FIAS Frankfurt Institute for Advanced Studies

2024

Content

FIAS

science for the reality of tomorrow

Dear colleagues,

Dear friends and supporters of our science,

Dear knowledge seekers,

Twenty years of the Frankfurt Institute for Advanced Science, a teenager has come of age. Obviously a reason to celebrate, to take stock of what has been achieved and to position FIAS for the future - and we have done so. This report is full of detailed descriptions of the various public engagements and examples of scientific research.

The highlight is undoubtedly the celebration in the university's casino, attended by dignitaries from the city of Frankfurt, scientists from the many collaborating institutions - and another jubilee: CERN is seventy years old. This Geneva-based laboratory is the epitome of particle and nuclear physics, one of the pillars of FIAS research. As a truly international laboratory, CERN is also a shining example of cooperation across borders, languages and political opinions. The Giersch Foundation honored this achievement by awarding a prize for Science Diplomacy to CERN, represented by Charlotte Warakaulle, Director of International Relations. The prize was presented by Timon Gremmels, Minister of State of Hesse.

FIAS is solemnly committed to promoting science and the free exchange of scientific arguments in a respectful manner. This is the basis of the work of the FIAS.

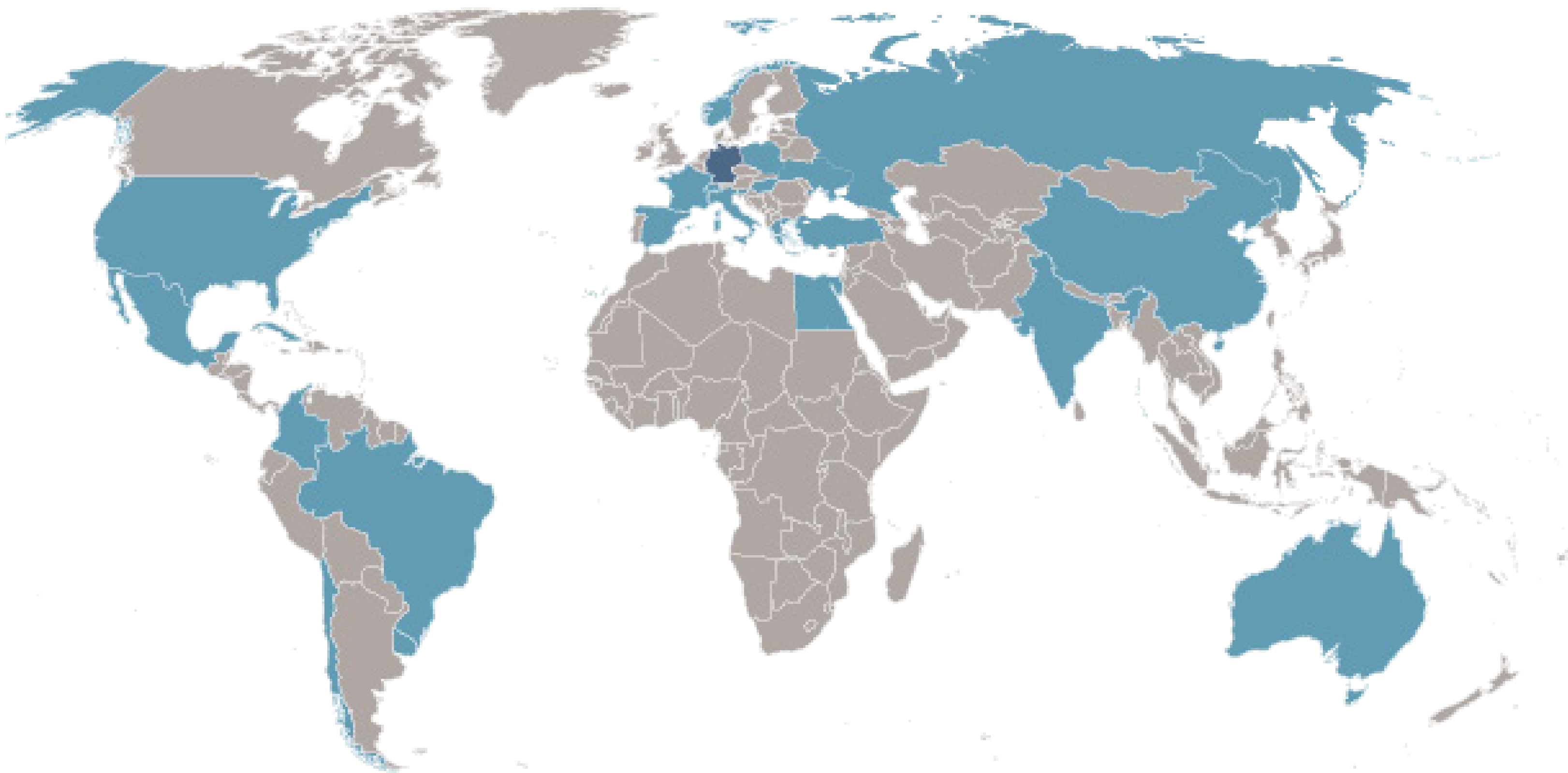
We look back to a very successful year. As well as the scientists, I would also like to thank the FIAS administration. They worked wonders to fit the many events into an already busy schedule.

Enjoy reading and re-living some of the highlights of 2024.

On behalf of all FIAS members,

Eckhard Elsen

FIAS 2024 in Numbers



32 Fellows
14 Postdocs
44 Doctoral students
13 Adjunct Fellows
14 Administration members
19 Undergraduate students
2 Student Assistants

138 people from **25** different countries

39%
female employees

7
new doctoral degrees

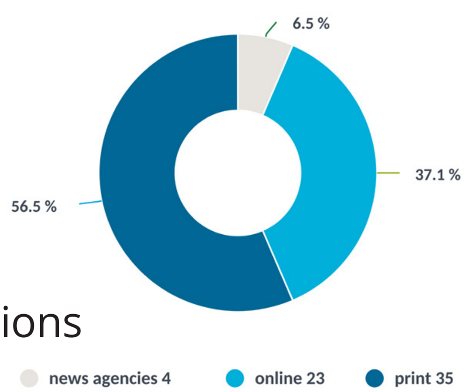
304
publications

6
workshops and conferences

4
seminar series

9
public events

62
press mentions



6229
coffeepads used

more than
5.9 Mio €
funding

20th Anniversary

20 Years FIAS

2024 was dedicated to the 20th anniversary of the Frankfurt Institute for Advanced Studies. Throughout the year, a series of special events showcased the institute's strong connection between research, society, and science communication. A key highlight was the official ceremony on December 5, celebrating the institute's development and the presentation of the Honorary Award for Science Diplomacy. However, the celebrations extended far beyond that evening: FIAS opened its doors to the public for the first time, engaged with the Frankfurt community, and participated in the Museumsuferfest. In addition, FIAS took part in "Frankfurt hat Hirn" and the Night of Science and hosted captivating FIAS Forum lectures, offering fascinating insights into cutting-edge research topics.

20 years of interdisciplinary excellence – and the journey continues.

Some impressions from the 20th anniversary celebrations, culminating in the official ceremony. Throughout the year, we also celebrated with the Frankfurt public, hosting our first Open Day and participating in the Museumsuferfest as a guest at the Museum Giersch of Goethe University.

FIAS Open House

For the first time in its 20-year history, FIAS welcomed visitors to explore its research and engage with science up close in an Open House. It featured hands-on experiments, short lectures, and a children's program, offering insights into topics such as particle acceleration, the role of light in drug control, and the impact of algorithms.

Many guests from the Riedberg neighborhood, along with longtime friends and supporters of FIAS, took the opportunity to visit the institute. Researchers explained their work in an accessible way, and interactive exhibits allowed visitors to experience scientific concepts firsthand. Over coffee and cake, attendees exchanged ideas and gained a glimpse into the interdisciplinary research at FIAS. The event highlighted the institute's ongoing commitment to sharing scientific knowledge and fostering curiosity across all generations.

FIAS at Museumsuferfest

Adults and children alike were captivated as they tried - unsuccessfully - to create rectangular bubbles, discovering firsthand how physics shapes these structures and how the fundamentals of surface tension work.

To celebrate its 20th anniversary, FIAS took part in the Museumsuferfest with a special interactive exhibition at the Museum Giersch of Goethe University (MGGU). Visitors of all ages were invited to explore the world of theoretical research in an accessible way. The exhibition introduced topics such as how algorithms work, how drugs can be controlled with light, and what a neutron star looks like. It also highlighted how FIAS researchers process large amounts of data - from molecules in cells to events in galaxies. Showing a fantastic comic strip FIAS Senior Fellow Martin Hansmann explained our immune system and his scientific research behind it.

Outside the museum, the FIAS stand offered hands-on science for curious minds. Visitors could take part in experiments and discover, for example, how soap bubbles can demonstrate mathematical and physical laws or what a vacuum actually is. Researchers were on hand to explain scientific concepts and guide participants through the experiments.

The Museumsuferfest provided a great opportunity to share insights into FIAS research with the public. Through interactive exhibits and experiments, the event made complex scientific topics more tangible and sparked curiosity among visitors of all ages.

Other highlights of the program included a speech by the Hessian Minister of Science and Art Timon Gremmels (right), a panel discussion (top) and contributions from young scientists (left).

Charlotte Warakaulle, CERN director for International Relations, was delighted to accept the award. The prize money will be used for science communication projects. (from left: Honorary Senator Carlo Giersch, Charlotte Warakaulle, Minister of State Timon Gremmels)

20 Years Celebration Event

What started as a bold vision two decades ago has become a thriving hub for interdisciplinary research. On December 5, 2024, FIAS celebrated its 20th anniversary with a ceremony at Goethe University's Casino, held in close partnership with its founding institution. The event highlighted our institute's unique role as a theoretical interface between disciplines, fostering groundbreaking insights into complex systems.

In a lively program, the evolution of FIAS and its innovative spirit took center stage. Special recognition was given to the funding institutions and private donors whose support - exceeding 100 million euros over the years - has enabled pioneering research in fields such as artificial intelligence, dense matter, and high-performance computing. As part of the celebration, the Honorary Award for Science Diplomacy was presented by Hesse's Minister of Science and Research, Art and Culture, Timon Gremmels to Charlotte Warakaulle. This award was made possible thanks to the generous support of the Giersch Foundation.

A panel discussion brought together key figures from the institute's history, including early visionaries, the newest Senior Fellow Roberto Covino, and PhD student Sigrid Traegenap. They reflected on FIAS's role as a "research speedboat", where interdisciplinary approaches drive scientific breakthroughs. As Scientific Director Eckhard Elsen noted: "For 20 years, FIAS has connected disciplines that seemed unrelated at first glance. The best ideas emerge from this exchange."

