FIAS Frankfurt Institute for Advanced Studies

2023

Content

FIAS

science for the reality of tomorrow

Dear colleagues,

Dear friends and supporters of our science,

Dear knowledge seekers,

New science results are emerging everywhere at FIAS and documented in high-level publications, in press releases and in specific outreach activities. Indeed, the portfolio of topics is so broad that it is difficult to reconcile all the investigations under one roof.

We tried nevertheless and organised a conference with the all-encompassing title: Condensed Complexity – The Essence of Information Processing and Cognition?, which turned out to become a highlight of the year at FIAS. The conference brought together experts from biology, chemistry, physics, neuroscience, and computing, including quantum computing, to expose their approach of understanding and the process of recognition. In doing so, they identified many commonalities and engaged in discussions about the current hype of artificial intelligence and the question of intelligence proper. The positions varied in a wide range: AI considered just a useful tool - to being on the verge of outsmarting humans and thus redefining research and understanding altogether. The culminating round table discussions provided a snapshot of the current developments and demonstrated the need for a better definition of cognition in the first place.

The conference has also been used to sharpen the discussion on the science strategy of the institute with a view of laying out its future course. In the wake of last year's changes in the management, FIAS is now preparing its scientific strategy and role in the Frankfurt scientific landscape. The overarching motivation of furthering scientific understanding finds a common basis in the use of digital twins, near-reality virtual models of the world that can be scientifically interrogated.

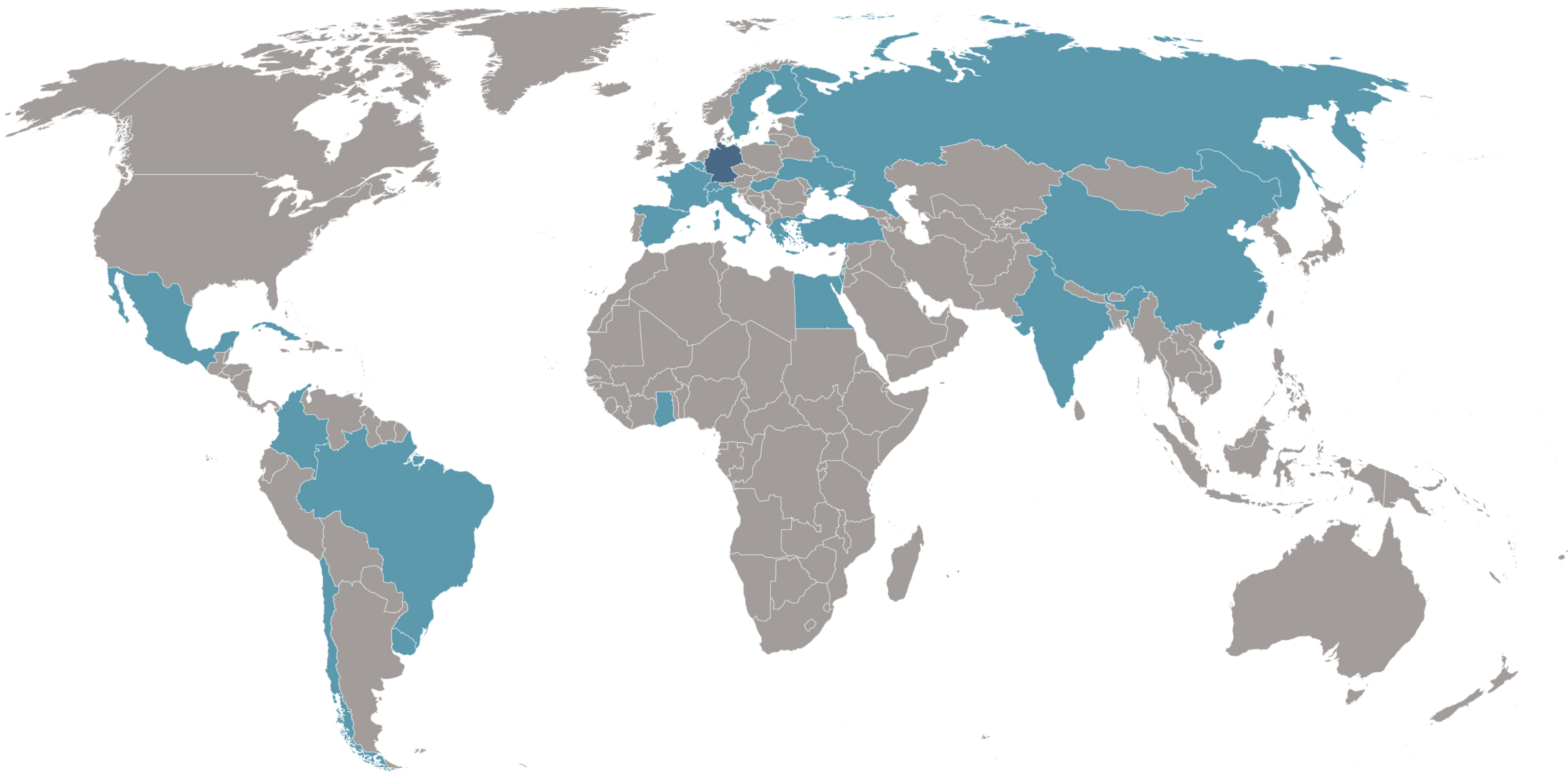
It is reassuring that the language of science forms a bridge across so many topics and so many personalities. Indeed, it is the diversity in science that fosters progress and understanding. In an increasingly fractured world with escalating extreme opinions a special role falls on scientists: to emphasise the importance of free and open exchange of differing opinions as the motor of societal development. FIAS takes a firm stance and opposes any restrictive or discriminating developments. We live and enjoy the open atmosphere at FIAS and cherish the many benefits that reach far beyond research.

My thanks go to all employees, to those who have contributed to this report and to those whose contribution is not directly visible, but without whom FIAS could not be what it is today.

Enjoy the reading.

On behalf of all FIAS members

FIAS 2023 in Numbers



133 people from

23 different countries

32 Fellows
17 Postdocs
46 Doctoral students
13 Adjunct Fellows
11 Administration members
14 Undergraduate students

19
visitig scientists

7
new doctoral degrees

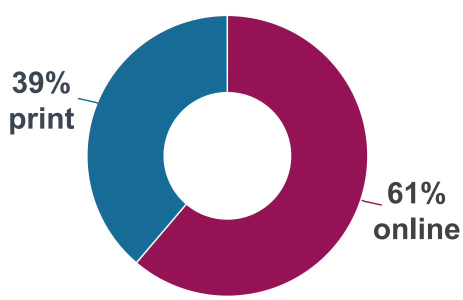
35%
female employees

360
publications

10
workshops and conferences

3
seminar series

26
external events



49
press mentions

more than
4.5 Mio €
project funding

HIGHLIGHTS 2023

A detailed analysis of the eruption behaviour of the island volcanoes Stromboli, Mount Etna (Italy), Yasur (Vanuatu), and Whakaari (New Zealand) was published by Darius Fenner from Nishtha Srivastava's team together with Patrick Laumann and Georg Rümpker. Such analyses of past major and minor events can help to understand volcanic eruptions, including the underlying physical and chemical processes.

Understanding island volcanoes and their threats

Nishtha Srivastava`s group employed a recently developed approach to detect seismo-volcanic events. It catalogues all small and large seismo-volcanic events including major eruptions continuously at stations near volcanoes. The automated and very powerful method "Adaptive-Window Volcanic Event Selection Analysis Module" (AWESAM), presented by the FIAS Seismology & Artificial Intelligence (SAI) working group last year, allows volcanic events to be detected quickly.

In their current research, the group extended their research by analysing the available data from up to fifteen years in detail, for example the time intervals between events, the amplitudes and the relationship between amplitude and frequency. This enabled them to identify differences and common patterns in volcanic events.

For example, they observed that there are more large eruptions on Stromboli than one might expect based on known distributions. Building on their previous findings, this study assesses and extends the understanding of this phenomenon based on a decade of data. For example, a certain pattern was found before and after the two heavy Stromboli eruptions in 2019, and the expanded dataset confirms the statistical significance of the results. However, so far this pattern has only been observed for Stromboli, which raises questions about its uniqueness.

Furthermore, the study classifies event types for Stromboli using an unsupervised machine learning approach. It reveals alternating patterns before and after paroxysms. The group was able to subdivide these patterns in more detail for the first time. Based on a clustering algorithm, they classified the frequencies of the events more precisely, for example. These patterns can be important for predicting large eruptions.

Using an identical approach for all four volcanoes, the group found similar behaviour despite different types and activities. At Whakaari, a certain pattern of repetition of large events was evident. As this observation is based on data from a single station, further in-depth investigations are needed as more data become available. "In a next step, we want to investigate if there are signatures prior to major eruptions", says first author Darius Fenner. "Our method offers a promising basis for more accurate volcano monitoring and for a better understanding of the underlying processes."

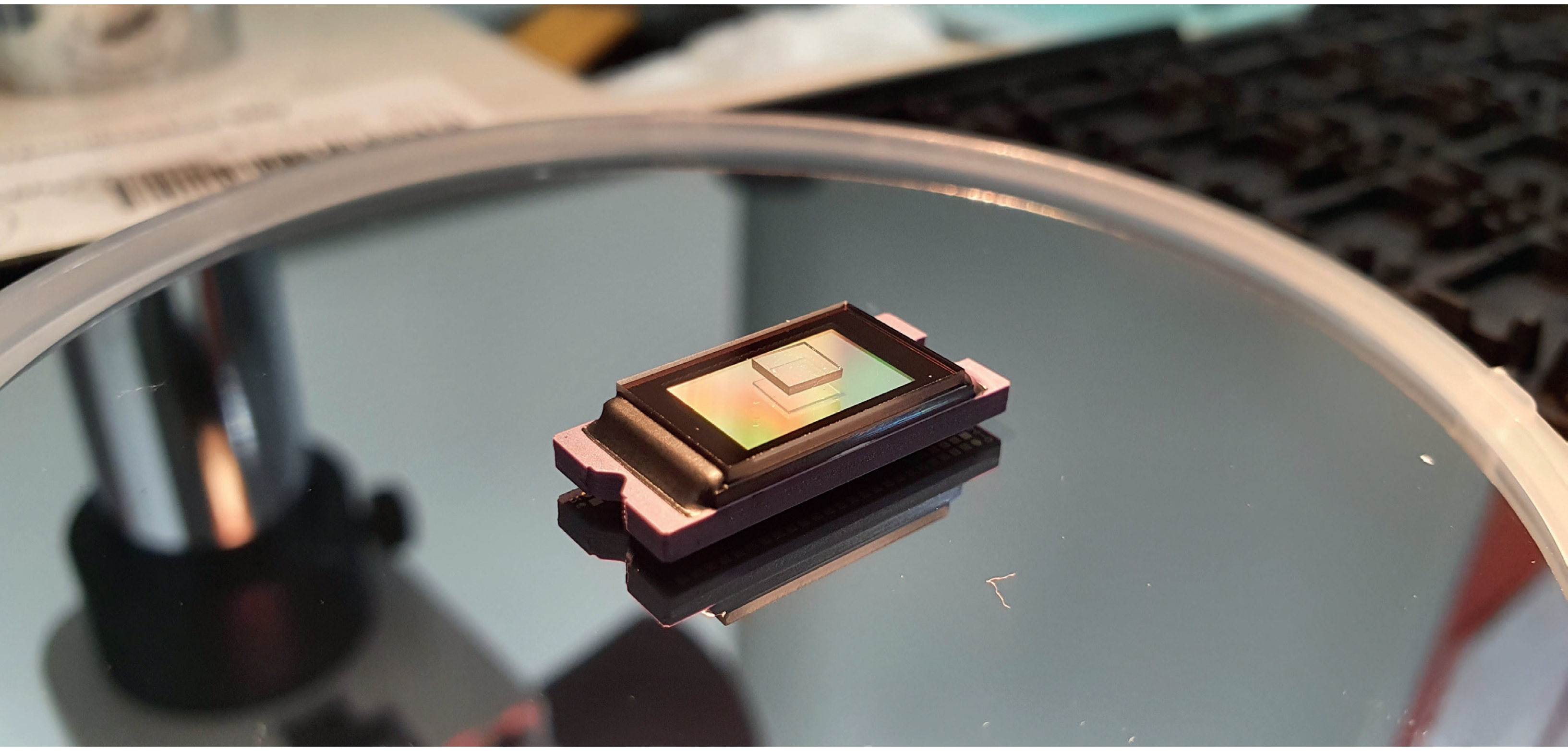
Publication: Darius Fenner, Georg Rümpker, Patrick Laumann, and Nishtha Srivastava, Amplitude and inter-event time statistics for the island volcanoes Stromboli, Mount Etna, Yasur, and Whakaari. Front. Earth Sci. 11:1228103, doi: 10.3389/feart.2023.1228103, https://www.frontiersin.org/articles/10.3389/feart.2023.1228103/full

Nobel prize winner Südhof new FIAS Laureate

Nobel Prize winner Thomas Südhof received the "FIAS Senior Fellow Laureatus" on 8 November 2023. The award ceremony had been postponed several times due to Covid. FIAS Director Eckhard Elsen was now able to hand over the certificate and cup. The prize money of 10,000 euros was donated by Stiftung Giersch.

Before the award ceremony, the prizewinner, head of Südhof Laboratory at Stanford University Medical School, gave a sophisticated lecture on his current research. In the packed hall at FIAS, the biochemist described detailed findings on the storage of information in memory. The basis for his research was the observation that mice prefer cocoa flavour to cinnamon flavour. A "lead mouse" with a preference for cinnamon can permanently change this preference in observing mice. Using elaborate experiments, Südhof's group was able to track and identify the molecular and genetic changes required for this in the mice's brains down to the details. The result is a confusing network of pathways across countless areas of the brain that are necessary at certain times to anchor the taste preference. "This is only one specific form of memory formation," Südhof qualifies the complex findings. But it is a complicated combination of odour, social factor, and permanence.

Nobel Prize winner Thomas Südhof (right) honoured by the Giersch Foundation's Chairman Stephan Rapp (left) and FIAS Director Eckhard Elsen (centre).



The first quantum computer at Goethe University will be installed under the direction of FIAS fellow Thomas Lippert. Quantum computing is a future technology that aims to master tasks in the field of computer simulation and AI that were previously too large or even unsolvable with digital methods.
Photo: NV Spin qubits on a photonic microchip (c) XeedQ GmbH.

Quantum computer coming to Frankfurt - headed by FIAS Fellow Thomas Lippert

The contract on the first Frankfurt quantum computer called "Baby Diamond" was signed in December. It will be delivered by the start-up XeedQ GmbH in the first quarter of 2024. The quantum computer uses a small artificial diamond, as known from industrial applications, in which nitrogen atoms are embedded. They each induce a defect that can be used as a central qubit. Spins of atoms can be controlled as further qubits around this defect. This makes practical quantum computing possible.

“With our entry-level system, we are pursuing the idea of a compact quantum computer that can already be used at room temperature, does not require any special cryogenic cooling, can be set up in a small laboratory and is particularly energy-efficient,” says Thomas Lippert, FIAS Senior Fellow and head of the Modular Supercomputing and Quantum Computing working group at Goethe University. “With the quantum computer, we are deliberately taking a stand against the current monopolisation of large companies that hide their systems behind paywalls. As it is a compact system, we can already train students hands-on and directly on the device. We have to use this momentum if we want to be fit for the future.”

The quantum computer is part of the Frankfurt roadmap, which aims to procure up to 16 high-quality qubits by 2025 and to gradually increase this number in the future. The pilot system will help to build an infrastructure that will closely link quantum computing with high-performance computing. The system is being developed by XeedQ GmbH, a company based in Leipzig, and at the DLR Innovation Centre in Ulm. XeedQ GmbH is funded by the DLR Quantum Computer Initiative to develop a scalable quantum computer technology.

The quantum computer will be located on the historic Bockenheim University campus, where Stern and Gerlach’s famous experiment more than 100 years ago laid the foundation for quantum computing today and was an important part of the first quantum revolution.

Ulrich Schielein, Chief Information Officer (CIO) and Vice President for Digitalisation at Goethe University, explains: “The treatment of completely new categories of problems from the world of finance, logistics in rail, air and road transport, medicine and biology, weather and climate research, but also from basic sciences such as physics and chemistry or the training of basic models of artificial intelligence seems to be feasible in just a few years”.

FIAS also shed light on this topic at the Giersch International Conference this year: Kristel Michielsen (Jülich) reported on her quantum simulator, i. e. a “classical” computer with GPUs set up as a quantum computer. Alberto di Meglio gave an overview of the quantum initiative at CERN. In a recent lecture at FIAS, Steven Rayan (Saskatchewan, Canada) explained the theoretical foundations of quantum computing and highlighted its significance for society.

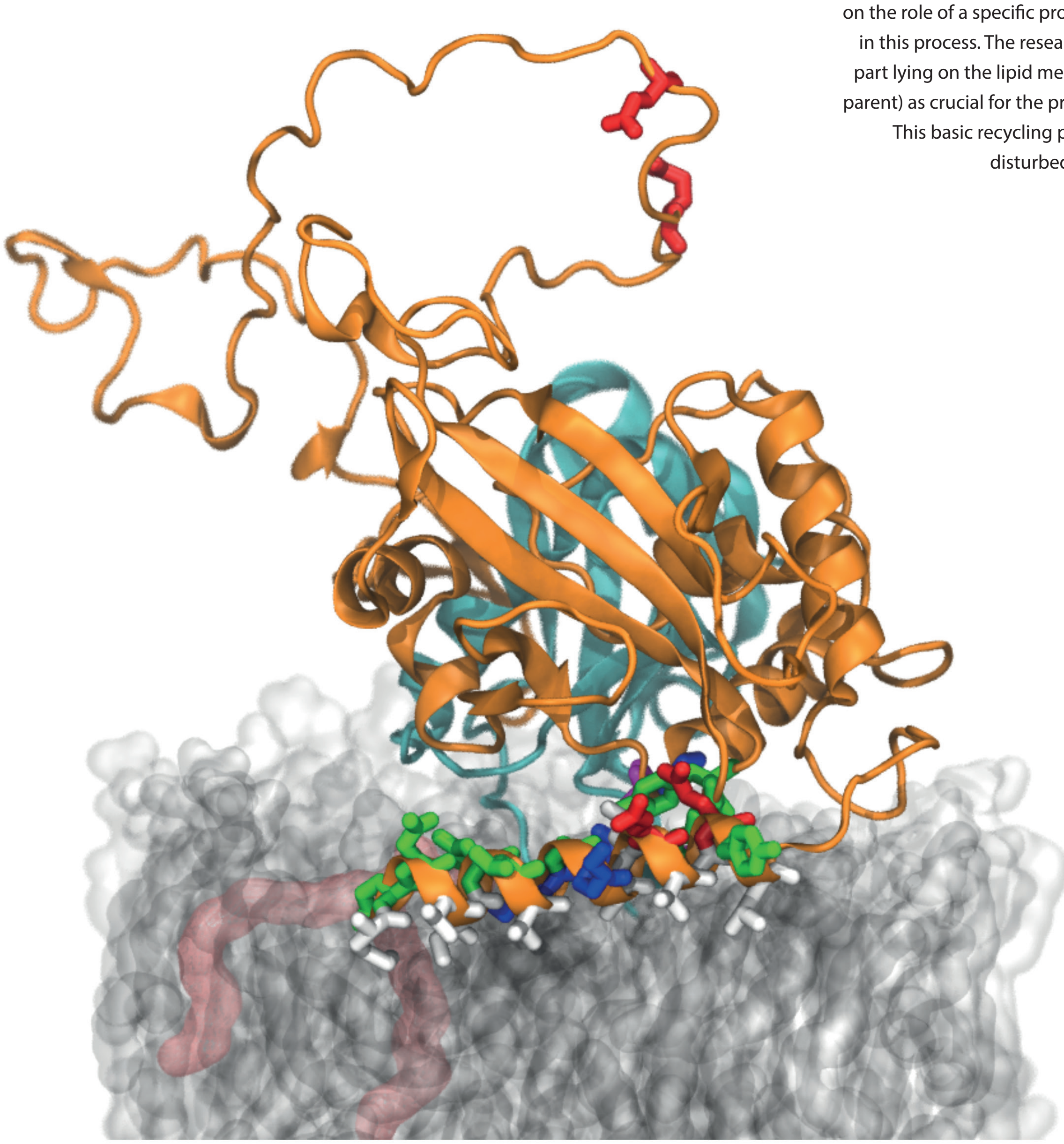
First place for “green” mainframe computer

The high-performance computer “Goethe NHR”, developed by FIAS Senior Fellow Volker Lindenstruth, achieved first place among the most energy-efficient mainframe computers in Germany and seventh place among the fastest. In the published rankings (November 2023), the mainframe is also far ahead in the worldwide “Green 500” comparison: thanks to its outstanding computing efficiency, it is in 9th place. This success is particularly remarkable in view of the significantly lower investment volume compared to other mainframes. Students and doctoral candidates from Lindenstruth’s research group are also involved in this success.

Volker Lindenstruth, FIAS board member and Fellow since 2007, is one of Germany’s most respected experts on the optimisation and energy efficiency of mainframe computers. Over the past ten years, computers designed by him have often occupied top positions in the national and world rankings of the most energy-efficient supercomputers, which are published every six months.

Frankfurt University’s President Enrico Schleiff congratulated Lindenstruth and Thorsten Kollegger on their success in the sustainable optimisation of mainframes: “Thanks to the outstanding work of this research group, Goethe University is a pioneer in the field of green mainframes in Germany and beyond”. Thanks to its efficient and sustainably produced computing power for research, Goethe University is very well positioned within the NHR consortium in Germany, he said.

FIAS researchers made a significant breakthrough in understanding the process of autophagy, a vital cellular mechanism responsible for the degradation and recycling of damaged cellular components. Their findings shed light on the role of a specific protein, ATG3 (orange), in this process. The researchers identified the part lying on the lipid membrane (grey/transparent) as crucial for the process of autophagy. This basic recycling process in our cells is disturbed in certain diseases.



Insights into the recycling of our cells

Biological cells developed a sophisticated "housekeeping" system called autophagy. Cells are made of numerous smaller components, ranging from small molecules, sugars, and individual proteins to lipids that assemble in large membranes. In a cell, all these components are organized in an enormously complex choreography, necessary for the correct cellular functioning and, ultimately, the health and survival of the whole organism. Sometimes elements of this choreography get damaged and the cell must eliminate them before they impede its normal functioning. In other situations, the cell can experience a lack of nutrients, such that it must recycle existing molecular complexes to focus on essential activities. In these situations, autophagy gets activated. From the Greek "self-eating," autophagy is a complex pathway that involves the concerted action of many regulatory proteins that control the formation of a large vesicle, which will contain the cellular content meant for recycling. The protein ATG3 plays a crucial role in forming autophagosomes, the structures that encapsulate the materials to be degraded.

The research team around FIAS Fellow Roberto Covino focused on a specific part of the ATG3 protein, known as the amphipathic α helix (AHATG3). They found that this component has unique biophysical properties that allow it to interact with membranes in a strictly controlled manner and are essential for the protein's function in autophagy. Using advanced computational techniques integrated with cell biology experiments, the researchers could observe the dynamics of the ATG3 protein and its interaction with membranes during the autophagy process. They found that the unique properties of ATG3 are crucial for a key step in autophagosome formation.

These findings provide a deeper understanding of the molecular mechanisms underlying autophagy, which could have significant implications for developing treatments for diseases associated with impaired autophagy, such as neurodegenerative disorders and cancer.

Publication: Taki Nishimura, Gianmarco Lazzeri, Noburu Mizushima, Roberto Covino, Sharon A. Tooze, Unique amphipathic α helix drives membrane insertion and enzymatic activity of ATG3, Science Advances 9:25, 2023, DOI: 10.1126/sciadv.adh128

Sensor enables analysis of important cellular scavenger

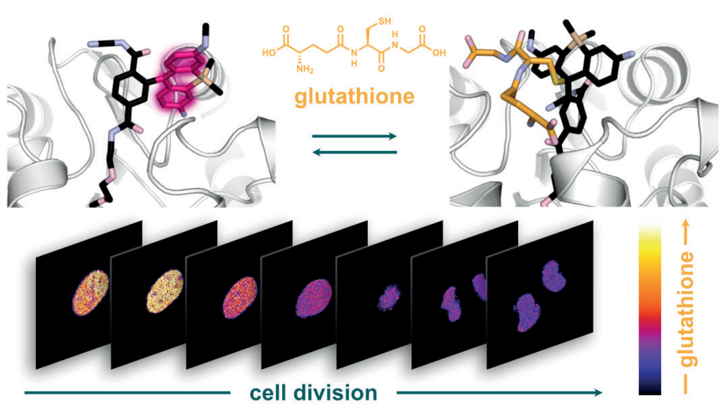
During the metabolism of cells, aggressive oxygen compounds are formed as side products that can damage proteins or DNA. To intercept these oxygen compounds, cells use the peptide glutathione. Researchers from FIAS and the University of Zurich developed a novel sensor to measure the glutathione concentration in cell organelles. The sensor allows precise observation of the important molecule in cell organelles and supports research into related diseases.

Glutathione is a small peptide consisting of three amino acids. It plays a key role in the detoxification of aggressive oxygen compounds and is involved in signal transmission in cells. It is present in the cells in a finely tuned balance of free glutathione and its dimer. Glutathione imbalances occur in cancer, diabetes and neurodegenerative diseases.

In order to better understand the glutathione balance and the associated disease triggers, methods are required to determine the amount of glutathione in cell organelles. So far, fluorescent proteins or small molecules are used as sensors that react with the glutathione molecules. However, the measurement in selected cell organelles has various weaknesses – e. g. the sensor has to cross the cell fluid and can already react with glutathione there.

Sebastian Thallmair and his team developed a glutathione sensor that is activated in cell organelles and thus allows reliable measurements of the glutathione concentration within cell organelles. They used a combination of protein and silicon rhodamine (SiR) dye. The fluorescence of the dye changes from "off" to "on" as soon as it binds to the HaloTag protein. Since HaloTag can be steered in a desired cell organelle before reacting with the dye, the sensor can be targeted in cell organelles.

The resulting hybrid sensor combines the advantages of genetically encoded sensors with the tunability, brightness, and photostability of small molecules. Unlike previous methods, the new sensor TraQ-G sensor only reacts in the organelle of interest. TraQ-G can also be linked to a redox-insensitive fluorescent protein. This allows quantitative measurements of glutathione concentrations in living cells. The researchers were thus able to show that during cell division, the glutathione concentration in the cell nucleus and the cellular fluid are regulated independently.



Publication: Sarah Emmert, Gianluca Quargnali, Sebastian Thallmair und Pablo Rivera-Fuentes, A locally activatable sensor for robust quantification of organellar glutathione, Nature Chemistry (2023). https://doi.org/10.1038/s41557-023-01249-3

Johannes Kirsch, Jürgen Struckmeier, Armin van de Venn, David Vasak and Vladimir Denk (from left to right) describe how the torsion of spacetime can explain the dark energy of standard cosmology. Publication: Armin van de Venn et al.: Torsional dark energy in quadratic gauge gravity, submitted to Eur. Phys. J., arXiv:2211.11868 [gr-qc].

Is “Dark energy” just contorted space-time?

A mathematically inspired extension of Einstein’s general theory of relativity provides new insights into space and time. In their recent publications, David Vasak et al. of Frankfurt Institute for Advanced Studies (FIAS) describe how the torsion of spacetime can explain the dark energy of standard cosmology.

Sponsors visiting FIAS - Presentations by funded scientists

In May, FIAS funders were guests to learn about "biomolecular function unraveled by the computational microscope" and "how computer-based simulations - playing an increasingly important role in the study of cellular processes - can be used". The FIAS working groups funded by the Alfons und Gertrud Kassel Foundation, the

Dr. Rolf M. Schwiete Foundation and the Johanna Quandt Foundation presented themselves. Roberto Covino and Sebastian Thallmair as well as their doctoral students Cristina Gil Herrero and Magnus Petersen introduced

their research areas in exciting lectures. Other doctoral students presented their research in elaborate posters. There was plenty of time for discussions and interested enquiries from the sponsors as well as speculation about

future research challenges, their organisation and social relevance.

FIAS thanks the foundations for their support and sustained interest in the research projects!

FIAS Forum is back

In the winter semester 2023/24 we resumed the popular public lecture series "FIAS Forum". On the first date in September Volker Mosbrugger, chairman of FIAS foundation board and president of the Polytechnische Gesellschaft Frankfurt, spoke about the sustainability crisis and its impact on the scientific landscape.

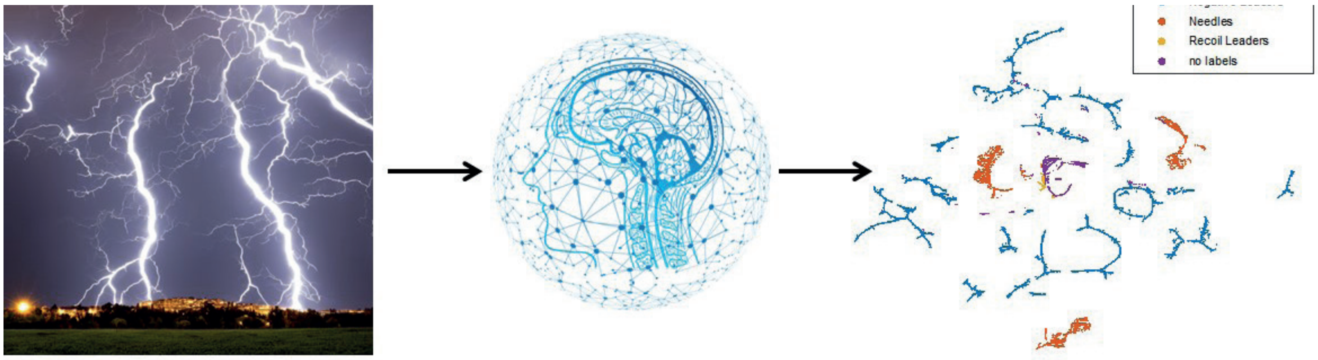
In the second talk, Eckhard Elsen, the Scientific Director of FIAS, introduced himself to the Frankfurt public with his lecture on "Dynamics of Scientific Research in Germany".

