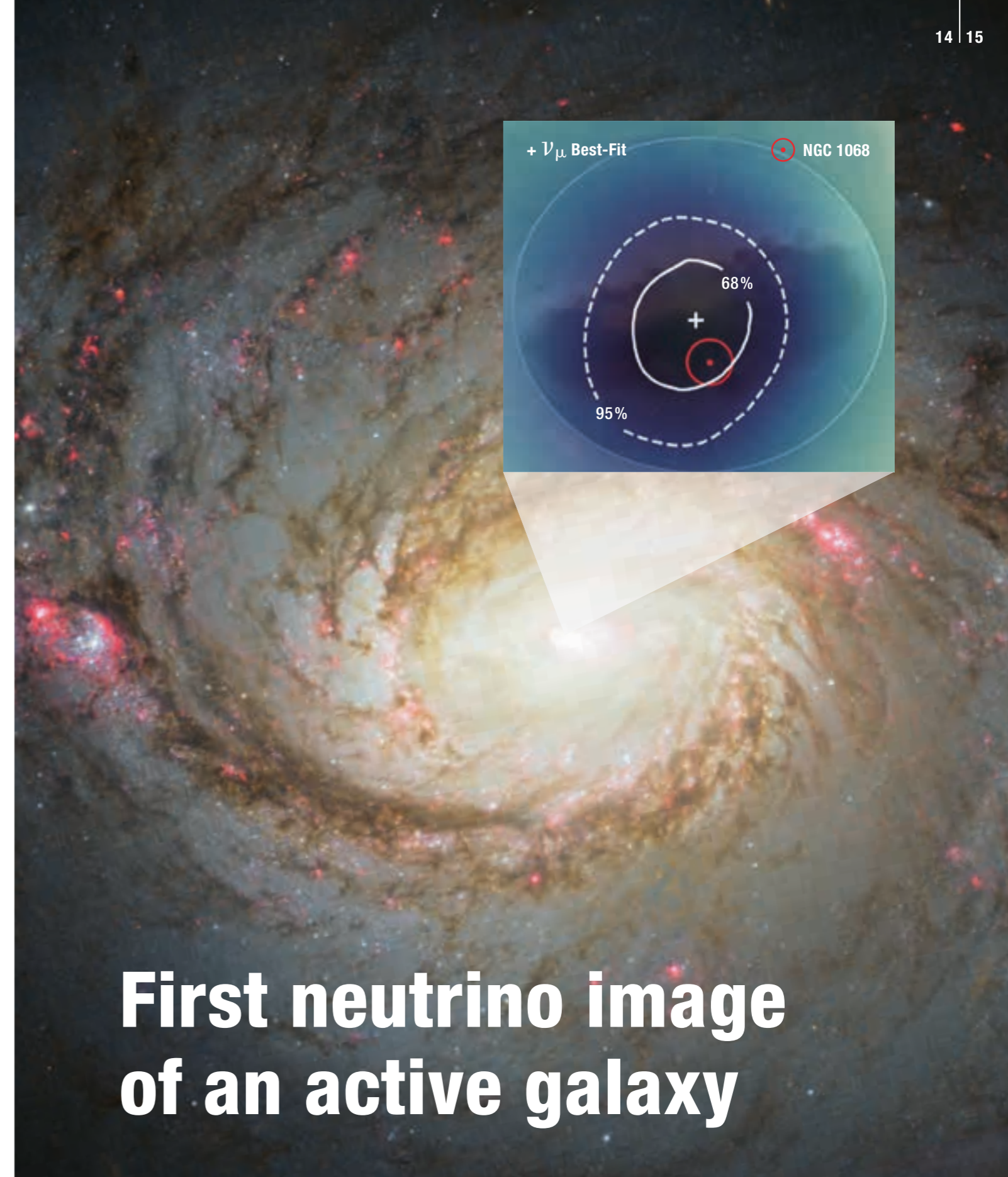
PUBLICATIONS

- * F. Oikonomou, K. Murase, P. Padovani, E. Resconi, P. Mészáros (2019), *MNRAS* 489, 3, 4347-4366
- * M. Agostini et al. incl. R. Gernhäuser, P. Padovani, E. Resconi, C. Spannfellner (2020), *Nature Astronomy*, 4, 913-915
- * P. Padovani, P. Giommi, R. Falomo, F. Oikonomou, M. Petropoulou, T. Glauch, E. Resconi, et al. (2022), *MNRAS*, 510, 2, 2671-2688
- * IceCube Collaboration (2022), *Science*, 378, 6619, 538-543
- * Padovani et al. (2023), in preparation
- * YouTube PR video (2022): www.youtube.com/watch?v=uV0eumyRlww



FUNDING INFORMATION

- * ORIGINS seed money funded project: P-ONE prototype
- * ORIGINS cluster funded PhD student: C. Spannfellner
- * MIAPbP is an ORIGINS infrastructure
- * Paolo Giommi was funded as ORIGINS guest for 3 months