The program's creative highlights included a poetry slam by PhD student Jonas Elpelt and an artistic lecture on the physics of snowflakes by FIAS Fellows Franziska Matthäus and Volker Lindenstruth - capturing the essence of FIAS: thinking beyond boundaries for 20 years.

In his speech, GU President Enrico Schleiff emphasized the close and inspiring collaboration between FIAS and Goethe University.

Franziska Matthäus used science to herald the start of winter with her lecture on the "snowflake".

Frankfurt Institute for Advanced Studies at 20

Eckhard Elsen's introductory address at the FIAS anniversary celebration on December 5, 2025 (abbreviated)

Frankfurt Institute for Advanced Studies - the name is suggestive of the famous Princeton Institute for Advanced Studies, where Einstein worked for many years. This sets the bar high. A research institute outside the narrow framework of a university's department, but with direct links to the university and neighboring research institutions, such as the Max Planck Society; research free from teaching commitments and administrative tasks; the possibility of guest visits by external researchers and contact with students.

Three visionaries - two scientists, Walter Greiner and Wolf Singer, and an energetic university president, Rudolf Steinberg - came together in 2003 and formulated the bold plan for an independent research institute. They wanted to combine heavy ion physics and brain research. A balancing act at the time, but in many respects almost natural today. FIAS was registered as a foundation under civil law in December 2004. The founder is Goethe University. It was crucial to secure private funding, which necessitated the formulation of research projects that appeared appealing to both public and private donors. The founders met enthusiastic supporters for their idea in Karin and Carlo Giersch. A building was erected on the Riedberg Campus, which has been the home of FIAS since 2007, right in the heart of the university's natural science departments.

Projects at FIAS are intentionally limited in time. The purpose is to test, mature, and, once sufficiently established, transfer topics to other institutes. Alternatively, if unsuccessful, the projects can be discontinued. In a figurative sense, FIAS serves as an exploratory speedboat for science topics. This approach involves significant risks but also the potential for substantial rewards.

Outstanding role of scientific computing

Frankfurt plays a crucial role as an Internet hub and home to several computing centers, including GSI, a leading facility in heavy ion physics. To support scientific computing, the Green IT Cube, a High-Performance Computer among the most powerful installations, was built at GSI. Volker Lindenstruth, an expert in scientific computing, was then appointed to Goethe University and FIAS. Scientific computing forms the foundation of most research at FIAS.

In physics, algorithms based on neural networks were established in the 1990s. Today, machine learning and artificial intelligence are popular topics, especially at FIAS. This year's Nobel Prizes for Physics and Chemistry honor these topics. Research topics have evolved over the past 20 years: In physics, gravitation has been added to nuclear physics following the discovery of gravitational waves. The neurosciences have been supplemented by the life sciences. One flagship project was CMMS, generously funded by the Hesse LOEWE Priority Programme. What is behind it?

Structural analysis methods now allow detailed descriptions of individual molecules. In some areas, we can use this knowledge to mechanistically describe reactions and transport phenomena in the body by putting the building blocks together. We play LEGO with the building blocks of life. But the diversity that emerges is overwhelming. The dynamics cannot yet be satisfactorily modeled experimentally. This is where simulation helps. The temporal development of an initial state is simulated according to scientific rules and the result is then compared with reality. These are experiments on the digital twin. From the many development possibilities, we select the scientifically valid ones and can then conduct more targeted experiments. This area will continue to play a major role at FIAS in the future. We're locating the digital twin for biological and human systems at FIAS and supporting the SCALE application as part of the DFG's Excellence Initiative.

What does FIAS stand for today?

FIAS, a research institute, focuses on basic research using theoretical methods in natural sciences and related fields. Through interdisciplinary collaboration, it advances scientific knowledge and addresses global challenges. Moreover, FIAS introduces students to scientific work, empowering them to shape the future responsibly. It produces future leaders who think broadly. That is our claim.

FIAS students remain affiliated with their home university, usually Goethe University, which awards degrees. However, research involves collaboration with graduate colleges, often outside FIAS, where students from diverse disciplines discuss projects and adopt methods and analysis techniques. For instance, biology uses physics methods, computer science mimics human brain behavior, and physics employs artificial intelligence to handle complexity.

Complexity is the essence of FIAS

Scientific research has successfully described fundamental phenomena using simple equations, expanding knowledge and leading to technical innovations. However, nature often presents complexity that yields fundamentally new properties, distinct from the fundamental system. For instance, a single molecule, characterized by location and speed, becomes a gas with state variables like entropy and establishes thermodynamics. Numerous other phenomena exemplify this complexity. Complexity is a hallmark of academic work at FIAS, where students from diverse cultures interact. English serves as the working language, fostering curiosity about foreign cultures. This cultural diversity promotes new ideas and approaches to solving scientific problems.

We must not limit ourselves to science. Close cooperation between people from different backgrounds requires respect, mutual support, and inclusivity. Recent press accusations of disrespect in dealings deserve clarification, protection for the affected, and presumption of innocence until proven guilty. At FIAS, we prioritize respectful interaction, which is the basis of our work. As Director, I am committed to this approach. We are currently drafting instructions and guidelines, inviting everyone, especially students, to participate. These rules will codify our daily interactions.

The future

Twenty years of successful research at FIAS, with thousands of publications and numerous scientists appointed to professorships. Roberto Covino, the latest example, shared his expectations at this meeting.

We live in a scientific world with unprecedented opportunities for deeper understanding. Experimental measurement methods provide ever more detailed data, allowing us to study biology, chemistry, and medicine at the atomic level. Personalized medicine and treatment are particularly promising. Quantum computers are coming, and FIAS can provide algorithms demonstrating their superiority. Particle physics and gravity, which push the limits of the universe, are supported at FIAS.

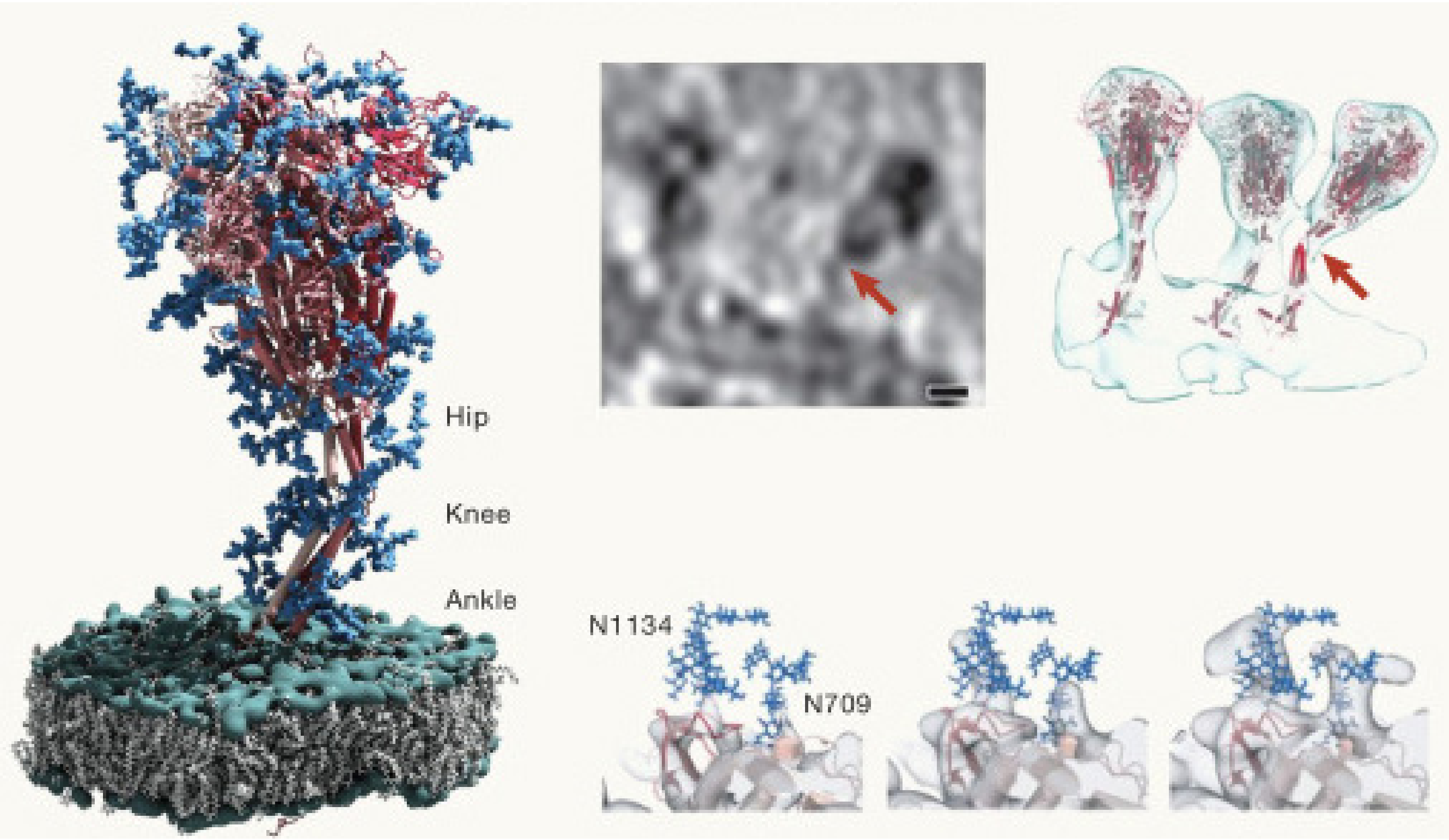
More pressing, however, are the questions about the sustainability of our world. So far, we have only carried out smaller projects on sustainability studies (resilience of distributed energy generation, optimisation of traffic flow, etc.). But what institute would be better suited than FIAS to dynamically take up such topics and also advise society?

We will not run out of topics. They are in good hands at FIAS. The future depends on the initiative of appointed scientists and private donors. However, FIAS delivers scientific success relatively inexpensively as a theoretical institute.

I am certain: If Frankfurt didn't already have a FIAS, it would be founded today.

more Highlights

A Digital Twin of SARS-Cov2 spike protein. The computer model of this infamous protein enabled an understanding of how the spike moves and evades the human immune system. Simulations predicted flexibility in three areas (hip, knee, and ankle), which electron microscopy confirmed.
from Martin Beck et al., CELL



FIAS researchers are playing a leading role in developing pioneering technology that will enter the next funding round as part of the excellence initiative.

Digital twins: The path to new discoveries in cells

In celebration of the 50th anniversary of the prestigious journal "Cell", FIAS Fellow Roberto Covino and his co-authors published an article discussing the future of structural and cellular biology. This piece delves into the limitations currently facing structural biology and shines a light on emerging technologies poised to revolutionize our understanding of molecular functions within cells. The authors introduce the concept of the virtual 4D reality of cells (3D plus time), poised to become a pivotal tool in the evolution of structural cell biology, which is also at the center of their SCALE excellence concept, selected for the next application stage.