Read more on page 26. FIAS Forum will continue in 2024.

Theoretical Sciences

Lightning is a natural phenomenon that has fascinated humans for centuries. However, understanding the complex structures of lightning has been a challenge for scientists due to the vast amount of data involved. In a recent study, researchers from FIAS and University of Groningen have developed a novel method to understand lightning structures using machine learning. This knowledge might also help to protect lightning dangers in the future.

Algorithms illuminate lightning structures



Electrical charge in the air creates a small ion pathway from the storm cloud towards the ground, the "leader". A newly discovered phenomenon are small, sharp pathways of charged air, the "needles". Lightning data from radio telescopes can be used to calculate their fine structure by artificial intelligence.
The photo was also generated by Artificial Intelligence (Lingxiao Wang).

Lightning is a natural phenomenon that has frightened and fascinated humans for centuries. However, understanding the complex structures of lightning has been a challenge for scientists due to the vast amount of data involved. In a recent study, researchers from FIAS and University of Groningen have developed a novel method to understand lightning structures using machine learning. This knowledge will also help us to avoid lightning threat in the future.

Analyzing lightning data can be very time-consuming and so far depends on photos for studying the structure of lightning. A single lightning flash contains hundreds of fine and complex structures and a myriad of different phenomena. To address this challenge, Lingxiao Wang and his colleagues Brian Hare, Horst Stöcker, Kai Zhou, and Olaf Scholten have developed a novel method to identify structures in lightning data using machine learning algorithms and correlation analysis. They used data from the Dutch-German radio telescope LOFAR (Low Frequency Array), a network of many individual antennas. "The exploration of the lightning structure is the first step to understand the occurrence and evolution of lightning phenomena", Wang explains. "If we understand such extreme phenomena better in the near future, it will help us to avoid lightning disasters".

The study, published in the Chaos, Solitons and Fractals journal, sheds light on the understanding of lightning structures and provides insights into the complicated correlation functions for different lightning phenomena. The use of machine learning algorithms can help identify structures from numerous spatio-temporal points in a high dimensional space, which is very time-consuming when done by-eye. This novel method is a powerful tool to search vast multidimensional data sets for unique structures.

The findings of this study have potential applications beyond the field of physics. The combination of algorithms used in this study (t-distributed stochastic neighbor embedding, t-SNE and a clustering algorithm) can be applied to search vast multidimensional data sets for unique structures in other fields beyond physics – "for example data of biological or medical methods, earthquakes, or human mobility", Wang says.

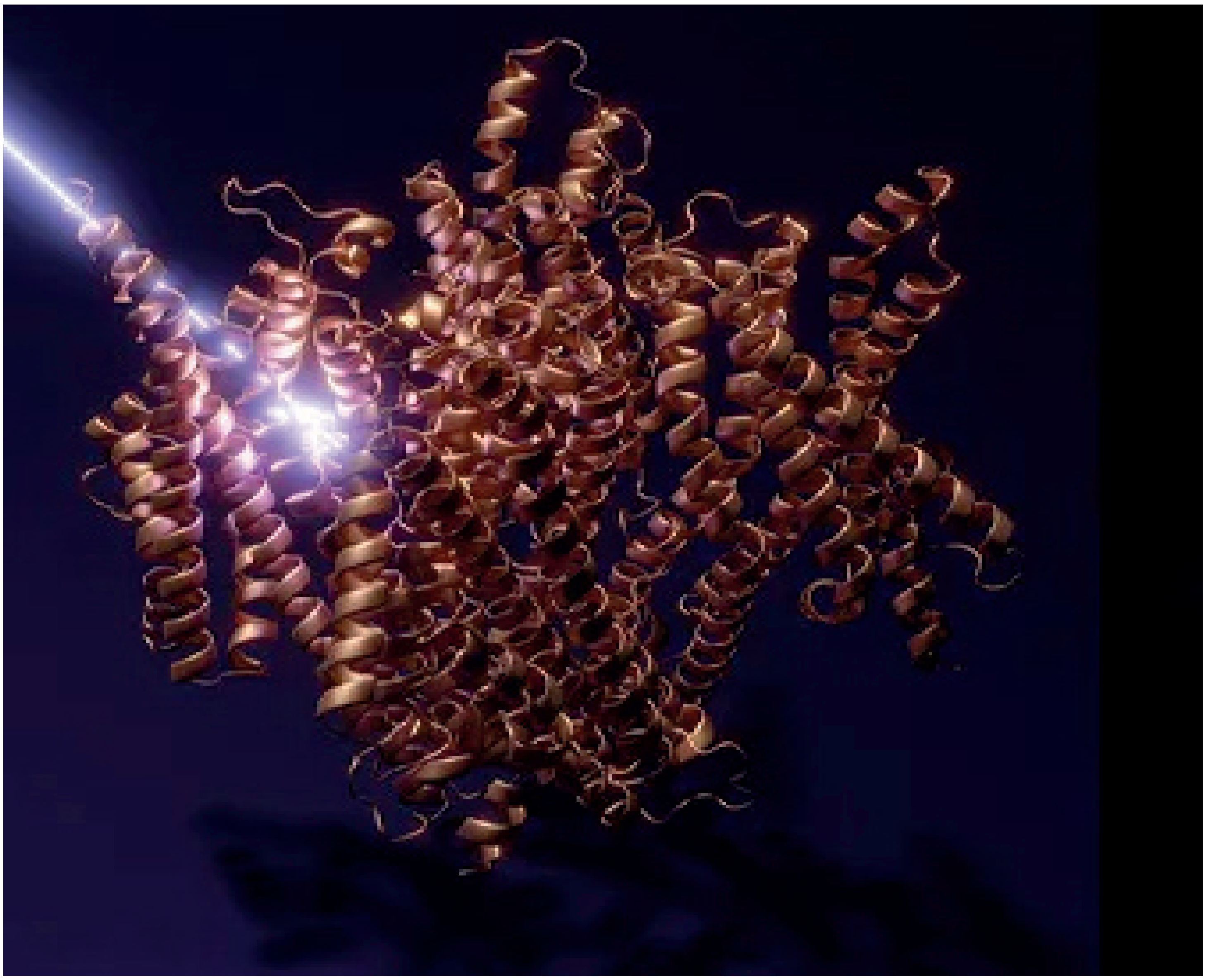
This research highlights the FIAS's commitment to advancing scientific knowledge through innovative research methods. By developing new tools and techniques to analyze complex data sets, our researchers are making significant contributions to our understanding of natural phenomena.

Publications:

Lingxiao Wang, Brian M. Hare, Kai Zhou, Horst Stöcker, and Olaf Scholten, Identifying Lightning Structures via Machine Learning, Chaos, Solitons & Fractals 170, 113346 (2023).

Brian M Hare, Olaf Scholten, Joseph Dwyer et al. Needle-like structures discovered on positively charged lightning branches, Nature, 2019, 568(7752): 360-363.

Life- & Neuro Sciences



A team from Frankfurt and New York elucidated a light-controlled ion channel with the aid of artificial intelligence. FIAS Fellow Gerhard Hummer and PhD student Serena Arghittu significantly contributed to the investigation of the structure of a novel light sensor of the nematode Caenorhabditis elegans (LITE-1-bronze: Lucy Reading-Ikkanda/Simons Foundation).

Sensing light without eyes

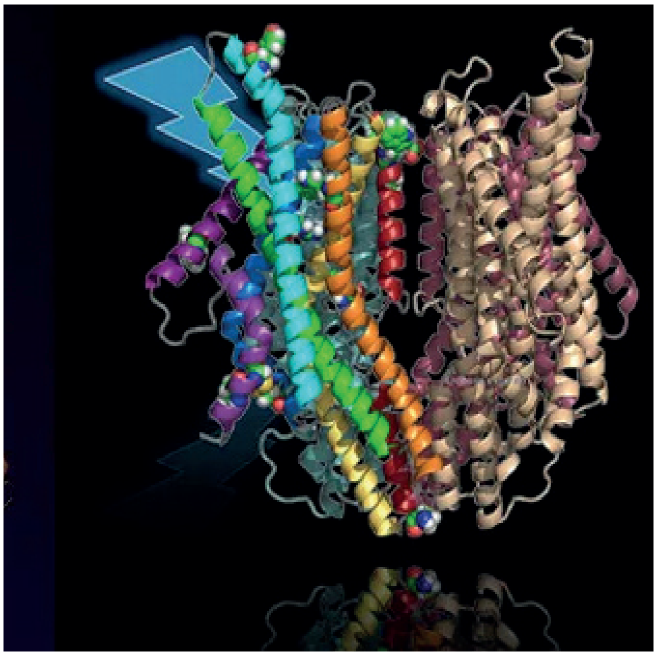
The small Caenorhabditis elegans nematode avoids light. While it does not have eyes, some of its cells contain a protein called LITE-1, which warns it of the sun, whose rays are dangerous for the animal. A team of scientists from Frankfurt and New York has now elucidated the structure of LITE-1 – a completely new type of light-controlled ion channel. Instead of biochemical experiments, the researchers used artificial intelligence to elucidate the structure and verified their structural model using biological experiments.

In a compost heap, the nematode Caenorhabditis elegans finds a richly laid table: at a length of just one millimeter, the worm feeds on bacteria that decompose organic material. It is essential that the animal avoids sunlight – and not just to ensure its body remains at an optimal temperature and does not dry out. Energy-rich blue and UV light can result in great damage to the cells of the transparent worm, causing the hereditary molecule DNA to mutate, or resulting in the formation of reactive oxygen species such as hydrogen peroxide (H2O2). The latter can, for example, prevent the correct production of proteins and drive cells to death. Laboratory observations show that Caenorhabditis elegans reflexively withdraws from a beam of light.

The nematode does not have eyes, but some of its sensory neurons contain the protein LITE-1, which converts light sensation into biochemical signals in a hitherto unknown manner, ultimately triggering the withdrawal reflex. A group of scientists led by Alexander Gottschalk (Goethe University), Gerhard Hummer (MPI Biophysics/Goethe University/FIAS), and Sonya Hanson (Flatiron Institute) elucidated the structure and function of LITE-1. They used the "AlphaFold2-Multimer" software, an artificial intelligence capable of predicting the structure of proteins and protein complexes based on the sequence of their amino acids. Their finding: LITE-1 is a so-called channel protein, located in the cell membrane and forms a pore through which charged particles (ions) can pass to cross the membrane.

"The AI worked really well and suggested a plausible structure for LITE-1," says Gottschalk. "In ensuing genetic experiments, we went on to check whether predictions based on this structure could also be verified in the live nematode and its response to light." To do so, the researchers specifically mutated individual amino acids in LITE-1 and observed the consequences on the light-evoked behavior. They found that, among other things, the replacement of amino acids that form the channel resulted in a complete loss of function of LITE-1. Additional mutation experiments revealed sites where the protein could interact with H2O2 and also uncovered a central amino acid that appears to be responsible for absorbing the energy generated by UV light.

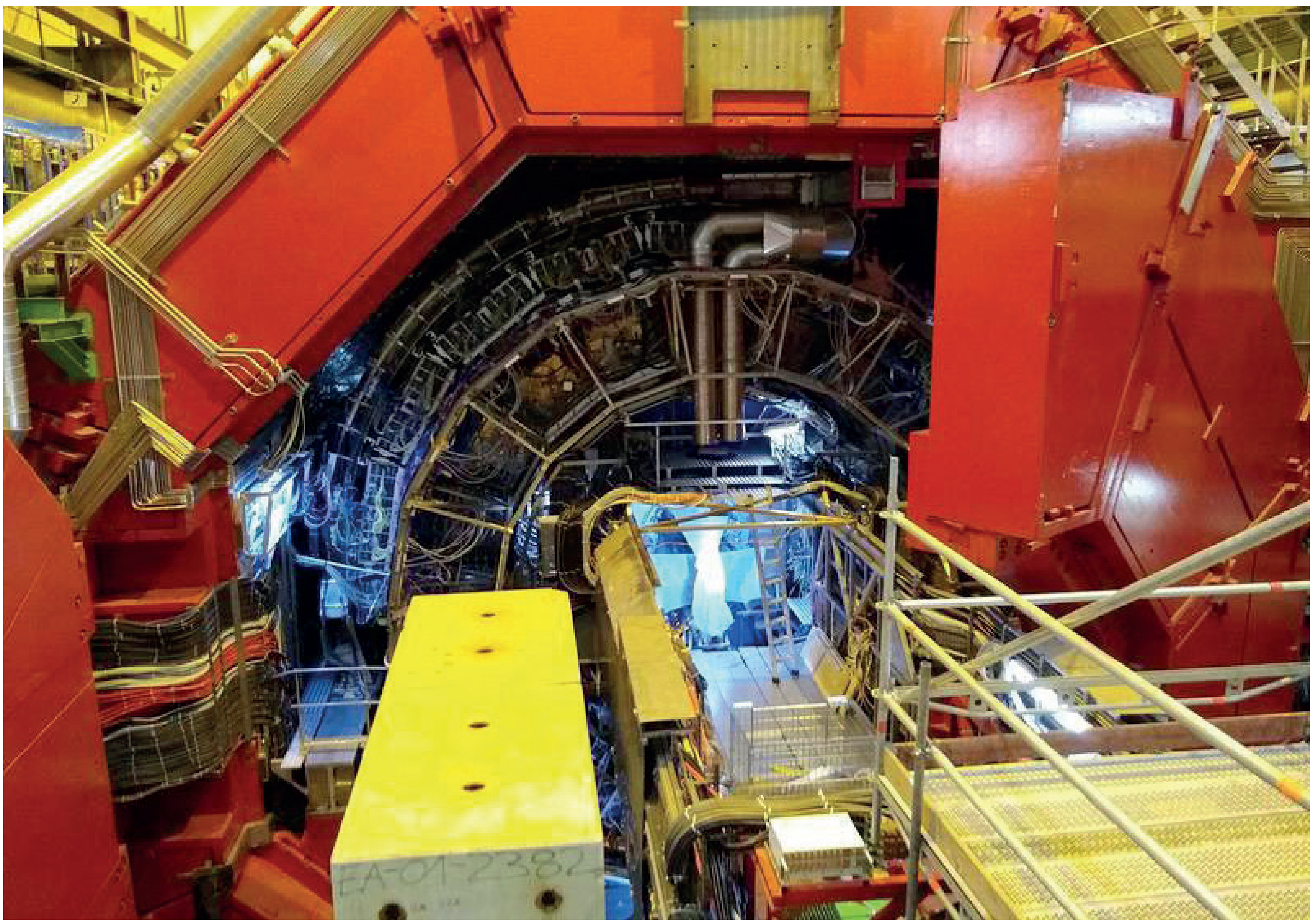
Hummer explains: "It appears as if LITE-1 contains a whole network of amino acids, aligned like antennas, to capture the energy of the UV photons and pass it on to a central position in the protein. Here, a cavity is located which in turn could serve as a binding pocket for a chromophore – i.e., a molecule that can absorb photons or their energy." The researchers' model posits that this as yet unknown chromophore is additionally stimulated directly by blue light, and then transfers all the energy to the LITE-1 protein, leading to the opening of the ion channel and the influx of ions into the cell. The higher ion concentration becomes the starting point for a biochemical-electrical signal that eventually triggers the recoil reflex.



The novel photosensor protein LITE-1 of the nematode Caenorhabditis elegans reacts as a danger sensor to UV and blue light. LITE-1 is a light-gated ion channel and is the second form of light-gated ion channel to be discovered to date after the long-known algal channel rhodopsin. (LITE-1-multicoloured: Alexander Gottschalk, Goethe University).

Publication:
Sonya M. Hanson, Jan Scholüke, Jana Liewald, Rachita Sharma, Christiane Ruse, Marcial Engel, Christina Schüler, Annabel Klaus, Serena Arghittu, Franziska Baumbach, Marius Seidenthal, Holger Dill, Gerhard Hummer, Alexander Gottschalk: Structure-function analysis suggests that the photoreceptor LITE-1 is a light-activated ion channel. Current Biology (2023), https://doi.org/10.1016/j.cub.2023.07.008.

Computer Science & AI Systems



A new measurement record was achieved at the CERN accelerator, recorded with the ALICE detector. The enormous amount of data is processed by a computing cluster headed by FIAS Senior Fellow Volker Lindenstruth. To carry out the upgrade, the ALICE detector had to be opened. Photo: Sebastian Scheid, Goethe University Frankfurt.

Measurement record: mimicking the Big Bang

After a five-year break, the large LHC accelerator at the CERN international research institute has once again brought lead ions to collision. The colliding matter dissolves into its components for an extremely short time, reaching a state similar to that of the universe a millionth of a second after the Big Bang. The particle tracks of the collisions are recorded by the house-sized ALICE detector, which researchers from FIAS and Goethe University have helped to improve. A new record was set in the first month alone: 20 times more collision events were registered than in the data collection periods of previous years combined.

Between the end of September and the end of October, the accelerator at the European Nuclear Research Centre CERN in Geneva generated lead-ion collisions at the world's highest-ever collision energy of 5.36 tera electron volts per colliding nuclear particle (nucleon-nucleon collision). Not only the collision energy, but also the collision rates were significantly increased. In addition to the collision energy, the collision rates also increased significantly compared to the data-taking periods of previous years. The specialised ALICE detector recorded 20 times more events than in the four one-month data collection periods since 2010 combined.

This is important because of the tremendous number of particles that are created and decay in a very short timeframe during the collisions. Recording the tracks of these particles allows conclusions to be drawn about exactly what happens at the moment of collision and shortly thereafter: The particles dissolve into their elementary components – quarks and gluons – and form a kind of "matter soup", the quark-gluon plasma. Immediately afterwards, new very unstable particles form again, which finally transform into stable particles in complex decay chains. In this way, researchers in the ALICE experiment are studying the properties of matter as it existed shortly after the Big Bang.

Frankfurt research groups are part of the experiments: The new record was first made possible because the world's most powerful particle accelerator, the Large Hadron Collider (LHC), was upgraded during the four-year reconstruction phase. The upgrades of the ALICE detector during the same timeframe enable it to record the traces of the LHC's higher collision rates.

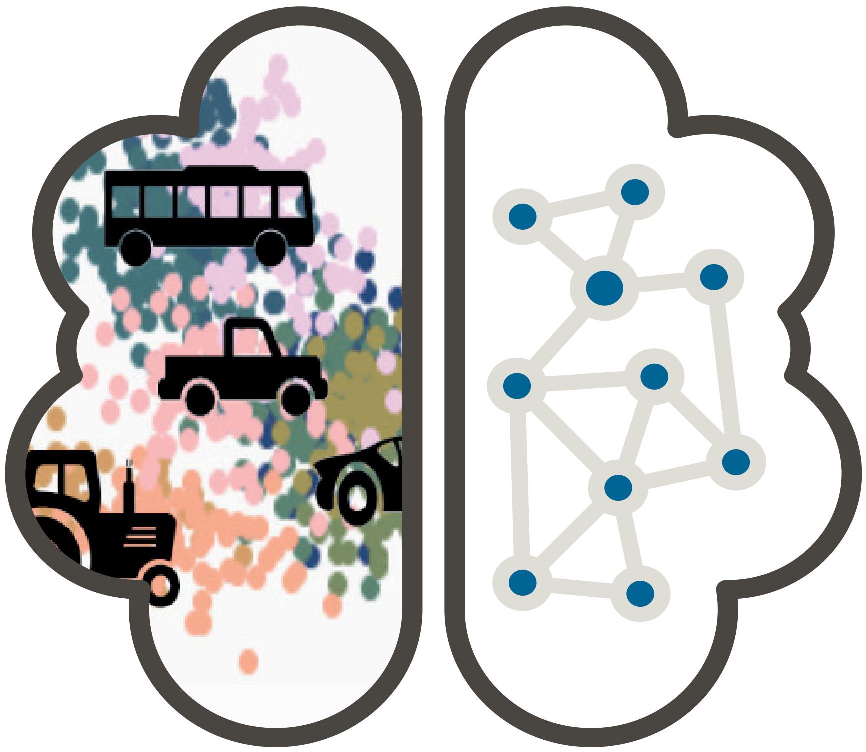
The enormous amount of data generated during the measurements – which reaches the range of terabytes per second for the TPC alone – constitutes a major challenge. To be able to sufficiently reduce the amount of data stored, this data stream must be processed in real-time, using effective pattern recognition methods. The Event Processing Nodes (EPN) computing cluster was set up specifically for this experiment. Based on both conventional computing cores (CPUs) and special graphics processors, the EPN project is led by Volker Lindenstruth, Senior Fellow at FIAS and Professor for High-Performance Computer Architecture at Goethe University.

More information on ALICE:

https://alice-collaboration.web.cern.ch/

ALICE detects quark-gluon plasma, a state of matter thought to have formed just after the Big Bang

Projects



The new FIAS project "Navigating Knowledge Spaces Using Cognitive Maps" (headed by Matthias Kaschube) aims to better understand the formation and utility of cognitive maps in the brain by developing new AI models. These models will utilize generative adversarial networks (GANs) to model cognitive maps for abstract representations. Additionally, the project will apply these models to category learning with limited data to examine the efficiency of the learning process.

Approved new Projects at FIAS 2023

Artificial intelligence for fast simulation of scientific data (KISS)
BMBF-Project, head Kai Zhou
03/2023-02/2026. 241.489,31€

The dynamic connectome 2: Dynamics of learning
DFG-Project, head Jochen Triesch
01/2023-12/2025. 192.850,00 €

Learning object representations via active exploration
DFG-Project, head Jochen Triesch
01/2023-12/2026. 390.048,00 €

Navigating knowledge spaces using cognitive maps
DFG-Project, head Matthias Kaschube
09/2023-08/2027. 390.048,00 €

A cortico-collicular network for hearing and noise avoidance responses in bats
DFG-Project, head Jochen Triesch
11/2023-10/2026. 216.253,00 €

EQUATE/SCALE (Combination of structural and computational approaches to determine the cellular architecture of membrane contact sites)
DAAD/HMWK-Project, heads Nishtha Srivastava, Sebastian Thallmair
01/2023-09/2024. 85.760,00 €

KISS: FIAS part of a joint project for AI simulation of scientific data

KISS enables faster, more flexible, and more efficient evaluation of research data based on AI simulations. With Kai Zhou as PI, FIAS is participating in the joint project "Artificial Intelligence for the Fast Simulation of Scientific Data" (KISS) funded by the Federal Ministry of Education and Research (BMBF).

Simulations play a key role in scientific research - from fundamental physics research to application areas such as biology, robotics, or climate modelling. Particularly in high-energy nuclear physics in the area of "Exploration of Universe and Matter" (ErUM), simulations are necessary starting from a detailed mathematical understanding of fundamental physical processes. This is the only way to achieve the physical goals of big infrastructures such as high-energy accelerators, which are particularly computationally intensive, resource-intensive and time-consuming. With the expansion of detectors and telescopes, computing capacities are reaching their limits. Thus, an increase in the efficiency of the related simulation algorithms is crucial for the successful operation of these large high-energy experiments.

As part of the "ErUM-Data" action plan, the BMBF is funding Zhou's research with 240.000 Euros for the next three years. In addition to Kai Zhou's working group, teams from Hamburg, Dortmund, Dresden, Göttingen, Heidelberg and Munich are involved. As part of KISS, the FIAS team will develop generative AI models that replace and accelerate classical detailed modelling of heavy ion collisions. This includes, for example, the high-resolution detector simulations (Geant4) for experiments such as "Compressed Baryonic Matter" (CBM) at GSI/FAIR or "A large Ion collider Experiment" (ALICE) at CERN. Zhou's group researches modern generative architectures such as Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs), Normalising Flows (NFs) and Diffusion Models (DMs) and creates the respective simulation task. These developments can largely mitigate the huge computational and memory demand in the physical exploration and data acquisition phases of experiments.

Such processes can also be applied to other important needs of society and industry, such as climate modelling and prediction, robotics simulations and 3D prototype design in industry. Two already successful and popular general applications for this kind of generative AI models are ChatGPT and DALL-E2.

FIAS part of Frankfurt physics academic ceremony

FIAS Director Eckhard Elsen called for social responsibility on the part of the research institutes at the Academic Celebration of the Department of Physics on 30 June. Prizes for the past year are awarded annually by the Department of Physics together with the Walter Greiner Society for the Promotion of Basic Physics Research and FIAS at an academic ceremony. Dean Roger Erb welcomed the finely dressed guests to what he called "the most beautiful department". University President Enrico Schleiff - based in biology - later put that into perspective with a smile to "one of the most beautiful".

Elsen emphasised that physics research must also follow social change and take up topics in which it is in demand with its expertise. As an example, he mentioned ChatGPT: "The methods of AI and machine learning are our competence, so we should also get involved in the societal discussion and take a stand on it".

Numerous donors support physics research, especially through the Walter Greiner Society. The physicist, who died in 2016, was one of the co-founders of FIAS.

The five best degrees were awarded, as well as the two best dissertations and the best teaching in physics. An important contribution is made by the Sandvoss scholarships, which help students in financial need, as well as the Germany scholarships, 14 of which went to Goethe physicists.

After an exciting lecture on "Three Trillion Degrees in the Shadow" by Heraeus Foundation Professor Gunter Roland, the guests celebrated and discussed and discussed over a casual dinner on the terrace of the Mensa Pi x Gaumen.

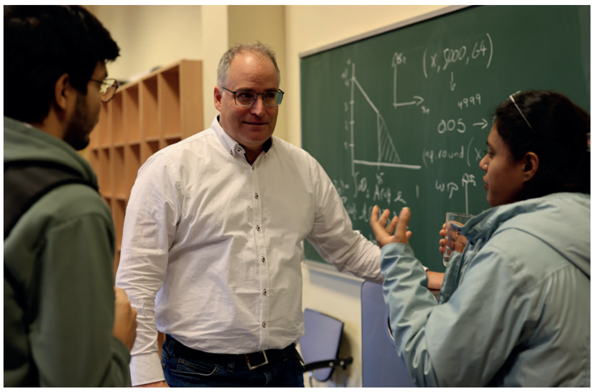
Events

Condensed complexity - the essence of information processing and cognition?

What do the human brain, biological networks, evolving organisms, the immune system, flocks of birds, AI systems and quantum devices have in common? Despite their outward differences, they share a remarkable property - they unfold their dynamics in high-dimensional state spaces. These systems have the amazing ability to reduce their complicated states in surprisingly simple ways to respond to specific stimuli. What is even more impressive is that these simplified states often emerge through simple interactions and combinations that create a balance between many possible solutions and the selection of the best solutions from these many options.

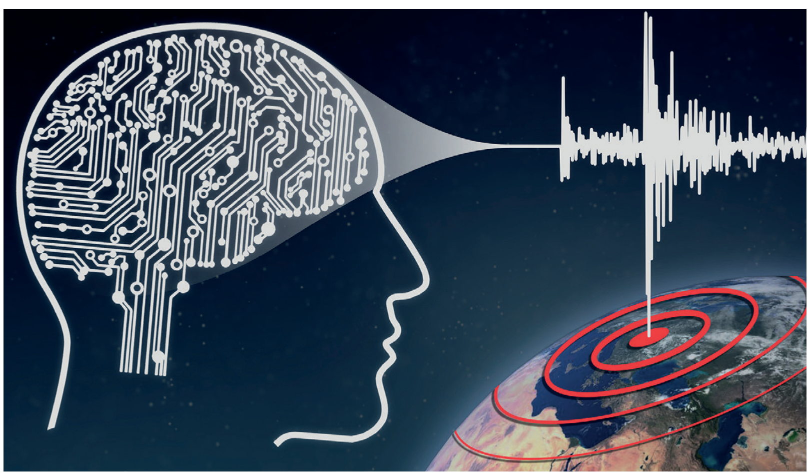
This ability to create new and meaningful system states seemingly out of nothing begs the question: Is this the origin of knowledge, cognition and information processing? At the "Condensed Complexity" conference, held at FIAS from November 6th to 10th, over 70 international scientists did address this question. They gave each other insights into their research and discussed which common principles influence these processes in different systems, regardless of their different fields of origin.

The event was part of the "Giersch International Conference" series and is generously supported by the GIERSCH Foundation.



Some impressions of the 5th International Giersch School and Conference. Experts from very different fields of research came to FIAS and enjoyed the exchange and the opportunity to gather impressions outside their own area.

Seismology & artificial intelligence workshop



The Seismology and Artificial Intelligence workshop, funded by the Federal Ministry of Education and Research (Bundesministerium für Bildung und Forschung - BMBF), was organized from the 13th to the 15th of September 2023 at the Frankfurt Institute for Advanced Studies (FIAS). This workshop was part of an established project, "Seismology and AI - SAI," conducted jointly by FIAS and the Institute of Geosciences at Goethe University.

The workshop aimed to address the complex nature of seismic events, which posed challenges in efficiently extracting information from geophysical data using classical statistical tools. Additionally, analytical methods faced limitations due to simplified assumptions. Recognizing this, cutting-edge research in Deep Learning/Machine Learning was already providing powerful tools for handling massive data and extracting desired features.