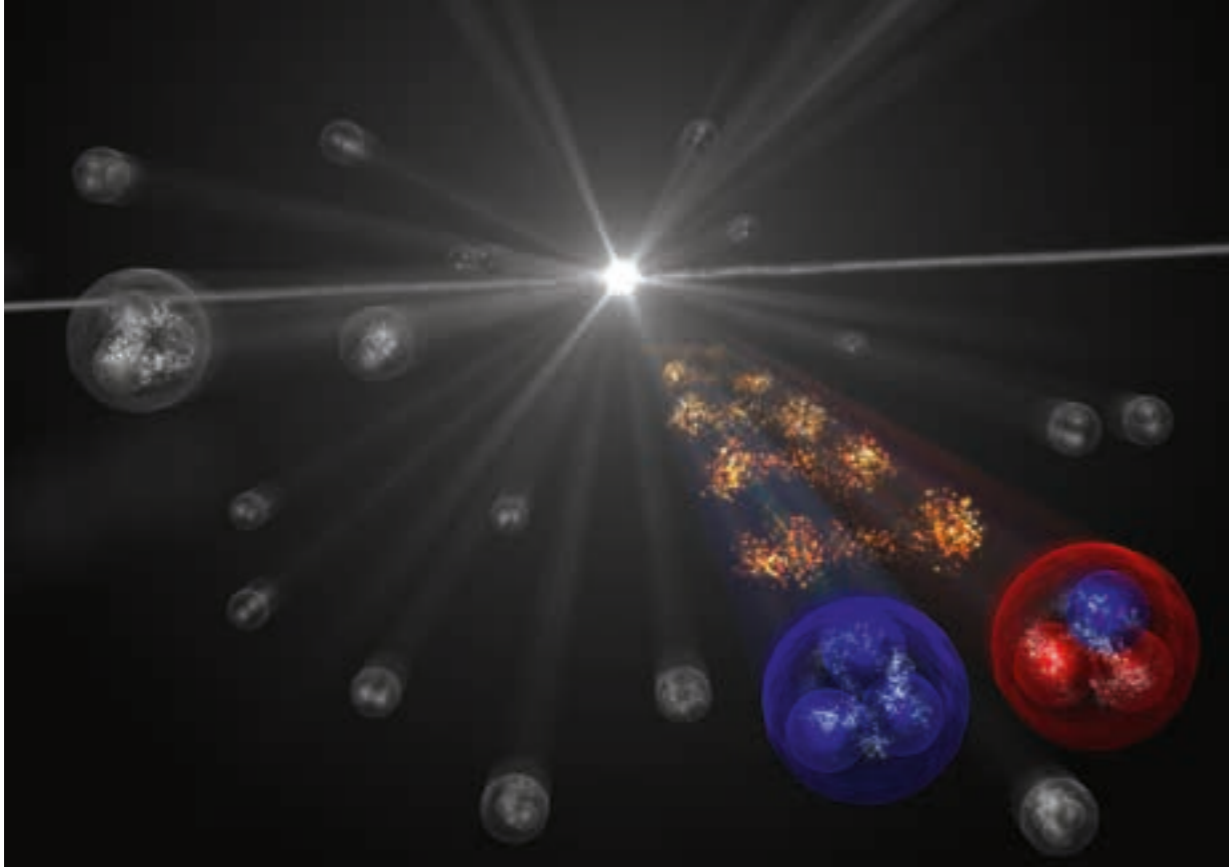


First neutrino image of an active galaxy

Combined image of NGC1068 (NASA, ESA & A. van der Hoeven) and the neutrino hot spot from IceCube (IceCube Collaboration, *Science* 378, 6619).

CN-6

COSMIC ACCELERATORS



Artistic representation of an ALICE particle interaction event. © CERN/D.Dominguez

Constraining the equation of state of neutron stars via precision hadronic interaction measurements

SUMMARY

The composition of the innermost region of neutron stars (NS) is unknown. They might consist of heavy subatomic particles with strange-quark content, called hyperons. The production of hyperons in the dense NS environment is energetically favoured. However, their presence results in a stiffening of the equation of state (EoS), unable to reproduce observed heavy NS. This problem can be resolved through precise knowledge of two- and three-body interactions for all hyperon and nucleon combinations. The necessary precision measurements of these interactions come from the ALICE experiment at CERN. Recently, a collaboration between experimentalists and theoreticians from the ORIGINS cluster started working on a realistic EoS of NS based on the ALICE data.



PUBLICATIONS

- * ALICE Collaboration, *Nature* 588, 232–238 (2020)
- * L. Fabbietti, V. Mantovani Sarti, and O. Vázquez Doce (2021), *Annu. Rev. Nucl. Part. Sci.* 71, 377-402
- * Robert Glas, H.-Thomas Janka, et al (2020), *Phys. Rev. D* 101, 063001 (2020)
- * Sajad Abbar, Francesco Capozzi, Robert Glas, H.-Thomas Janka, and Irene Tamborra (2020), *Phys. Rev. D* 103, 063033
- * J. Ehrling, S. Abbar, H.-T. Janka, G. Raffelt, I. Tamborra, (2023), *Phys. Rev. D*, arxiv:2301.11938
- * Video English: www.youtube.com/watch?v=u8uL2pA3tul
- * Video German: www.youtube.com/watch?v=8ALOMhqWypc&t=103s



FUNDING INFORMATION

- * 1.5 years of postdoc (Robert Glas) funded in CN-7 by ORIGINS
- * 3.0 years of PhD (Jakob Ehrling) funded in CN-7 by ORIGINS

THE STORY

Neutron stars (NS) are one of the most compact and dense astrophysical objects in our Universe. They are the results of supernova explosions and typically characterised by masses between 1.2 and 2.2 solar masses, and radii of the order of 10 km. The relation between the mass and the radius depends on the nuclear equation of state (EoS), which in turn hinges on the nature of the constituents and their interactions. The possible appearance of hyperons in the innermost region of neutron stars is still under debate. The production of strange hadrons becomes energetically favourable with the increasing density inside the star, which exceeds even nuclear saturation density by a factor three to four. On the other hand, the inclusion of hyperons in the EoS leads to NS configurations that cannot reach the current highest mass limit from observations. A key element for the solution of this puzzle is the interaction of hyperons with the surrounding medium. More precise knowledge of the hyperon-nucleon two- and three-body interactions leads to better knowledge of the hyperonic content inside NS. An improved description of the EoS of dense hadronic matter helps in understanding a plethora of phenomena in astrophysics, ranging from gravitational waves to the dynamics of supernova explosions and binary NS mergers.

This motivated a collaboration within ORIGINS of the experimental group of Laura Fabbietti (TUM) and experts in the theory of dense hadronic matter, such as Norbert Kaiser (TUM). They aim to build a realistic model for the EoS of NS based on new high-precision measurements performed by ALICE collaboration at the LHC. Fabbietti demonstrated that the femtoscopy method

can provide new insight into interactions between nucleons and hyperons through momentum correlations of hadrons emitted in small colliding systems at the LHC. Here, the average distances of the produced particles are of order one femtometer. This experimental technique allowed Laura Fabbietti to precisely probe hadronic interactions, which were poorly understood or not at all accessible by past scattering experiments. For example, the correlation of $p-\bar{\Xi}$ and $p-\Omega$ pairs, with strangeness $S=-2$ and $S=-3$, has been measured and is used to test Lattice QCD calculations. A review with the results has been published in 2021. Norbert Kaiser is currently working with Valentina Mantovani Sarti, a postdoc in Fabbietti's group and member of the ORIGINS cluster, on modelling the EoS, including all the hyperon-nucleon interaction models, which have been tested and validated by the ALICE measurements. In parallel, the femtoscopy technique has been extended by Fabbietti's group to investigate for the first time hadronic interactions in three-body systems aiming to experimentally isolate the contributions of genuine three-body interactions. The latter represents one of the most important missing pieces for the understanding of dense nuclear matter.

The resulting EoS for neutron-rich dense matter at finite temperature will permit astrophysicists from the group of ORIGINS PI Thomas Janka (MPA), to investigate the consequences of improved nuclear-matter models in extreme cosmic phenomena involving compact objects such as core-collapse supernovae and compact binary mergers. In fact, the EoS of hot NS is a crucial input for dynamical models of