Despite the recent surge in high-resolution data detailing the minutest cell components, our comprehension of how cells function remains incomplete. Digital twins represent precise virtual counterparts of biological cells, encompassing all existing information. These sophisticated models meticulously replicate cellular structures at the molecular level, accounting for changes over time and enabling the simulation of molecular processes that are fundamental to cellular life. This approach paves the way for groundbreaking predictions that can be experimentally verified, offering new insights into cellular functions.

This publication also highlights the strategy underpinning the "SCALE: Subcellular Architecture of Life" Cluster of Excellence initiative, which has just been selected for the second round by the German Research Foundation. Covino, as a core Principal Investigator (PI) of the SCALE initiative and a leader in the development of the Digital Twin technology, is at the forefront of this pioneering endeavor.

Publication: Martin Beck, Roberto Covino, Inga Hänelt, Michaela Müller-McNicoll, Understanding the cell: Future views of structural biology, CELL perspective, Vol 187,2, s. 545-562, 2024, doi: https://doi.org/10.1016/j.cell.2023.12.017

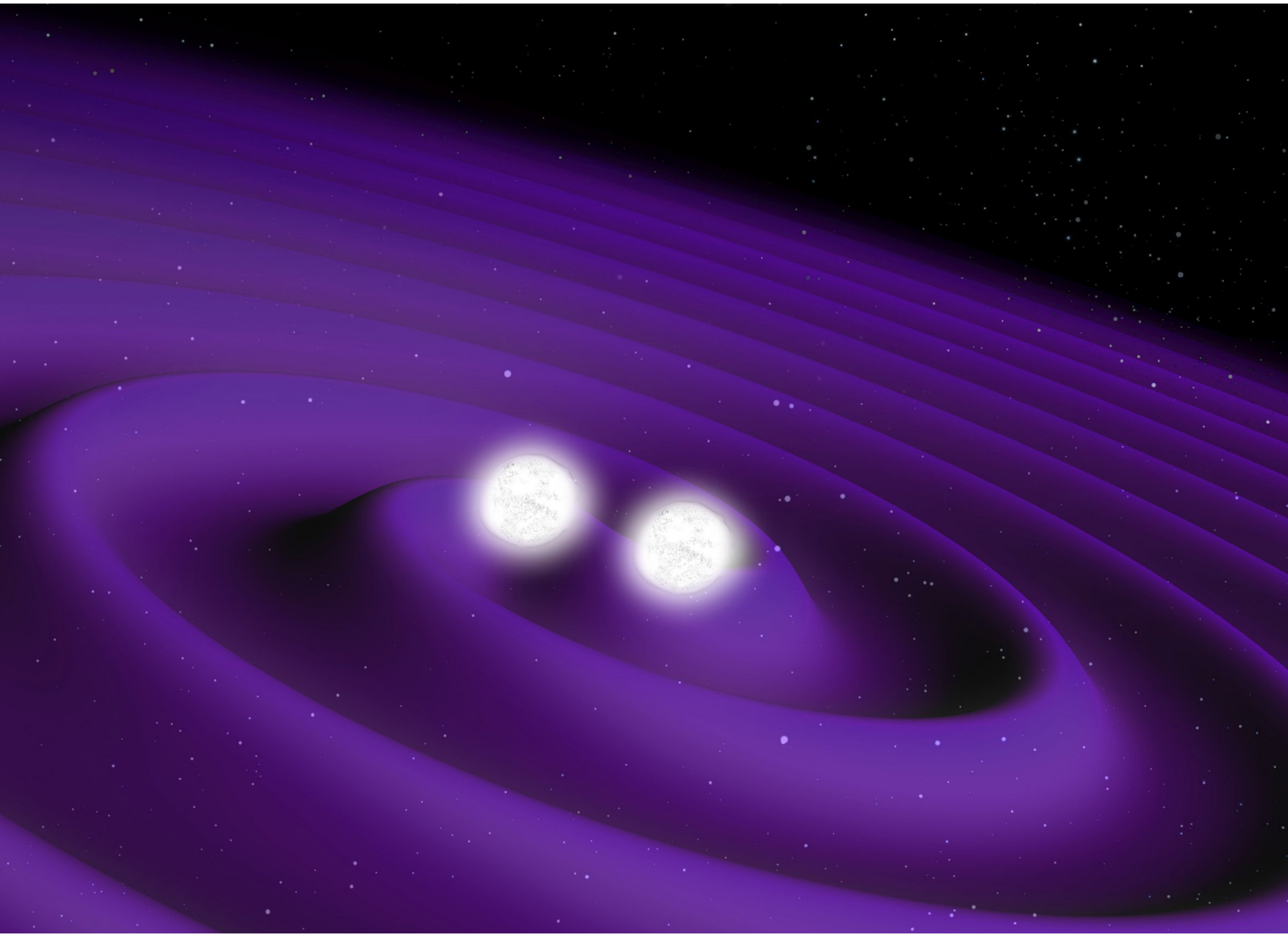
Scientific Advisory Board at FIAS

In March, FIAS presented itself to the Scientific Advisory Board (SAB) - in talks, posters, and intensive discussions. Every three years, the Scientific Advisory Board visits FIAS to evaluate its progress and provide strategic recommendations. During their recent visit, the board engaged in in-depth discussions and compiled a comprehensive expert report on FIAS's scientific trajectory. Their initial assessment was positive, emphasizing a sharpened research focus. The SAB highlighted the significant benefit of maintaining an independent institute, notably its agility in quickly responding to scientific developments, particularly across faculty boundaries.

The Scientific Advisory Board will support the strong standing of FIAS in the Frankfurt science landscape. IIn the meantime, there have been regular exchanges between the SAB Chairman and the FIAS management.

SAB visiting FIAS. From the right: Aneta Koseska, Volker Dötsch (speaker until April 2024), Owe Philipsen, Arndt von Haeseler (speaker as of May 2024), Edda Klipp, Reinhard Schneider and FIAS director Eckhard Elsen; missing on the picture: Alberta Bonanni, Ulrich Achatz and Luciano Musa.

Artist's impression of two neutron stars – the compact remnants of what were once massive stars – spiralling towards each other just before merging. The collision of these dense, compact objects produced gravitational waves – fluctuations in the fabric of spacetime – that were detected by the LIGO/Virgo collaboration in 2017. A couple of seconds after that, ESA's Integral and NASA's Fermi satellites detected a burst of gamma rays, the luminous counterpart to the gravitational waves emitted by the cosmic clash. © ESA



The direct observation of cosmic events such as the merging of black holes or neutron stars has long been a scientific challenge. Electromagnetic radiation (like light) can be affected by dust, gas and other objects in the universe, but gravitational waves penetrate these obstacles. This allows us to obtain more precise information about distant events. In a new study, Shriya Soma, together with Kai Zhou and Horst Stöcker made progress in our understanding of gravitational waves by successfully using deep learning to analyze gravitational waves from binary mergers.

Progress in gravitational wave research

The team investigated whether gravitational waves can be alternatively detected by classifying simulated signals from binary black holes, binary neutron stars and noise signals. While the classification of signals from different sources has already been done using DL by other research groups as well, Shriya Soma's focus was on the estimation of crucial parameters from signals of binary neutron star mergers. The developed DL methods are not only computationally efficient, but also enable more precise estimates of the masses and tidal deformabilities of neutron stars - two key parameters for studying the behavior of these dense celestial bodies and the properties of strongly interacting matter under extreme conditions.

The results of Shriya Soma and her colleagues underline the potential of DL techniques for the further development of gravitational wave analysis. In particular, the signal detection and parameter estimation methods developed in this work can be combined in the future to find a holistic solution for the analysis of gravitational wave signals. As an interdisciplinary research institute, FIAS has been an early mover in the application of artificial intelligence in various fields of research, particularly physics. With their approach, the institute's researchers were able to circumvent the computational challenges of conventional analysis methods. The paper was published in the renowned Journal of Cosmology and Astrophysics.

Publication: Mass and tidal parameter extraction from gravitational waves of binary neutron stars mergers using deep learning, Shriya Soma et al., JCAP01(2024)009, https://doi.org/10.1088/1475-7516/2024/01/009

Tidal deformabilities: When a neutron star passes close to another massive object, such as another neutron star, or a black hole, it is deformed by its tidal forces. The term "tidal deformability" is used to describe how strongly a neutron star reacts to these forces and how easily it can be deformed. It is therefore an important parameter for understanding the behavior of extremely dense states of matter in neutron stars and provide insights into the fundamental properties of astrophysical objects.

Nobel prize winners' research related to FIAS

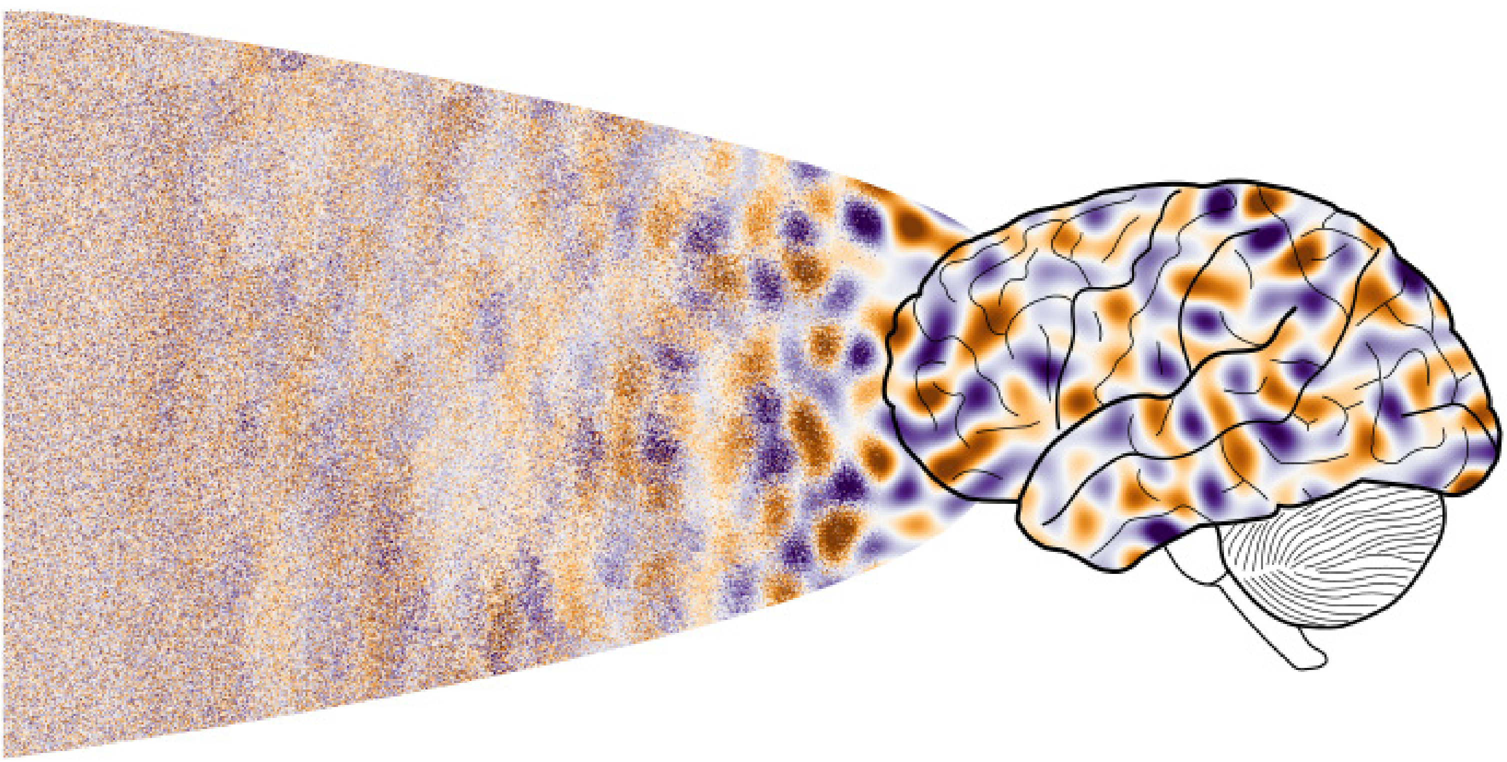
FIAS congratulated the Nobel Prize winners 2024 in Physics and Chemistry, whose work is directly related to research at FIAS. The fundamental findings of John Hopfield and Geoffrey Hinton on artificial neural networks, together with the massive progress in computing, have laid the foundation for today's AI revolution.