During the three-day event, experts, early career researchers, and experienced scientists from both Artificial Intelligence and various domains of Seismology came together. Their objective was not only to explore the numerous unique, novel, interdisciplinary methods, and computational solutions offered by these approaches but also to envision the future direction and associated challenges in seismic research and artificial intelligence applications in the field.

Volker Mosbrugger gave a thought-provoking talk entitled "The great transformation towards sustainability - challenges for science and education".

FIAS Forum

After a three-year hiatus due to Covid, the FIAS Forum returned, presenting hot topics to the public once again. Volker Mosbrugger, Chairman of the FIAS Board of Trustees, opened the series with a discussion on necessary sustainability changes, stressing the importance of balancing costs, consumption, and damage in the economy.

Mosbrugger highlighted the need for innovative, globally-oriented science to address the trinity of planet-society-economy. He emphasized the urgency of accelerating necessary innovations, such as better funding for startups, citing the low rate of new businesses founded at German universities. Drawing from FIAS examples, Mosbrugger illustrated sustainable research approaches, including the energy-efficient Green Cube and earthquake research contributing to planet understanding. He referenced the CMMS team's work on "digital twins" in biology, which aids efficient research on virtual replicas, a central topic at FIAS. Acknowledging the transformative process's challenges, Mosbrugger advocated for proactive measures, emphasizing the importance of growth and evolution in preserving the planet and humanity. He highlighted the significance of transdisciplinarity, particularly for creative young minds.

The second FIAS Forum talk, delivered by FIAS Scientific Director Eckhard Elsen focussed on the dynamics of scientific research in Germany. He emphasized the crucial role of universities as pillars of research but also highlighted the necessity for larger institutes to conduct extensive and long-term research projects. Additionally, he addressed the evolving global research landscape and the need for research funding to adapt to emerging themes and agile institutions. He offered some valuable insight into current global developments through concrete examples, addressing questions about sustainability, the importance of basic research, and the potential of research locations.

On both evenings discussions continued over pretzels and wine at the FIAS Faculty lounge. We were delighted to be able to open FIAS to the public again this year. Not only visitors but also our scientists enjoy the exchange on such special events.

Eckhard Elsen introduced himself to the public.

CMMS Summer school in the Eifel

In July, CMMS project members, including doctoral students, postdocs, and subproject leaders, gathered for a week-long retreat in the scenic Eifel region. Supported by Hessian LOEWE funding, CMMS focuses on understanding molecular processes to organism behavior, integrating high-resolution data into simulations.

Organized by FIAS Fellow Franziska Matthäus, the retreat featured crash courses for interdisciplinary collaboration and a workshop on research data management. A writing course provided valuable insights into scientific writing.

Afternoons allowed for recreational activities at Lake Rursee in Eifel National Park, like swimming, hiking, and kayaking, fostering team bonding.

More events at FIAS 2023

Special lectures on quantum computing:

The options of quantum computing and benchmarks of some of the most powerful supercomputers were presented in a talk by Kristel Michielsen in October.

Also in October, FIAS and Goethe University hosted a joint colloquium under the heading “Science Perspectives”. Professor Steven Rayan, University of Saskatchewan, spoke about “Quantum Innovation at the Interface of Materials and Information”.

CMMS Talks

The CMMS Collaboration seminar was also very popular in 2023. 13 internal and external speakers from the field of CMMS research were invited.

SPP2041 Status meeting

In March, SPP 2041 gathered to discuss “Computational Connectomics.” This project explores brain structure and function by studying nerve cell networks at various scales, emphasizing computational methods to bridge brain wiring diagrams with functional understanding.

SAI online seminar

THe SAI Group organzied a Online Course on Single-Station Earthquake Monitoring using Deep Learning-based Python Package SAIPy.

IQbio Career Day

Within the scope of our graduate program, the IQbio Career Day took place on Nevember 14th, to present possible fields of employment to doctoral students.

Special FIAS Seminar in Theoretical Physics

In 2023 5 scientics where invited to speak at the “Special FIAS Seminar in Theroretical Physics”. For example Prof. Tomoi Koide from University Rio de Janeiro spoke about “Hydrodynamics incorporating field theoretical quantum fluctuations”.

Public Relations

Algorithmen analysieren Blitze

FRANKFURT Eine Methode, um die Struktur von Blitzen besser zu verstehen, haben Forscher des Frankfurt Institute for Advanced Studies und der Universität Groningen entwickelt. Das Verfahren nutzt Künstliche Intelligenz und soll dabei helfen, die von Gewittern ausgehenden Gefahren zu verringern. Die Wissenschaftler werteten Daten von Blitzen aus, die das niederländisch-deutsche Radioteleskop LOFAR (Low Frequency Array) aufgezeichnet hatte. Bei der Anlage handelt es sich um ein Netzwerk aus vielen Einzelantennen. Mithilfe von Algorithmen des maschinellen Lernens und Korrelationsanalysen untersuchten die Forscher die Strukturen der Entladungen. Mit Künstlicher Intelligenz sei es schneller als mit bloßem Auge möglich, viele räumlich-zeitliche Punkte in einem hochdimensionalen Raum zu identifizieren. Die neue Methode könne auch außerhalb der Physik angewandt werden, etwa in Biologie und Medizin, bei der Erforschung von Erdbeben oder zur Analyse der menschlichen Mobilität. zos.

WISSEN — 9. März 2023 DIE ZEIT Nº 1

Hirnforschung

Es schwingt in unserem Kopf

Das Gehirn – was für eine Wundermaschine! Wolf Singer hat sie sein Leben lang erforscht. Bis heute fragt er sich: Was ist Bewusstsein? Und wie entsteht das Ich?

T: Herr Singer, mehr als 50 Jahre haben
mit dem Gehirn beschäftigt. Lassen Sie
Ihrem 80. Geburtstag – gemeinsam eine
den Kopf antreten, an Ihren großen
gsfragen entlang, von der Wahrnehmung
rfindung des Ich. Vor uns auf dem Tisch
Brille. Wie erkennen wir sie als solche?
ger: Wir setzen sie in unserem Gehirn zu-
Wenn draußen in der Welt Strukturen
m auftreten, wie zum Beispiel die Kanten
nen dieser Brille, werden im Gehirn die
ngen zwischen jenen Nervenzellen nach-
tärkt, die auf diese Strukturen reagieren.
er aus dem Muster der Verstärkung muss ja
nen folgen: Diese Strukturen bilden eine
e eine Großmutter. Es gab die Theorie, am
Signalkette im Gehirn meldet eine be-
elle: Ich sehe Großmutter. Sie haben – der
größte Durchbruch in Ihrer Forscher-
herausgefunden, dass wir die »Großmutter-
nicht brauchen.
: müsste dann ja nicht nur eine Groß-
e geben, sondern Zellen für alle Menschen
nstände, die wir kennen, samt deren
zueinander. Dies würde zu einer kombi-
n Explosion der notwendigen Zahl von
ren.
ind auf überraschende Rhythmen im Ge-
en. Welche Rolle spielen die?
r haben die Aktivität von Neuronen im
essen und beobachtet, dass sie im Gleich-
wenn sie auf Merkmale reagieren, die in
häufig gemeinsam vorkommen. Diese
gemeinsame Aktivierung verstärkt die
en zwischen den Neuronen. Auf diese
Wissen über die Struktur der Welt in der
der Nervenverbindungen gespeichert.
rankfurter Labor gab es 1986 einen

ZEIT: Auf einem Kongress von Philosophen h
Sie vor vielen Jahren einmal erklärt, es gebe ke
freien Willen – und damit eine enorme Debatte
gelöst. Eine bewusste Provokation?
Singer: Im Gegenteil, ich wollte lediglich aufkl
bin aber gründlich missverstanden worden. I
FAZ folgerte ein Redakteur: Wenn alles determi
ist, dann gibt es keine Schuld und ohne S
keine Strafe. Das führt direkt in die Anarchie.
ZEIT: Kein freier Wille, das klingt einfach
einer massiven Beleidigung des menschlichen
Singer: Ich habe nie nachvollziehen können, w
manche das als Angriff auf die Menschen
begriffen haben. Die Evidenz ist doch erdrü
Alles, was in uns und um uns herum geschie
Einfluss auf das Gehirn. So wie dieses Gespräc
re Gehirne im Augenblick, aber auch in alle Z
verändert. In dem Sinne sind wir neurobiolog
terminiert. Aber natürlich müssen wir uns se
schreiben – wem denn sonst? –, was wir tun, u
verantworten. Und ebenso selbstverständlich
wir belangt werden, wenn wir gesellschaftlich
brechen. Der freie Wille ist eine Zuschreib
wir in unser Selbstmodell integrieren konnte
die Vorgänge in unserem Gehirn, die uns
scheidungen vorbereiten, nicht wahrnehm
nen. Aber wie gesagt: Solche Zuschreibunge
ihre eigene Realität und sind wirkmächtig.
ZEIT: Haben wir die Welt zu sehr entmysti
Singer: Zu Beginn der Aufklärung ist die
schaft angetreten, einen Gottesbeweis zu e
Wir haben das Gegenteil erreicht. Wir ha
vieles entmystifiziert, was man früher tran
talen Mächten zuschrieb.
ZEIT: Und damit die Autoritäten außer
Reichweite des Menschen demontiert.
Singer: Stimmt. Das ist ein Problem, wei
solcher Autoritäten Regeln eine nicht hinte
Gültigkeit bekamen. Ich kann mir keine wi
Autorität vorstellen, als eine, die nicht a
Man kann ihr nicht widersprechen.

The many activities at FIAS as well as the exciting research are reflected in many publications, on websites, TV broadcast, Social Media, and in public lectures. Newspapers such as Frankfurter Allgemeine Zeitung, and the local TV station Hessischer Rundfunk (HR) as well as other national and local publishers reported on FIAS events and scientific publications.

TAGESSPIEGEL

RERUM COGNOSCERE CAUSAS

Die Macht der Blitze

KI soll helfen, das Phänomen besser zu verstehen

Von Ralf Nestler

Wenn ein Sommergewitter losbricht, ist Vorsicht geboten: Blitze haben eine enorme Kraft, können Brände auslösen und Menschen töten. Wie sie entstehen und was sie gemeinsam haben, ist bis heute nicht vollständig verstanden. Allein in Deutschland schlagen jährlich

te, Höhe und Zeit", erklärt Wang. Es entsteht also ein räumliches Bild über mehrere Kilometer, dessen Veränderung sich über die Zeit verfolgen lässt. Wobei Zeit hier lediglich den Bruchteil einer Sekunde bedeutet, die aber nun verlangsamt und in Einzelschritten dargestellt werden kann.

Dank der Algorithmen können die Wissenschaftler verschiedene Strukturen innerhalb von Blitzen

rig, sagt Finke. „Die … den besser und erfass… ze – ob es real mehr si… zu sagen." Grundleg… man, dass mit erhöht… die Luftfeuchtigkeit … es mehr Gewitter ge… len Durchschnitt ma… aber wie sich das r… ckelt, ist schwer abz…

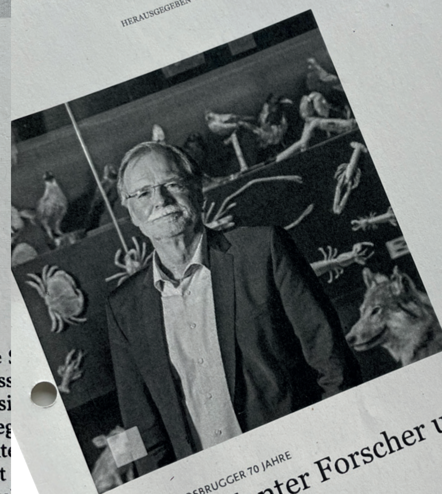
Zumindest für die … es nun genauere Za…

THEMEN TICKER ARCHIV STELLENMARKT

Volker Mosbrugger 70 Jahre: Ein exzellenter Forscher und Vermittler

Frankfurter Allgemeine

HERAUSGEGEBEN VON GERALD BRAUNBERGER, JÜRGEN KAUBE, CARSTEN KNOP, BERTHOLD …



VOLKER MOSBRUGGER 70 JAHRE

Ein exzellenter Forscher und Vermittler

AKTUALISIERT AM 10.07.2023 - 19:32

Elf Jahre lang stand Volker Mosbrugger an der Spitze von Senckenberg. Von seinen Fähigkeiten als Kommunikator profitiert Frankfurt noch immer. Am Mittwoch wird der Paläontologe 70 Jahre alt.

Wie Zellen Müll entsorgen

FRANKFURT Wie funktioniert die „Müllabfuhr" in Körperzellen? Forscher des Frankfurt Institute for Advanced Studies haben neue Erkenntnisse über die sogenannte Autophagie gewonnen – einen Entsorgungs- und Recyclingprozess, der in Krebszellen (Foto) und bei neurodegenerativen Erkrankungen gestört ist. Wichtig für diesen Prozess sind die Autophagosomen, eine Art Bläschen, in denen zum Beispiel defekte Proteine eingekapselt werden. Eine entscheidende Rolle bei der Bildung der Autophagosomen spielt ein Protein namens ATG3. Die Frankfurter Wissenschaftler haben eine Seitenkette dieses Eiweißstoffs untersucht und festgestellt, dass sie über einzigartige biophysikalische Eigenschaften verfügt. Sie ermöglichen es dem Protein, streng kontrolliert mit Zellmembranen zu interagieren. Nach Ansicht der Forscher könnte diese Entdeckung die Behandlung von Krankheiten erleichtern, bei denen die Autophagie beeinträchtigt ist. zos.

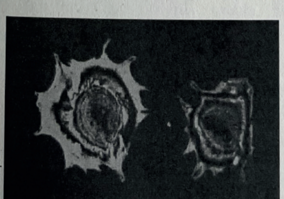


Foto Okapia

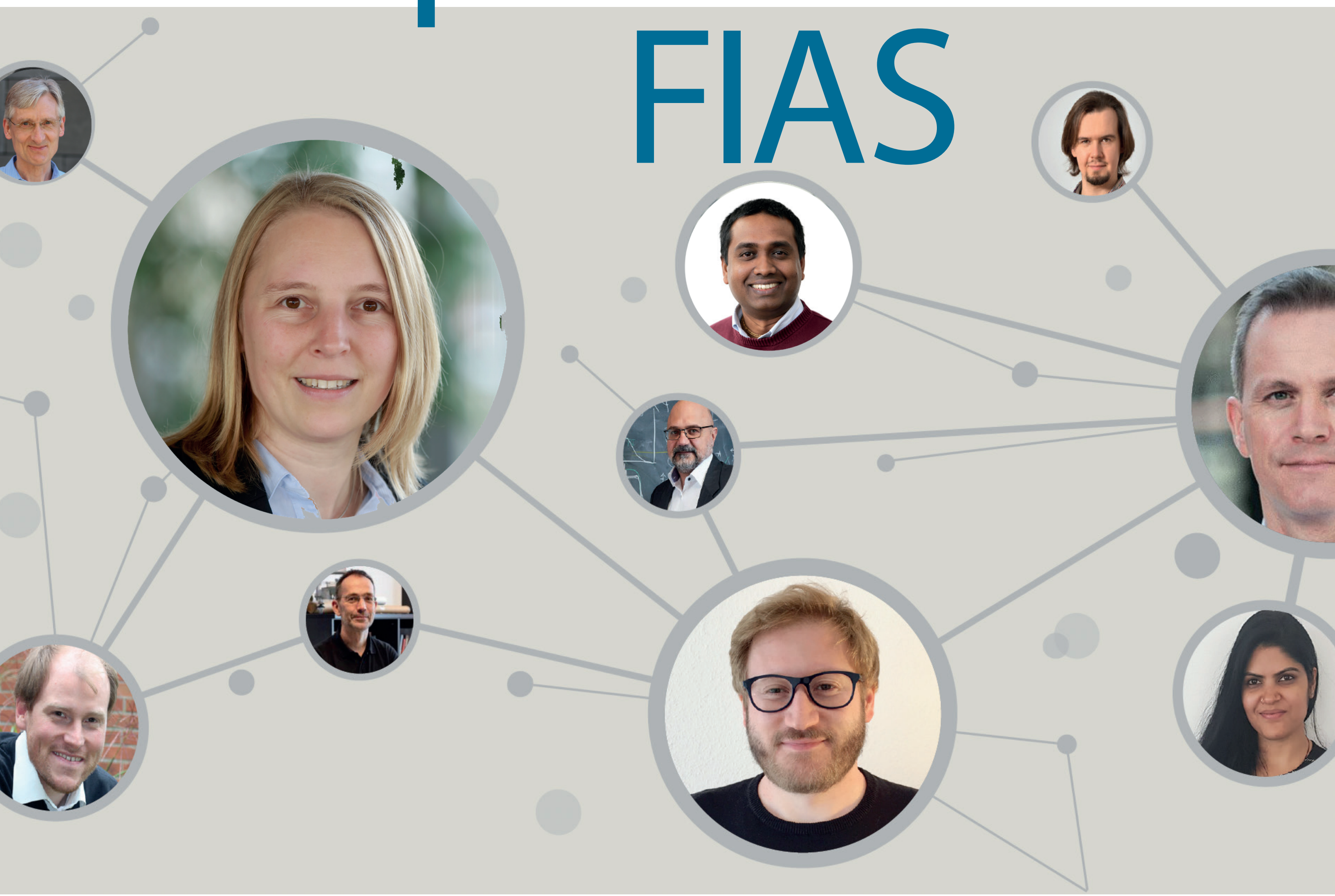
Lingxiao Wang (left) and his team attracted the attention of TV channel Hessischer Rundfunk. In the programme "Alle Wetter" Anja Störiko from FIAS press office (right) presented, how the group tries to understand lightning structures using machine learning (see page 16).

NOBELPREISTRÄGER SÜDHOF NEUER FIAS-LAUREATUS

Nobelpreisträger Thomas Südhof (2. v. r.), Universitätspräsident Enrico Schleiff (r.), der Vorstand der Stiftung Giersch Stephan Rapp (links) und FIAS-Direktor Eckhard Elsen (2. v. l.). Foto: FIAS

Nobelpreisträger Thomas Südhof erhielt am 8. November 2023 die Auszeichnung „Senior Fellow Laureatus" des Frankfurt Institute for Advanced Studies (FIAS). Vor der Verleihung hielt der Preisträger, Leiter des Südhof-Labors an der Stanford University Medical School, einen anspruchsvollen Vortrag über seine aktuelle Forschung. Der Vortrag war eingebettet in die diesjährige „Giersch International Conference" am FIAS, die sich unter dem Motto „Verdichtete Komplexität – die Essenz der Informationsverarbeitung aus Kognition?" mit den gemeinsamen Prinzipien Wissen/Bewusstsein und Informationsverarbeitung vieler Forschungsgebiete befasst. Eine großzügige Spende der Stiftung

People at FIAS



The performance of a scientific institute depends decisively on the people who work there. The same is true at FIAS; our researchers, with their enthusiasm and commitment, are the foundation of our success. With their work, they not only ensure the scientific operation but also attract with their applications the third-party funding that is so important for research activities.

Fellow status is based on scientific experience. **Senior Fellows** are experienced scientists with an outstanding publication record (comparable to W3 status). They form the FIAS Faculty. **Fellows** are high-potential researchers with a strong publication record (comparable to W2 status). **Research Fellows** are research associates with their first own research group (comparable to W1 status). **Adjunct Fellows** are internationally renowned scientists who regularly collaborate and publish with FIAS researchers. These fellows are appointed for three years or the duration of their project; renewal is possible.

Gordon Pipa new FIAS Fellow: Understanding information processing in the brain

FIAS has recruited the neuroinformatician Prof. Dr. Gordon Pipa as a new Fellow. The Chair of Neuroinformatics and Director of the Institute of Cognitive Science at the University of Osnabrück focuses on information processing in the brain. In doing so, he uses methods ranging from mathematical description and computer-based methods to machine learning and artificial intelligence.

The aim of his research is to understand the principles of neuronal information propagation and to implement them in artificial systems. In doing so, his group primarily investigates information processing by nerve cells. They use very short electrical impulses, the action potentials. This property of our brain makes it possible to implement information processing extremely efficiently, also with regard to the necessary energy consumed by the system. A special role is played by the collection of incoming information in the dendrite, fibrous extensions of the nerve cells that function like complex antennae of the system.

Pipa's research group investigates the processing of information in the dendrite and creates conceptual models to understand the function of dendritic information processing in the context of the large neuronal network. In addition, neuroinformatics deals with the experimental methods of virtual reality, sleep research, especially lucid dreaming, the emergence of intelligence in cognitive systems, and machine learning to infer dynamic systems on experimentally observed data. In this area, the group is currently modelling the spread of infectious diseases such as COVID-19, with unprecedented spatial resolution.

Pipa studied in Frankfurt am Main and was a junior fellow at FIAS many years ago; he later conducted research at MIT in Cambridge, and at Massachusetts General Hospital in Boston (USA). "Research is the fulfilment of my life's dream," says Pipa. He enjoys trying every day, together with others, to understand concepts of information processing in complex systems like our brain. "This is how we make new, better and more efficient technologies possible".

Two FIAS poster prizes at international meeting

EBSA poster prizes, photo montage: left Cristina Gil-Herrero, right marked Gianmarco Lazzeri

Gianmarco Lazzeri and Cristina Gil-Herrero, FIAS PhD students, each received one of the coveted poster prizes of the European Biophysical Societies' Association (EBSA) - a remarkable achievement at a conference with more than 1200 participants.

At the international meeting of the European Biophysical Societies' Association (EBSA) in Stockholm from 31 July to 4 August, two FIAS PhD students won prestigious awards for their posters.

Cristina Gil-Herrero from the research group of FIAS Fellow Sebastian Thallmair received the prize for her poster "Ligand Flip-Flop on a GPCR Surface", which deals with transport across cell membranes and opens up possibilities for the transport of drugs into cells.

Gianmarco Lazzeri from the research group of FIAS Fellow Roberto Covino deals with "Accurate rare-event kinetics from AI-assisted molecular dynamics simulations".

Scientists hoping for peaceful life and research: Roman Poberezhnyuk (left), Zhanna Khuranova (right), centre: first picture of the Ukrainian scientists at FIAS 2022 (Maria Khelashvili - Oleh Savchuk - Oleksandr Stashko - Roman Poberezhnyuk - Mark Gorenstein).

FIAS as a temporary home for Ukrainian researchers

FIAS hosted seven Ukrainian researchers after the attack on their country last year. How are they doing today?

Dr. Roman Poberezhnyuk praises "the great working environment" at FIAS. He had already spent several months as a visiting scientist at FIAS before the war. So he was able to use his scientific contacts and immediately find support and accommodation here. Poberezhnyuk has been cooperating for years with researchers from Prof. Horst Stöcker's group at FIAS to understand the thermodynamic properties of dense elementary matter. Finding an appartement was not easy, he says, and getting the residence permit took long. But apart from that, Poberezhnyuk and his girlfriend, who also lives here, are completely content. He wrote four publications during his stay; two more are in preparation. The physicist wants to continue his career in the USA next year, where he has been offered a post-doctoral position at a colleague's institute. A return to Ukraine depends on research opportunities after the war. Before the Russian attack, he observed a positive development in funding, which made it possible to live from research: "How this will develop in the future is completely open".

His colleagues Oleksandr Stashko and Oleh Savchuk have already moved on to the USA as PhD students. They had both found temporary accommodation at FIAS and were “very grateful for the full support of the research stay” in Frankfurt.

Prof. Mark Gorenstein, on the contrary, returned to Kyiv in April. The head of the department of High Energy Density Physics at the Bogolyubov Institute for Theoretical Physics at the National Academy of Sciences of Ukraine had fled to Germany with his family last year in the face of the bombardments in Kyiv. “Even today we don’t sleep well, there are bombings every night,” Gorenstein describes the oppressive atmosphere in Kyiv. Fortunately, little is destroyed - thanks to air defence. Why did he return anyway? “The support - for which I am very grateful to FIAS and the Alexander von Humboldt Foundation - ended. I could have stayed in Germany as a refugee, but I wanted to continue my work in Kyiv.” He has not regretted this step. The institute in Kyiv and the researchers on site are working, even though most of the seminars take place online. In 2001 Gorenstein was Alexander von Humboldt Awardee for his research on phase transitions and their signatures in cooperation with FIAS and GSI in Darmstadt. He had received a fellowship from the Alexander von Humboldt Foundation in 2022 and lived in Frankfurt with his wife, daughter and granddaughter. Gorenstein praises the fruitful cooperation with FIAS scientists, the support and helpfulness of all the staff. “We published seven papers during my stay in Frankfurt”.

Should I stay or should I go? - Science counts.

His colleague Prof. Dmytro Anchyshkin from the Kyiv Bogolyubov Institute, on the other hand, decided to stay in Germany. He had worked as FIAS visiting professor for four months. Now he and his wife are taking advantage of state support to continue working at FIAS, which provides him with a workplace. They are considering returning to Kyiv to work there and manage a group of young scientists and Ph.D. students. But when they visited Ukraine around Christmas, life was hard: “Due to the bombing there was no electricity, internet, heating, and even water supply for hours”. Anchyshkin greatly appreciates the warm hospitality and support provided by the FIAS administration and scientific community, especially by Horst Stöcker.

Zhanna Khuranova had completed her master’s degree in physics in 2020. She wanted to apply for a PhD position in Germany anyway - the war made this wish concrete. Oleh Savchuk arranged contacts for her at FIAS; last August she met PD Dr Benjamin Dönigus. She has been working on her doctorate with him at the Department of Physics at Goethe University since the beginning of the year, on the prediction and measurement of tiny particles called hadrons. “I am glad that Horst Stöcker from FIAS supported me; and I am very happy with my current research topic, my supervisor and the support from the federal government,” says Khuranova. She doubts that she will ever return to Ukraine: “My family lives in the USA”. And a stay at CERN in Geneva lures her scientifically.

Maria Khelashvili had started her doctorate on ultra-light dark matter at the Bogolyubov Institute. She was very happy to continue her research at FIAS, thanks to a scholarship from the Polytechnic Society Foundation. She is currently continuing her work on ultra-light and axion-like dark matter candidates as a visiting PhD student at Princeton University (USA). “All that would not be possible without initial and very prompt support from FIAS”, she adds with gratitude.

Danylo Batulin completed his doctorate at FIAS a few weeks ago. He came to Germany from occupied Luhansk region back in 2016. Some of his friends and family members have been wounded or killed since the invasion, he says; his family’s real estate units have been destroyed. At first, he says, it was hard to live in a society where life continues as normal - with festivals, music and celebrations. “What saved my mental state was supporting Ukraine volunteer projects from here”. He praises: “It was amazing how fast and effectively the FIAS administration responded to the invasion. I was very moved by the symbolic large Ukrainian flag over FIAS”. He is enthusiastic about his PhD supervisor Jochen Triesch, in whose research group he published two papers.

“FIAS will continue to support scientists who are under threat at home and unable to conduct their research at home,” emphasises FIAS Director Eckhard Elsen. The cooperation with funders such as the Alexander von Humboldt Foundation, Foundation of the Polytechnic Society and the DFG makes it possible to give a home to researchers from all over the world - at least temporarily. The primary goal, of course, remains to recreate a desirable working environment at home in the long term and to strengthen this through cooperation. For example, FIAS is considering cross-country and cross-disciplinary conferences.

Happy Birthday!

A marvellous cake for the 86th anniversary of our FIAS sponsor Carlo Giersch: A gift from Goethe University and FIAS as a thank you to him and his wife for their many years of ongoing support, such as Giersch Conference, Laureatus Award, Giersch Excellence Awards and scholarships for young scientists.

80th birthday of Rudolf Steinberg

Rudolf Steinberg, an outstanding figure in the field of education and science, turned 80 in June 2023. The former president of Goethe University and long-time chairman of the Foundation Board of FIAS made significant contributions to the promotion of cutting-edge research and academic excellence during his career.

During his tenure as president of Goethe University, Rudolf Steinberg not only made a decisive contribution to the transformation of Goethe University into a foundation university under public law. During this time, he was also instrumental in establishing the FIAS Foundation. After his tenure at Goethe University, he remained closely connected to FIAS. Thus, first as a member, and later as chairman of the Foundation Board, he played a major role in shaping the development of our Institute. His dedication to the advancement of science left a lasting impact on FIAS and laid a foundation for its sustained success. Steinberg's work and dedication have garnered numerous awards and recognitions. Among others, he was awarded the Order of Merit of the Federal Republic of Germany in 2020 for his work.

70th birthday of Volker Mosbrugger

Volker Mosbrugger was appointed to the FIAS Board of Trustees in 2021 and elected its chair last year. He was born in Constance on 12 July 1953. He studied biology and chemistry for the teaching profession in Freiburg and later obtained his doctorate there. He habilitated at the Institute of Palaeontology at the University of Bonn in 1989 and followed a call to the University of Tübingen one year later. Mosbrugger investigated ecological and climatic changes in the Earth's history.

In 2005, Mosbrugger came to Frankfurt as director of the Senckenberg Research Institute and Nature Museum. From 2009 to 2020, he was Director General of the "Senckenberg Gesellschaft für Naturforschung". He promoted the timely topics of climate and environmental protection in research and at the Senckenberg Museum and brought biodiversity research into focus. Under his leadership, the museum and the research institute were rebuilt and expanded.