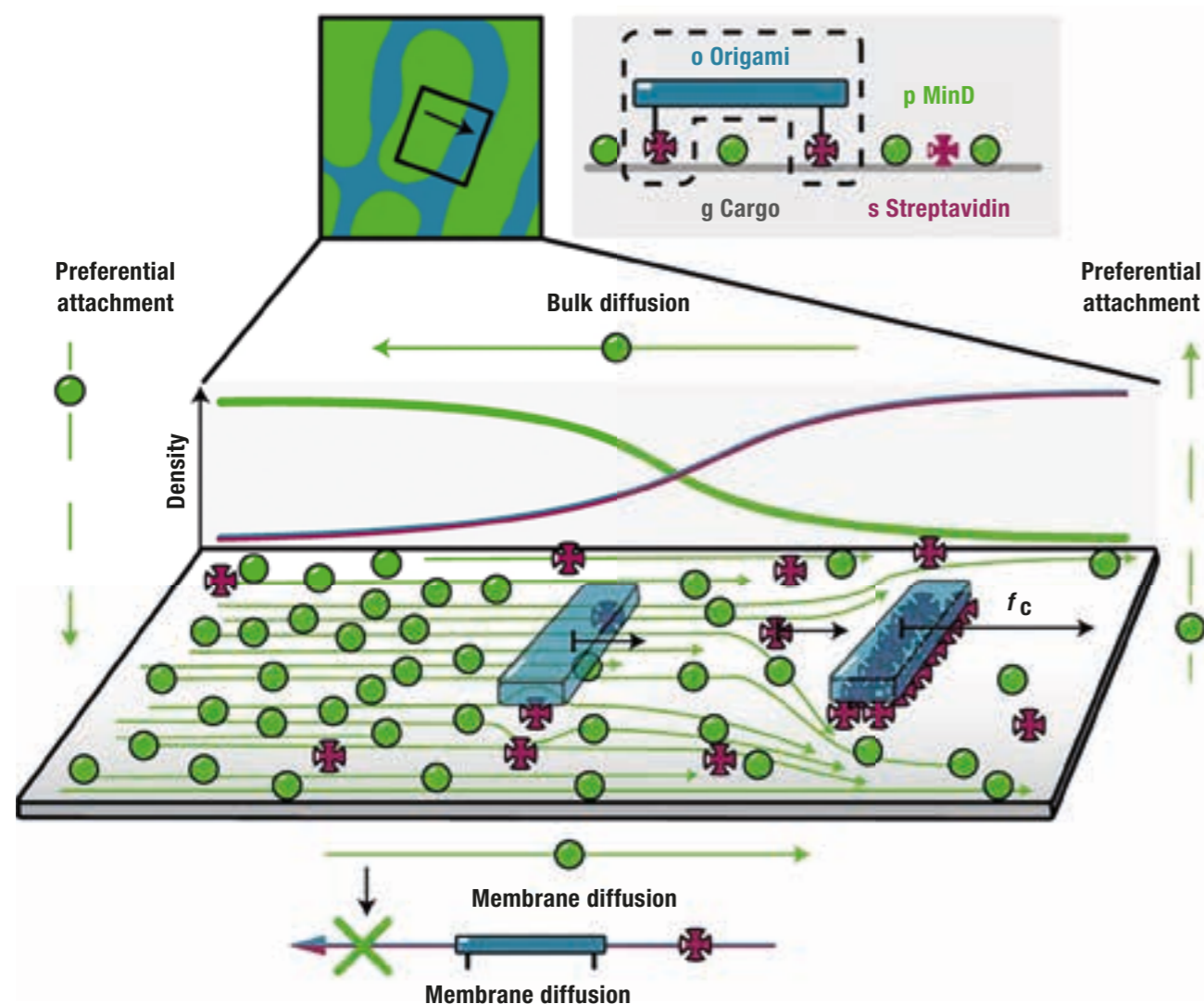
supernova explosions and NS mergers, which can be probed through signals of neutrinos and gravitational waves. The tools are observations of the associated astronomical transients (supernovae and kilonovae), and the comparison of observed chemical element abundances in the Universe with the nucleosynthesis predictions for their explosive sites of creation. The construction of a new 3D Monte Carlo neutrino transport code for supernovae (including first code tests) has been a master thesis project in Janka's group and continues as a PhD project since October 2022.

Supernovae and compact binary mergers also generate extreme neutrino densities, which permit collective neutrino flavour oscillations. Georg Raffelt (MPP) from ORIGINS studied the physics of this intriguing quantum mechanical phenomenon. Corresponding studies involved 3D supernova models of Robert Glas as a postdoc in Janka's group, as well as the first hydrodynamical supernova models that include the impact of this phenomenon, carried out by PhD student Jakob Ehrling (jointly supervised by Raffelt and Janka). Potentially, also the production of beyond-standard-model particles could play an important role or may be constrained by linking astrophysical source models (based on nuclear physics inputs) with astronomical observations. These are concrete examples for interdisciplinary highlights of the ORIGINS Connector 7, demonstrating the necessity to combine expertise of astrophysics and particle physicists.

CN-7

MATTER UNDER EXTREME CONDITIONS

Self-organisation and molecular transport in simple cell membranes



Schematic of the phenomenological MS-type model. MinDE protein density gradients are determined by a closed cycle of reactive fluxes (dashed green arrows) and diffusive fluxes (green arrows). Mediated by hydrodynamic or direct interactions, the diffusive MinD membrane fluxes exert a frictional force (black arrow) on the cargo molecules.

© B. Ramm et al. (2021)



PUBLICATIONS

* B. Ramm, A. Goychuk, A. Khmelinskaia, P. Blumhardt, H. Eto, K. A. Ganzinger, E. Frey & P. Schuille (2021), *Nat. Phys.* 17, 850-858



FUNDING INFORMATION

* Beatrice Ramm, ORIGINS PhD Award 2020

SUMMARY

An interdisciplinary collaboration between the groups of Petra Schuille (MPIB) and Erwin Frey (LMU, Coordinator CN-8) discovered that protein patterns can move synthetic cargo even without motor activity. They identified the underlying mechanism as diffusiophoresis driven by non-equilibrium currents. This mechanism may represent a new mode of general transport in cells that has never before been described in biology. This is particularly important for simple biological life forms such as prokaryotes and early life forms, as they lack the highly complex motor proteins of higher organisms. Studying such simple and robust variants of today's sophisticated biological functions is key to discovering the origins of life.

THE STORY

In order to fulfil their biological functions, cells must ensure that molecular cargoes reach their destination in time. To this end, cells employ sophisticated transport mechanisms, usually based on specific interactions in which energy-consuming motor proteins deliver the cargo to its destination.

In a joint effort of experiment and theory, ORIGINS scientists assisting Beatrice Ramm with her PhD uncovered an additional transport mode driven by pattern-forming reaction-diffusion systems. They showed that ATP-driven protein patterns can trigger diffusiophoresis of other, completely independent biomolecules through a true nonequilibrium coupling. Their results suggest a rudimentary and purely physical transport process not previously described in biological systems that does not rely on specific interactions and is therefore robust to mutations.