The work of Demis Hassabis and John Jumper uses such neural networks to predict the structure of almost all known proteins, and David Baker uses AI to create completely new proteins.

Artificial intelligence methods are playing an increasingly important role at FIAS. For example, it helps scientists at FIAS to better understand highly complex processes in cells, such as the molecular mechanisms of diseases. FIAS is also researching AI systems that even mimic the learning processes in the brains of small children.

Nobel Prize physics (John Hopfield, Geoffrey Hinton) and chemistry (David Baker, Demis Hassabis, John Jumper) 2024, © Niklas Elmehed, Nobel Prize Outreach

Life- & Neuro Sciences



During brain development, regular patterns form, as known from sand or fish.
Source: FreeImages.com

Like ripples in the sand: the young cerebral cortex forms spontaneous patterns

The cortex allows us humans to think, perceive our environment, and act purposefully. Certain patterns of brain activity enable this; they emerge early in brain development through dynamic processes of self-organization. This is shown by researchers from the University of Minnesota (UoM) and FIAS in a study published in Nature Communications. They found that the networks of the young cortex convert unstructured input into highly organized activity patterns. The organization of these patterns is therefore not determined externally (e. g. by sensory input), but arises through interaction between the nerve cells and follows dynamic laws.

The international research team's findings confirm a decades-old theoretical hypothesis of brain development. "Our results suggest that brain activity in the early cerebral cortex is self-organized," explains FIAS Senior Fellow Matthias Kaschube. Neighboring nerve cells activate each other, while more distant groups of them are suppressed. This spontaneously leads to the formation of regular patterns of brain activity, and the brain uses such patterns later in development to process sensory stimuli.

"What makes this transformation so important is that it appears to occur entirely within the cortex itself", adds Gordon Smith (UoM Medical School). The cortex can apparently organize its own function during development.

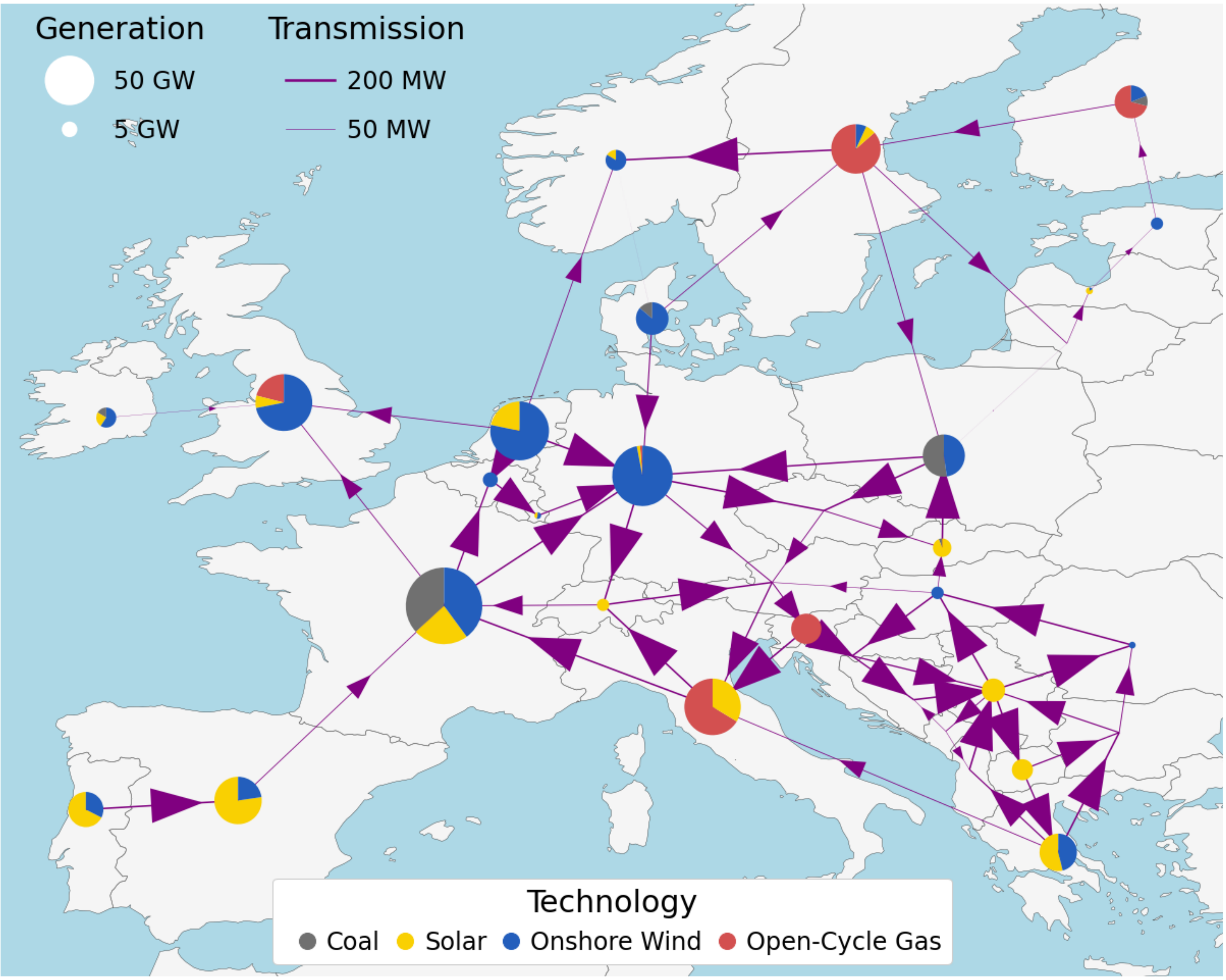
In a self-organizing system, even simple interactions generate complex organization. Examples are wave patterns on sand dunes, dot patterns on some fish, spiral nebulae of the Milky Way, or flocks of birds. By closely linking theory and experiment, the research team was able to show that similar mathematical rules that apply to the patterns in a variety of living and non-living systems also control the development of the brain.

The research team used optical instruments developed at the UoM that directly visualize how the large-scale structure of developing brain activity emerges from the networks themselves. Kaschube analysed this data at FIAS and compared it with the predictions of mathematical models of the self-organization of brain activity.

The researchers are currently investigating how changes in these self-organized neuronal activity patterns at the beginning of development affect later sensory perception.

Publication:
Haleigh N. Mulholland, Matthias Kaschube* and Gordon B. Smith* (*shared equally), Self-organisation of modular activity in immature cortical networks. Nat Commun 15, 4145 (2024). https://doi.org/10.1038/s41467-024-48341-x

Theoretical Sciences



Power generation and transmission solution for the 33-node European power system model. The AI approach by Chen Li et al. links power generation from different sources, including conventional and renewable resources (shown in pie charts in different locations), as well as power transmission (shown by arrows connecting the pie charts) and immediately ensures that power demand is met everywhere based on the input weather conditions. Grafic: Chen Li

AI solution avoids weather-dependent fluctuations in the power system

The high amount of solar and wind energy makes it difficult to ensure a stable power supply. A state-of-the-art AI system developed by FIAS researchers compensates for these weather-dependent fluctuations. It ensures efficient and reliable distribution of electricity from sources such as solar and wind to meet energy needs even in changing weather conditions while minimizing costs.

In a breakthrough study, PhD student Chen Li, supervised by FIAS Fellow Kai Zhou, presents a new AI technology that could revolutionize the incorporation of renewable energy into the power grid. Integrating renewable energy sources such as wind and solar power is not easy. Changes in the weather have a rapid impact on power generation and require frequent adjustments to the power grid. For example, even a single cloud over a photovoltaic system can cause major fluctuations in electricity within a very short space of time. Traditional methods face difficulties in dealing with this variability, especially in large power systems. The FIAS research team developed a cutting-edge, physics-informed machine learning method that can quickly adapt to changing conditions, making it ideal for real-time applications.

Based on electricity demand and weather patterns, the team's approach offers a solution for the immediate equalization of fluctuations. It is based on innovative neural networks based on graphical data on weather and power demand, the graph attention networks. It identifies the key nodes in the power grid, that mainly influence the pattern of power dispatch. The method also improves transparency in AI decision-making and provides insights how neural networks interpret data to make optimal decisions on energy distribution.

The current publication demonstrates the superiority of this method over existing data-driven techniques in two different scale scenarios for renewable energy systems. The new approach not only provides prompt and feasible solutions, but also maintains interpretability, which is crucial for understanding and trusting AI-based systems.