In 2022, the City of Frankfurt awarded him the Goethe Plaque. He had made outstanding contributions to the city's museum and science landscape, the laudation said. FIAS director Eckhard Elsen praised his "creative activities and communicative exchange". Mosbrugger also promoted this spirit as Chairman of the FIAS Board of Trustees. This "Stiftungsrat" supervises the Board of Directors and appoints its members. It decides on the budget of FIAS and advises the Board of Directors in all matters of strategic importance. In recent years, for example, it contributed significantly to the successful restructuring of the research areas at FIAS and accompanied this process. Mosbrugger is also the honorary president of the Polytechnische Gesellschaft Frankfurt. FIAS looks forward to continued constructive and creative cooperation for the benefit of our institute!

Seven new doctorates at FIAS

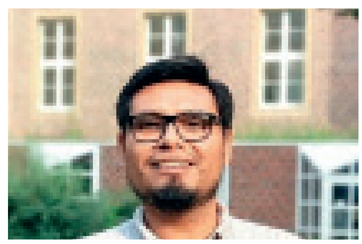
Josephine Tetteh, Danylo Batulin, Manjunath Omana Kuttan, Gustavo Hernandez Mejia, Vinzent Steinberg, Michael Florian Wondrak and Oleksandr Stashko sucessfully ended their doctoral thesis at FIAS. Congratulations to all new PhDs - and their supervisors!

Josephine Naa Ayeley Tetteh, from the group of Esteban Hernandez-Vargas, defended her doctoral thesis in April. Her doctoral studies focused on the application of mathematical and computational techniques to model the development of resistance in infectious diseases.

Danylo Batulin (middle) from the group of FIAS fellow Jochen Triesch (middle) defended his doctoral thesis in June. He studied epilepsy disease development and the role of neuro-immune interactions. During his PhD he also volunteered as a FIAS student representative.

Manjunath Omana Kuttan finalized his PhD in October in the Deepthinkers group, supervised by FIAS Senior Fellow Horst Stöcker and FIAS Fellows Jan Steinheimer and Kai Zhou. His topic was artificial intelligence in heavy ion collisions, thereby linking theory and experiment. One of his articles in a long list of publications was highlighted as Editors' Suggestion in the journal Physical Review Letters.

Gustavo Hernandez Mejia from Esteban Vargas' FIAS research group, supervised by FIAS Fellow Franziska Matthäus, defended his doctoral thesis in December. During his doctorate, he studied affinity mechanisms of broad protection against influenza infections and developed strategies that contribute to the paradigm of personalized medicine. His work resulted in many publications.



"Best FIGSS Talk" prizes awarded

The "Best FIGSS Talk " was awarded for the first time by the Frankfurt International Graduate School for Science (FIGSS) at FIAS. In the bi-weekly FIGSS Seminar, doctoral students present their research to a scientific audience including their fellow doctoral students at FIAS.

Last winter semester, nine doctoral students presented their projects. Talks were evaluated by Coordinators Sebastian Thallmair and Doris Hardt (right).

The first prize for the "Best FIGSS Talk" was awarded to Mariia Golden (GU) and **Marc Pereyra** (FIAS, left). Their tandem talk on embryonic development of insects convinced the jury with a coherent presentation of the joint theoretical and experimental work to characterize cell motion during the development of the red flour beetle Tribolium castaneum. The smooth transitions between the alternating speakers illustrated the close collaboration in this research project embedded in the Center for Multiscale Modeling in Life Sciences (CMMS).

Pamela Osuna (second from left) won the second prize of the "Best FIGSS Talk" with her talk on the details of the machine learning-based approach which she uses used to detect dendritic spines which play an important role in the communication between neighboring neurons. The clear presentation and the detailed discussion of the challenges as well as an example application convinced the jury.

FIAS Postdoc Bastian Eppler as expert in a school chat

Can artificial intelligence be dangerous for us? Pupils from grades 7 to 12 asked FIAS postdoc Bastian Eppler and other scientists these and other questions. He was part of a panel of experts on the topic of artificial intelligence (AI) from the non-profit organisation "Wissenschaft im Dialog" (science in dialogue).

The online offer "I'm a Scientist, Get me out of here!" enables students to exchange ideas directly with researchers. From 25th to 29th of September 2023, a thematic round on the topic of AI took place, for which Eppler volunteered (https://imascientist.de/). The neuroscientist himself researches how neuronal networks function - both in the brain and the "black box" of artificial neuronal networks. "I answered the questions of interested students on the homepage and in the live chat and liked their great interest," reports Eppler. The topic of AI seems to occupy the students a lot, and they deal with it on many different levels, he observes.

"The curiosity and knowledge of the students I had contact with impressed me deeply," says Eppler. They not only asked questions about AI, but also showed great interest in the impact of this technology on our world. With great pleasure, he answered their questions and discussed with them how AI will influence our future. He answered questions from school classes in two half-hour live chats and also replied to questions from students on the homepage every morning.

One of the questions was: In which areas will we deal with AI in the near future? So the students are aware of the rapid integration of AI into our daily lives. Of course, AI already has a big impact in many areas of our lives, such as healthcare and transport, but we are also likely to see more AI applications in education soon.

The students also had the opportunity to ask questions beyond science, e. g. about the daily work of a scientist, as well as about things like Eppler's favourite football club (FSV Frankfurt). "Questions like these help students, who otherwise have no contact with scientists in their environment, to understand that we are only human," the scientist smiles. He also hopes to show them that a career in science is possible and can be a lot of fun.

Eppler found his participation in "I'm a Scientist, Get Me Out of Here!" a remarkable experience: "It showed me how important it is to make science and research accessible to young people and to encourage their curiosity". This platform allows the 35-year-old to connect with the next generation of researchers and share their enthusiasm for the world of AI. He recommends this experience to all scientists. Eppler says he would be happy to participate again next time: "I look forward to getting more students excited about the fascinating world of artificial intelligence."

By the way, he denied the question posed at the beginning, "Can artificial intelligence become dangerous for us?" - at least as far as an omnipotent AI dominating humanity is concerned. He considers the careless or deliberate use of AI by humans to be more dangerous, for example in the production of fake news images or discrimination by AI that reproduces racism by humans, for example, because it only uses data generated by humans.

Future Groove Slam with FIAS PhD student

The 'ON/NO FUTURE FESTIVALS' of the Heinrich Böll Foundation Hesse on 24 November was all about the next generation. FIAS doctoral student Jonas Elpelt hosted the U20 Science Slam and successfully took part in the "Future Groove Slam".

By just one point Elpelt missed out on the final round of the "Future Groove Slam" at Frankfurt's Haus am Dom. The candidates performed impressive texts to the sound of live improvised music. Elpelt rapped his profound thoughts on the new biotechnological generation, accompanied by electric guitar and drums. Although AI now is able to write poetry faster than humans, he said: "The dignity of man is: incredible!" (citing the German constitution: Die Würde des Menschen ist unantastbar/unfassbar). He endet playing with German words: "Wollen wir die sein - oder die, die designen? Oder einfach nur die, die sind" ("Do we want to be them - or the ones who design? Or just the ones who are").

Prior to this, the 25-year-old moderated the U20 Science Slam, in which four tenth-graders from Marienschule Offenbach presented scientific topics from the STEM field.

Jonas Elpelt is currently working in the research group of FIAS Senior Fellow Matthias Kaschube in the field of theoretical neuroscience. He uses computer-aided data analysis and modelling to investigate the spontaneous activity of neuronal networks and their effects on processes of forgetting. It is not only in his scientific work that he tries to track down the cognitive foundations of creativity; he also devotes his freelance work to the study of memory. Eight years ago, he came to poetry slam, a modern form of poetry competition that began in the USA in the 1980s. In addition to several successful participations in championships at regional and national level, Elpelt now also organises regular events in the Rhine-Main region.

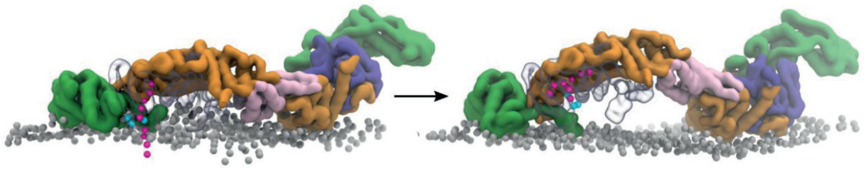
Science slams are derived from the popular format of the poetry slam and describe a competition in which scientists present their research topics to a wide audience within a given time. The origins of the science slam in Germany lie in Darmstadt, where the first such event took place almost 20 years ago.

"With this form of entertaining science communication, I want to reach an interested audience outside of professional community and facilitate dialogue," says Elpelt. The bioinformatician is convinced that successful research should not only be guided by interdisciplinary collaboration in an academic environment, but also by networked thinking in the context of society as a whole. "I would like to take part in science slams more often in future and make my research understandable and accessible to a wider audience in this way," says Elpelt, who working on his doctorate at FIAS since last year.

FELLOW REPORTS 2023

From a bacterial Trojan horse to a lipid Robin Hood

The protein P116 from *Mycoplasma* while it steals a lipid. Preprint at: https://doi.org/10.1101/2023.10.24.563710



The last year was the busiest and most productive year of our young group so far. Between journals and preprint servers, we published 13 scientific articles. This was only possible thanks to the passion and engagement of the young scientists in the group, and to the network of fantastic collaborators of which we are part. In our research we focused on tackling exciting molecular challenges adopting a multidisciplinary approach.

To name a few examples. Together with scientists at Goethe University, we explored how parasites use subtle techniques to interact with their hosts - us humans! We were able to determine the mechanism that the intracellular pathogen Listeria uses to gain access to our cells. A small protein acts as a Trojan horse, tricking some receptors on the surface of our cells to open the gates, otherwise heavily guarded. Integrating our molecular simulations with cutting-edge single molecule experiments, we were able to determine the structure of the protein that opens the gate with a precision of few nanometers. In another story, we looked at Mycoplasma, another human pathogen. This bacterium does not produce cholesterol, even though it needs it to survive. The solution to this problem is to steal it from our cellular membranes. But how? Mycoplasma has an invasion protein that binds to our membranes, makes holes to dig out cholesterol molecules, and then shuttles them back to the pathogen. Without consuming energy (!). Our simulations were instrumental in understanding how this occurs.

We also continued our effort to develop new computational methods. We proposed a new computational framework that integrates physical molecular simulations with deep learning to obtain mathematical models of how proteins and other biomolecules spontaneously reorganize between different structures, which is often necessary to perform their biological function. We also built on state-of-the art generative Artificial Intelligence methods that became famous for producing realistic images from nowhere. We modified these methods to generate, instead, trajectories containing the dynamics of biomolecules, without need to simulate them with computationally expensive physical simulators.

Group outing in the Odenwald.

Prof. Dr. Roberto Covino

He studied physics and theoretical physics at the University of Bologna and moved to Trento University for his PhD in physics. Afterwards he joined the Department of Theoretical Biophysics at the MPI of Biophysics in Frankfurt. He started his independent research group at FIAS in 2020. His group develops novel computational methods integrating physics-based models, molecular simulations, and machine learning to study how biomolecules perform their function in the cell. In 2023 he was appointed W3 professor for Artificial Intelligence in Protein Science at the University of Bayreuth.

Highlight

Roberto Covino brings a different manifestation of marzipan to group meetings every time.

Projects at FIAS: 4

Staff

PhD students: Gianmarco Lazzeri, Elena Spinetti, Lars Dingeldein, Serena Arghittu, Magnus Petersen, Francesco Carnovale (visiting); Master's students: Gabriel Hella, Emil Jackel; achelor's students: Rafael Heinz, Kai Stock

Collaborations

Sebastian Thallmair, FIAS
Mike Heilemann, Achilleas Frangakis, Michaela Müller-McNicoll, Volker Dötsch, Christoph Welsch, Inga Hänelt, Gemma Roig (Goethe Uni)
Robert Ernst (Saarland Uni)
Elif Karagöz (Max Peruz, Vienna)
Sharon Tooze (Crick Labs, London)
Taki Nishimura (Tokyo Univeristy)
Michael Woodside (University of Alberta, Canada), Pilar Cossio (Flatiron Institute, New York).

Dr. Hermann Cuntz

In the year 2013 he received the prestigious Bernstein Award with a prize money of around 1.25 million Euros to establish a group at FIAS and the Ernst Strüngmann Institute. He is approaching cellular neuroanatomy in a similar comparative manner as Santiago Ramón y Cajal one of the founders of the field of Neuroscience. Instead of using pen and paper as in his beautiful drawings Hermann Cuntz now takes advantage of computer models to reproduce dendritic structures from simple general principles.

Highlight

The lab has received two small grants to improve the TREES Toolbox, our Matlab software package for dendrite modelling. We look forward to wrapping up version 2.0 in the very near future.

Projects at FIAS: 1

Collaborations

Peter Jedlicka, ICAR3R – Interdisciplinary Centre for 3Rs in Animal Research, University Gießen
Gaia Tavosanis, Center for Neurodegenerative Diseases (DZNE), Bonn
Albert Gidon, Charité Universitätsmedizin, Humboldt University, Berlin
Jonathon Howard, Department of Molecular Biophysics & Biochemistry, Yale University
Stefan Remy, Leibniz Institute for Neurobiology, Magdeburg

The biological complexity of single neurons

Dendrites are the beautifully branched input structures that shape a neuron's connectivity and the computations that it performs. We work with computer models that describe the morphology and electrophysiology of such dendrites. While the morphology is well described by simple optimal wiring criteria, the electrophysiological behaviour depends on a complex composition and spatial distribution of a large variety of different ion channels (see Figure 1, for a dentate gyrus granule cell model).

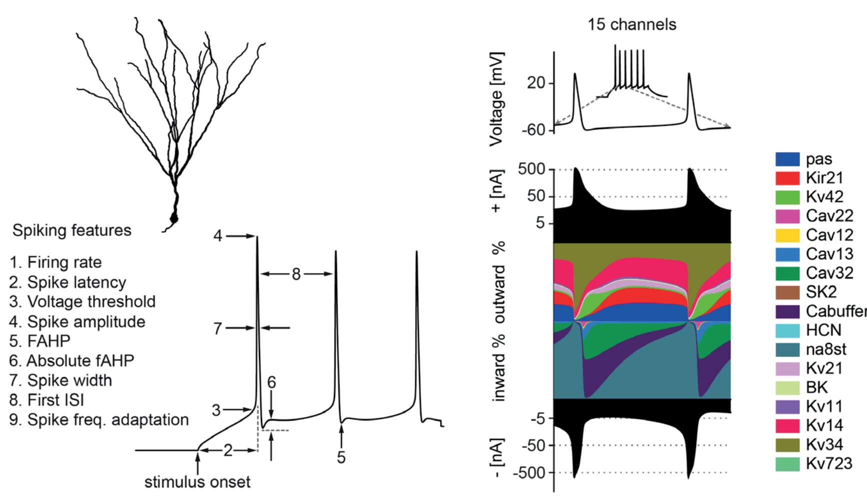
We explored here how the high dimensional parameter space describing the electrophysiology of dentate granule cells may come about. Each ion channel type in the dendrite has a conductance value per surface membrane, which can be thought of one parameter in the model.

Intriguingly, we found that the electrophysiological behaviour of a granule cell could be easily reproduced with a much smaller set of ion channels: A much smaller number of knobs, therefore, to tweak. Shouldn't this simpler model then be easier to tune?

We found the surprising result that choosing parameters randomly in the more complex model increased the chances of achieving the target spiking by 5x. Any putative neuron, therefore, producing the proteins for ion channels and sending them into the dendrites in a somewhat stochastic manner may be more likely to perform the desired computation in the model with higher ion channel complexity. It turns out that, in a way, the higher complexity actually may make it easier to tune the model.

Original publication:
Schneider M, Bird AD, Gidon A, Triesch J, Jedlicka P+, Cuntz H+ (2023) Biological complexity facilitates tuning of the neuronal parameter space. PLoS Computational Biology, 19(7):e1011212.

Dendrites are the beautifully branched input structures that shape a neuron's connectivity and the computations that it performs. We work with computer models that describe the morphology and electrophysiology of such dendrites. While the morphology is well described by simple optimal wiring criteria, the electrophysiological behaviour depends on a complex composition and spatial distribution of a large variety of different ion channels (see Figure 1, for a dentate gyrus granule cell model).



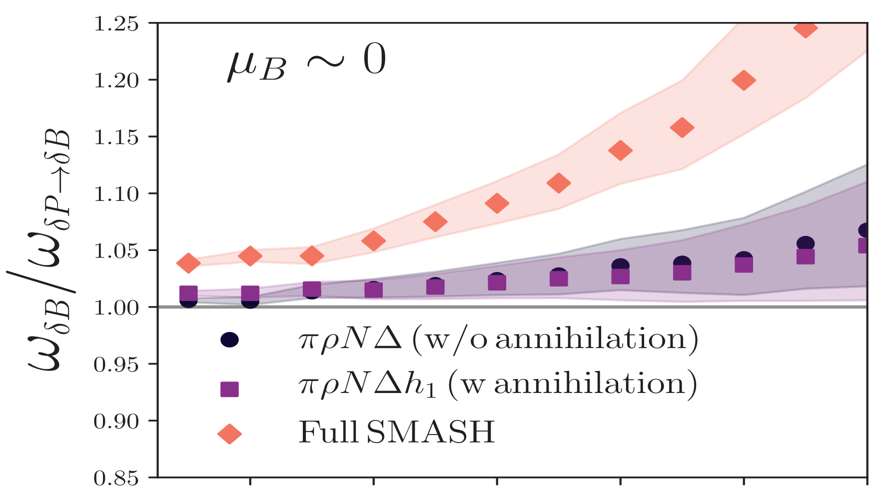
Fluctuations of conserved charges in heavy-ion collisions

One of the main goals of heavy-ion research is the quest for structures in the phase diagram of strongly-interacting matter. Similar to water that exists in different phases (fluid, ice and steam), the smallest constituents of matter form different structures depending on temperature and density. At high temperatures and small densities, theoretical calculations within quantum chromodynamics are performed on the lattice and concluded that there is a cross-over between the hadron gas and the quark-gluon plasma phase. At moderate temperatures and high densities as they are explored in low energy heavy-ion collisions as well as neutron star mergers, effective theory calculations suggest a first order phase transition. The potential critical endpoint motivates experimental efforts like the beam energy scan at the Relativistic Heavy Ion Collider (RHIC) and the future FAIR CBM program.

The most important signature for the passage of matter through the critical endpoint is a change in correlation length and associated different fluctuations of conserved charges. Unfortunately, the system is very dynamic and many assumptions in theoretical calculations cannot be directly verified experimentally. For example, instead of the net baryon number fluctuations, only proton fluctuations can be measured. In [1] we have shown that the suggested mapping between protons and net baryons only works for small volumes (see Fig. below), while for larger volumes non-trivial dynamic scatterings play a role. Furthermore, the fate of fluctuations in the hadronic rescattering phase has been investigated in [2]. If the coupling of the critical mode to the baryons is large enough, the signature for criticality survives the rescattering as simulated within the SMASH hadronic transport approach.

Publications: [1] Phys.Rev.C 107 (2023) 4, 044910 e-Print: 2202.11417
[2] e-Print: 2310.06636

Fig. (part of Fig. 9 from [1]): Ratio of the scaled variance of baryons and baryons when mapped from the protons $\omega_{\delta B} / \omega_{\delta P \to \delta B}$ as a function of the size of the subvolume. Three different systems with increasing number of degrees of freedom and interactions are shown.



Prof. Dr. Hannah Elfner

She is coordinating the theory pillar and head of the department "Hot and dense QCD matter" at GSI, professor for Theoretical Physics at Goethe University and FIAS fellow since 2013, in 2022 promoted to Senior Fellow. She obtained her PhD degree at Goethe University in 2009 sponsored by Deutsche Telekom Stiftung and spent three years as a Humboldt fellow and visiting assistant professor at Duke University. In 2016, she received the Heinz Maier-Leibnitz prize by the DFG and BMBF. In 2018, she was awarded the Zimanyi medal at the Quark matter conference, the highest recognition of young theoretical heavy ion physicists. In 2021, she received the award "Scientist of the year" by the Gertrud and Alfons Kassel foundation (GU).

Highlight

The Hard Probes 2023 conference: Renan Hirayama won a flash talk with his poster on elliptic flow of dileptons in low energy heavy ion collisions as they are measured at GSI, Darmstadt.

Projects at FIAS: 3

Staff

Jan Hammelmann (DFG SinoGerman), Renan Hirayama (HFHF), Carl Rosenkvist (F&E), Alessandro Sciarra, Gabriele Inghirami, Hendrik Roch, Justin Mohs, Niklas Götz, Nils Saß, Antonio Bozic, Timo Füle, Martha Ege, Robin Sattler

Collaborations

JETSCAPE collaboration, USA
MUSES collaboration, USA
Marlene Nahrgang, Marcus Bluhm, Subatech, Nantes, France
Sören Schlichting, Bielefeld

Dr. Nadine Flinner

She studied bioinformatics and worked on the structure and phylogeny of membrane proteins during the diploma thesis. In her PhD, finished in 2015, she investigated the behaviour of membrane proteins using molecular dynamic simulations.
Nadine Flinner started her PostDoc at FIAS investigating the migration of immune cells and is now interested in understanding the correlation between cell morphology and the underlaying molecular features. She is FIAS Fellow since 2020.

Highlight

Ingvild Mathisen joined our group, working on the prediction of molecular subtypes in bladder cancer.

Projects at FIAS: 1

Staff

Robin Mayer
Ingvild Mathisen
Marina Kurtz
Jessica Darling

Collaborations

Peter Wild, Jochen Triesch, Martin Hansmann, FIAS
Henning Reis, Sylvia Hartmann, GU

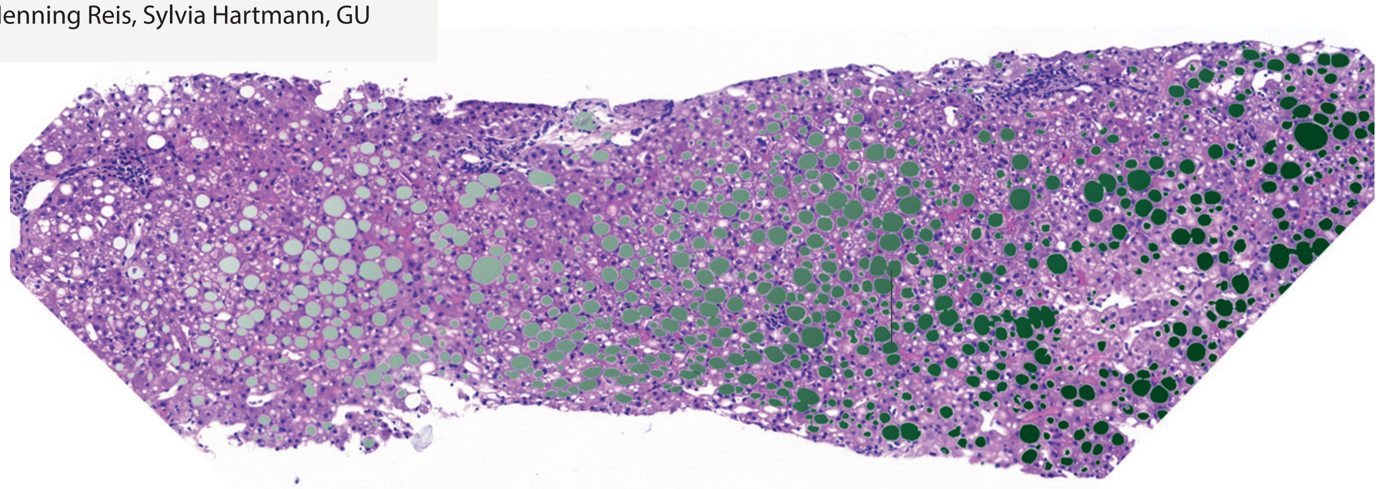
Quantitative assessment of steatosis in liver disease

In pathology, the number of affected cells is often required to make a diagnosis: In MASLD (metabolic dysfunction-associated steatotic liver disease), for example, one factor is the number of fatty hepatocytes. However, as a tissue section contains several thousand of cells, this number cannot be counted but is estimated by the pathologist. This leads to high intra- and interobserver variability.

We have therefore developed an algorithm that automatically recognizes fat in tissue sections and can then relate it to the total area of the tissue or the cells it contains. The area-based approach yielded a stronger correlation to the manual pathologist evaluation than nucleus-based method (Ø Spearman Rho (ρ) = 0.92 vs. 0.79). The inclusion of information on the tissue composition (presence of collagen and/or immune cells) reduced the average absolute error for both area- and nucleus-based predictions by 0.5%, and 2.2%, respectively.

An addition we have shown that the automatically determined values can guide pathologists in manual analysis and therefore have the potential to minimize interobserver variability, which can improve the quality of patient care in the long term.

Hematoxylin and Eosin (HE) stained tissue section of a liver biopsy. Fat appears as white circles in the image (left), which will be automatically recognized and highlighted in green (right). From: Tim Liebisch, PhD thesis, Generation of an Efficient Agent-Based Framework for the Simulation of 3D Multicellular Systems. Aufnahme: Jessica Darling, GU.



Immune system in 3D and 4D including molecular analytics

The focus of my research group's scientific activities in 2023 continued to be the immune system and specifically the human lymph node. The laser technologies we established were again used to create 3D and 4D, i.e. also moving, images of the human lymph node. These were the starting point for further calculations of B-cell regions (16), T-cell states (11) and strategic considerations in lymph node diagnostics (3). The movement characteristics of different cell types were also documented and interpreted (12). Machine learning methods were also used for the calculations (10). Checkpoint and receptor analyses were carried out to gain a better understanding of cell interactions (13, 4). A special place was taken by work dealing with mutations, molecular and cytogenetic analyses and mRNAs in different types of lymphoma (1, 6, 7, 8, 15). A very interesting result was obtained by analysing reactive CD30-positive, activated B cells in human lymph nodes. Here it was shown that these cells are probably essential in the B cell reaction, but generally do not exhibit any particular additional potential for malignant transformation (8). Finally, we continued to work on our overarching model of a virtual lymph node using a Petri net approach (5).

Overall, we were able to use both bioinformatic and molecular methods to gain further insight into the development and spread of malignant lymphomas and take further steps towards our goal of creating a virtual lymph node model.

Publications: Novel insights into the pathogenesis of follicular lymphoma by molecular profiling of localized and systemic disease forms. Kalmbach S. et al, Leukemia. doi: 10.1038/s41375-023-01995-w. // Clonal T-cell proliferations occasionally occur in Kikuchi-Fujimoto disease. Hartmann S. et al, Hum Pathol. doi: 10.1016/j.humpath.2023.06.003 // 3D/4D strategic lymph node diagnostics: The 4D representation of the human lymph node enables the observation and interpretation of the immune system in space and time]. Hansmann ML. Pathologie (Heidelb). doi: 10.1007/s00292-023-01265-7 // B-cell receptor reactivity against Rothia mucilaginosa in nodular lymphocyte-predominant Hodgkin lymphoma. Thurner L. et al. Haematologica. doi: 10.3324/haematol.2023.282698 // Holistic View on the Structure of Immune Response: Petri Net Model. Scharf S. et al. Biomedicines. doi:10.3390/biomedicines11020452 // Identification of two unannotated miRNAs in classic Hodgkin lymphoma cell lines. Ustaszewski A. et al. PLoS One. doi: 10.1371/journal.pone.0283186 // Clonal composition and differentiation stage of human CD30+ B cells in reactive lymph nodes. Küppers R. et al. Front Immunol. doi: 10.3389/fimmu.2023.1208610. // Immune phenotypes and checkpoint molecule expression of clonally expanded lymph node-infiltrating T cells in classical Hodgkin lymphoma. Ballhausen A. et al. Cancer Immunol Immunother. 72(2):515-521. doi: 10.1007/s00262-022-03264-8. // The RHOA Mutation G17V Does Not Lead to Increased Migration of Human Malignant T Cells but Is Associated with Matrix Remodelling. Merk-Ahmad K. et al. Cancers 15(12):3226. doi: 10.3390/cancers15123226 // Three-dimensional human germinal centers of different sizes in patients diagnosed with lymphadenitis show comparative constant relative volumes of B cells, T cells, follicular dendritic cells, and macrophages. Schemel CM et al. Acta Histochem. 125(7):152075. doi: 10.1016/j.acthis.2023.152075. // Tumour cell characteristics and microenvironment composition correspond to clinical presentation in newly diagnosed nodular lymphocyte-predominant Hodgkin lymphoma.

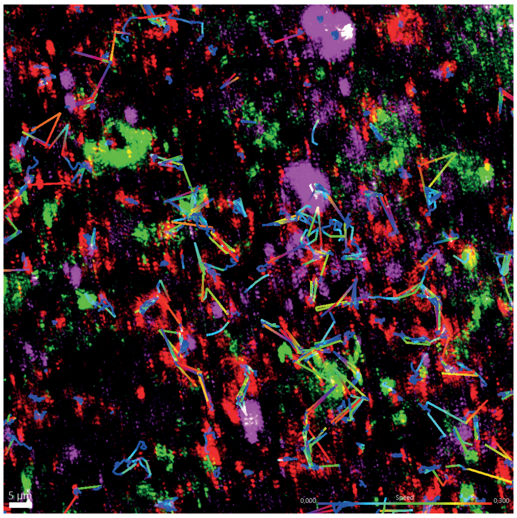


Illustration of various immune cells in human tissue and their movement tracks. Green CD20, purple CD4 and red CD8. Track colour is an indicator of speed.

Prof. Dr. Martin-Leo Hansmann

He studied medicine and biology in Bonn. After recieving his diploma in 1974 and his medical state examination in 1977, he received his doctorate in 1982 and habilitated in 1987. From 1990 to 1996 he was Professor at the Institute of Pathology at the University of Cologne and since 1996 Professor at the Senckenberg Institute of Pathology at the Goethe University.
Hansmann joined FIAS in 2016. His main expertise lies in haematopathology, the molecular pathology of malignant lymphomas.