Specifically, they studied the *E. coli* MinDE reaction-diffusion system, a model for self-assembled pattern formation that has been studied in detail for nearly 20 years. Until now, it was

generally assumed that the sole purpose of the oscillations generated by MinDE in the cell was to position the FtsZ inhibitor MinC at the cell poles, forcing FtsZ to the centre of the cell. Recent experiments showed that the MinDE system can also regulate other unrelated membrane-bound proteins in a non-specific manner, but the broader biological implications and, more importantly, the underlying physics remain unclear. To fill this gap and explain how MinDE patterns can trigger active transport of biomolecules, theorists from Erwin Frey's group, in collaboration with Petra Schuille's research laboratory at the Max-Planck Institute for Biochemistry (MPIB), have developed a highly controllable in-vitro platform. They mimicked the formation of MinDE patterns on artificial membranes and developed a modular synthetic cargo: a DNA origami scaffold with multiple streptavidin building blocks. With these nanostructures, they were able to show that transport depends on the effective size of the cargo (which also works for small molecules like single streptavidin) and that MinDE can even sort molecules by size. These well-controlled experiments allowed them to determine the underlying transport mechanism using a theoretical analysis in which they tested the predictions of several possible mechanisms based on either thermal

equilibrium effects or true nonequilibrium dynamics. They found that the experiments could only be explained by diffusiophoresis driven by nonequilibrium currents from ATP-consuming active proteins. Such nonequilibrium currents occur in pattern-forming systems in the form of reactive currents that establish a gradient and diffusive currents. In their case, diffusive currents couple to cargo on the membrane via effective mesoscopic friction, driving diffusiophoretic transport.

Diffusiophoresis was first described by Derjaguin 50 years ago and has long been demonstrated for colloidal suspensions. As other physicochemical mechanisms such as liquid-liquid phase separation come to the fore in biology, diffusiophoresis may represent a new type of general transport mechanism in cells that has not yet been described in biology. This mechanism may be particularly important in simpler biological systems such as prokaryotes and early life forms, which lack the highly complex motor proteins of higher organisms. Beatrice Ramm received the 2020 ORIGINS PhD Award for this outstanding discovery in molecular and cellular biophysics that has the potential to change textbook knowledge.

CN-8

EMERGENCE AND NON-EQUILIBRIUM

Classification of the exotic quarkonium state X(3915) at the Belle experiment

SUMMARY

At the heart of understanding the structure of visible matter lies the interpretation of the zoo of newly observed hadrons that contain heavy quark-antiquark pairs. The technologies to uniquely determine the quantum numbers of their quantum mechanical states require both the expertise to perform complex spin-parity analyses and the knowledge of how to extract the rather small sample of well identified events from the large data set of the Belle experiment. This technical know-how is indeed present at the ORIGINS cluster, however in the context of very different scientific projects. In this recently started collaboration theorists and experimentalists from ORIGINS repurpose their skills to tackle the classification of an exotic quarkonium state.

THE STORY

Within the last 15 years a plethora of new mesons have been discovered carrying two or more heavy quarks of the flavours Charm and/or Bottom. These systems of heavy quark pairs have stunned theorists and experimentalists alike and turned the field of flavour physics – long thought to be well under control – into one of the most active research areas in particle physics, specifically in quantum chromodynamics (QCD), the theory of strong interactions. Since most excitations of such heavy-heavy systems have been identified and found to be in good agreement with all model calculations, the structure of the new mesons remains an unsolved problem. Thus, new topological structures and flavour structures ranging from tetraquark-systems to molecular type 2-meson bound states have been discussed.

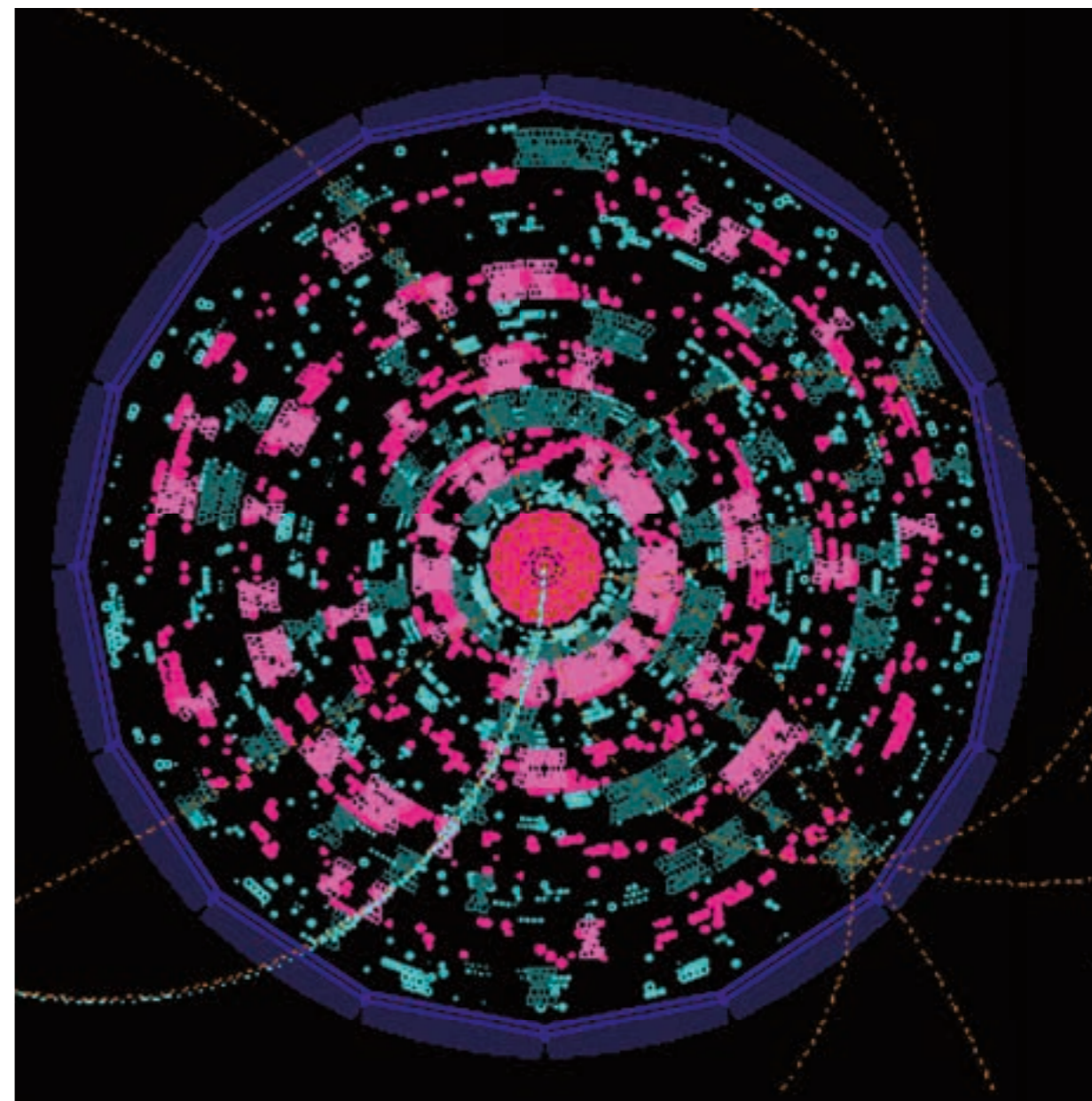
The exact knowledge of the spin and parity of such states (the quantum-mechanical fingerprints of hadrons) allows to strongly constrain interpretations and also to build families of

new states with supposedly similar structures. However, the techniques to identify these fingerprints are not developed within the community who conducts the (often simplistic) searches for new hadrons. Moreover, data samples are scarce and the evaluation of angular distributions and correlations requires a large number of events.