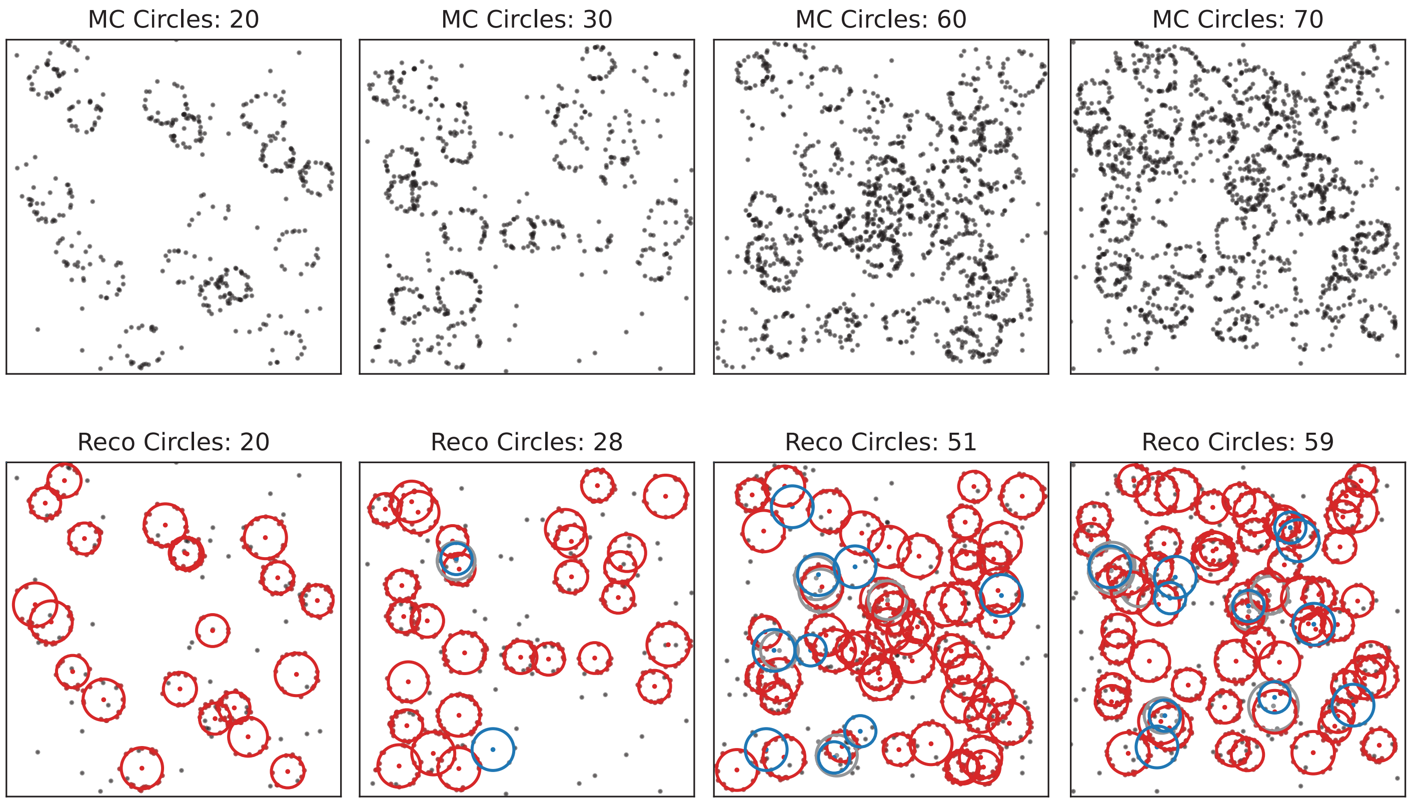
This technology is still at an early stage. It has mainly been tested on small and medium-sized power grids. "But it will change modern energy systems," Chen Li is convinced: "It enables the seamless integration of distributed energy sources into the grid, primarily solar cells and wind turbines". This will make renewable energies more reliable and easier to use. The system improves the efficiency, reliability and sustainability of electricity distribution and enables intelligent management and regular adjustment of the electricity grid. It also lays the groundwork for economic optimisation by considering a comprehensive range of physical factors and the dynamics of the energy market.

"As we continue to explore and improve this technology, we move closer to a cleaner, greener, and more sustainable future," says physicist Li. The team wants to further develop the system to include energy storage solutions with the help of AI.

Publication:

Chen Li, Alexander Kies, Kai Zhou, Markus Schlott, Omar El Sayed, Mariia Bilousova, Horst Stoecker, Optimal Power Flow in a Highly Renewable Power System Based on Attention Neural Networks, Applied Energy 359 (2024) 122779, https://doi.org/10.1016/j.apenergy.2024.122779

Computer Science & AI Systems



The accurate reconstruction of ring structures in high-energy physics experiments is crucial for identifying electron signatures and improving event classification. The integration of artificial intelligence into ring reconstruction processes has opened new ways for efficiency and accuracy improvements.

Hybrid GNN-Transformer Approach for Ring Reconstruction in High-Density Regions

The group of FIAS Fellow Ivan Kisel developed a novel hybrid approach that leverages Graph Neural Networks and Transformer architectures for enhanced ring center finding. The study is particularly relevant in the context of the Compressed Baryonic Matter experiment at FAIR (Facility for Antiproton and Ion Research at Darmstadt) where reconstructing Cherenkov rings in the RICH detector is a significant challenge. The hybrid method provides superior performance in detecting and reconstructing ring centers compared to traditional techniques.

This approach combines the strengths of Graph Neural Networks, which excel at learning from graph-structured data, and Transformers, which efficiently capture long-range dependencies through self-attention mechanisms. Each event is represented as a graph, where nodes correspond to detected hits, and edges are created between nodes using k-nearest neighbors and radius search. A Graph Neural Network-based encoder processes node and edge features, creating a latent representation for each hit. The edge attributes encode local geometric relationships and ring properties. The latent features are passed through a multi-head self-attention mechanism that learns global relationships between hits, refining the ring center predictions. The final model output includes ring center candidates, their probabilities, and estimated parameters such as radius.

The model was evaluated on a custom dataset created to resemble the simulated CBM RICH detector data, benchmarking against traditional ring reconstruction techniques such as Elastic Net and Hough transform. The hybrid approach achieved a high ring reconstruction efficiency, with the Graph-Transformer model reaching approximately 96.5 percent efficiency in identifying rings with more than 14 hits. The method maintains strong performance even in high ring density scenarios, demonstrating robustness against increasing event complexity.

The figure on the adjacent page shows the input and output corresponding to 4 samples consisting of 20, 30, 60 and 70 rings. Each sample is also added with utmost 40 random noise points. The top row of the figure displays raw hit distributions, which serve as input to the model. These distributions contain ring-like patterns corresponding to particle interactions in the detector. The bottom row highlights the true ring centers, which are used as ground truth labels for training the model. In the bottom row, we also draw rings using the center and radius parameters found from our model. The reconstructed circles that match with simulated circles are shown in red color and the missed simulated circles are shown in blue.

The distribution of hits in each sample varies significantly, reflecting realistic conditions encountered in the CBM experiment. The presence of noise hits challenges conventional reconstruction algorithms, whereas the hybrid model effectively suppresses such noise. The model successfully differentiates between true ring structures and spurious signals, improving detection reliability.

This hybrid GNN-Transformer model provides a powerful solution for real-time ring reconstruction in high-energy physics experiments. The approach demonstrates superior performance in terms of efficiency and accuracy. Future work will focus on integrating this method into experimental pipelines and extending it to multi-detector ring detection scenarios.

Publication:

I. Kisel and A. Mithran, „RCNet — U-Net and Hybrid GNN-Transformer based Ring Center Finder for RICH Ring Reconstruction", CBM Note, will be published, 2025

Projects

First step towards the Excellence Initiative

FIAS researchers are part of the cluster initiatives that were successful in the first application step: SCALE will develop radically new experimental techniques to map and simulate the inside of cells and predict their behavior. TAM aims to understand fundamental processes of human perception, thought and behavior that enable us to adapt to constantly changing conditions. The next step was the full proposal in August. The decision is expected in May 2025.

SCALE - From single molecule to cell function

The SCALE consortium with FIAS Fellows Gerhard Hummer, Roberto Covino and the participants Eckhard Elsen, Volker Lindenstruth, Franziska Matthäus, and Sebastian Thallmair combines technological expertise from cell biology, biophysics, molecular biology, neurobiology, chemistry, bioinformatics, and mathematics. They will develop radically new experimental techniques to map and simulate the inside of cells and predict their behaviour. This research will provide important new insights into bacterial resistance, inflammation, neurodegenerative diseases and immune defence. For details see https://scale-frankfurt.org/.

TAM - The Adaptive Mind

The TAM cluster initiative with FIAS Senior Fellow Jochen Triesch aims to understand fundamental processes of human perception, thinking, and behavior that enable us to adapt to constantly changing conditions. It is coordinated by the Justus Liebig University Giessen, the Philipps University Marburg, and the Technical University Darmstadt. Triesch is one of three Frankfurt scientists involved in the initiative as PIs. TAM brings together researchers from psychology, cognitive science, and neuroscience with experts in artificial intelligence (AI), machine learning, and robotics to decipher universal principles of human adaptability. The findings will be implemented in computer models that can mimic, predict and explain both the spectacular successes and tragic limitations of the human mind, with implications for basic research, mental health and the development of safe AI and robotics technology.

Future perspectives in multiscale modeling at FIAS

CMMS

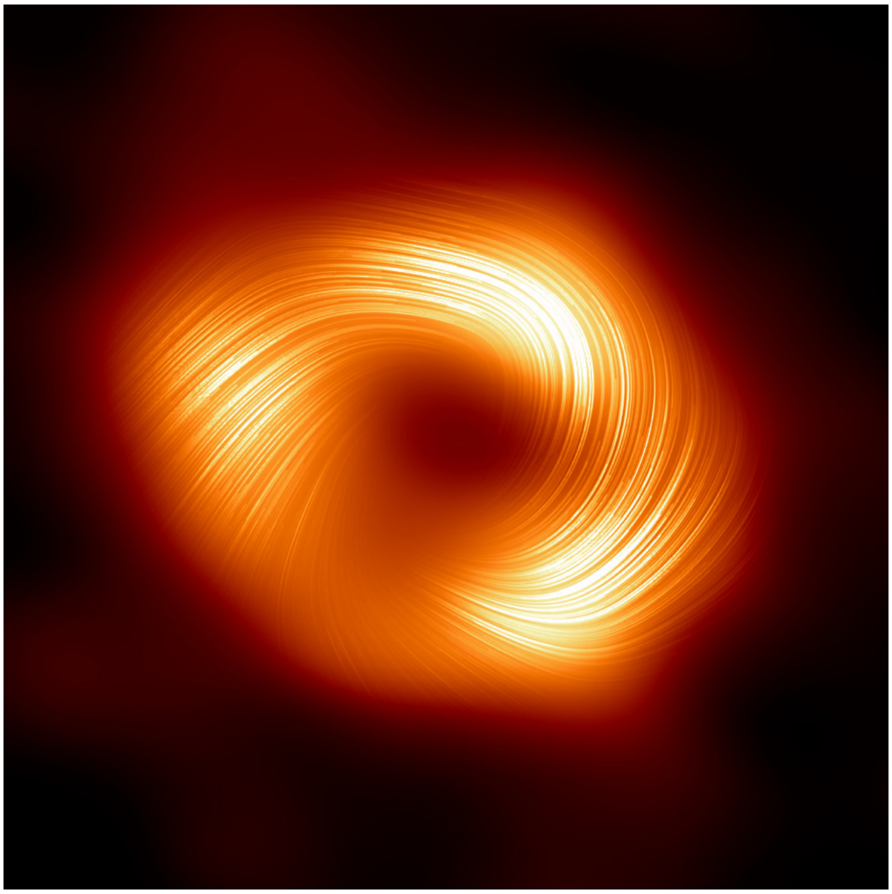
At the end of 2024, LOEWE funding for the Center for Multiscale Modeling in the Life Science (CMMS) at FIAS ended. We are looking back at a collaborative project, which strongly influenced the research at FIAS in the past five years. At the beginning of the funding period, four additional junior research groups were set up and integrated into CMMS. They enriched the field of research, strengthened our focal points, and intensified the interlinking of the subprojects. CMMS also acted as a catalyst for the core project - the digital twin of the cell - in the successful new excellence initiative SCALE, in which several CMMS PIs are involved. Digital twins - multiscale models with a strong quantitative orientation, a focus on the virtual representation of the system; and hybrid modeling approaches (like integrating mechanistic and AI approaches) are already an important new core topic at FIAS.