Highlight

Results of the group were presented both in the FIAS colloquium lecture and in the lecture by Hendrik Schäfer.

Projects at FIAS: 1

Staff

Hendrik Schäfer
Patrick Wurzel
Sonja Scharf

Collaborations

Emmanuel Donnadieu, Institut Cochin Paris; Patrick Wagner, Fraunhofer Heinrich Hertz Institute Berlin & TU Berlin; Klaus-Robert Müller, TU Berlin; Frederick Klauschen, Ludwig-Maximilians-Universität München & Charité-Universitätsmedizin Berlin; Ralf Küppers, Institute of Cell Biology Esse; Evelyn Ulrich, Klinik für Kinder- und Jugendmedizin des Universitätsklinikums Frankfurt

Prof. Dr. Gerhard Hummer

He studied physics and received his PhD at the University of Vienna, Austria, for work done at the Max Planck Institute for Biophysical Chemistry, Göttingen. He joined the Los Alamos National Laboratory (NM, USA) as a postdoc (1993-1996) and group leader (1996-1999). In 1999, he moved to the National Institutes of Health (MD, USA), where he became Chief of the Theoretical Biophysics Section and Deputy Chief of the Laboratory of Chemical Physics, NIDDK. Since 2013 he is director of the Department of Theoretical Biophysics at the Max Planck Institute of Biophysics in Frankfurt/M. Since 2016, he is also Professor of Biophysics at the Goethe University in Frankfurt. Since 2015 he is FIAS-Senior Fellow.

Highlight

In 2023, the Hummer group used molecular dynamics simulations to visualize the dynamic network of FG nucleoporins mediating the transport in and out of the cell nucleus.

Projects at FIAS: 1

Collaborations

Roberto Covino
Sebastian Thallmair

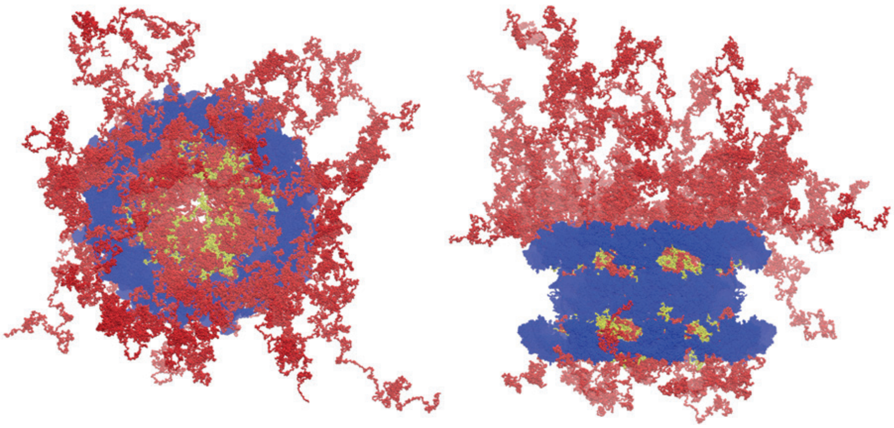
Molecular simulations of cellular machineries – guided by AI

2023 was another exciting year for our group with publications in Nature (3), Nature Computational Science, Nature Structural and Molecular Biology, Cell Chemical Biology, Nature Chemical Biology, Nature Communications (2), Current Biology, and other journals. As a highlight on the methods side, we collaborated with Roberto Covino at FIAS to develop an AI method that autonomously learns the mechanisms of complex molecular self-assembly processes and reactions (Jung, Covino et al., Nat. Comput. Sci. 3, 334, 2023).

The AI agent repeatedly runs molecular dynamics (MD) simulations, makes a wager on their outcome, records the actual outcome and, over time, improves the predictions to learn what makes a reaction happen and what not. In this way, the AI agent builds an ever deeper understanding of the reaction mechanism, uses this knowledge to achieve maximum efficiency in sampling reaction events, and distills the knowledge extracted into human-understandable analytic mathematical expressions.

On the applications side, we teamed up with the groups of Edward Lemke in Mainz and Martin Beck in Frankfurt to visualize the FG nucleoporins (Nups) in the central pore of the nuclear pore complex (NPC). In an integrative approach, we used information on the anchoring positions of the FG-Nups to position these long and mostly disordered proteins in the NPC and on distances from in-cell fluorescence measurements (Yu, Heidari et al., Nature 617, 162, 2023).

By matching the interaction strength between the FG-Nups to the experimental data, we could show that the FG-Nups are near the critical point to phase separation between a dense protein condensate and a dilute protein solution. Criticality appears to ensure a highly dynamic network that acts as a molecular filter for most proteins but can, if needed, accommodate also very large cargo such as mRNA. This work sets the stage for detailed explorations of the transfer of gene regulatory factors into the nucleus and of gene products out of the nucleus.



FG nucleoporins (red, yellow) form a dynamic network that seals the center of the nuclear pore complex (blue) to gate the molecular traffic between the cell nucleus and cytosol. Their structure could be resolved by integrating molecular dynamics simulations with fluorescence measurements (Yu, Heidari et al., Nature 617, 162-169, 2023; Image: Maziar Heidari).

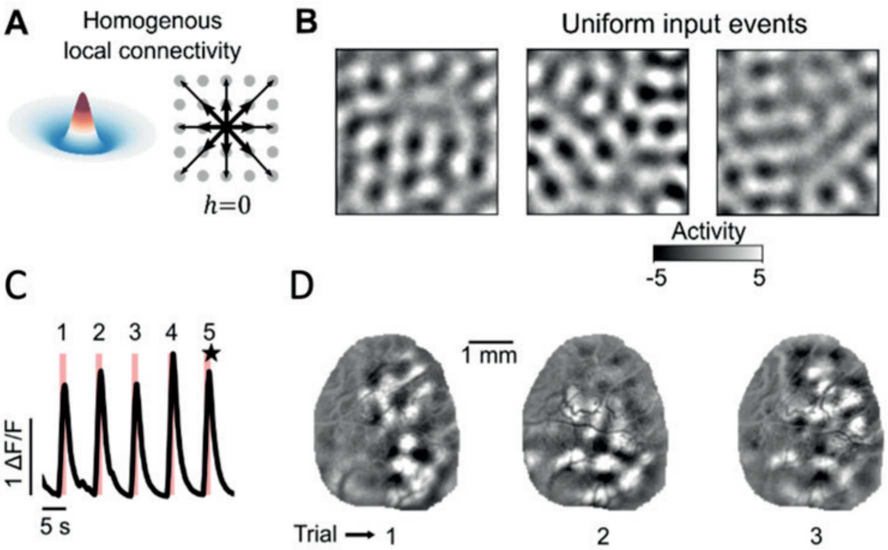
Universal origin of cortical representations

In order to deal with a complex environment, the brain forms a diverse range of neural representations that vary across cortical areas, ranging from largely unimodal sensory input to higher-order representations of goals, outcomes, and motivation. The developmental origin of this diversity is currently unclear, as representations could arise through processes that are already area-specific from the earliest developmental stages or alternatively, they could emerge from an initially universal functional organization shared across different cortical areas.

In a recent study in PNAS, conducted together with neurobiologist Gordon Smith at the University of Minnesota, we leveraged ongoing spontaneous activity to show that a distributed and modular functional architecture with long-range correlations, known for many years to exist in visual cortex, is in fact a common feature of the developing cortex. The high degree of quantitative similarity across cortical areas suggests that similar design principles might operate throughout the early cortex. Thus, a common modular organization might serve as a generic cortical substrate upon which later area-specific influences generate the functional specificity found in the mature brain.

What mechanism could shape such universal modular activity structure early in cortex? For more than five decades scientists hypothesized that such modular activity patterns, first observed in the visual cortex of primates and carnivores, could arise via a Turing mechanism – a widespread mechanism for the self-organization of near periodic patterns in biology. By combining computational modelling with direct optogenetic cortical activation in ferret visual cortex, we showed that cortical networks transform unstructured uniform stimulation into a diverse set of structured modular activity, confirming key predictions of a Turing mechanism. Our work provides the first direct in vivo demonstration of a Turing mechanism operating in the developing brain and was selected for an oral presentation at 2023 COSYNE conference (top 3% of submissions).

(A) Circuit model of visual cortex. (B) The model produces Turing patterns. (C, D) Repeated uniform cortical optogenetic activation (pink vertical lines in (C)) drives diverse modular patterns (D), consistent with a Turing mechanism shaping cortical activity.



Prof. Dr. Matthias Kaschube

He studied physics at Universities Frankfurt and Göttingen, graduated in 2000 and obtained his doctoral degree 2005. He carried out his thesis at the Max Planck Institute for Dynamics and Self-Organization in Göttingen. In 2006, he earned a scholarship at the Bernstein Center for Computational Neuroscience in Göttingen. 2006-2011 he worked at Princeton University as a Theory Fellow at the Lewis Sigler Institute for Integrative Genomics and as a Lecturer in the Physics Department. 2011 he became Professor for Computational Neuroscience and Vision in the Department of Computer Science and Mathematics at Goethe University and is Senior Fellow at FIAS.

Highlight

Diverse cortical representations emerge in development from a universal functional organization shared across the early neocortex.

Projects at FIAS: 5

Staff

Lorenzo Butti, Jonas Elpelt, Bastian Eppler, Santiago Galella, Deyue Kong, Thomas Lai, Pamela Osuna, Sigrid Trägenap, Maren Wehrheim

Collaborations

David Fitzpatrick, Max Planck Florida Institute, USA; Gordon Smith, University of Minnesota, USA; Simon Rumpel, University Mainz; Ben Scholl, University of Pennsylvania, USA; Gilles Laurent, Max Planck Institute for Brain Research; Ernst Stelzer, Biology, Goethe University (GU); Amparo Acker-Palmer, Biology, GU; Christian Fiebach, Psychology, GU

Prof. Dr. Udo Kebschull

He studied computer science at the Technical University of Karlsruhe (today KIT) and graduated in 1989. From 1989 to 1990 he worked as a scientific employee at the FZI in Karlsruhe. After working in Leipzig and Heidelberg, in 2010 Udo Kebschull became head of the University Computer Center of the Goethe University Frankfurt in connection with a chair for infrastructures and computer systems in information processing.

Highlight

Completion of the dataflow template library for high level synthesis for FPGAs.

Projects at FIAS: 6

Staff

Philipp Lang
Franca Speth
Felix Hoffmann
Diyar Takak
Thomas Janson
David Schledt

Collaborations

SVA System Vertrieb Alexander GmbH und dem Deutsches Zentrum für Luft- und Raumfahrt (DLR); HZD Hessische Zentrale für Datenverarbeitung; ekom21 - KGRZ Hessen; BMBF (ALICE, CBM)

To Mars with artificial intelligence

Have you ever thought about the fact that radio signals from Mars to Earth take between 3 and 22 minutes? If, for example, a fire were to break out during a manned mission to Mars, a control room on Earth would only find out about it after this time. The response to the accident would then take the same amount of time to arrive on Mars. This could already be too late. On the other hand, astronauts on Mars cannot be kept busy operating a control room around the clock. It therefore makes sense to automate the operation of a Mars station using artificial intelligence. This is precisely what is being investigated in a new project by Franca Speth from Kebschull's group. She is developing the AI components of a multi-agent system that will recognize and analyze various system states. Based on the data, the system provides recommendations for action in the event of problems. Simulated and operational data from the Columbus module of the International Space Station (ISS) is used as a data base to test how efficient and safe such a system would be in real ISS operations. The results can be transferred to other missions in space.

Blockchain technology remains a controversial topic. Another aim of the working group is to find answers here, whether it be new application possibilities or the reduction of energy requirements. This year, Philipp Lang was able to submit his dissertation on the use of blockchain technology for public administrations in the context of the RADIUS protocol. His work deals with the granting and revocation of rights and authentication. Diyar Takak investigated another application of blockchain technology in collaboration with ekom21 and the ONCE consortium. This involves the electronic archiving of hotel registration certificates secured by a blockchain. This approach can be extended to control access to confidential data stored on cloud storage. In his dissertation, Felix Hoffmann develops the approach of a proof-of-useful-work consensus algorithm, as well as alternative distributed computing approaches that allow the donation of computing power. In the field of high-energy physics (HEP), this approach will help to cope with the required and computationally expensive data in the CBM project at FAIR.

Thomas Janson is working on the development of a modern C++ data flow template library for the implementation of algorithms on FPGA accelerator cards. The aim is to implement concepts from data flow programming with the help of high-level synthesis. The results of his work will make it easier to develop, test, and use algorithms, e. g. used for detector readout in high-energy experiments at CERN. David Schledt is developing algorithms based on FPGAs for online feature extraction for the CBM-TRD detector. CBM data acquisition operates in a triggerless free-streaming mode, which requires online data selection. It brings the required feature extraction for the TRD data to the readout FPGA. Feature extraction includes decoding raw data, reconstructing energy and time, and finding clusters.

In the summer semester 2023, the lecture "Computer Hacking" and the blockchain seminar were held with the help of Takak and Hoffmann. Both courses will be offered again in 2024. In September 2023, the textbook for the lecture "Computer Hacking" for the lecture of the same name was published by Springer-Vieweg.

In 2023, a total of 13 Bachelor's and Master's theses were supervised in the working group and one doctorate was completed.

Image of the control room of the Columbus Control Centre (Col-CC), where real-time monitoring takes place, at DLR in Oberpfaffenhofen (photo: Franca Speth)

Enhancing interpretability of artificial neural networks

A key goal of the future CBM experiment at the FAIR facility is to explore the quark-gluon plasma (QGP) properties through heavy ion collisions at low energies. Given the low probability of QGP formation at these energies, identifying collisions that result in QGP becomes crucial.

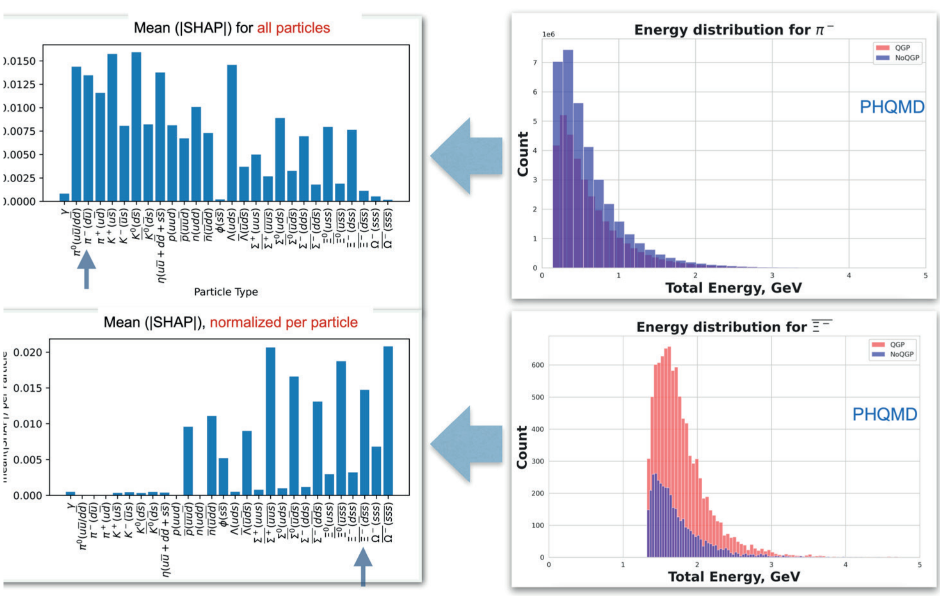
To address this challenge, we have developed both fully-connected and convolutional neural networks to detect QGP presence in central Au+Au collisions at 31.2 A GeV, using the PHQMD model for simulation. The convolutional network, in particular, has demonstrated superior performance, achieving over 95% accuracy in identifying QGP events in the test datasets.

Yet, the critical question remains: How does the neural network make these selections? To demystify the decision-making process of the network and move beyond treating it as a "black box," we employ the Shapley Additive Explanations (SHAP) method. This technique, rooted in cooperative game theory, enhances the interpretability of machine learning models by assigning a SHAP value to each feature, representing its average impact on the outcome when included in various subsets of features.

Our analysis reveals intriguing insights. The top left image illustrates the absolute SHAP values for all particle types generated in a typical heavy ion collision, indicating their importance in predicting QGP formation. For instance, the right-side chart highlights how pions, which are less abundant in QGP events, serve as a key indicator for the network.

Similarly, the bottom left image presents these SHAP values normalized by particle type frequency, underscoring the significant role of heavy anti-baryons. Despite their rarity, their increased production in QGP events, as shown in the right-side chart, is a critical factor for the network.

Through SHAP analysis, it's evident that the neural network has successfully learned the critical signatures of QGP formation, offering a reliable method for identifying relevant collisions in the CBM experiment.



Interpreting Artificial Neural Networks with Shapley Additive Explanations (SHAP) method. For details see text.

Prof. Dr. Ivan Kisel

He works on data reconstruction in high-energy and heavy-ion experiments. His approach based on cellular automata allows to develop parallel algorithms for real-time physics analysis using HPC. He received his PhD in physics and mathematics from the Joint Institute for Nuclear Research (Dubna, 1994). Then he worked at the University of Heidelberg, where he gained his habilitation in physics, in 2009, and at the GSI Helmholtz Centre for Heavy Ion Research. Since 2012, he is a professor for software for HPC at the Goethe University and a fellow at FIAS.

Highlight

QGP trigger for the CBM experiment.

Projects at FIAS: 3

Staff

Artemiy Belousov
Akhil Mithran
Oddharak Tyagi
Robin Lakos
Gianna Zischka

Collaborations

CBM
ALICE
STAR

Prof. Dr. Volker Lindenstruth

He studied physics at TU Darmstadt and received his doctorate in 1993 at Goethe University. He spent his Postgraduate years at the Lawrence Berkeley National Laboratory and UC Space Science Laboratory. In 1998, he returned to Germany as a Professor at the University of Heidelberg. In addition, he has been the head of the ALICE HLT project at the LHC since 2000. In 2009 he joined Goethe University as professor, and at FIAS he held the position of Fellow but became a Senior Fellow soon thereafter.

Highlight

On-line processing of first heavy ion collisions at the highest collision energies ever.

Projects at FIAS: 4

Staff

Gvozden Neskovic
Johannes Lehrbach
Felix Weiglhofer
Andreas Redelbach
Grigory Kozlov
Alexander Schröter

Collaborations

CERN
GSI

Fast data processing at large scale research

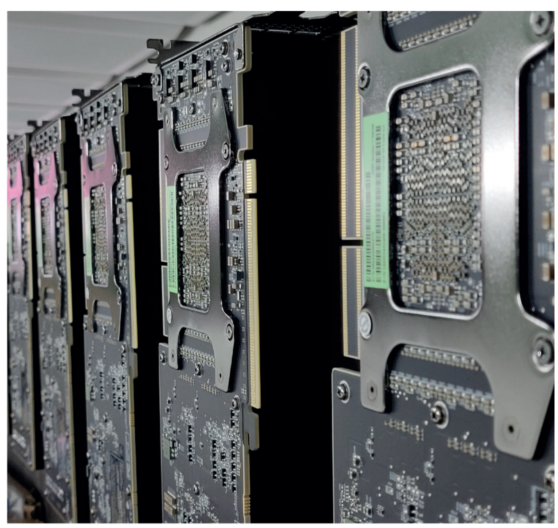
The team led by Volker Lindenstruth at FIAS continues to pioneer the use of GPUs in online data compression and processing in high-energy physics. In 2023, the updated data processing framework and the ALICE Event Processing Node farm proved successful in handling high-rate lead–lead collisions in real time.

During a long pause of operations (2019–2022), both the LHC and the experimental facilities performed maintenance and upgrades in preparation for the LHC's higher luminosity era. For the ALICE experiment, this included major upgrades to some detector systems, a new computing model, and new computing infrastructure. With these improvements, ALICE can now process lead–lead collisions, at an interaction rate of 50 kHz, in a continuous readout mode and the online (synchronous) and offline (asynchronous) data processing are now merged into a single software framework.

The new computing infrastructure includes the Event Processing Node (EPN) project, led by Prof. Dr. Volker Lindenstruth. The EPN farm of 350 servers, totaling to 2,800 GPUs and 24,640 CPU cores, is optimized for fast TPC track reconstruction – the bulk of the synchronous processing. Since the detector data arriving to the farm cannot be buffered, the EPN compute facility can handle raw data rates up to 1.3 TB/s and provide 90% of compute power via GPU processing.

In contrast to the data processing mode of past data-taking periods, the object processed is no longer a single collision event but is instead a predefined timeframe (TF) data structure. The Data Distribution software (developed at FIAS) orchestrates the building of the TFs. It starts by collecting all partial TFs sent by individual detectors and schedules the building of the full TF. Following the data transfer, each EPN receives and subsequently processes a full TF that contains data from all ALICE detectors. In addition to processing, the EPN farm compresses the data to a manageable size, and further ships it off to the CERN distributed storage system at a rate 170 GB/s.

In July of 2022 the LHC returned to full operations, with proton–proton collisions at a record center-of-mass of 13.6 TeV, starting of the so-called Run 3. But for the ALICE experiment – the LHC's heavy-ion enthusiasts – the most anticipated collisions and the biggest test of the new systems was the high-rate lead–lead collisions, which commenced on the 26th of September 2023 at the highest-ever center-of-mass energy of 5.36 TeV. Within the five-week data-taking period ALICE recorded nearly 12 billion collisions, 40 times of that collected in the previous collection periods from 2010 to 2018.



A batch of AMD GPUs, which are used extensively for the online processing of ALICE data.

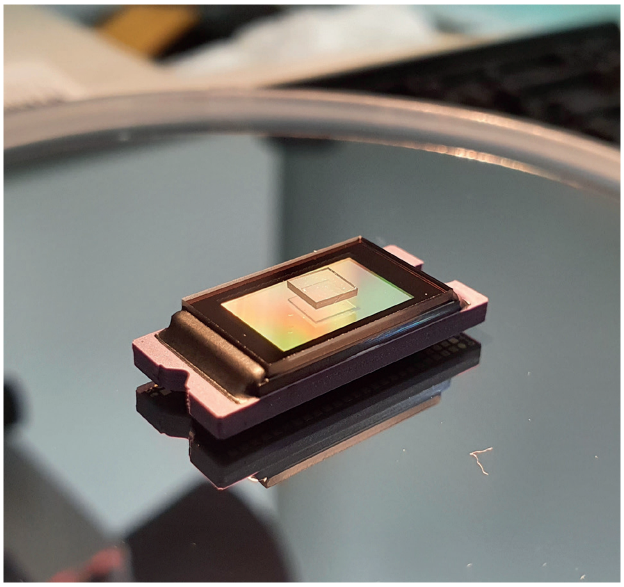
Modular supercomputing and quantum computing

In 2023, the MSQC group has substantially intensified its research and development activities in the area of quantum computing while simultaneously forebringing research in modular supercomputing. The group is commissioning Goethe University's first 5-qubit quantum computer named "Baby Diamond" which is based on NV-Centre Technology that works at room temperature settings (see page 10).

We extended our academic outreach by hosting a workshop in the FIAS building on Applied Quantum Computing, attended by students affiliated with the NHR alliance from all across Germany. Another workshop tailored for the industry was offered to Bundesbank at their location. Overall, we were able to start discussions about potential collaborations with partners from NHR, Deutsche Bank, ING Bank, d-fine GmbH, XeedQ GmbH, Quantagonia GmbH, Deutsche Bahn (DB Systel GmbH), and others.

Our group members published papers, presented posters, and participated in international conferences with topics related to quantum-classical variational algorithms and applications of quantum annealers. We continue to closely collaborate with the Jülich Supercomputing Centre (JSC), in particular with its unified quantum computing platform JUNIQ in order to offer quantum computing at the CSC beyond our own quantum hardware. We also filed an invention disclosure relating to a new hybrid quantum computing method to Goethe University's patent office at Innovectis GmbH.

In the modular supercomputing research area, we explored novel architectures and programming paradigms to enable this innovative technology, working on projects with EUPEX (European Pilot for Exascale) and NHR (Nationales Hochleistungsrechnen). Projects include empirical roofline models for Extreme-Scale I/O workload analysis, steps toward a modular workflow for network performance characterization, and modular and automated workload analysis for HPC systems. Our postdoc in this research area, Dr. Sarah Neuwirth, was awarded the 2023 PRACE Ada Lovelace Award for HPC. She left the group to become a professor at the University of Mainz.



NV Spin qubits on a photonic microchip - basis for the new quantum computer in Frankfurt.
(c) XeedQ GmbH

Prof. Dr. Dr. Thomas Lippert

He received his diploma in Theoretical Physics in 1987 from the University of Würzburg. He completed PhD theses in theoretical physics at Wuppertal University on simulations of lattice quantum chromodynamics and at Groningen University in the field of parallel computing with systolic algorithms. He leads the research group for Modular Supercomputing and Quantum computing at Goethe University Frankfurt and was appointed Senior Fellow at FIAS in March 2020. He is director of the Jülich Supercomputing Centre at Forschungzentrum Jülich, member of the board of directors of the John von Neumann Institute for Computing (NIC) and of the Gauss Centre for Supercomputing (GCS). He is Vice Chair of the Research and Innovation Advisory Group RIAG of the EuroHPC JU. His research interests cover the field of modular supercomputing, quantum computing, computational particle physics, parallel and numerical algorithms, and cluster computing.

Highlight

The group participated at the Supercomputing Conference 2023 in Denver, USA.

Projects at FIAS: 1

Staff and Collaborations

Arne Nägel, Manpreet Singh Jattana, Sarah Neuwirth, Zhaboin Zhu, Niklas Bartelheimer, Philip Döbler, Lucas Menger, Cedric Gaberle, Julian Hilbert, Junxi Wang, Benedikt Schröter

Prof. Dr. Franziska Matthäus

Following her studies in biophysics at the Humboldt University of Berlin, including one year research stay at UC Berkeley (USA), Franziska Matthäus spent five years in Warsaw (Poland) on her PhD and scientific research. Between 2005 and 2016, she held two postdoc positions and a group leader position at IWR, University of Heidelberg. In 2016, she received a junior professorship at CCTB, University of Würzburg. Since October 2016, she holds a W2 position in bioinformatics, funded by the Giersch-Foundation. In 2021 her position was made permanent at FB 12 of Goethe University.

Highlight

Since April 2023 Franziska Matthäus is part of the founding board of the newly established Center for Critical Computational Studies of the Goethe University.

Projects at FIAS: 3

Staff

Zoë Lange
Tim Liebisch
Marc Rereyra

Collaborations

Ernst Stelzer (GU)
Thomas Sokolowski (FIAS)
Alf Gerisch (TU Darmstadt)
Kevin Painter (Politecnico di Torino (Italy)
Mingfeng Qiu and Francis Corson, (LPENS, France)

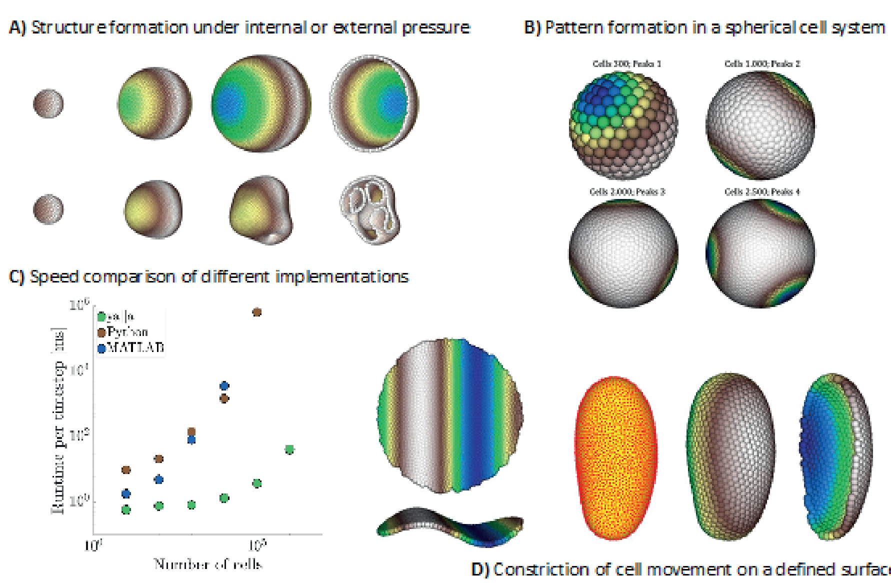
Speeding up stochastic particle simulations

To identify basic principles of complex behavior in multicellular systems, the Matthäus group uses agent-based models. These describe each cell as a discrete object with features (such as position, velocity or size), which are described by a system of stochastic differential equations. Agent-based models are very versatile, can incorporate biomechanical properties of cells, but also internal signaling processes, cell-cell interaction or the interaction with a chemical or mechanical environment. However, with the number of cells also the system of equations grows, and stochastic simulations become computationally expensive.

To overcome limitations attributed to these computational costs, Tim Liebisch dedicated intense work to an extension of the recently published GPU framework ya||a from the group of James Sharpe (EMBL Barcelona). He used a three-month research stay at EMBL Barcelona, funded by an EMBO short term fellowship, to established a fruitful collaboration with the Sharpe group and familiarize himself with the software. Since his return he successfully implemented all core features of our modeling approaches, as well as several new extensions. Comparisons with the previous implementations in Matlab and Python demonstrate an immense speedup, especially for large cell numbers. For instance, simulations involving 10^5 cells achieve a speedup of over 170.000-fold on the GPU in contrast to the Python implementation.