In principle the necessary tools have been developed to disentangle the spectra of light-flavoured hadrons, and ORIGINS scientists working with COMPASS are at the forefront of such techniques. This project brings together Boris Grube (TUM, formerly working in the group of Stephan Paul) and Thomas Kuhr (LMU) and thus uniquely combines the expertise of performing spin-parity analysis with the expertise of singling out clean samples of heavy hadrons at the Belle experiment at KEK. In order to collaborate, Grube joined the Belle experiment and together they trained a new PhD student, Yaroslav Kulii (LMU), in performing such an analysis that is novel at particle colliders

such as B-factories. The cross-disciplinary funding and mentoring of PhD students is only possible in a research network like ORIGINS.

Kulii is now two years into the project and has mastered many unforeseen difficulties, mostly related to verifying previous analysis on this state and the complex simulation work, for which the framework was non-existent within this collaboration. With the data and formulism at hand, Kulii is at the verge of performing fits to the extracted experimental distribution to return the answer of the quantum nature of the X(3915) state. There is no result available yet, but the project is already a big success in terms of analysis-technology development. It requires a strong engagement of Kuhr and Grube, who committed to this project despite his new obligation at the JLAB US Natl. Laboratory. If successful, this technique can easily be transferred to other exotic heavy quark systems and thus become a powerful tool to understand the nature of exotic quarkonia.



Visualization of charged particles traversing the drift chamber of the Belle II experiment. © Belle II/SuperKEKB



PUBLICATIONS

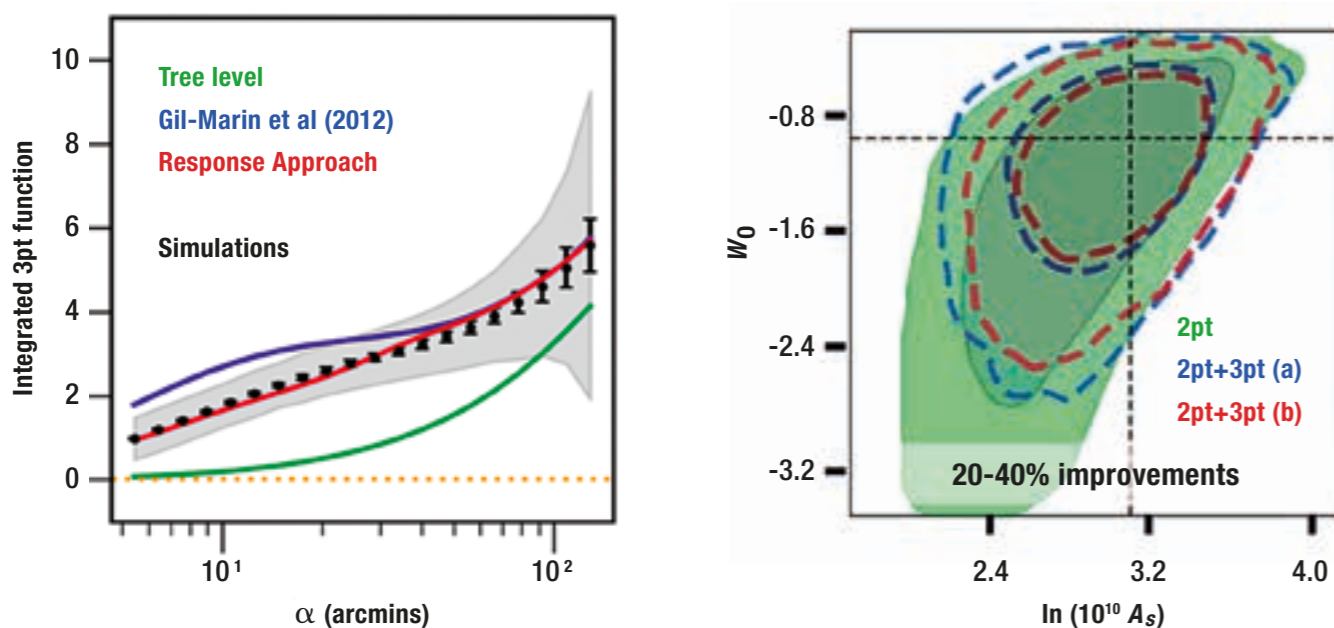
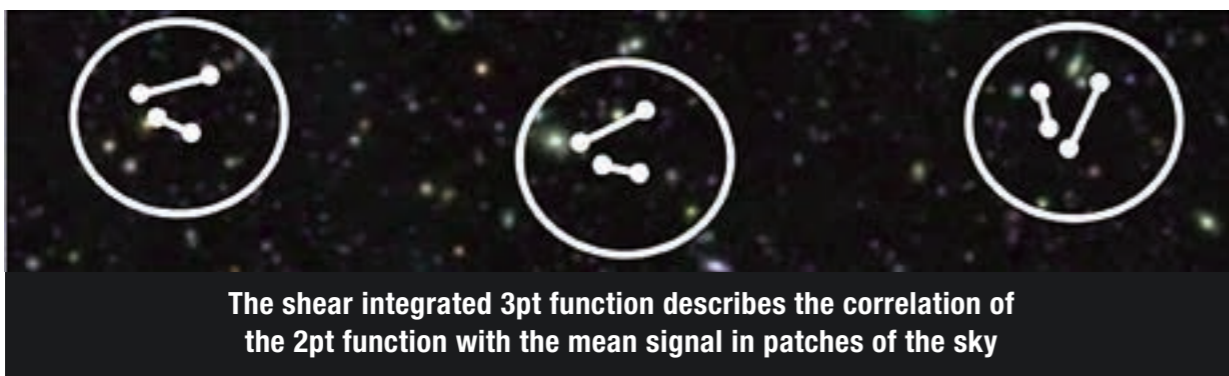
* Y. Kulii, B. Grube, T. Kuhr
(in preparation)



FUNDING INFORMATION

* PhD student Yaroslav Kulii
funded by ORIGINS

Cosmology beyond the 2-point function



The integrated shear 3-point function is a new cosmic shear statistic that is easy to measure and can be predicted robustly in the non-linear regime. Researchers at ORIGINS have shown that adding this non-Gaussian information in data constraint analyses can significantly improve the precision on cosmological parameters like the amplitude of fluctuations A_s or the dark energy equation of state w_0 . These works have pointed to a new path towards the systematic exploration of non-Gaussian information in LSS surveys.

SUMMARY

The cosmic energy density is not uniform but show ripples: macroscopic traces of quantum fluctuations that hint at an inflationary period in the early Universe. Popular tools to extract information encoded in this large-scale structure (LSS) are 2-point statistics which characterise the probability of observing pairs of galaxies as a function of their absolute separation. However, 2-point statistics cannot describe non-Gaussian density fluctuations that stem from a non-linear evolution of the density field. A recent collaboration of researchers at ORIGINS has developed a framework based on a new higher-order statistic called the integrated 3-point correlation function. In the context of a simulated parameter likelihood analysis for a survey like the Dark Energy Survey Year 3, this new statistic is able to lead to improvements of 20–40% in parameter constraints.