Numerous career successes of CMMS members are associated with the funding period. These include professorship offers to Tatjana Tchumatchenko, Ulrich Meyer, Roberto Covino, and our associate members Cornelia Pokalyuk, and Gemma Roig, the appointment of Enrico Schleiff as President of Goethe University, the appointment of Ulrich Meyer and Franziska Matthäus as members of the founding board of the new Center for Critical Computational Studies, the successful application of Nadine Flinner for a Mildred Scheel Junior Research Group, two ERC grants (to Gilles Laurent and Tatjana Tchumatchenko), and also a prize for efficient algorithms to Ulrich Meyer, and prizes for the best posters and best presentations to our doctoral students.

Overall, the CMMS supported the development and focus of FIAS to a high degree, and the FIAS is now excellently positioned both internally and internationally in the field of multiscale modeling in the life sciences and the development of digital twins of biological systems.

Part of a retreat during the five-years-project Center for Multiscale Modeling in the Life Science (CMMS), that ended this year. Photo: Franziska Matthäus

Spiral magnetic fields around a black hole



The black hole SgrA*: The magnetic fields spiral around the central shadow of the black hole. Image: EHT Collaboration

Images from the Event Horizon Telescope (EHT) team show that the black hole Sagittarius A* (Sgr A*) in the centre of our Milky Way is surrounded by strong, spiral-shaped magnetic fields. The team led by FIAS Senior Fellow Luciano Rezzolla played a key role in this study.

The first image of the black hole Sgr A* - roughly 27,000 light years away from Earth - was published by the collaboration in 2022, revealing that the supermassive black hole at the centre of our Milky Way is more than a thousand times smaller and less massive than that of the galaxy M87, of which the EHT collaboration published the first image of a black hole in 2019. Nevertheless, Sgr A* and M87* look remarkably similar. To find out whether the two black holes share any other common features, the EHT team decided to study Sgr A* in polarised light. It was already known from M87* that the magnetic fields around the giant black hole enable it to send a strong jet of particles into space. The new images show that the same could apply to Sgr A*.

Imaging black holes in polarised light is not easy, especially for Sgr A*. This is because the gas, or plasma, in the vicinity of the black hole orbits Sgr A* in just a few minutes, and because the particles of the plasma swirl around the magnetic field lines, the magnetic field structures change rapidly during the recording of the radio waves by the EHT. Sophisticated instruments and procedures were therefore required to image the supermassive black hole.

Luciano Rezzolla, theoretical astrophysicist at Goethe University Frankfurt and FIAS Senior Fellow, explains that magnetic fields influence the polarised radio waves. Examining the degree of polarisation of the observed light shows how the magnetic fields of the black hole are distributed. However, in contrast to a standard image, which only requires information about the intensity of the light, it is much more difficult to show the polarisation. “In fact, our polarised image of Sgr A* is the result of a careful comparison between the actual measurements and the hundreds of thousands of possible image variants that we can create using advanced supercomputer simulations,” explains Rezzolla. “Similar to the first image of Sgr A*, these polarised images represent a kind of average of all measurements.”

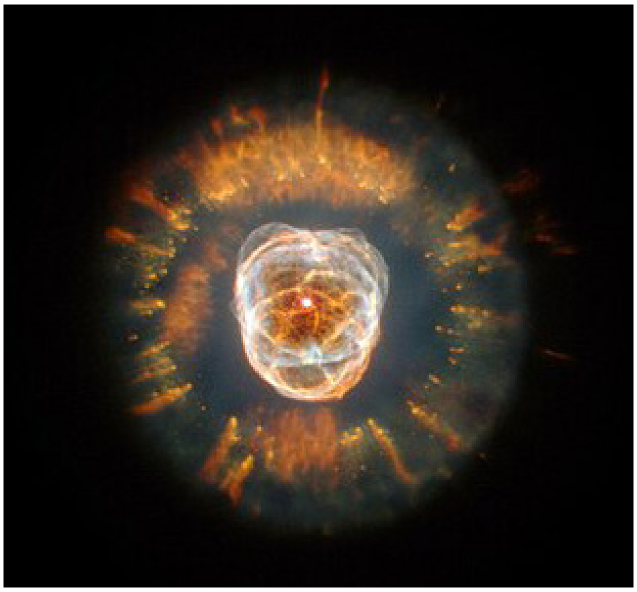
Publications:

First Sagittarius A* Event Horizon Telescope Results. VII. Polarization of the Ring. Astrophysical Journal Letters (2024) https://iopscience.iop.org/article/10.3847/2041-8213/ad2df0

First Sagittarius A* Event Horizon Telescope Results. VIII. Physical Interpretation of the Polarized Ring. Astrophysical Journal Letters (2024) https://iopscience.iop.org/article/10.3847/2041-8213/ad2df1

Understanding dense matter & compact stars

The research project 'Investigation of compact stars with heavy baryons and quarks' by FIAS Fellow Armen Sedrakian entered its third funding period in May 2024. The German Research Foundation (DFG) approved the application for research funding for a further two years.



White Dwarf, a compact star (NASA, ESA, A. Fruchter).

Sedrakian's new project aims to help better understand the nuclear systems in general and, more specifically, the properties of compact stars. In an extension of the work carried out in the previous periods, the research will now focus on the link between the first-principle description at the level of elementary particles (nucleons) and a more macroscopic description based on a phenomenological relation between the density and energy of the system. With this insight, the team will analyze the properties of compact stars (mass, radius, etc) consisting of nucleons and their more massive sisters known as hyperons (collectively known as baryons). The team will also investigate the possibility that the baryons are crashed into their constituents - quarks - at very high densities reached in compact stars.
"We hope to gain a better understanding of the deep interiors of compact stars through a combination of theoretical work with observations in terrestrial laboratories, and with telescopes on Earth and its orbit", says Sedrakian.

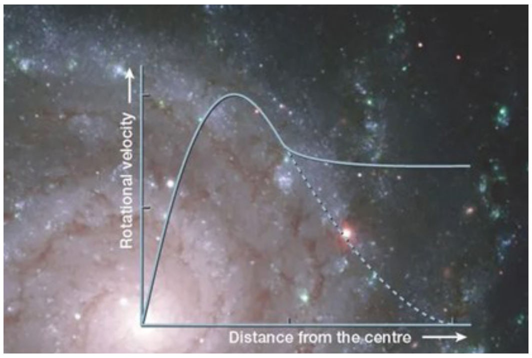
Dark Energy inside the galaxies?

The universe is shaped by two mysterious forces: dark matter, which attracts and pulls galaxies together, and dark energy, which repels and drives them apart, causing the universe to expand. Dark matter accounts for about 26% of the universe's energy, while dark energy makes up roughly 68% (the other 6% are the known baryonic matter that we and the stars are made of). These forces, one attractive and the other repulsive, have long been considered the primary influences on the structure and evolution of the cosmos.

New research by David Benisty and David Vasak from the groups of FIAS Fellows Jürgen Struckmeier and Horst Stöcker suggests that dark energy's effects can also be detected within galaxies, a much smaller scale than previously considered. By analyzing the rotation curves (velocity vs. distance of stars, see figure above) on dwarf galaxies, they found that the upper limit of dark energy's influence is surprisingly close to known values - just two orders of magnitude higher.