This strong reduction in computation time also allowed for the efficient inclusion of further modeling aspects, such as the generation of an additional force field restricting the motion of the cellular agents to any curved surface or arbitrary volume, either through shape parametrization or discretization of image data. This efficient, flexible and modular GPU implementation now opens doors for the analysis of a variety of biological systems, as well as AI-based parameter estimation, e.g., simulation-based inference.

Showcase simulations for several model extensions, such as the interaction of a growing structure with a mechanical environment (A), the inclusion of chemical substances subject to reaction and transport between cells (B), or the constriction of the cell dynamics to a previously defined surface (D). The graphics shown in (C) displays the large difference in computational cost between implementations in Matlab, Python or Cuda.



Network models and Big Data

Network models play a crucial role in various fields of science and their applications far surpass the original scope of explaining features observed in the real world. A common use case of such random graphs is to provide a versatile and controllable source for synthetic data to be used in experimental campaigns. As such, they can provide valuable insights during the design and evaluation of algorithms and data structures — in particular, in the context of large problem instances. Generating such graphs at scale, however, is a non-trivial task in itself. We are interested in algorithmic aspects of generating massive random graphs - especially in the context of cache-efficiency and parallelism.

In this context we published the following results in 2023:

* Parallel global edge switching for the uniform sampling of simple graphs with prescribed degrees. (J. Parallel Distributed Comput. 174: 118-129 (2023))

* Parallel and I/O-Efficient Algorithms for Non-Linear Preferential Attachment. (ALENEX 2023)

These papers were an integral part of the PhD thesis of Dr. Hung Tran, who defended in 2023 and is currently a postdoc at FIAS. Some of the generators have also been applied in the research work on k-shortest paths by GU-group member Dr. Alexander Schickedanz, who completed his PhD thesis in 2023 as well.

Furthermore, we took part in the PACE 2023 challenge, which asked to design and implement practical algorithms to compute contraction sequences of small twin-width. Together with our colleagues from Holger Dell's group (GU) and Frank Kammer's (THM) group we contributed the winning heuristic solver and placed second in the exact track. The results were published at IPEC 2023.

Further research cooperations at FIAS include CMMS (Project "Construction, analysis and dimensional reduction for binary networks", together with Prof. Dr. Tatjana Tchumatchenko) and DFG FOR 2975 ("Algorithms, Dynamics, and Information Flow in Networks" - two subprojects with connections to network generation: one at FIAS and one at FB12).

Prof. Dr. Ulrich Meyer

He joined FIAS in January 2020. He has been a full professor at Goethe University Frankfurt since 2007. Meyer is currently also a director for research at the new Center for Critical Computational Studies (C3S) founded in 2023. From 2014 to 2022 he was the spokesperson of the DFG priority program SPP 1736 "Algorithms for Big Data". Ulrich Meyer received his PhD in computer science from Saarland University in 2002. Subsequently he was a postdoc and eventually senior researcher (W2) at Max Planck Institute for Computer Science in Saarbrücken.

Highlight

Within DFG FOR 2975 we co-organized a successful summer school on Algorithm Engineering at Hasso-Plattner Institute (Potsdam) in 2023. All talks were recorded and are available under https://hpi.de/ae2023/.

Projects at FIAS: 2

Staff

Yannick Gerstorfer
Hung Tran

Cooperations

CMMS
DFG FOR 2975

Summer school on Algorithm Engineering at Hasso-Plattner Institute (Potsdam).

Prof. Dr. Igor Mishustin

He studied theoretical physics and astrophysics at the Moscow State University. He obtained his PhD and then the Doctor of Sciences degree (habilitation) at the Kurchatov Institute in Moscow. After longterm stays in the Niels Bohr Institute (Denmark) and the University of Minnesota (USA), he joined the newly-established Frankfurt Institute for Advanced Studies, in 2004. Here he leads the group of theoretical subatomic physics and astrophysics.

Highlight

Fruitful scientific collaborations with several Ukranian postdocs.

Projects at FIAS: 2

Collaborations

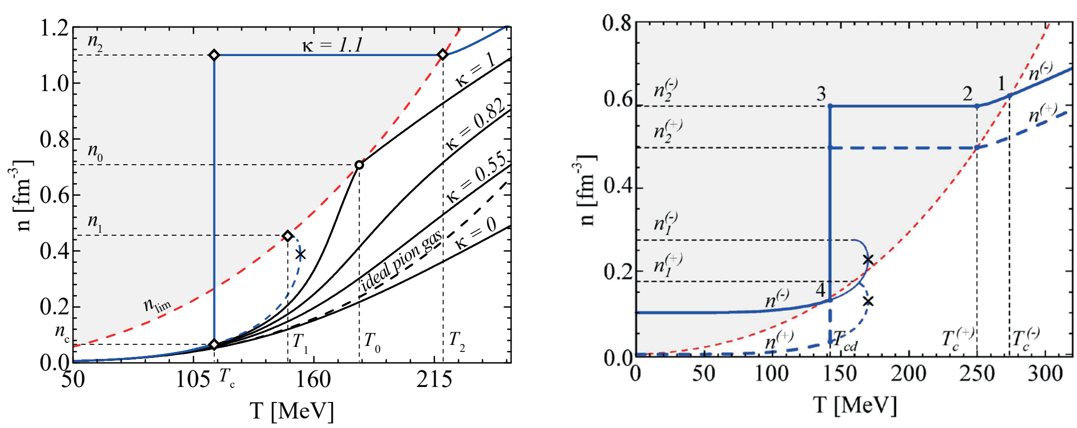
Horst Stoecker
Mark Gorenstein
Leonid Satarov

Phase transitions in the interacting relativistic Boson systems

The thermodynamic properties of the interacting particle-antiparticle boson system at high temperatures and densities were investigated within the framework of scalar and thermodynamic mean-field models. We assume isospin (charge) density conservation in the system. The equations of state and thermodynamic functions are determined after solving the self-consistent equations. We study the relationship between attractive and repulsive forces in the system and the influence of these interactions on the thermodynamic properties of the bosonic system, especially on the development of the Bose-Einstein condensate. It is shown that under “weak” attraction, the boson system has a phase transition of the second order, which occurs every time the dependence of the particle density crosses the critical curve or even touches it. It was found that with a “strong” attractive interaction, the system forms a Bose condensate during a phase transition of the first order, and, despite the finite value of the isospin density, these condensate states are characterized by a zero chemical potential. That is, such condensate states cannot be described by the grand canonical ensemble since the chemical potential is involved in the conditions of condensate formation, so it cannot be a free variable when the system is in the condensate phase.

This automatically leads to the fact that the Grand Canonical Ensemble, where the chemical potential μ_I is a free variable, can be adequate to describe the bosonic system only in the thermal phase. In the condensate phase, an adequate tool for describing this phase is the Canonical Ensemble, where the chemical potential $\mu_I(T,n_I)$ is a thermodynamic quantity that depends on free variables. It should be noted that this statement fully corresponds to our conclusion about the description of the ideal bosonic gas in the condensate phase obtained in the introduction.

Interacting particle-antiparticle boson system in the thermodynamic mean-field model. Left panel: Particle densities vs. temperature at conserved isospin (charge) density n_I=0.1 fm−3 as the solid blue line consisting of several segments (π− mesons) and the dashed blue line consisting of several segments (π+ mesons). The vertical segment for both dependencies indicates a phase transition of the first order with the creation of the condensate. In the condensate phas μ_I=0. A dashed red line is the critical curve n_I lim(T). Right panel: particle-number densities vs. temperature at n_I=0 (or μ_I=0):(1) the supercritical attraction κ =1.1 is shown as a solid blue line consisting of several segments, the vertical segment (solid blue line) indicates a phase transition of the first order with the creation of the condensate; (2) particle densities at “weak” attraction κ≤1 are shown as solid black lines in the thermal phase. A dashed red line is the critical curve. Crosses on both panels separate metastable and non-physical states.



Gravity at Work

Astrophysicist Samaya Nissanke is an International Fellow at FIAS hosted at the University of Amsterdam active in the development of novel techniques to extract fundamental physics from astronomical data and thus paving the way for the era of gravitational-wave multi-messenger astronomy. Her research aims at understanding strong-field gravity astrophysics with compact objects — an essential ingredient in understanding the origin and evolution of the Universe. The evolution of our Universe on all scales, from the life-cycle of individual stars to the Universe in its entirety, is inextricably linked with gravity.

Specifically, her group addresses fundamental questions such as: how do the laws of physics interact with each other in strong-field gravity? What is the fate of binary stellar evolution, and how can we detect electromagnetic and multi-messenger signatures, such as gravitational waves of their merger events? What is the physics that drives the most ubiquitous energetic events in the Universe — jets, accretion disks, mergers and explosions? What is the origin and evolution of the Universe?

In particular, her work aims to explain the physics driving the merger of compact object binaries (black holes, neutron stars and white dwarfs) and to map out the expansion history of the Universe by using electromagnetic and gravitational wave measurements. As a member of the Virgo Collaboration, Einstein Telescope collaboration and LISA Consortium she works with a slew of time-domain telescopes and surveys from the Zwicky Transient Facility, the Neil Gehrels Swift Observatory, the Vera Rubin Observatory's LSST to LOFAR and the JVLA. Her work spans gravitational wave source modelling, data analysis, and multi-messenger astronomy, where she played a role in the remarkable discovery in 2017 of the merger of two neutron stars. – The work nicely complements the activities in the Physics Theory Department at GU that focuses on the dynamical description of the mergers.

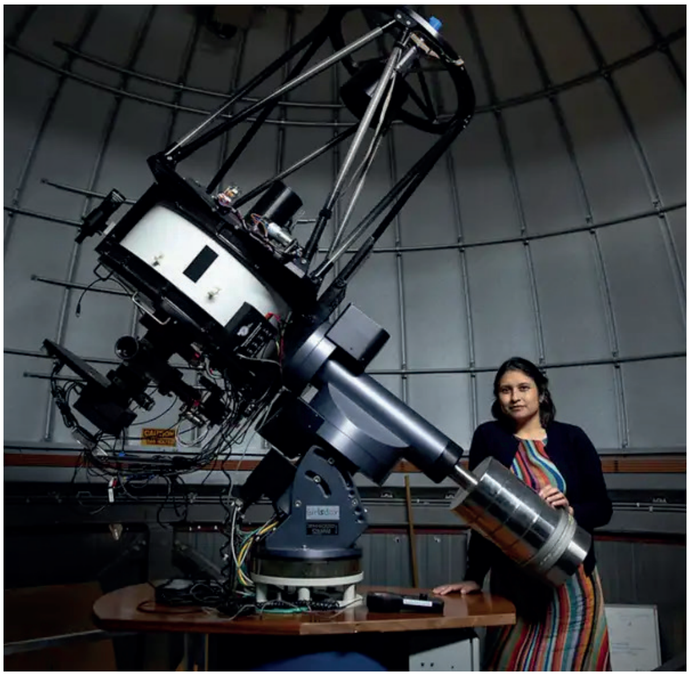
Prof. Dr. Samaya Nissanke

She joined FIAS 2023 as International Fellow, working on gravitational wave astrophysics, physics and multi-messenger astronomy. Nissanke is an associate professor at GRAPPA, the research center for gravity and astroparticle physics at the University of Amsterdam. Since 2018, she has been working in a joint appointment both for the Anton Pannekoek Institute and for the Institute of Physics – and through the latter is a staff member of the National Institute for Subatomic Physics Nikhef in Amsterdam. In 2020, she was awarded the Breakthrough Prize Foundation's New Horizon Prize in Physics for her work on the new techniques she helped develop. In 2021, she won a Suffrage Science Award from the London Medical Council for her efforts on behalf of women in the natural sciences.

Highlight

Measuring the Hubble constant with dark neutron star–black hole mergers.

Projects at FIAS: 1



Samaya Nissanke in front of an optical telescope, (c) Bas Uterwijk.

Prof. Dr. Gordon Pipa

He became Full professor (W3) and chair of the Neuroinformatics department at Institute of Cognitive Science at the University of Osnabrueck in Germany at the age of 36. Before he had held a Group leader postion in Prof. Wolf Singer Department of Neurophysiology, Max Planck Institute for Brain Research, Frankfurt am Main, Germany and a Junior fellow position at the Frankfurt Institute for Advanced Studies (FIAS), Frankfurt am Main, Germany. Between 2007 and 2009 he was a Research fellow with Prof. Emery Brown with an joint appointment at the Dep. of Brain and Cognitive Sciences at the MIT, Cambridge, and the Dep. of Anesthesia and Critical Care at Massachusetts General Hospital, Boston.

Highlight

Neuroinspired dendritic computing on Memristors.

Projects at FIAS: 1

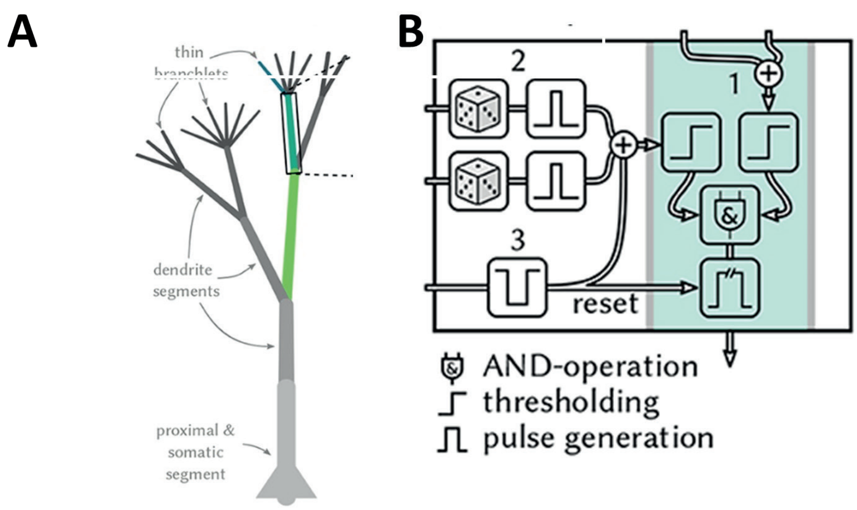
Collaborations

Kwabena Bohema Stanford, Palo Alto, US
Pawn Sinha, MIT Cambridge US
Paul Strachan, FZ Jülich

AI helps prediction of rain, infections, and neural transmission

In 2023 the Neuroinformatics group focused on two main themes. Firstly, we finalized three research projects, based on combining dynamical modelling with machine learning. In the first project we used machine learning to increase the spatial resolution of rain predictions that are generated by weather modelling based on coupled differential equations. We demonstrated that we can significantly improve the spatial resolution. Secondly, we improved predictions of the spread of infectious diseases by using machine learning to estimate unknown factors from data, such as contact rate or spatial spreading across scales in two DFG funded projects that ended in 2023.

A second research focus was on using neuro inspired computational models for conceptualizing and building new neuro inspired hardware. Here the first project started its preparation in 2023 and lead to a DFG funded project starting in 2024 that will follow up on the initial results. In this project we are designing a Memristor based computer chip to implement adaptive computations on timeseries, that are mimicking neuronal computation in dendrites, a model that was published by the group in 2023. This project also led to cooperation with the Group of Kwabena Boahen from Stanford University, that explores time scale adaptation based on neuroinspired learning to maximize the information processing capacity of spiking neuronal networks.



A stylized neuron (A) with dendritic arbor and the algorithmic approximation of a dendrite segment in (B)

Exciting news from black holes and neutron stars

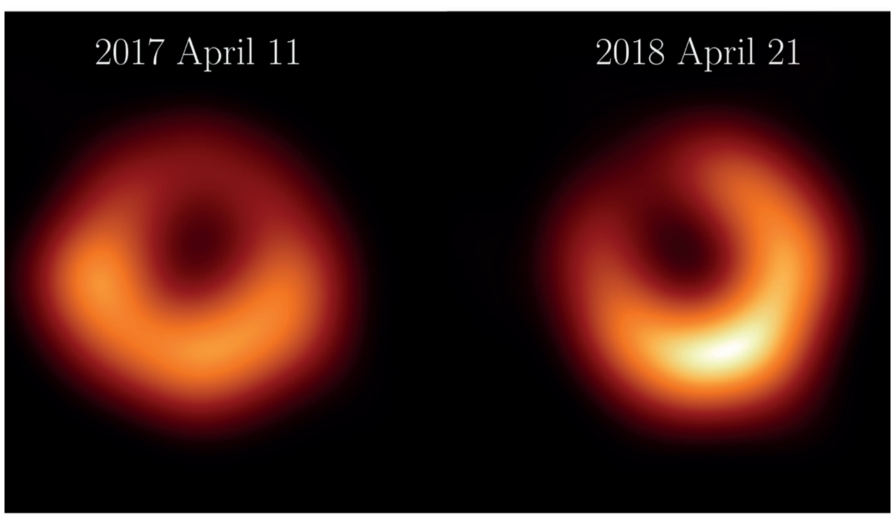
The first picture of a black hole ever recorded appeared only in 2019 using data collected in 2017. The publication of the Event Horizon (EHT) Collaboration, with my team as leading theory members, achieved what at first sight appears as a contradiction: Black holes that distort the surrounding spacetime so dramatically that no light can escape from within the event horizon, can actually be photographed. Indeed there is no contradiction, and the image that the EHT produced showed light from matter that is still outside the event horizon and hence can reach a distant observer. At the same time, the image showed the presence of a „shadow", a dark central region in the image, which is the evidence for the existence of black holes, as first proposed by Frankfurt physicist Karl Schwarzschild. In 2023, the EHT collaboration published a second picture of M87*, with data taken 2018. The new image reveals a familiar ring the same size as the one observed in 2017. This bright ring surrounds a deep central depression, the shadow, as predicted by general relativity. Excitingly, the brightness peak of the ring has shifted by about 30° compared to the images from 2017, which is consistent with the theoretical understanding of variability from turbulent material around black holes. This second image of M87* may not seem very different from the previous one. However, for science, it is an extremely important confirmation. While the excitement in science obviously comes with the discovery, the confidence in science comes from the confirmation of previous results. Hence, the new image testifies that the analysis behind first image of a black hole was indeed correct and accurate.

Important progress has been obtained also when considering neutron stars and their collisions in binary systems. In collaboration with Horst Stoecker and his team, we showed that binary mergers and heavy-ion collisions are related through the properties of the hot and dense nuclear matter formed during these extreme events. In particular, low-energy heavy-ion collisions offer exciting prospects to recreate such extreme conditions in the laboratory. As a way to understand similarities and differences between these systems, scientists at FIAS performed a direct numerical comparison of the thermodynamic conditions probed in both collisions. In this way, they found that laboratory heavy-ion collisions at the energy range of 0.4 - 0.6 A MeV probe states of matter that are very similar to those created in binary neutron-star mergers, thus making these astrophysical events also probes of regimes that cannot be accessed in laboratories. In collaboration with Christian Ecker, we showed that setting bounds on the maximum mass of a nonrotating neutron star, constrains tightly the behaviour of the pressure as a function of the energy density and moves the lower bounds for the stellar radii to values that are significantly larger than those constrained by the NICER measurements, rendering the latter ineffective in constraining the EOS. This result confirms once more the importance of studying the most massive neutron stars as they represent gateways to matter under extreme conditions of density and gravity.

Prof. Dr. Luciano Rezzolla

He received his PhD in Astrophysics at the SISSA in Trieste, Italy in 1997. After a number of years at the university of Illinois at Urbana-Champaign, he moved back to SISSA for a tenured position.
In 2006 he moved to the Max-Planck Institute for Gravitational Physics in Potsdam as Head of the numerical-relativity group. In 2013 he moved to Frankfurt and was awarded an ERC Synergy Grant and is the recipient of the 2017 Karl Schwarzschild Prize from the Walter Greiner Foundation. Luciano Rezzola was a Senior Fellow from 2015-2018, he rejoined the institute in September 2020.

Projects at FIAS: 1



First and second images of the black hole M87*: The diameter of the shadow enclosed by the ring is identical. As expected, the brightness distribution of the radiation emitted by the matter swirling around the black hole has shifted. Photos: EHT Collaboration.

Prof. Dr. Georg Rümpker

After studying geophysics at the University of Münster, Georg Rümpker received his PhD degree in seismology from Queen's University (Canada) in 1996. He continued his career as a postdoctoral fellow at the Carnegie Institution of Washington and later at GeoForschungsZentrum Potsdam as a research scientist. Since 2004, Rümpker has been professor of geophysics at the Institute of Geosciences at Goethe University Frankfurt. He joined FIAS in May 2020.

Highlight

Field campaign for the deployment of land-based seismic arrays to study the submarine Kavachi volcano in the Solomon Islands.

Projects at FIAS: 1

Cooperations

Department of Geology, Ministry of Mines, Honiara, Solomon Islands

Institute of Seismological Research, Gandhinagar, India

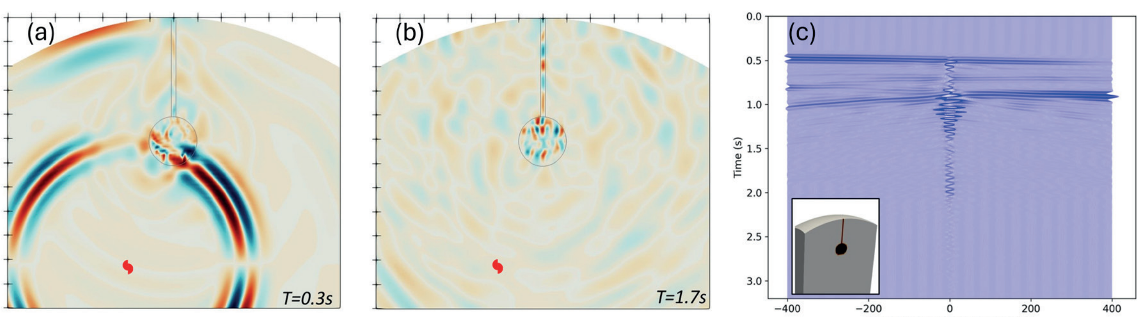
Modeling seismic resonances within volcanoes

The properties of the magmatic system within a volcanic edifice are fundamental for characterizing volcanoes and enhancing our understanding of eruptive processes. Seismic wavefields can offer valuable insights into the internal structure of the volcanic edifice due to their sensitivity to the heterogeneous seismic velocity distribution related to magma chambers and magmatic conduits. Seismic signals observed at volcanoes encompass volcano-tectonic events, relatively long-period signals, and tremors, all of which are recorded in various volcanic regions worldwide. Tremors, in particular, are thought to result from seismic events induced by magma movements within the volcanic system.

In a recent study (Limberger & Rümpker, 2023), we employed 3-dimensional numerical modeling to simulate seismic resonances in a volcanic edifice, arising from the interaction of an externally excited wavefield with a magma chamber-conduit system. The resultant wavefield holds the potential to provide significant insights into the properties of the magmatic system. Contrary to previous assumptions of requiring an internal seismic source, our findings indicate that the magma chamber and conduit efficiently capture the incident high-frequency wavefield excited by micro-earthquakes located within the edifice. Due to multiple internal reflections off the boundaries of the chamber and the conduit, prolonged reverberations occur, which are guided along the conduit.

Temporal and spectral analysis of synthetic seismograms illustrates that the size of the magma chamber and the width of the conduit are critical in determining the magnitude and dominant frequencies of seismic resonances. Specifically, models with larger magma chambers and wider conduits consistently produce larger resonance amplitudes at distinct frequencies. At greater distances from the conduit, we observe an intensified scattered wavefield with a broad frequency range, indicative of a substantial magma chamber within the volcanic edifice. In general, these externally initiated resonances may manifest as tremor-like signals at seismic stations located on the edifice. Our results show that analyzing these signals can provide detailed information on the internal structure of volcanoes.

Literature: Limberger, F. & Rümpker, G. (2023). 3-D seismic modeling of "calabash-resonances": Conduit-guided-wave excitation by magma-chamber wavefield capturing, 28th International Union of Geodesy and Geophysics General Assembly, Berlin.

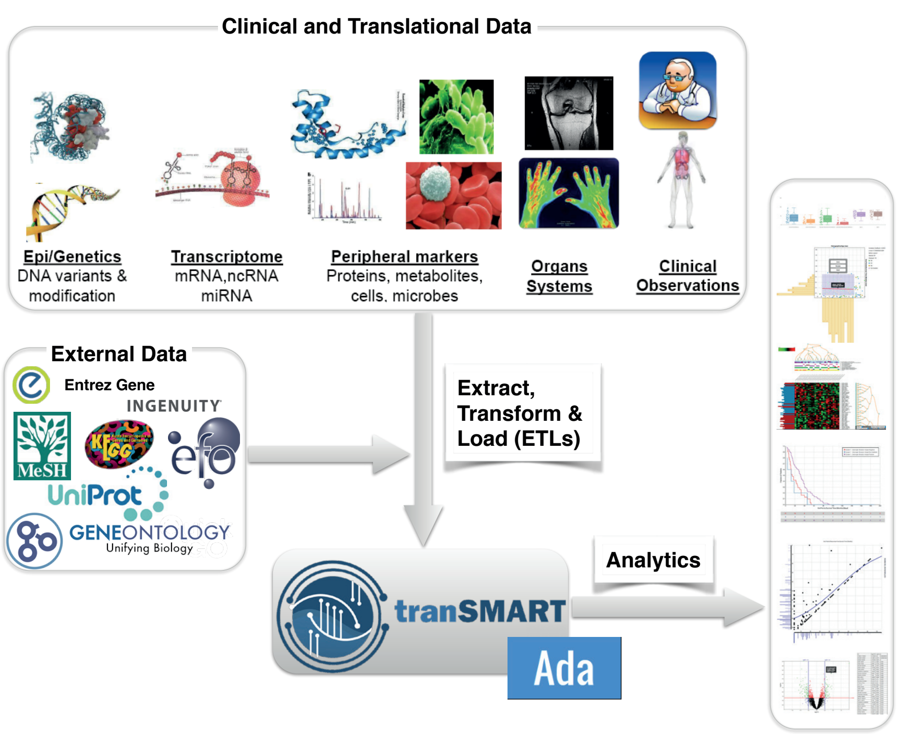


Snapshots of the seismic wavefield for the 3-dimensional simplified model of the volcanic edifice, featuring a magma chamber with a radius of R=100 m and a conduit width of D=20 m. The wavefield is excited by a micro-earthquake, indicated by a red S-shaped symbol. The reduced seismic velocities within the magma chamber and conduit lead to the trapping of the incident wavefield, which reflects at its internal boundaries, as shown in panels (a)-(b). The reverberations within the magma chamber-conduit system induce resonances that can potentially be observed in seismogram recordings from densely distributed seismic stations positioned across the edifice, as depicted in panel (c).

Clinical and translational medicine informatics

My research focuses on applying information technology solutions, data science and bio-medical informatics towards development of a knowledge-based clinical and translational medicine domain, aiming at expediting the discovery of new diagnostic tools and treatments by using a multi-disciplinary, highly collaborative, "bench-to-bedside" approach and bridging the gap between research and clinical care. In my studies I am developing methodologies for the integration of multiple high dimensional datasets that capture the molecular profiles of patients, as well as detailed clinical information collected at multi-site/hospital clinical studies. In this area, I investigate into best optimal strategies and methodologies necessary to consistently collect, curate/harmonise, integrate the data, annotate with consistent and useful ontologies/terminologies, apply semantic web solutions (Satagopam et al, Big Data, 2016; Gu et al, Drug Discovery Today, 2021). I also work on application of Natural Language Processing (NLP), text-mining based approaches to transform unstructured Electronic Health Records (EHRs) and free text data into structured data.

In the area of data analysis, I investigate into integrated analysis of multi-layer clinical, molecular, imaging and mobile/senor data from different clinical cohorts and EHRs by applying sophisticated bio-medical informatics, statistical and advanced Machine Learning (ML) for unravelling disease aetiology, co-morbidities, disease trajectories, stratification of patients, early detection of biomarkers, clinical decision support for diagnosis, prognosis and treatment of diseases. I also lead a team of scientific programmers and developers to build innovative and intuitive user interfaces, reporting systems and visual analytics solutions for exploration, slicing/dicing, analysis of integrated multi-dimensional data through graphical user interfaces tailored for patients, clinicians, and bench scientists.



Clinical and translational medicine data integration and analysis to unravel disease mechanisms as well as patient stratification and biomarker discovery.

Dr. Venkata Satagopam

He is FIAS Fellow, Senior Research Scientist and Deputy Head of Bioinformatics core facility, LCSB, University of Luxembourg; Technical Coordinator (TeC) of ELIXIR-Luxembourg Node and CTO & Co-founder of ITTM S.A. Luxembourg. 2004-2012 he worked as a Senior Bioinformatics Scientist at EMBL, Heidelberg. Before he worked as a Bioinformatics Scientist at LION bioscience AG, Heidelberg from 2001 after obtaining Masters in Pharmaceutical Sciences from Andhra University, Visakhapatnam, India. He obtained his PhD from Technical University Munich (TUM), Munich, Germany in the field of Bioinformatics. He is an associate editor of Frontiers in Systems Biology, co-chair of ISCB Education Committee as well as ELIXIR Health Data Focus Group, executive committee member of several European projects and Data Access Committees (DACs) involved in the organisation of several conferences, workshops, code/data hackathons.

Highlight

Engaged in the preparation of the EMTHERA ("Emerging THERApeutic strategies against infections, inflammation and impaired immune mechanisms") project proposal.