THE STORY

The distribution of mass and energy in the Universe on large scales, called the large-scale structure (LSS), encodes a wealth of information on the main components of the current standard model of cosmology: dark energy, dark matter, inflation and gravity. Current methods to extract this information from LSS data are based on analyses of the 2-point correlation function (2PCF), and as a result fail to capture important cosmological information in higher-order N-point functions.

Recently, a collaboration between the ORIGINS researchers Alex Barreira (ORIGINS Fellow), Oliver Friedrich (LMU), PhD student Zhengyangguang (Laurence) Gong (LMU), PhD student Anik Halder (LMU) and Stella Seitz (LMU) has started a program towards a robust and systematic exploration of non-Gaussian information in the LSS. They proposed a new higher-order statistic called the integrated shear 3-point correlation function (3PCF). Cosmic shear observations probe the total density field along the line-of-sight between the observer and background source galaxies. This new statistic describes the correlation of the local 2PCF with the mean value of the shear field in patches of the survey (Figure, top panel), which is sensitive to squeezed configurations of the 3PCF.

This statistic enjoys two key advantages relative to other higher-order statistics. The first is that it is easy to measure: it requires only the estimation of the (i) mean field and (ii) 2PCF in patches of the survey, for which there are very efficient and well-tested estimators. The second is that it admits accurate theoretical predictions as a function of cosmological and baryonic physics parameters using a formalism known as the Response Approach to Perturbation Theory. The response approach was developed in 2017 by Alex Barreira and Fabian Schmidt (MPA). Anik Halder has recently used it to build an accurate theoretical model for the integrated shear 3PCF (Figure, bottom left). In a subsequent paper led by Gong, the group developed an analysis pipeline for cosmological constraints using this new statistic. This included the use of simulations to build realistic cosmic shear survey mocks with the Dark Energy Survey Year 3 (DES-Y3) specifications, which accounts for important observational systematics in the theory model (intrinsic alignments, photometric redshift uncertainties and multiplicative shear biases). Moreover, they developed a machine learning-based emulator to speed up the calcu-

lation of the theory predictions as a function of the model parameters. Using a Monte-Carlo Markov Chain simulated likelihood analysis, this work shows that, relative to conventional 2PCF analyses, the integrated shear 3PCF can lead to improvements of 20–40% on the constraints of parameters like the amplitude of fluctuations A_s (or σ_8) and the dark energy equation of state parameter w_0 (Figure, bottom right). Crucially, these are improvements that can be obtained for existing publicly available data. With the usefulness of the integrated shear 3PCF established with this analysis pipeline, this collaboration will apply it to data from DES-Y3 in upcoming works to investigate the potential of this new statistic and to improve cosmological constraints using real cosmic shear data.

Overall, this work opened the door to the systematic exploration of information beyond the 2PCF in cosmic shear surveys. In an upcoming paper led by Halder, the same group of researchers will generalize this statistic to include also the foreground galaxy distribution and its cross-correlations with the cosmic shear field.



PUBLICATIONS

- * A. Barreira & F. Schmidt (2017), JCAP 06 (2017) 053, arXiv:1703.09212.
- * A. Halder, O. Friedrich, S. Seitz & T. Varga (2021), MNRAS(506), arXiv:2102.101780.
- * A. Halder & A. Barreira (2022), MNRAS(515), arXiv:2201.05607.
- * L. Gong, A. Halder, A. Barreira, S. Seitz & O. Friedrich (2023), preprint, arXiv:2304.01187.
- * A. Halder et al, in preparation.



FUNDING INFORMATION

- * ORIGINS Fellow Alex Barreira is funded by ORIGINS.
- * These works made use of the Computational Center for Particle and Astrophysics (C2PAP), which is an ORIGINS infrastructure.

Multi-Scale Star- and Planet Formation

SUMMARY

A recent collaboration among observers and theorists from ORIGINS showed that star and planet formation is intimately coupled to the large scale turbulent interstellar medium (ISM) by gas streamers. The streamers originate in the ISM on spatial scales of parsecs (206265 astronomical units, AU) and directly feed protostars in formation and their surrounding protoplanetary discs on AU scales, bridging up to 6 orders of length scales. This demonstrates the intimate coupling of processes on very different scales in the Universe and the importance to self-consistently bridge those scales.

THE STORY

The standard paradigm of gas and planet formation has been that stars and their surrounding protoplanetary discs form by gravitational collapse of dense clumps of cold molecular gas. A clump condenses out of the ISM and becomes self-gravitating, developing a roughly spherical shape and a centrally concentrated density distribution. The clump itself is kinematically quiet with internal subsonic irregular motions, embedded in the turbulent, highly supersonic ISM environment. When the clump reaches a critical mass it disconnects completely from the environment and collapse. Low angular momentum gas now settles into a central star while gas with higher angular momentum accumulates around the star and forms a homogeneous protoplanetary disc. The disc in later phases could develop structure, e. g. due to gravitational and magneto-rotational instabilities. In addition, planets grow in the disc by dust coagulation and open gaps that have been detected e. g. with the Atacama Large Millimeter Array (ALMA).

In a recent Nature paper ORIGINS scientists Paola Caselli and Bo Zhao from

MPE demonstrated that this scenario is oversimplified. They observed one of the youngest protoplanetary discs in a stellar binary system and detected for the first time a very long, dense gas streamer that connects the disc on AU scales to the large-scale gas environment. ORIGINS cluster funded postdoc, Stefan Heigl (LMU), was working at that time on the origin of turbulent molecular filaments in the ISM of galaxies. He found that his filaments can condense into molecular cloud cores which inherit turbulent motions from the filament within which they form. Motivated by the results of Pineda et al. he then zoomed into his gravitationally collapsing cores and indeed detected a protoplanetary disc surrounding a young protostar.

This demonstrates that collapsing cores are not isolated and spherically symmetric, but that they interact with the filamentary, turbulent ISM environment which produces irregularities that generate streamers. These streamers then funnel gas over several orders of magnitudes in length directly into the discs. Both, observations and

the numerical simulations find that chemically fresh material, infalling through the streamers, leads to a highly structured disc with strong implications for disc chemistry, disc evolution and the formation of planets. They open a new window in our understanding of the multi-scale, interconnected physics of the universe where processes on very different length scales are intimately coupled and need to be considered in combination and self-consistently.

Within an ORIGINS seed funded collaboration between Til Birnstiel (LMU) and Klaus Dolag (LMU) and Petra Schulle (MPIB), as well as Andreas Burkert (LMU) and Torsten Enßlin (MPA), 3D printed cubes were developed for education and visualisation of complex 3D structures. Heigl's simulation of a prominent, streamer-fed protoplanetary disc, even including magnetic field lines, has been printed and provides an excellent tool in order to study and better understand the complex physics of star- and planet formation.