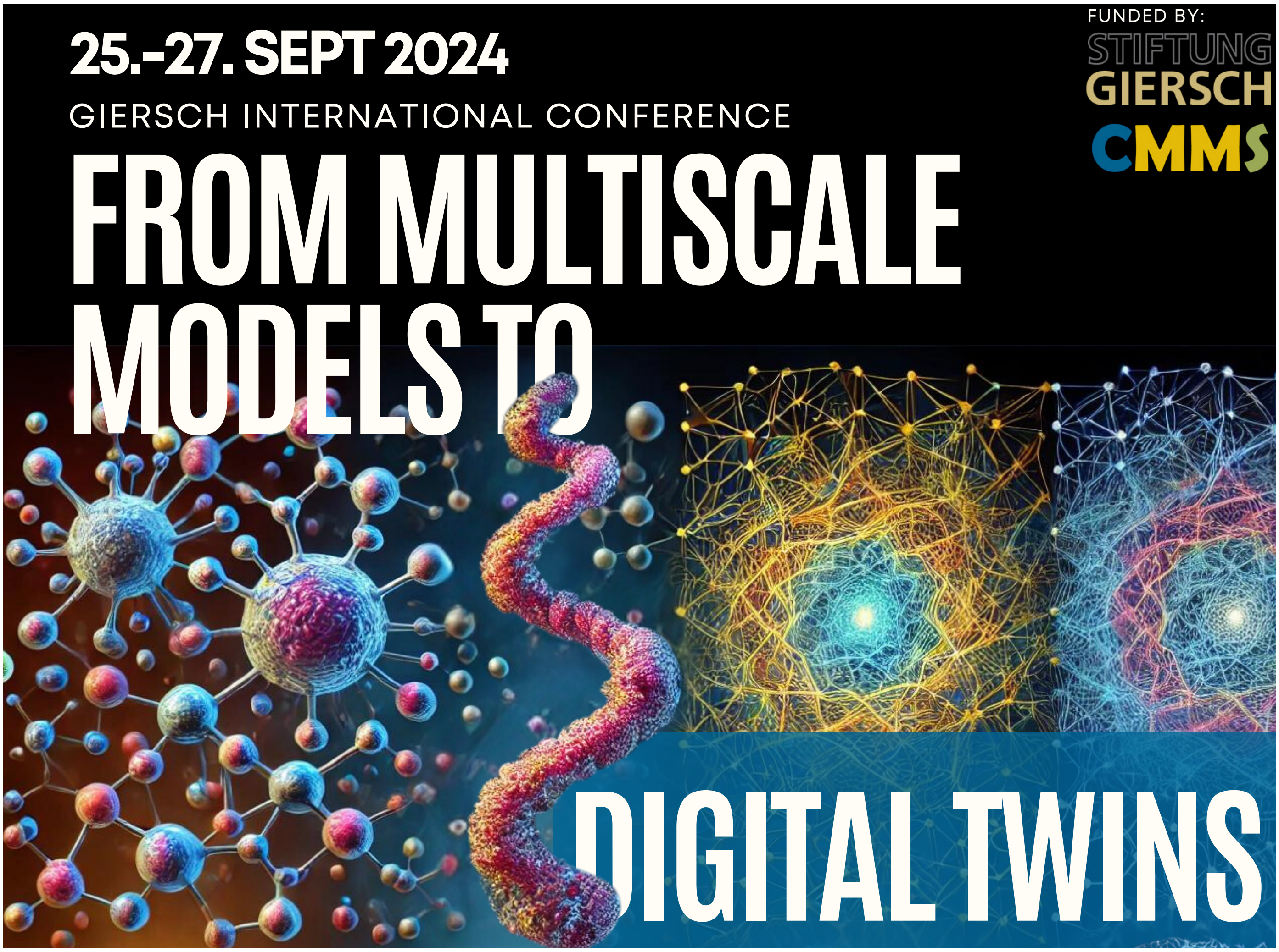
This groundbreaking discovery implies that dark energy has a more significant impact on galaxy dynamics than previously believed, potentially disrupting the balance between dark matter's gravitational pull and dark energy's push, leading to galactic instability. The research funded by Carl Wilhelm Fueck-Stiftung and Margarethe und Herbert Puschmann-Stiftung opens new avenues for studying dark energy within galaxies, offering fresh insights into its relationship with dark matter. The results challenge previous assumptions, suggesting that dark energy has an impact on much smaller scales than considered before.

The research shows that in galaxies with large orbital periods, the impact of dark energy reduces the velocity in the outskirts. Therefore, the researchers claim that with future measurements focused on the outer regions of galaxies, it will be possible to detect dark energy on much smaller scales than we currently imagine. This could lead to a profound shift in our understanding of the universe's fundamental forces.



The graph shows the velocity versus distance for stars in galaxies. Without dark matter, the velocity should follow the dashed line, decreasing with distance from the center. However, the observed velocity follows a near flat line, indicating that galaxies contain dark matter to explain this higher-than-expected velocity at larger distances. Photo: Gemini Observatory.

Events



Giersch Conference 2024

In September 2024, the international Giersch Conference From Multiscale Models to Digital Twins took place at FIAS. Over 70 scientists from various disciplines gathered to discuss the application of digital twins in the life sciences. Topics ranged from molecular simulations and tissue modeling to AI-driven medical digital twins.

Funded by the Giersch Foundation and the Hessian LOEWE-CMMS program, the conference provided a valuable platform for young researchers to present their work and connect with experts in the field. The interdisciplinary exchange sparked new ideas and perspectives on the use of digital twins in science and medicine.

Digital twins have the potential to overcome experimental limitations and offer deep mechanistic insights with improved control and reproducibility. Originally developed in industry and engineering, they are now transforming the life sciences. By integrating rigorous multiscale modeling with AI-driven approaches, researchers can better understand complex biological systems. The conference fostered discussions on how to enhance existing models and develop digital twins that are both accurate and efficient. Given its success, a continuation of the conference series is planned for the coming year.

FIGSS Retreat in Marburg

In October 2024, FIAS doctoral candidates of the Frankfurt International Graduate School for Science (FIGSS) participated in a four-day retreat in Marburg, building on insights gained from the From Multiscale Models to Digital Twins conference. Renowned experts shared perspectives on digital twin technology, sparking discussions on interdisciplinary applications. Working groups encouraged collaboration, while social activities, including a city tour and a scenic hike, strengthened the FIAS community. The retreat provided fresh perspectives and new ideas, leading to the establishment of a regular working group on digital twins at FIAS.

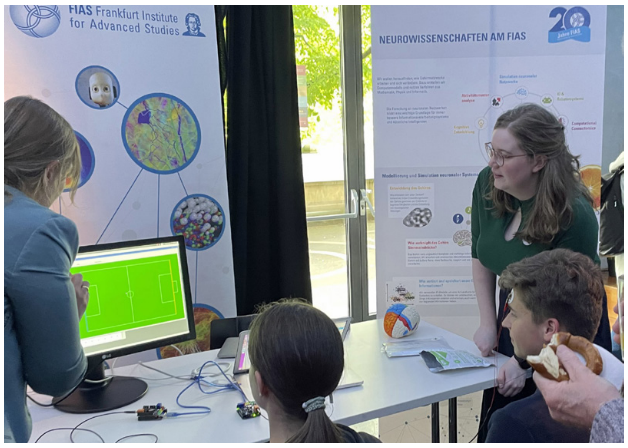
FIAS Forum

In 2024, the FIAS Forum continued to connect leading researchers with the public, offering insights into current scientific topics and their societal relevance. On March 14, Dr. Sebastian Thallmair explored how light-switchable molecules could revolutionize medicine by enabling precise drug control. On May 16, Prof. Dr. Judith Simon discussed the ethical and epistemological challenges of machine learning, emphasizing trust and responsibility in the digital age. On September 19, Charlotte Warakaulle, former Director for International Relations at CERN, highlighted CERN's role in science diplomacy and international collaboration. Finally, on November 21, Dr. Nadine Flinner and Prof. Dr. Peter Wild presented innovative applications of artificial intelligence in precision medicine and tissue diagnostics.

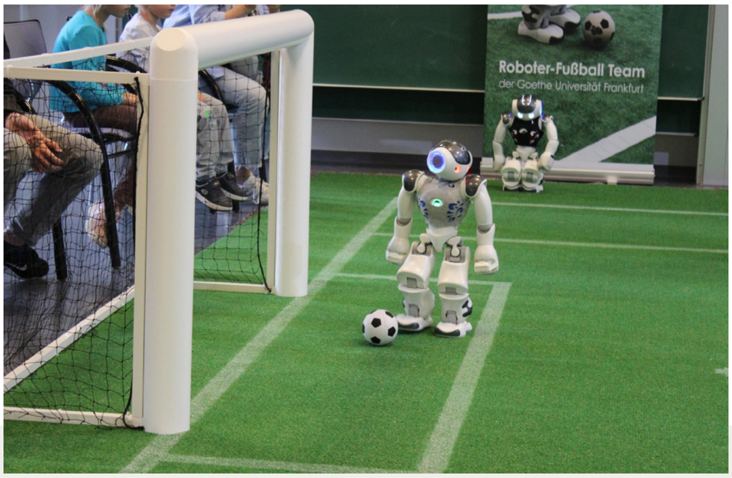
The FIAS Forum fostered interdisciplinary dialogue and strengthened the connection between science and society, continuing its tradition of engaging discussions and open exchange.

“Frankfurt hat Hirn – live”

The event organized in collaboration with the Hertie Foundation and Frankfurt neuroscience institutions, captivated a packed audience at the Jugendkirche St. Peter. Researchers from all instituions, including FIAS doctoral candidates Bastian Eppler and Jonas Elpelt, presented topics like brain rhythms, memory storage, and gut-brain interactions in a vivid and accessible way. Interactive exhibits and live demonstrations rounded out an evening that showcased the fascinating complexities of the human brain.



At the FIAS booth, visitors to “Frankfurt hat Hirn” were able to compete against each other in “brain soccer”.



The Bembelbots from GU Frankfurt played a “soccer match” against a group from Berlin in the packed FIAS lecture hall every hour.

Night of Science

On June 21, 2024, the Riedberg campus once again transformed into a hub of scientific discovery during the Night of Science. With talks, tours, and hands-on activities stretching late into the night, the event attracted curious visitors eager to explore cutting-edge research.

FIAS was part of the program, offering an interactive exhibition on the fourth floor with a stunning view over Frankfurt. Here, visitors delved into key research topics and engaged directly with scientists. A particular highlight was the Bembelbots robot football tournament, where guests could cheer on autonomous robots as they prepared for the World Championships.

How can we actually measure and analyze the amount of data generated in a particle collision? Our interactive exhibition answers these and other questions.

The Bernstein Network

The research alliance in the field of computational neuroscience "Bernstein Network" organized a PhD symposium in October at FIAS. It focused on the topic of transitions, providing young neuroscientists with a platform to discuss career changes, research communication, and adapting to new professional environments. With engaging talks, interactive sessions, and networking opportunities, the event successfully fostered exchange and inspiration for the next generation of researchers. "The participants were very enthusiastic," sums up Jonas Elpelt (FIAS) from the organising team with doctoral students Sigrid Trägenap (FIAS) and Lisa Haxel (Tübingen). "We hope to welcome them back to FIAS next year."

The participants of the doctoral symposium were able to exchange on scientific and social topics in the FIAS Faculty Lounge.

AvH Study Tour

As part of their summer tour, around 60 Alexander von Humboldt Foundation scholars visited FIAS to learn about its research through expert lectures. Director Eckhard Elsen and his deputy Volker Lindenstruth welcomed them and reported on the aims and research projects at the institute. FIAS postdocs Sahila Chopra and Claudia Quinteros Cartaya then gave an insight into the range of research at FIAS. Chopra herself holds an AvH scholarship.

The conference did not take place at FIAS but in the beautiful vineyard town of Oppenheim.

Bridging Fields in Creativity Research

In November 2024, the interdisciplinary Creativity Conference took place in Oppenheim, focusing on the neurobiological foundations and enhancement of creativity. Leading scientists presented the latest research findings, while workshops provided practical strategies for fostering creativity. The conference encouraged exchange between neuroscience, psychology, and the arts to develop a deeper understanding of creative processes.

Public Relations

Markus Schlott (left) and Chen Li presented a technology developed at FIAS on HR television. In the programme "Alle Wetter" they explained their AI solution to avoid weather-dependent fluctuations in the power system. This could stabilise the use of renewable energies in the grid (see details on page 20).