Projects at FIAS: 1

Prof. Dr. Armen Sedrakian

He received his physics degree from the University of Rostock (1989), PhD at Yerevan State University (1992) and Habilitation from Tübingen University (2006). He held research positions at the Max-Planck Institute for Nuclear Physics (Heidelberg-Rostock), Cornell University (USA), Groningen University (The Netherlands) and Tübingen University. Since 2007, he teaches at Goethe University at the Institute for Theoretical Physics and since 2017, he has the position of Fellow at FIAS. In parallel he holds Professorships at Yerevan State University (2011) and at Wroclaw University (2018).

Highlight

We found amazing features of the fourth family of compact stars formed due to multiple phase transitions.

Projects at FIAS: 1

Collaborations

Mark Alford (Washington University, St. Louis)
Fridolin Weber (San-Diego State University)
Arus Harutyunyan (Byurakan Astro. Observatory)
Peter Rau (INT, Washington University)
Jia-Jie Li (Chongqing Unversity)

Exploring fundamental physics with tiny stellar-like objects

We have worked on a range of topics related to neutron star physics including

(a) Universal relations for integral parameters of such stars

(b) equations of state for astrophysical simulations

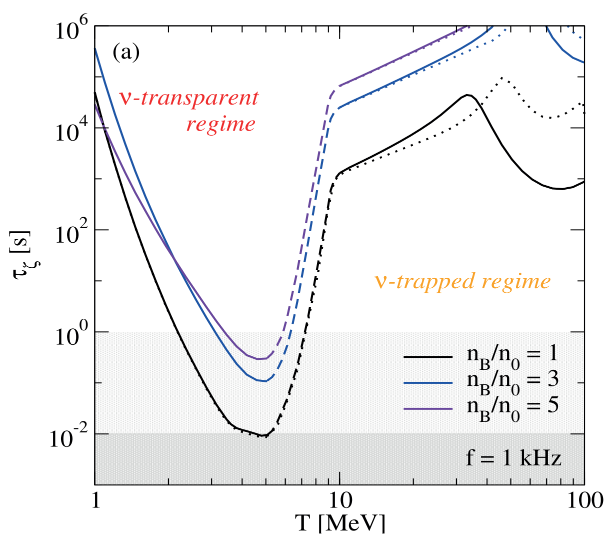
(c) structure and properties of stars featuring phase transition to quark matter

(d) bulk viscosity of dense hot matter in neutron star binary mergers.

We have extended the formulations of the second-order relativistic hydrodynamics to multi-flavor fluids. This allowed us to derive new diffusion coefficients of fluids moving with respect to each other, which are absent in the standard Israel-Stewart theory.

We have reviewed the dense phase of quark matter and conjectured the possible structure of the phase diagram which can contain a tri-critical point.

Effects of bulk viscosity on the damping of oscillations in binary neutron star mergers are characterized by the damping timescale shown in the figure as a function of temperature for various densities. The oscillation frequency is fixed at 1 kHz. The solid lines show the results obtained with isothermal and the dotted lines - with adiabatic susceptibilities. The dashed lines interpolate between the results of neutrino-transparent and neutrino-trapped regimes.



Fading memory as bias in residual recurrent networks

The power of deep neural networks for pattern recognition tasks lies in their universal approximation abilities, and their theoretical expressivity is well-studied. Practical expressivity, however, the space of solutions attainable by a given network through gradient descent training, is known to lag behind theoretical expressivity. Network performance achieved in practice is determined by a set of inductive biases such as architectural constraints and the learning process itself.

In particular, residual connections have been proposed as architecture-based inductive bias to mitigate the problem of exploding and vanishing gradients and increase task performance in both feed-forward and recurrent networks (RNNs) when trained with the backpropagation algorithm. Yet, little is known about how residual connections in RNNs influence their dynamics and fading memory properties.

To study the effect of residual connections on RNN dynamics, we introduce weakly coupled residual recurrent networks (WCRNNs) in which the residual connections result in well-defined Lyapunov exponents.

This allows for studying properties of their dynamics and fading memory. We investigate how the residual connections of WCRNNs influence their performance, network dynamics, and memory properties on a set of benchmark tasks (adding problem and sequential MNIST).

We show that several distinct forms of residual connections yield effective inductive biases that result in increased network expressivity (see figure). In particular, those are residual connections that (i) result in network dynamics at the proximity of the edge of chaos, (ii) allow networks to capitalize on characteristic spectral properties of the data, (iii) result in heterogeneous memory properties.

In addition, we demonstrate how our results can be extended to non-linear residuals and introduce a weakly coupled residual initialization scheme that can be used for Elman RNNs.

Taken together, our analyses not only show the influence of RNN dynamics on their practical expressivity, but also allow for giving functional interpretations of some hallmark properties of cortical dynamics such as criticality, and oscillatory dynamics.

Prof. Dr. Dr. h.c. mult. Wolf Singer

He studied Medicine in Munich and Paris, received his PhD from the LMU Munich and his habilitation at the TU Munich. He was one of the directors of the MPI for Brain Research, as well as founding director of FIAS and the Ernst Strüngmann Institute for Neuroscience. His research is devoted to the exploration of neuronal foundations of cognitive functions. Central to his research is the question how the dynamics of neuronal networks like the cerebral cortex contribute to computations.

Highlight

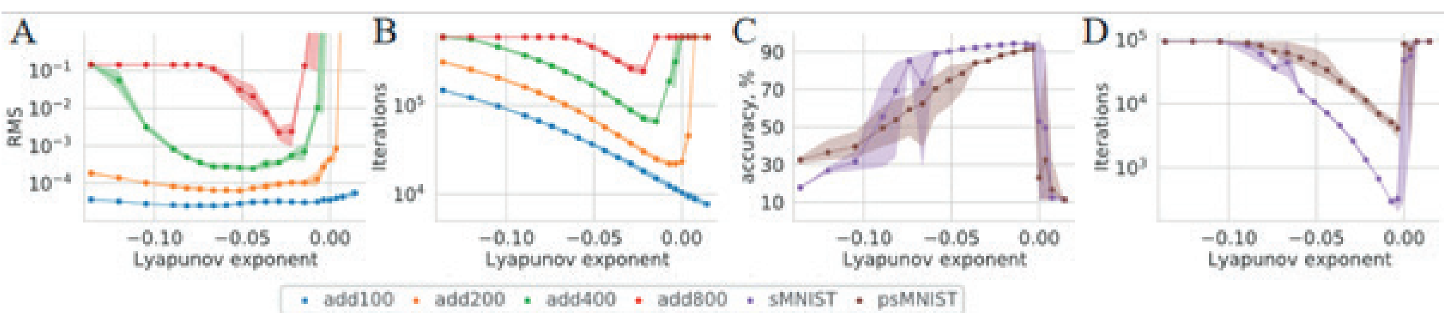
The discovery that natural neuronal networks use computational strategies resembling some of those implemented in quantum computers.

Projects at FIAS: 1

Staff

Igor Dubinin

Dependence of WCRNN performance for ADD and sMNIST datasets for different distances to the critical transition as measured by Lyapunov exponents. A. Best test error(RMS error, lower is better) for ADD datasets. B. Learning speed defined as number of iterations to reach a minimal level of performance for ADD datasets. C. Best test accuracy (higher is better) for sMNIST. D. Learning speed for sMNIST.



Understanding information processing in cells and tissues

Dr. Thomas Sokolowski

He studied physics and mathematics at Saarland University, already specializing in Theoretical Biophysics. He completed his PhD in Computational Biophysics in 2013 at AMOLF (Amsterdam), graduating from the Vrije Universitet (VU). From 2014 until 2020 he was a Postdoc at IST Austria, with a focus on optimizing spatial-stochastic models of biophysically constrained cellular information processing, mainly in developmental biology. In April 2020 he started as a group leader and fellow at FIAS.

Highlight

Completion and parametrization of the first genuinely spatial-stochastic model of early mouse embryogenesis with the help of event-driven simulation and machine learning.

Projects at FIAS: 1

Staff

Michael Ramírez Sierra

Niklas Heuser

Collaborations

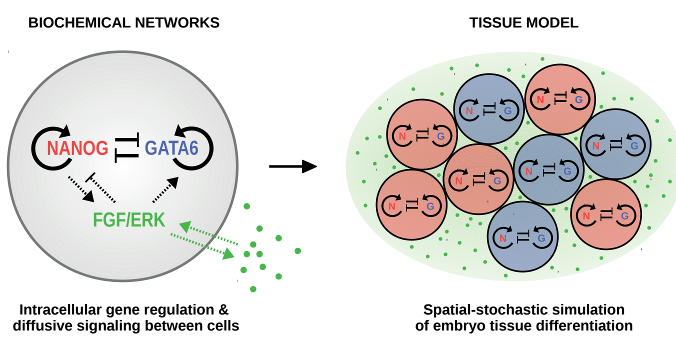
William Bialek, Princeton
Gašper Tkačik, IST Austria
Thomas Gregor & Ben Zoller, Princeton / Institut Pasteur (Paris)
Marcin Zagórski & Maciej Majka, Jagiellonian University (Cracow)
Pieter Rein ten Wolde, AMOLF (Amsterdam)
Sabine Fischer, Uni Würzburg
Franziska Matthäus, Kai Zhou (FIAS)

Living organisms are able to process information reliably and efficiently, both inside cells and at tissue and organism levels. Though relying on fundamentally stochastic biochemical processes, cellular information processing can attain astonishingly high precision and reproducibility, in particular in early embryo development. Here, timely and accurate cell fate assignment is crucial while material and temporal resources are limited, meaning that successful information processing relies on efficient noise-control mechanisms optimized by evolution.

Our group studies such mechanisms with numerical and analytical models that accurately incorporate the biophysical and resource contraints faced by the cells. Such models rely on realistic descriptions of the fundamental stochastic processes that determine the biological noise levels, which quickly can become intractable both mathematically and numerically. Our approach therefore builds on event-driven simulations, smart mathematical approximations, problem-specific numerical optimization techniques, and AI-aided inference for reducing the computational cost associated with realistic biophysical models.

In 2023 we carried out a thorough analysis of several variants of our model of early mouse embryo development, combining event-driven spatial-stochastic simulations with simulation-based inference (SBI), a recent inference technique based on machine learning. This allowed us to obtain a prediction for the structure and biophysical parameters of the core regulatory network driving the associated cell differentiation processes, and - most importantly - also to assess its robustness to stochastic and systematic perturbations. This confirmed and quantitatively characterized the crucial role of spatial coupling between the differentiating cells via the signaling modelecule FGF4. Moreover, our analysis revealed that this coupling is driving a tissue-level feedback mechanism that implements effective buffering against different forms of perturbations. To our knowledge, our work is the first truly spatial-stochastic description of this paradigmatic developmental system. In an associated side project, we studied how FGF4 can be efficiently transmitted between the differentiated cells of the emerging tissue, identifying strategies that increase the transmission efficiency.

We intensified our collaboration with the group of Thomas Gregor with a project that analyses state-of-art dynamical expression data in the early fly embryo, investigating the mechanisms of expression initiation and how they vary for different genes and activator levels. Moreover, we internally established closer ties with the group of Kai Zhou, in order to augment their machine-learning approaches in epidemiology by our spatial-stochastic modeling techniques.



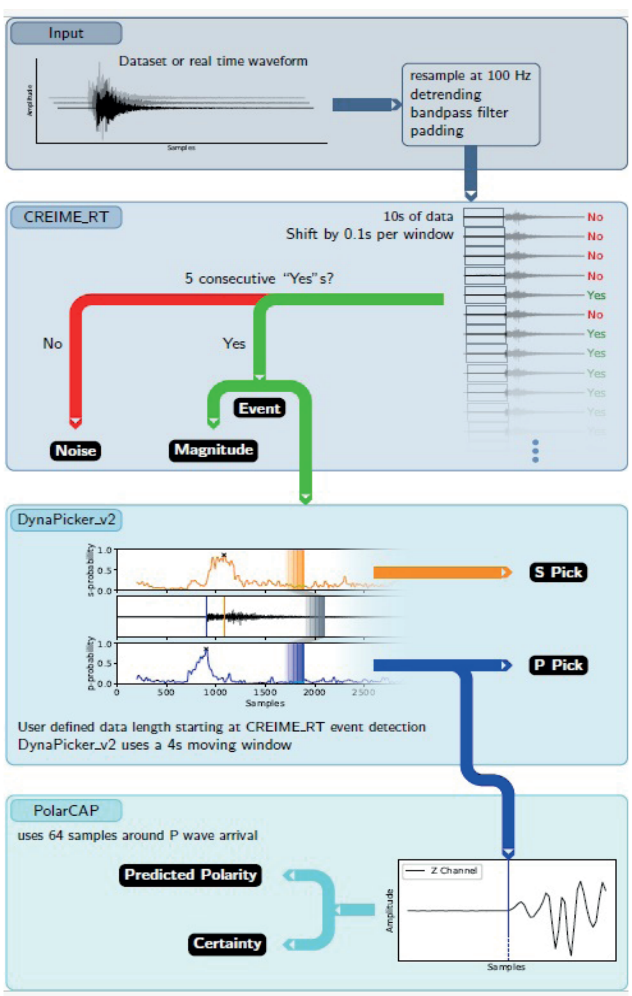
Nanog and GATA6 mutually repress each other in the early mouse embryo tissue, specifying exclusive cell fates. Spatial signaling via protein Fgf4 implements a tissue-level biochemical feedback that regulates the cell fate ratio and buffers noise.

SAIPy: Python package for earthquake monitoring using AI

Early Warning Systems are expected to identify the potentially damaging events, to estimate the extent of its effects and to disseminate the warning issued. My current research primarily focuses on the potential of Deep/Machine learning in the identification of potentially disastrous seismic events, earthquake forecasting. My team has developed one of the first open source deep learning based python package SAIPy which provides a user-friendly pipeline for fast seismic waveform data processing.

SAIPy offers solutions for multiple seismological tasks such as earthquake detection, magnitude estimation, seismic phase picking, and polarity identification. This brings together the capabilities of previously published models such as CREIME (for magnitude estimation of the earthquake), Dynapicker (for seismic phase picking) and PolarCAP (for polarity estimation) and introduces upgraded versions of previously published models such as CREIME_RT capable of identifying earthquakes with an accuracy above 99.8% and a root mean squared error of 0.38 unit in magnitude estimation.

These upgraded models outperform state-of-the-art approaches like the Vision Transformer network. SAIPy provides an API that simplifies the integration of these advanced models with benchmark datasets like STEAD and INSTANCE. The package can be implemented on continuous waveforms and has the potential to be used for real-time earthquake monitoring to enable timely actions to mitigate the impact of seismic events.



Schematic diagram for SAIPy. The input (continuous waveform or sample from a dataset) is resampled and preprocessed. Then CREIME_RT uses 10 s windows shifted by 0.1 s to detect earthquake signals. Once five consecutive windows are found to contain an earthquake signal, the magnitude will be determined and an event trigger is placed. As long as there are no 5 consecutive windows found to contain earthquakes, the trace is considered noise. An earthquake signal is processed with DynaPicker_v2 in the next step. There, moving 4 s windows are used to determine the P- and S- wave arrivals. The end of the 4 s moving window is shown by the vertical line in the middle panel of the DynaPicker_v2 box. As a final step, the P-pick is used to select the Z-Channel data of 31 samples before and 32 samples after, which is then fed to PolarCAP for polarity prediction. All model outputs are marked in black boxes.

Dr. Nishtha Srivastava

She finished her Bachelor's in Mathematics and Masters in Exploration Geophysics at Banaras Hindu University, India. Afterwards Srivastava joined the Advanced Computational Seismology Laboratory at the Indian Institute of Technology (IIT) Kharagpur, India where she was part of various seismological projects and wrote her doctoral thesis in seismology to study the site effects due to the impact of both near and far field earthquakes. In 2018 she joined FIAS as a postoctoral researcher and became a Research Fellow in 2020.

Highlight

The group organized Seismology and Artificial Intelligence workshop funded by BMBF in September. We brought together experts, early career and experienced scientist, from both Artificial Intelligence and various domains of Seismology to explore methods and computational solutions and to envision the future direction and associated challenges.

Projects at FIAS: 2

Staff

Claudia Cartaya
Jonas Köhler
Javier Andres Quintero Arenas
Abel Daniel Zaragoza Alonzo

Collaborations

Institute of Seismological Research Gandhinagar, India
CentraleSupelec Paris, France
Centro de Investigación Científica y de Educación Superior de Ensenada, Baja California, Mexico

Dr. Jan Steinheimer-Froschauer

He graduated in physics in 2008 with a diploma in theoretical physics from Goethe University Frankfurt. After three more years, he earned a PhD from the Goethe University. He then received a postdoctoral position at FIAS from 2011-2012, before moving to the Nuclear Science Division of the Lawrence Berkeley National Laboratory, Berkeley, USA. Since 2013, he has been working at FIAS as a postdoc and was appointed Research Fellow in 2017.

Highlight

Organized a successful MAGIS23 workshop in India (see photo) and two noteworthy publications in PRL. Successful Disputation of Manjunath Omana Kuttan.

Projects at FIAS: 2

Staff

Tom Reichert (postdoc, funded by STPG and FIAS), Roman Poberezhnyuk (Postdoc, funded by AvH), Manjunath Omana Kuttan (doctoral student and now Postdoc in KISS project of Kai Zhou).

Collaborations

HADES collaboration, GSI Darmstadt Benjamin Dönigus, IKF Goethe Universität; Marcus Bleicher and Elena Bratkovskaya, Goethe-Universität; Abhijit Bhattacharyya, Calcutta University, Kolkata, India; Christoph Herold, Suranaree University, Nakhon Ratchasima, Thailand; Volker Koch, LBNL Berkeley, USA; Yasushi Nara, Akita International University, Akita, Japan; Toru Nishimura, Osaka University; Volodymyr Vovchenko, Houston University, Texas, USA; Pia Jakobus and Bernhard Müller, Monash University, Australia

QCD equation of state in heavy ion and astrophysical collisions

This year our group made significant progress in the study of the properties of dense and hot matter as it can found in collisions of heavy nuclei at accelerators (e.g. at GSI, RHIC and the LHC) and in macroscopic astrophysical objects like neutron stars and core-collapse supernovae. The figure below shows the phase diagram of strongly interacting matter as simulated with models from the FIAS group. Parts of the figure were created using generative AI.

Within our, Alexander von Humboldt foundation funded, group linkage project we organized a successful workshop MAGIC23 in Kerala-India, in which many relevant topics of gravitational wave astrophysics and heavy ion collisions where discussed. Many high-quality and high-impact talks from local groups in India as well as invited international speakers where given.

The research of our group, and our international collaborators, on the high density QCD equation of state in heavy ion collisions and core-collapse supernovae was published in several in several papers. Noticeable here where two papers on Physical Review Letters, the most prestigious journal in physics, of which one was even selected as editors' choice and featured the front page of the journals issue.

In this publication a Bayesian inference was used to constrain the density dependence of the QCD equation of state, using flow data from heavy ion reactions as input. In the second PRL a novel signal in gravitational waves, emitted from large core-collapse-supernovae, sensitive to the equation of state was first identified.

Conference dinner at MAGIS23 workshop in India.

MAGIC and AI for science

We focused on two interdisciplinary research fields: MAGIC (Matter, Astrophysics, Gravitation, Ion Collisions) and AI4Science (Applications of AI for Science). MAGIC is a collaboration, at FIAS and with international partners as in the US, BITP, XFiJRC, GU and GSI, between the groups of Jan Steinheimer, Kai Zhou, the late Stefan Schramm and Luciano Rezzolla: A direct comparison of Binary Neutron Star Mergers and Heavy Ion Collisions, employing the selfconsistent Chiral Mean Field EoS for hot and dense QCD Matter in two Frankfurt 4-Dim fully relativistic hydrodynamic Codes for the Macro and Micro case, showed that the values T=50 MeV, n = 3 n_0, S/A = 2, are nearly identical, for (1.4+1.4) M_s BNSM and HIC at HADES energies: Cosmic Matter can indeed be probed quantitatively on earth, in the GSI Laboratory.

AI4Science is our multidisciplinary collaboration between the FIAS-groups of Nishtha Srivastava, Kai Zhou, Jan Steinheimer: Seismology-AI, AI4QCD, AI4Life Science (Inflammation, Infections, Viral Spreading in body and continents, nable), Climate-/ EnergySys-AI, and AI4Technology, etc. Some references, e. g.:

- Identifying lightning structures via machine learning
- Fourier-Flow model generating Feynman paths
- Approaching epidemiological dynamics of COVID-19 with physics-informed neural networks
- Reconstructing the neutron star equation of state from observational data via automatic differentiation
- Neural network reconstruction of the dense matter equation of state from neutron star observations
- The QCD EoS of dense nuclear matter from Bayesian analysis of heavy ion collision data
- CREIME: A Convolutional Recurrent model for Earthquake Identification and Magnitude Estimation
- Tracking influenza virus infection in the lung from hematological data with machine learning
- EPick: Attention-based multi-scale UNet for earthquake detection and seismic phase picking
- A study on small magnitude seismic phase identification using 1D deep residual neural network
- Regional-Local Adversarially Learned One-Class Classifier Anomalous Sound Detection in Global long-term space
- SMTNet: Hierarchical cavitation intensity recognition based on sub-main transfer network
- An acoustic signal cavitation detection framework based on XGBoost with adaptive selection feature engineering

Front cover of PRL issue which displayed a figure of the group on the cover and ighlighted the article as an editor's suggestion.

**Prof. Dr. Dr. h. c. mult.
Horst Stöcker**

He studied physics at Goethe University and was awarded the Dr. phil nat. in Walter Greiner's Institute. He did his Postdoc at GSI Darmstadt and at LBL Berkeley, USA, as a DAAD-NATO Fellow. 1982-1985 he held his first faculty position at MSU, USA. In 1985 he returned to Frankfurt as Professor for Theoretical Physics at GU, where he still holds the Judah M. Eisenberg Professur Laureatus for Theoretical Physics. 2000-2007 Stöcker was repeatedly Vice-President of the GU. 2007 -2018 he was head of the Theory Experiment Simulations group and Director General of GSI and, helped founding the Helmholtz Institutes in Mainz and Jena, and the international research facility FAIR in Europe. He has over 600 publications and graduated more than 60 early career scientists to doctorates. He holds several patents. 2003-2006, he served as founding director and CEO of FIAS and the graduate school FIGSS. He served as member of the FIAS Board (Vorstand) for two decades.

Highlight

Placement on the front page of PRL, by far the world's most prominent physics journal (see photo).

Projects at FIAS: 6

Staff

Mariia Bilousova
Omar El Sayed
Shriya Soma
Manjunath Omana Kuttan
Anton Motornenko
Leonid Satarov
Markus Schlott
Nan Su
Laszlo Csernai
Jörg Aichelin

Prof. Dr. Jürgen Struckmeier

After finishing his diploma in physics 1978, he got an appointment as staff scientist at GSI in Darmstadt, where he obtained his PhD in 1985. In 2002, his habilitation thesis was accepted at the Physics faculty of Goethe University Frankfurt. Having worked as a lecturer, he was appointed there as "Extracurricular Professor" in 2010. In 2016, he joined FIAS as Fellow.

Highlight

Gauge-theoretical derivation of the spin-torsion coupling for fermions and interpretation of Dark Energy

Projects at FIAS: 3

Staff

David Benisty, Ben-Gurion University of the Negev, Beer-Sheva, Israel (postdoc at Cambridge University, UK, subsequently FIAS)
Vladimir Denk (PhD student)
Matthias Hanauske
Johannes Kirsch
Horst Stöcker
Armin van de Venn (PhD student)
David Vasak

Collaborations

Eduardo Guendelman, Ben-Gurion University of the Negev, Israel
Peter Hess, Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico
Friedrich Wilhelm Hehl, University Cologne
Frank Antonsen, Copenhagen University
Andreas Redelbach, Goethe Univ.
Tomoi Koide, University Rio de Janeiro
Marcelo Netz Marzola, University Sao Paulo

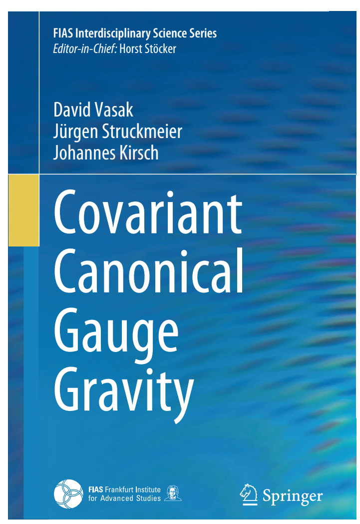
Covariant canonical gauge theory of gravitation (CCGG)

The paper "Torsional dark energy in quadratic gauge gravity" discusses the quadratic term in the Riemann–Cartan tensor CCGG formulation of gravity which a priori includes non-metricity and torsion. For a totally anti-symmetric torsion tensor, the resulting equations of motion in a Friedmann–Lemaître–Robertson–Walker (FLRW) Universe are analytically derived. In the limit of a vanishing quadratic Riemann–Cartan term, the arising modifications of the Friedmann equations are shown to be equivalent to spatial curvature. It is shown how the accelerated expansion of the Universe can be understood as a geometric effect of spacetime through torsion, rendering the introduction of a cosmological constant redundant. We compute expected values of the involved coupling constants and provide a lower bound on the vacuum energy of matter.

The paper "Torsion driving cosmic expansion" is a numerical study of the cosmological model based on the canonical Hamiltonian transformation theory. Using a linear-quadratic approach for the free gravitational De Donder-Weyl Hamiltonian, the model contains terms describing a deformation of an AdS spacetime and a fully anti-symmetric torsion in addition to Einstein's theory. In this way, it is shown that torsion can explain phenomena commonly attributed to dark energy, and thus can replace Einstein's cosmological constant.

The paper "Torsion waves in Covariant Canonical Gauge Theory of Gravity" analyzes the dynamics of propagating torsion field sourced by fermion spin. We show for the first time that in the weak field limit the torsion axial vector field obeys a wave equation with an effective mass term. Possible measurable effects such as neutron star mergers could act as a dipole or quadrupole for torsional radiation. An analysis of radiation of pulsars could lead to a detection of torsional wave background radiation.

During the MAGIC23 conference we presented the paper "On CCGG, the De Donder-Weyl Hamiltonian formulation of canonical gauge gravity" giving a brief overview of the manifestly covariant canonical gauge gravity (CCGG) that is rooted in the De Donder-Weyl Hamiltonian formulation of relativistic field theories, and the proven methodology of the canonical transformation theory. That framework derives, from a few basic physical and mathematical assumptions, equations describing generic matter and gravity dynamics with the spin connection emerging as a Yang Mills-type gauge field. The key elements of this approach are discussed and its implications for particle dynamics and cosmology presented. Among the results are especially:
- Anomalous Pauli coupling of spinors to curvature and torsion of spacetime
- Spacetime with (A)dS ground state, inertia, torsion and geometrical vacuum energy
- Zero energy balance of the Universe leading to a vanishing cosmological constant and torsional dark energy.

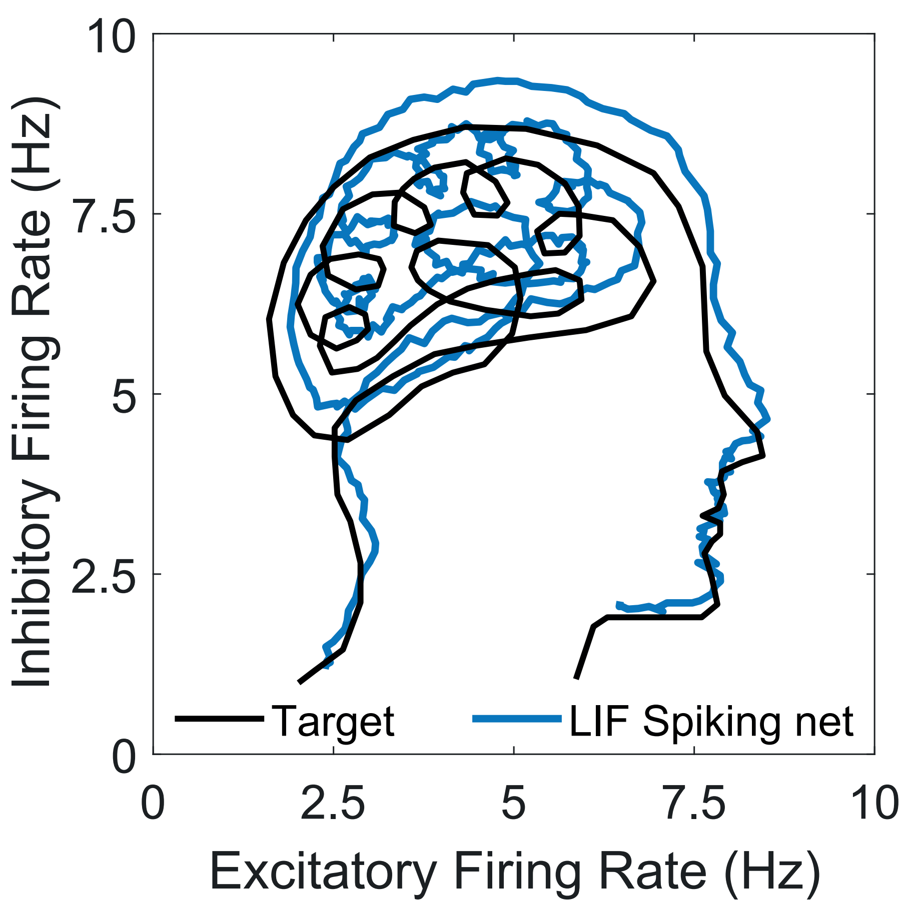


In the book "Covariant Canonical Gauge Gravity" (available now) we have compiled past works on the covariant canonical gauge theory of gravity and added sections on the underlying mathematics and the vierbein version of gauge gravity. This gives a concise overview of this novel, mathematically rigorous gauge approach to gravity.