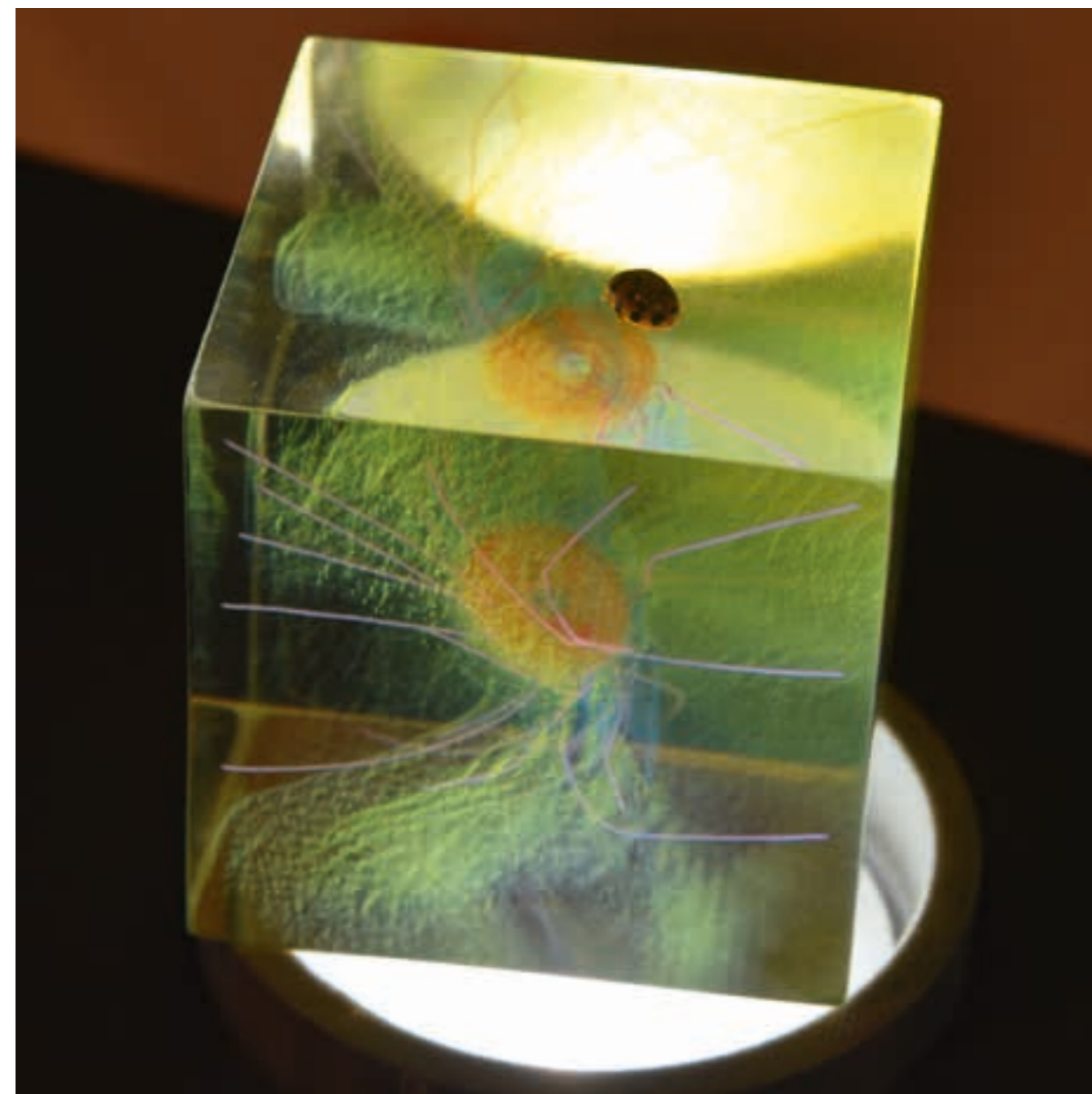


Fig. 1

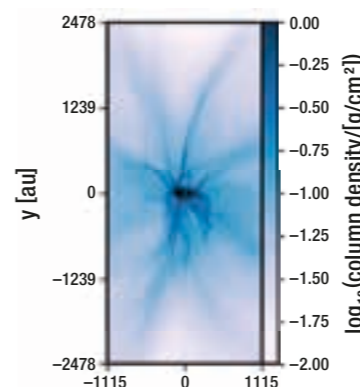


Fig. 2

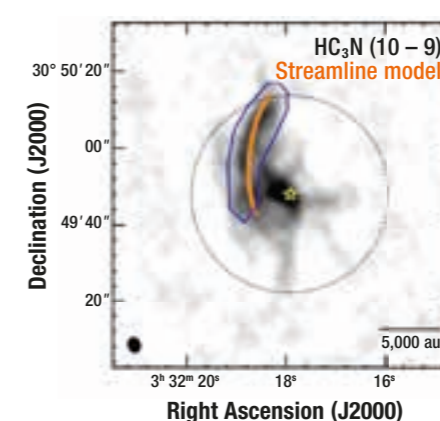


Fig. 3

Fig. 1:
3D printed cube of a simulation of a streamer-fed protoplanetary disc. And a ladybug.
© Ina Haneburger / ORIGINS Cluster

Fig. 2:
Simulation of a streamer. © Heigl et al., 2023 in prep

Fig. 3:
Observation of Per-emb-2 (IRAS 03292+3039), a protostellar system in the Perseus molecular cloud. It hosts a young close stellar binary system that is still in the process of formation. © Pineda et al., 2020



PUBLICATIONS

- * S. Heigl et al., 2023 in preparation



FUNDING INFORMATION

- * ORIGINS Seed-Project (SP2022-1)
- * ORIGINS funded postdoc Stefan Heigl

RU-D

GALAXIES, STARS AND PLANETS

Physical non-equilibria for prebiotic nucleic acid chemistry

SUMMARY

A recent interdisciplinary collaboration among biophysicists (Braun, Gerland, Mutschler), astrophysicists (Ercolano) and geoscientists (Scheu) from the Excellence Cluster ORIGINS reported state-of-the-art perspectives about physical non-equilibria for prebiotic nucleic acid chemistry. The authors show how the interplay of replication chemistry with the strand separation and length selectivity of non-equilibrium physics can be provided by plausible geological environments. Such environments are characterized by gradients in temperature, salts, pH, ultraviolet irradiation or CO₂. Air-water interfaces that are exposed to a plausible CO₂-rich atmosphere enable a) sense and antisense RNA replication as well as b) template-dependent synthesis and c) catalysis of a functional ribozyme in a one-pot reaction. Especially dew in a simulated heated rock pore in a CO₂-rich early Earth atmosphere was identified as key component kick-starting molecular evolution. This accelerates otherwise intolerably slow reactions involving polymerases, which are the enzymes that make the nucleic acids of DNA or RNA.

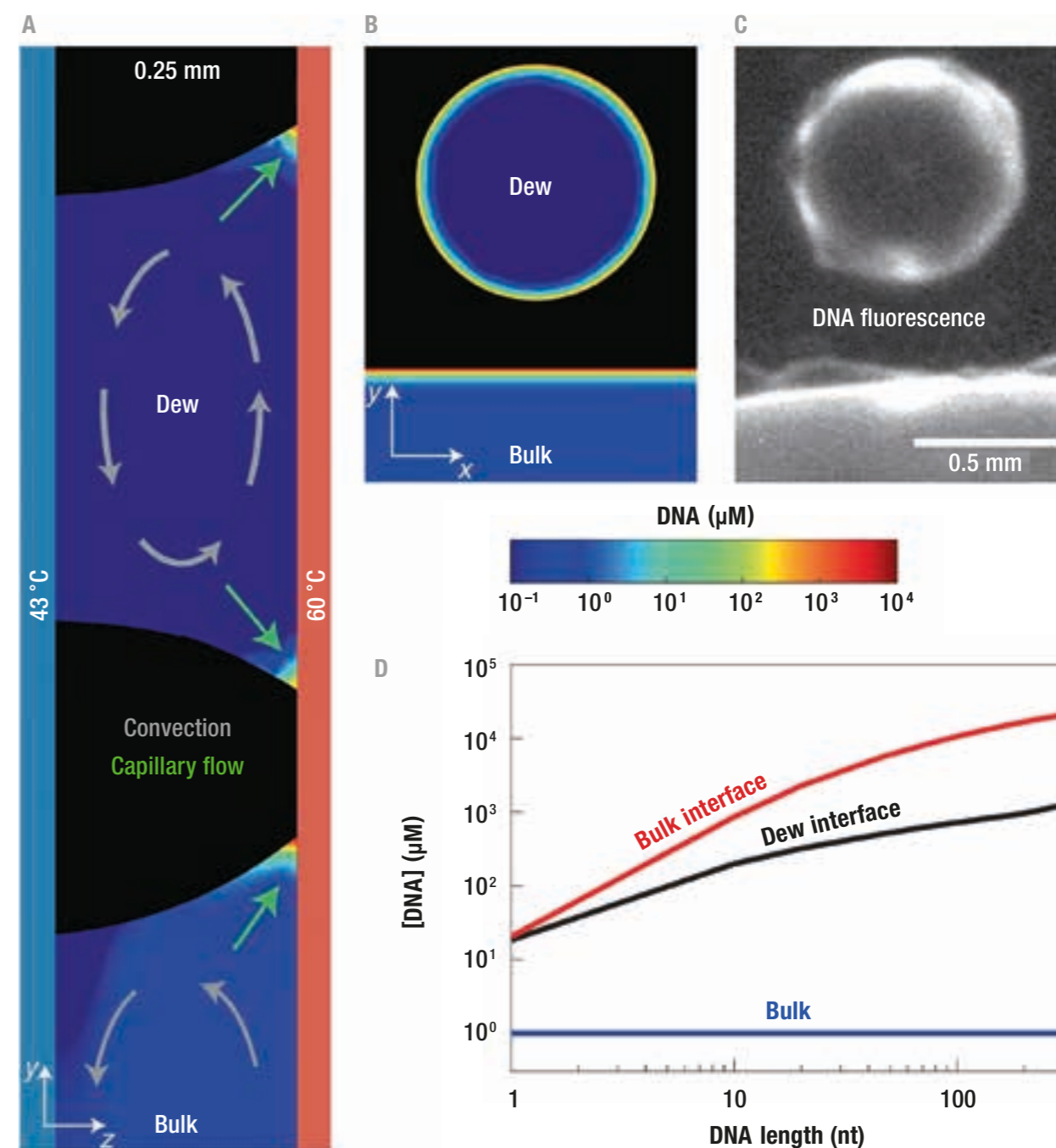
THE STORY

The understanding of possible mechanisms for the origin of life requires the study of environmental conditions suitable to generate and sustain the first stages of molecular evolution. Geological systems of the early Earth are sources of local non-equilibrium conditions, driven by the slowly cooling early Earth under a young faint Sun. By entropy arguments, such non-equilibria are essential because life could not have originated under equilibrium conditions. These non-equilibria – such as concentration gradients, salt and pH cycles, irradiation or temperature differences – actively drive the system towards a continuous and dynamic self-organization. They could be provided by external

forces such as geothermal heating, solar and isotopic irradiation, day-night cycles and atmospheric phenomena. Brief, physical non-equilibria drive molecular evolution.

The identification of suitable and early Earth-realistic environmental conditions that trigger physical non-equilibria enabling molecular evolution, e.g. of RNA/DNA sequences thus is essential. The ORIGINS PI groups Braun, Gerland and Mutschler (former ORIGINS PI, now at TU Dortmund) showed the importance of CO₂-dew droplets in molecular evolution. They enable sense and antisense RNA replication as well as template-dependent synthesis and

catalysis of a functional ribozyme in a one-pot reaction. The experimental CO₂ dew chamber mimics the ubiquitous setting of a heated rock pore in a CO₂-rich Hadean atmosphere. CO₂ dew droplets strongly increase the concentrations at gas-water interfaces. During wet-dry cycles, they induce fluctuations between low and high salt concentration and a periodic change between acidic and neutral pH. The combination of the above processes enhances the replication of oligonucleotides with increasing lengths. This opens the door to open-ended Darwinian evolution.



Simulations verify the accumulation of longer DNA at gas-water interfaces as observed in the fluorescence image. Due to their lower diffusion coefficient, longer strands are favoured and accumulate more strongly. © Ianeselli et al (2022).



PUBLICATIONS

- * A. Ianeselli, A. Salditt, C. Mast, B. Ercolano, C. L. Kufner, B., Scheu & D. Braun (2023). Physical non-equilibria for prebiotic nucleic acid chemistry. *Nature Reviews Physics*, 1-11.
- * A. Salditt, L. Karr, E. Salibi, K. Le Vay, D. Braun & H. Mutschler (2023). Ribozyme-mediated RNA synthesis and replication in a model Hadean microenvironment. *Nature Communications*, 14(1), 1495.
- * A. Ianeselli, M. Atienza, P.W. Kudella, U. Gerland, C. B. Mast & D. Braun (2022). Water cycles in a Hadean CO₂ atmosphere drive the evolution of long DNA. *Nature Physics*, 18(5), 579-585.



FUNDING INFORMATION

- * PhD Anna-Lena Salditt is partially funded by ORIGINS
- * PhD Leonie Karr is partially funded by ORIGINS
- * IDSL state of the art "ORIGINS of Life" Lab mostly funded by ORIGINS
- * ORIGINS PhD Prize winner 2022 – Alan Ianeselli – for his thesis "Hadean water-dew cycles drive the evolution of DNA and protocells"
- * Hannes Mutschler (Prof. at TU Dortmund) is a former PI of ORIGINS
- * Alan Ianeselli funded by ERC Advanced grant "AutoEvo" and the Simons collaboration on the Origins of Life

RU-E

PREBIOTIC MOLECULES AND LIFE



CONTACT: Excellence Cluster ORIGINS · Boltzmannstr. 2 · D-85748 Garching
Tel: +49 89 35831-7100 · info@origins-cluster.de · www.origins-cluster.de

DFG Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)
under Germany's Excellence Strategy – EXC-2094 – 390783311.