Modelling large recurrent networks

In 2023, the Tchumatchenko group has continued to study neural network activity and synaptic plasticity. We looked at how the binary activation function of neurons and the recurrent network connectivity can give rise to the different collective activity regimes such as bistability, supersaturation etc.

We found that the size of the network has an important influence on the activity regime of the network. Growing the network can mediate a transition of different activity regimes, but the connections can be rescaled ensure that the network stays in the same activity regime as before and if necessary the input current will need to be adjusted. These insights can help understand how to make recurrent neural networks exhibit a particular firing rate for a given input and can help in the training of these networks.



The time course of the E and I firing rates in the LIF network follows the target trajectory and results from designed dynamical inputs.

Prof. Dr. Tatjana Tchumatchenko

She did her PhD 2006-2011 at the University of Göttingen, and a Postdoc at Columbia University, NYC (USA) 2011- 2013. Tchumatchenko is a computational neuroscientist and professor at the Institute for physiological chemistry, University of Mainz Medical Center, and group leader at the Institute of Experimental Epileptology and Cognition Research, University of Bonn Medical Center. Tchumatchenko's group models address the molecular, synaptic, and neuronal mechanisms underlying neuronal circuit computation. How are neural circuit computations controlled by synaptic dynamics? How does activity relate to functional output, and what changes at the level of activity and synaptic dynamics when tasks shift?

Highlight

Publication of a PloS Comp Neuroscience article (https://doi.org/10.1371/journal.pcbi.1011097).

Projects at FIAS: 1

Staff

Pierre Ekelmans

Collaborations

Ulrich Meyer, FIAS

Dr. Sebastian Thallmair

He studied chemistry and biochemistry at the LMU Munich, where he completed his PhD in theoretical chemistry in 2015. After a short period as postdoctoral researcher in Munich, he joined the University of Groningen (Netherlands) in 2016. His research focused on modeling of biological processes and method development for coarse-grained molecular dynamics. He joined the FIAS as a Fellow in October 2020. Since 2022, he is also scientific coordinator of the Frankfurt International Graduate School for Science (FIGSS) at FIAS.

Highlight

Cristina Gil Herrero received a poster prize at the international meeting of the European Biophysical Societies' Association (EBSA) - a remarkable achievement at a conference with more than 1200 participants.

Group Members

Cristina Gil Herrero (PhD student)
Marieli Gonalves Dias (visiting PhD student)
Saara Lautala (Postdoc)
Thilo Duve (Master student)
Charlie Müller (Bachelor student)

Projects at FIAS: 2

Collaborations

Roberto Covino (FIAS)
Stefan Knapp, Clemens Glaubitz, Irene Burghardt, Jens Bredenbeck (GU Frankfurt); Balázs Fábián, Gerhard Hummer, Florian Wilfling (MPI Biophysics Frankfurt)
Dominik Oliver (University Marburg)
Paulo C. T. Souza (CNRS Lyon)
Pablo Rivera-Fuentes (Univ. of Zürich)
Ana C. Migliorini Figueira (University of Campinas)

Understanding, controlling, and inhibiting protein function

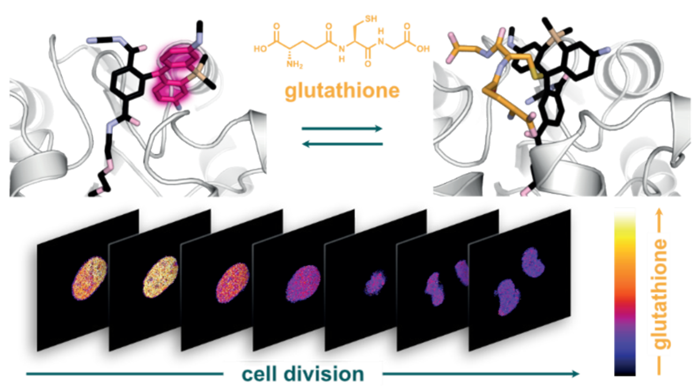
In 2023, we continued our research on light-switchable molecules and their application in biology. We started working on lipid molecules with tails that can be switched between a straight and a bent conformation. In doing so, light can be used to modify the properties of lipid membranes. This could be used to control the release of drugs locally and spatially or as a starting point to develop novel antibiotics. In addition, we continued our collaboration with the groups of Wiktor Szymanski and Ben Feringa at the University of Groningen (NL) to develop light-switchable inhibitors for bacterial proteins.

In another joint experimental and computational study in collaboration with the group of Dominik Oliver at Philipps University Marburg, we were able to show that the Tubby protein localizes to contact sites between endoplasmic reticulum and plasma membrane. It binds to specific lipids as well as to a protein, which only occurs in these contact sites. Within the initiative "Subcellular Architecture of Life" (SCALE) by the Goethe University, Saara Lautala joined our group as postdoc to further investigate the role of the Tubby protein in membrane contact sites in close collaboration with Florian Wilfling (MPI for Biophysics) and Dominik Oliver.

Together with researchers from the University of Zurich, we developed and characterized a quantitative sensor for glutathione (see Figure). Glutathione plays an important role in cells: it regulates the cellular redox potential and is involved in signaling processes. The sensor can be applied selectively in cellular substructures, so-called organelles. Our results were published in Nature Chemistry.

In March, Charlie Müller joined our group for his Bachelor Thesis and David Grantz visited us from the University of Groningen. In October, Saara Lautala joined us as postdoc and Thilo Duve started with his Master Project on light-switchable kinase inhibitors. Sadly, we had to say goodbye to Marieli Goncalves Dias, because her one-year research visit came to an end at the end of October – time flies!

In 2023, Sebastian Thallmair was invited for a keynote lecture at the "10th European Symposium on Plant Lipids" in Amsterdam (NL) and presented the work of the group among others in seminars at the University of Zurich (CH) and the University of Münster. Cristina Gil Herero presented her results on G-protein coupled receptors at the international meeting of the European Biophysical Societies' Association (EBSA) and won a coveted poster prize.



The HaloTag bound, fluorescent silicon rhodamine dye loses its fluorescence when reacting with glutathione (top). Using the novel sensor, we showed that the glutathione concentration in the cell nucleus varies strongly during cell division (bottom). Reproduced from S. Emmert et al., Nat. Chem. 15, 1415 (2023).

Cognitive development in artificial minds

Human intelligence and human consciousness emerge gradually during the process of cognitive development. Understanding this development is an essential aspect of understanding the human mind and will facilitate the construction of artificial minds with similar properties. Importantly, human cognitive development relies on embodied interactions with the physical and social environment, which is perceived via multiple complementary sensory modalities such as vision, hearing, touch, smell, and proprioception. Interacting with the world allows the developing mind to probe the causal structure of the world. This is in stark contrast to the dominant machine learning approach, e.g., for large language models such as ChatGPT, where the learning system is merely passively "digesting" large amounts of training data, but is not in control of its sensory inputs. This makes it much harder to infer cause and effect relationships and truly understand the world. We have argued that in order to build more human-like and capable artificial intelligence, embodied interactions with the environment cannot be neglected. However, computational modeling of the kind of self-determined embodied interactions that lead to human intelligence and consciousness is a formidable challenge. To address this, we have presented MIMo, an open-source multi-modal infant model for studying early cognitive development in a reproducible fashion through computer simulations. MIMo's body is modeled after an 18-month-old child with detailed five-fingered hands. MIMo perceives its surroundings via binocular vision, a vestibular system, proprioception, and touch perception through a full-body virtual skin, while he uses simulated muscles to control his body. With MIMo we have started to study the computational and learning mechanisms that drive the emergence of human intelligence and human consciousness.

MIMo, the multi-modal infant model, is a research platform for studying the development of human-like intelligence and consciousness through computer simulations.

Prof. Dr. Jochen Triesch

He is the Johanna Quandt Professor for Theoretical Life Sciences at FIAS. He also holds professorships at the Dept. of Physics and the Dept. of Computer Science and Mathematics at Goethe University Frankfurt. Before joining FIAS in 2005, he was Assistant Professor at UC San Diego, USA. Originally trained as a physicist, he discovered his passion for studying the brain and building brain-like artificial intelligence already during his graduate education.

Highlight

Jochen Triesch has been studying cognitive development in the lab and in his spare time (see photo above).

Projects at FIAS: 6

Staff

Arthur Aubret
Francisco López,
Antony N'Dri
Philip Sommer
Alexandra Stoll
Petros-Evgenios Vlachos
Xia Xu
Zhengyang Yu
Markus Ernst
Marius Vieth
Mitra Hani
Marcel Raabe

Collaborations

Elke Hattingen (Frankfurt)
Jürgen Jost (Leipzig)
Matthias Kaschube (Frankfurt)
Lucia Melloni (Frankfurt)
Felix Rosenow (Frankfurt)
Simon Rumpel (Mainz)
Bert E. Shi (Hong Kong)

Prof. Dr. Christoph von der Malsburg

He studied physics at the universities of Göttingen, Munich and Heidelberg, with PhD work at CERN, Geneva. He worked as research scientist at a Max Planck Institute in Göttingen, served as professor for computer science, neuroscience and physics at USC in Los Angeles, co-founded the Institute for Neural Computation at Ruhr-University in Bochum and is, since 2007, Senior Fellow and, since 2022, Fellow Emeritus at FIAS. He co-founded two companies and received a number of national and international awards.

Highlight

A new theory of consciousness, presented at the Conference Mathematics of Consciousness, Oxford, Sept 2023 https://youtu.be/IcxD-7oIOPE.

Projects at FIAS: 1

Collaborations

Benjamin Grewe, Rodney Douglas and Matthew Cook at the Institute for Neuroinformatics, University Zurich, ETH Zurich
Thilo Stadelmann, Zurich Hochschule für Angewandte Wissenschaften

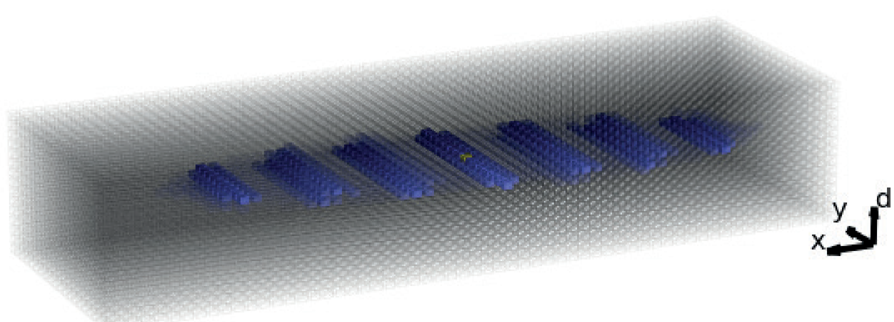
How is mental content represented in the brain?

According to the currently dominating view meaning has the form of hierarchies of discrete propositions (features), each neuron representing a fixed feature. To solve fundamental problems with this view we are pursuing the idea that, above fundamental feature units, meaning is carried by network fragments, sets of neurons that support each other by mutual excitatory ("lateral") connections. As neurons can belong to a number of fragments, they don't carry fixed meaning (such as individual pixels are to be interpreted differently in different contexts).

In an application to stereo vision (the perception of surface shape on the basis of comparing images in the two eyes) we demonstrate the ability of net fragments to represent continuous surfaces. As in long-established models, our system is composed of binocular units that represent local image depth behind or in front of the fixation point, and it filters out depth units that represent a continuous surface with the help of lateral short-range connections ("regularization"). The regularizing connectivity patterns can be interpreted as a simple form of net fragments.

By adding longer-range lateral excitatory connections we construct net fragments of higher specificity that respond to smooth surfaces of specific inclination. To represent surface inclination we don't introduce new feature neurons but use a sparse selection of the basic binocular units that together sample the inclined surface and just connect them appropriately with each other (see the figure). Surfaces of different steepness or orientation are represented by different, possibly overlapping, sub-sets of binocular units. By using inhibition periodically varying in time, our system creates a phase in which only those neurons are active that together represent a continuous surface with the correct inclination. This can be read out at further layers with the help of homeomorphic net fragments.

Connectivity of a single neuron that takes part in a net fragment specific to a particular inclination. Shown is a block (gray-haze) of binocular units that differ in image position (x, y) and in stereo depth (d). A single unit (yellow) is connected with a selection of other units (blue) that belong to surfaces within a narrow range of inclinations, thus forming this unit's net fragment.



Deciphering new prognostic markers for prostate cancer

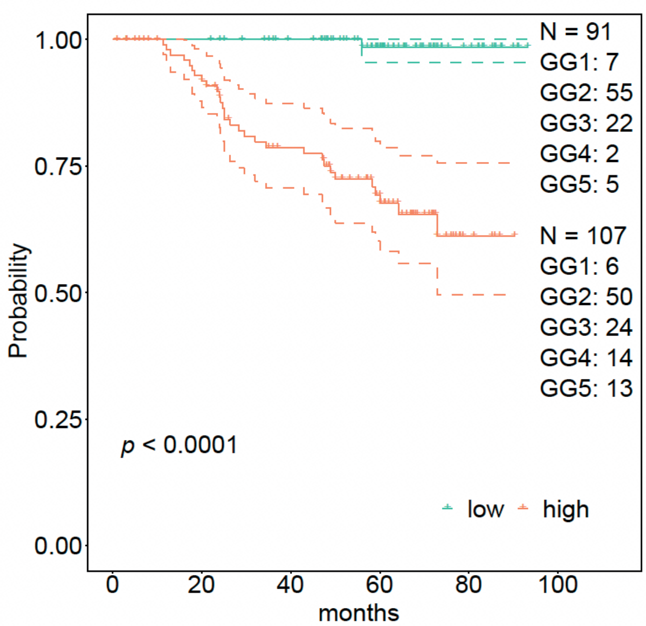
In 2023, the Wild research lab made huge progress in deciphering new prognostic markers for intermediate-risk prostate cancer (PCa) patients (Zhong et al., Life Sci Alliance 2023).

PCa is a highly heterogeneous disease, and so far, most of the treatment-decision algorithms depend on risk stratification based on the tumor stage, the prostate-specific antigen (PSA) level at the time of diagnosis, and the Gleason grade group (GG). Although this clinical risk stratification is of prognostic and predictive value, better biomarkers are still required to improve patient stratification, as intermediate-risk patients diagnosed in the Gleason grade group (GG) 2 and GG3 can harbor either aggressive or non-aggressive disease, resulting in under- or overtreatment of a significant number of patients.

In this study, we performed proteomic, differential expression, machine learning, and survival analyses for 1,348 matched tumor and benign sample runs from 278 patients. Three proteins were identified as candidate biomarkers in patients with biochemical recurrence. Multivariate Cox regression yielded 18 proteins, from which a risk score was constructed to dichotomize prostate cancer patients into low- and high-risk groups. This 18-protein signature is prognostic for the risk of biochemical recurrence and completely independent of the intermediate GG.

Our results suggest that markers generated by computational proteomic profiling have the potential for clinical applications including integration into prostate cancer management.

Kaplan–Meier (KM) curves for biochemical recurrence–free survival (BCRFS) for PCa patients in all Gleason grade groups. KM curves with 95% CIs of the low- and high-risk groups based on the 18-protein risk score, along with respective numbers of samples corresponding to each GG (Gleason grade group). Vertical lines illustrate patients who were censored at the time of their last clinical follow-up visit. The P-value shows the significance of the difference between survival estimates evaluated by the log-rank test. Coloured values represent the number of patients in each group under risk. Reference: Qing Zhong et al., Life Sci Alliance, doi: 10.26508/lsa.202302146. PMID: 38052461; PMCID: PMC10698198).



Prof. Dr. Peter Wild

After finishing medical school and residency in pathology in Regensburg, Hamburg-Eppendorf and Zürich, Peter Wild did a postgraduate training at the University of Heidelberg. He became assistent professor in 2012 at ETH Zürich. In 2016, he became a Full-Professor for Systems Pathology at the University of Zürich. He has been Director of the Dr. Senckenberg Institute of Pathology at University Hospital Frankfurt since 2018. Furthermore, he is a professor at Goethe University Frankfurt a. M. and is employed as a specialist pathologist at Wildlab (UKF MVZ GmbH). He is a Senior Fellow at the FIAS.

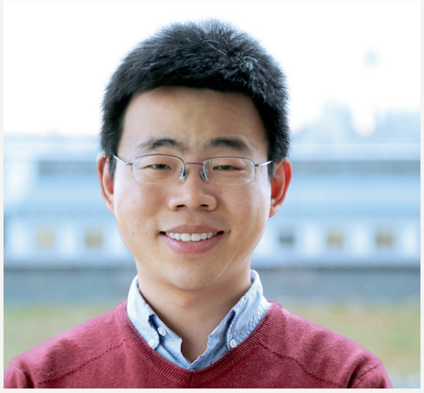
Highlight

Digital transformation of Senckenberg Institute of Pathology and setup of the Senckenberg Biobank (SBB) as a digital, integrated, structured database for whole slides images, fresh frozen tissue collections, molecular data, and clinicopathological data.

Projects at FIAS: 1

Collaborations

Venkata Satagopam, University of Luxembourg & FIAS
Felix Chun, University Frankfurt
Marco Eichelberg, OFFIS e. V., Oldenburg
Johannes Lotz, Fraunhofer MEVIS, Bremen
Norman Zerbe, Charité Berlin
Tiannan Guo, Westlake, China
Qing Zhong, University of Sidney, Australia



Dr. Kai Zhou

He received the BSc degree in Physics from Xi'an Jiaotong University, in 2009, and his PhD degree in Physics with 'Wu You Xun' Honors from Tsinghua University, in 2014. Afterwards he went to Goethe University Frankfurt to do postdoctoral research work at the Institute for Theoretical Physics (ITP) . Since August 2017, he is a FIAS Research Fellow focusing on Deep Learning (DL) application research.

Highlight

The group developed machine learning and Bayesian Inference pipeline to explore QCD matter under extreme conditions.

Projects at FIAS: 3

Staff

Lingxiao Wang
Manjunath O. K.
Shriya Soma
Mingjun Xiang
Shuai Han
Yu Sha
Jannis Koeksel
Lukas Stelz
YiLin Cheng

Collaborations

Gert Aarts, Swansea Uni., UK
Yu-Gang Ma, Fudan Uni., China
Long-Gang Pang, CCNU, China
Xin-Nian Wang, Berkely, USA
Shuzhe Shi, Tsinghua Univ., China

AI for Science and Extreme QCD matter Exploration

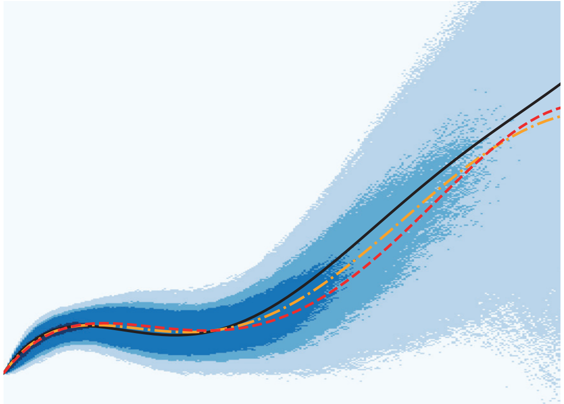
In 2023, we further advanced our several developed directions within AI for Science domain, and got accordingly many interesting results, across extreme QCD matter exploration [1,2,3,4,], physics-informed Generative AI [5,6], Lightning structure investigation[7], Neutron Star EoS [8] and Gravitational wave analysis[9], Terahertz holography smart imaging [10], infectious dynamics [11] and also optimal power flow [12] speeding up with machine learning.

In the area of QCD matter properties study, we well developed the Bayesian inference pipeline with gaussian process emulator to be applied in heavy ion collision physics inference, specifically two groundbreaking studies were conducted in our group along this line: (1) one focused on estimating the deformation parameters of nuclei using Bayesian techniques from heavy ion collision accessible data[3], which offers a deeper insight into the nuclear structure exploration with HICs, emphasizing the potential of Bayesian analysis in uncovering complex nuclear behaviors in high energy nuclear physics studies. (2) the other one which published in the prestigious Physical Review Letters as Editors suggestions used Bayesian analysis to constrain the density-dependent QCD equation of state of dense nuclear matter with heavy-ion collision flow and mean transverse mass measurements [4], showcasing a similar peak structure of the speed of sound square as evidenced from analysis with neutron star observations and marking a substantial advancement in understanding dense nuclear matter's state under very dense conditions.

In the area of atmospheric science, we developed a novel method combining machine learning algorithms to analyze Very High Frequency (VHF) lightning data [7]. By using a t-distributed stochastic neighbor embedding (t-SNE) algorithm and unsupervised Density-Based Spatial Clustering of Applications with Noise (DBSCAN) algorithm, we successfully identified structures in vast multidimensional data sets, providing a promising approach to studying lightning phenomena.

[1] Progress in particle and Nuclear Physics, 104084 (2023); [2] Nuclear Science and Techniques 34, 88 (2023); [3] Physical Review C 107, 054917 (2023); [4] Physical Review Letters 131, 202303 (2023); [5] Physical Review D 107, 056001 (2023); [6] NeuIPS 2023: Machine Learning and the Physical Science Workshop; [7] Chaos, Solitons & Fractals 170, 113346 (2023); [8] Physical Review D 107, 083028 (2023); [9] Journal of Cosmology and Astroparticle Physics 01, 009 (2024); [10]IEEE Transactions on Terahertz Science and Technology, 1-9 (2023); [11] Mathematical Modelling, Simulations and AI for Emergent Pandemic Diseases; [12] Applied Energy 359 (2024) 122779

Bayesian analysis of the QCD equation of state for dense nuclear matter. Color represents the probability for the chemical potential at a given baryonic density.



Donors and Sponsors

To ensure the greatest possible independence and flexibility, FIAS was established as a foundation. A large part of the research activities is funded by the public German and European research sponsors, but without the extraordinary commitment of private sponsors, foundations, and companies, FIAS would not exist and could not continue its work. In recent years, various endowed professorships have been made possible at FIAS and Goethe University.

Alexander von Humboldt Stiftung / Foundation

Alfons und Gertrud Kassel-Stiftung

Bundesministerium für Bildung und Forschung

DAAD

DFG Deutsche Forschungsgemeinschaft

Dr. Rolf M. Schwiete Stiftung

Margarete und Herbert Puschmann-Stiftung

Freunde der Universität

Rudolf Steinberg-Fonds

Goethe Universität Frankfurt am Main

GSI

Helmholtz Spitzenforschung für grosse Herausforderungen

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Johanna Quandt Stiftung

Samson

Stiftung Giersch

Stiftung Polytechnische Gesellschaft Frankfurt am Main

VolkswagenStiftung

Walter Greiner Gesellschaft zur Förderung der physikalischen Grundlagenforschung e. V.

Endowed Professorships:

2016: Giersch Stiftungsprofessur Prof. Dr. Franziska Matthäus
2007: Johanna-Quandt-Stiftungsprofessur Prof. Dr. Jochen Triesch

Endowed Fellowships:

2022: Quandt Research Group on Mathematical Immuno-Epidemiology Prof. Dr. Gemma Roig
2020: Quandt Research Group on Simulation of Biological Systems Dr. Roberto Covino
2020: Kassel-Schwiete Research Group on Development of phamacological Probes Dr. Sebastian Thallmair

FIAS PhD students


Jonas Elpelt is interested in computational models of forgetting and creativity and the characteristics of spontaneous activity in the brain.


Armin van de Venn is modifying Einstein's General Relativity by allowing more general geometric structures (torsion and non-metricity) and higher order curvature.

The focus of **Chen Li**´s work is currently on optimizing energy systems using machine learning techniques to address the challenges posed by renewable resources.

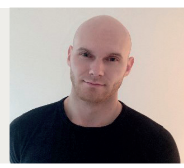

Lars Dingeldein uses simulation-based inference to solve inverse problems in molecular biophysics.

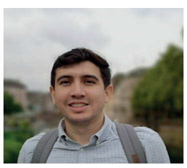


Blending artificial intelligence and thermodynamics to investigate biomolecular systems with computer simulations. Physics, chemistry, biology, informatics: **Gianmarco Lazzeri** combines them.


Zoë Lange studies how organs and organisms get their final shape, using statistical inference to extract cell-scale forces from fluorescence microscopy data to learn about epithelial tissues.

Serena Arghittu explores mechanistic insights into receptor signalling and lipid transport during pathogenesis.


Magnus Petersen`s research involves applying deep generative modeling to improve the efficiency and scope of molecular dynamics simulations.



Michael Ramirez-Sierra combines computational power with biophysical principles to illuminate the intricate dance of cell signaling and decision-making in embryo development.


Vladimir Denk is working on generalized theories of gravity, where he specifically studies the impact of dynamical torsion on matter and spacetime.

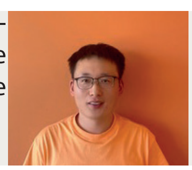
Elena Spinetti focuses on computational biophysics, involving computer-based methods to study the behavior of molecules in living organisms, esp. membrane proteins and their dynamic properties.


Robin Lakos is working on a neural-network-based 4-dimensional track finding and event building approach for the future heavy-ion experiment "Compressed Baryonic Matter" at GSI/FAI, Darmstadt.



Akhil Mithran`s field of research is the analysis of heavy ion collisions in the CBM experiment using artificial neural networks.

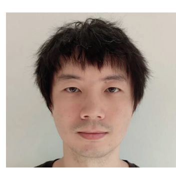

Shriya Soma analyzed simulated signals of gravitational waves from binary neutron star and black hole mergers for signal detection and parameter estimation, using deep learning techniques.

Shuai Han researches how to use artificial intelligence technology to study the spread dynamics of epidemiology in time and space.


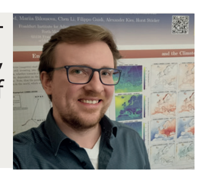
Mingjun Xiang focuses on machine learning for terahertz imaging, including tasks such as phase recovery, depth reconstruction, and super-resolution in THz holography and Fourier imaging.



Cristina Gil Herrero studies the interaction between small molecules resembling pharmaceutical compounds and proteins by classical and coarse-grained molecular dynamics simulations.


Xia Xu studies the effect of integration of action information in time-contrastive representation learning, resulting in an invariant contrastive and equivariant predictive learning paradigm.

Yannick Gerstorfer is working on the generation of random graphs and their application for the generation of synthetic data sets.


Markus Schlott investigates the impact of climate change on the stability, resiliency, and economic efficiency of electricity and energy systems.



Sigrid Trägenap's research highlights the dynamic nature of cortical network development, illustrating how sensory experience refines and organizes activity in the visual cortex.


Oddharak Tyagi is investigating Graph Neural Network based approaches to particle tracking for the Compressed Baryonic Matter(CBM) experiment at GSI-FAIR.

Jonas Köhler is creating millions of real looking earthquake catalogs (using the ETAS model) and training a Deep Learning model in differentiating earthquake mainshocks from their aftershocks.


Tim Liebisch works on agent-based models to analyse how properties on the individual-cell scale contribute to the emergence of complex behaviours on tissue scale in developmental contexts.



Lukas Stelz uses machine learning and mechanistic models to study the spread of infectious diseases in-host and on population-level and how these models perform with limited amounts of data.


Megha Chakraborty was studying the application of deep learning algorithms in the rapid characterization of earthquake parameters with a focus on earthquake early-warning.

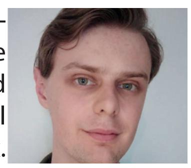
Artemiy Belousov studies the mechanisms of Quark-Gluon Plasma formation in high-energy collisions through the application of deep learning and neural networks.


Francisco López studied how binocular eye movements develop autonomously in infants to explain eye-hand coordination and saccade-vergence interactions.



Petros E. Vlachos studies the mechanisms of homeostatic and functional synaptic plasticity and what allows long-term stable memories to be maintained in the changing, dynamic brain.


Lorenzo Butti studies the cortical networks in the early stage of the brain development.

Igor Dubinin investigates how the dynamics of recurrent networks influence their computations, to better understand the inner workings of artificial and natural neuronal networks, e.g. the cerebral cortex.


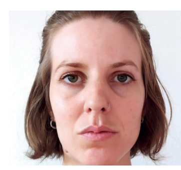
Manjunath O. Kuttan developed AI techniques to analyze data collected in experiments that collide heavy nuclei, to study how matter interacts through nuclear force under density/temperature.



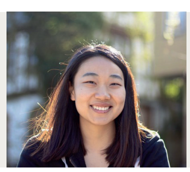
Santiago Gallela studies the nature of abstract representations and cognitive maps in the brain and in artificial neural networks.


Marina Kurtz studies the connection between metabolites and genes in the differentiation of filamentous cyanobacteria when they are exposed to environmental stress, e. g. nitrogen deprivation.

Marc Pereyra quantifies motion and morphology of multicellular systems by analysis of 3D time lapse microscopy data.


Camile Kunz focuses in her PhD project on pattern formation in embryonal systems.



Pamela Osuna Vargas applies and develops deep learning models to enable large-scale analyses of synapses in the brain and their dynamic changes.


Deyue Kong studies the properties of neural activity in the early cortex, how it changes over development, and how it respond to external perturbations.

Thomas Lai investigates why neural representations of sensory stimuli change over time by looking at the dynamics of neuronal activity and measures of connectivity.


FIAS PhD students

We are FIAS

An adhoc snapshot in February 2024 of the administrative team that supports the FIAS scientists in all aspects of their research including computing. Our FIAS team thrives on people and change: As every year some staff set off for new shores, and new faces joined us in 2023.

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Michaela Hofmann - Project Coordination, Research Funding, Support with applications
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Patricia Vogel - Public Relations, Webmaster, Graduate programs

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