KI soll für stabile Stromnetze sorgen

FRANKFURT Schwankungen, die in Stromnetzen durch das Einspeisen erneuerbarer Energien entstehen, soll eine Künstliche Intelligenz (KI) ausgleichen, die Forscher des Frankfurt Institute for Advanced Studies entwickelt haben. Weil die Leistung von Photovoltaik- und Windkraftanlagen wetterabhängig ist, muss die Netzsteuerung flexibler reagieren als früher: Schon eine einzige Wolke über einem Solarpark kann zu einem Einbruch führen, der schnell kompensiert werden muss.

Um das zu ermöglichen, haben die Frankfurter Forscher neuronale Netze entwickelt, die auf grafischen Daten zu Wetter und Energiebedarf beruhen. Sie erkennen Schlüsselknoten im Stromnetz, die das Muster der Stromabgabe entscheidend beeinflussen. Die Methode ermöglicht es auch, nachzuvollziehen, wie die KI ihre Entscheidungen trifft. Bisher wurde das Verfahren hauptsächlich in kleinen und mittleren Stromnetzen getestet. zos.

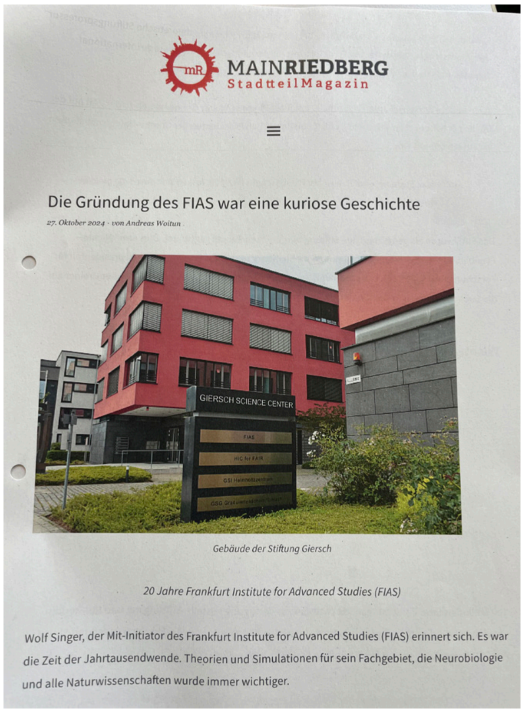
Foto dpa

FAZ 27.2.2

The topic was also covered by Frankfurter Allgemeine Zeitung (FAZ).

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.

The FIAS anniversary was highlighted in various media.



MAINRIEDBERG StadtteilMagazin

Die Gründung des FIAS war eine kuriose Geschichte

27. Oktober 2024 · von Andreas Woitun

Gebäude der Stiftung Giersch

20 Jahre Frankfurt Institute for Advanced Studies (FIAS)

Wolf Singer, der Mit-Initiator des Frankfurt Institute for Advanced Studies (FIAS) erinnert sich. Es war die Zeit der Jahrtausendwende. Theorien und Simulationen für sein Fachgebiet, die Neurobiologie und alle Naturwissenschaften wurde immer wichtiger.

UniReport | Nr. 5 | 10. Oktober 2024 — Aktuell 3

Das Schnellboot der Forschung

20 Jahre Frankfurt Institute for Advanced Studies (FIAS)

20 Jahre FIAS – das sind
- 72 Fellows
- über 100 Promotionen
- 3 Stiftungsprofessuren
- 15 eng kooperierende Adjunct und International Fellows
- über 20 fördernde Stiftungen und Sponsoren
- jährlich rund 150 forschende Gäste aus über 25 Ländern

Klein, aber fein – interdisziplinär und international: das aktuelle FIAS-Team. Foto: Störiko/FIAS

Wolf Singer, Mitbegründer des FIAS. Foto: privat

Das markante rote FIAS-Gebäude (links) am Riedberg wurde 2007 bezogen. Foto: Störiko/FIAS

Wenn die Nacht der Wissenschaft gehört

NIEDERURSEL/RIEDBERG Am Campus Riedberg zeigen schlaue Köpfe, was sie können und versetzen Gäste ins Staunen

VON HANS HOFELE

Die Bembel Bots können sogar Fußball spielen.

Goethe, Deine Forscher

FRANZISKA MATTHÄUS, BIOINFORMATIKERIN

FAZ, Frankfurter Rundschau and other media also covered FIAS events, research, and scientists.

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). **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.

Roberto Covino appointed Senior Fellow at FIAS and Professor at Goethe University

Roberto Covino has been appointed Senior Fellow at FIAS in August. He has been a research group leader and Fellow at FIAS since 2020.

Covino simulates cellular processes at the molecular level and thus enables a deeper understanding of the cell. "This was unthinkable until recently and is now a new field of research to be established and ventured at FIAS," says FIAS Director Eckhard Elsen. Covino embodies the spirit of FIAS and promotes it through his research. His previous group leadership proves he is more than up to the new challenge as a Senior Fellow. This includes, for example, his commitment to the CMMS project and his intensive promotion of young researchers.

Roberto Covino (left) receiving his certificate of appointment from GU-President Enrico Schleiff.

Covino develops theoretical models and innovative computer simulation methods. He merges physics-based and machine-learning methods to understand the dynamic organization of complex biomolecular systems.

Covino's successful and highly committed research led to a W3 professorship of Computational Life Science at the Institute of Computer Science at Goethe University in May. This will further support the networking of FIAS and the university.

"We want to understand how biological cells work," says Covino. Cells are the basic unit of all life forms on Earth. And they are incredibly complex. "Understanding them is not only an exciting scientific challenge but would also help us to come up with better solutions for diseases and grand social challenges.

Particle physics prize for FIAS director

The Scientific Director of FIAS, Eckhard Elsen, will be awarded the W. K. H. Panofsky Prize in Experimental Particle Physics 2025 by the American Physical Society (APS) together with Robert Klanner. The two particle physicists are being honored for their pioneering work on the large particle accelerator HERA (Hadron-Electron Ring Facility) at DESY (Deutsches Elektronen-Synchrotron). Both scientists were professors at the University of Hamburg and conducted research together at DESY.

Elsen was Professor of Experimental Physics at the University of Hamburg and a senior scientist at DESY for around 25 years, including as spokesperson for the H1 experiment, one of the four experiments at the HERA accelerator. Robert Klanner was deeply involved in setting up, operating, and analyzing the ZEUS experiment and was research director at DESY.

Elsen and Klanner receive the award for their key contributions to science at DESY's largest particle accelerator HERA, which was in operation from 1992 to 2007. HERA was used primarily to study the structure of the proton in detail. The knowledge gained is not only of central importance for the general understanding of the proton and its components, but is now incorporated into the daily work of researchers from all over the world who are involved in the Large Hadron Collider (LHC) at the CERN research center in Geneva, where Elsen conducted research for several years.

Elsen is particularly pleased "to be part of a long line of friends and colleagues who have received the Panofsky Prize over the past 30 years". He names stories and joint discussions about almost every prizewinner.

The Panofsky Prize is considered one of the most important prizes in particle physics. It is awarded annually at the Spring Meeting of the American Physical Society, which will take place in Anaheim, California (USA) in mid-March 2025. The two particle physicists will receive the prize of 10,000 US dollars for their "pioneering work in establishing the HERA physics programe and detectors".

New impetus: Stephan Huber joins FIAS Board

Entrepreneur Stephan Georg Huber has been appointed as a new member of the FIAS Board of Trustees (Stiftungsrat). Over the next five years, he will help shape our independent scientific institution for basic theoretical research.

Stephan Huber has been a successful entrepreneur and investor in medium-sized manufacturing companies for many years. These include the Upper Palatinate-based manufacturer of precision technology Hör and the Austrian high-tech company Pichler & Strobl GmbH. The 59-year-old also works as an advisor for the corporate finance company CRESCAT Advisory GmbH in Frankfurt. The entrepreneur, who lives in Königstein im Taunus, has gained extensive experience in the fields of consulting and management during his career.

As an entrepreneur and consultant, Huber brings a broad range of expertise to the Board of Trustees. The graduate aeronautical and industrial engineer held various management positions and played a key role in shaping medium-sized companies. With his strategic expertise and flair for innovation, he will actively support FIAS in meeting future challenges.

Huber succeeds Ekkehardt Sättele (see below). FIAS is looking forward to working with Stephan Huber.

Ekkehardt Sättele retires from Board of Trustees

The Board of Trustees and the FIAS Board of Directors bid farewell to Ekkehardt Sättele (third from left).

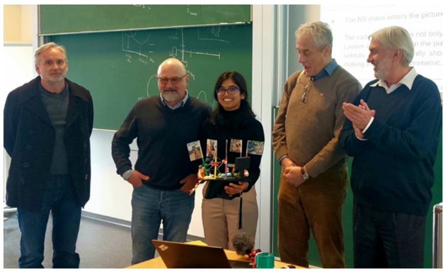
Ekkehardt Sättele stepped down from the FIAS Board of Trustees (Stiftungsrat) at the end of his term of office at the Board of Trustees meeting in May 2024. Since 2004, his expertise as an auditor and his extensive experience in the foundation sector have been invaluable to FIAS.

Sättele has supported the institute from its very beginnings and made a significant contribution to strategic planning and ensuring the institute’s financial stability. After 20 years of valuable commitment, he is leaving the FIAS Board.

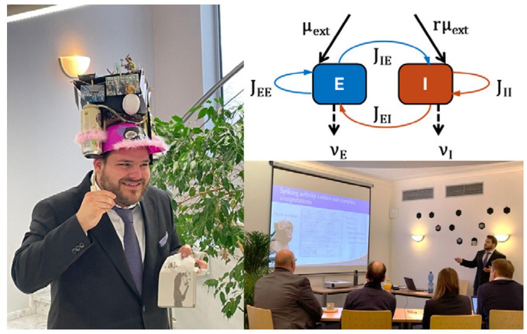
The Board of Trustees and the FIAS staff thank Ekkehardt Sättele for his 20 years of commitment and strategic engagement for science!

Seven new doctorates at FIAS

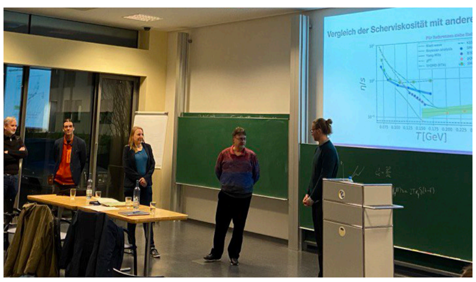
Shriya Soma, Pierre Ekelmans, Jan Hammelmann, Johannes Lehrbach, Megha Chakraborty, Solveig Plomer and Tim Liebisch successfully ended their doctoral thesis at FIAS. Congratulations to all new PhDs - and their supervisors!



Shriya Soma successfully defended her thesis in April. Her PhD on constraining the neutron star equation of state using deep learning techniques was supervised by FIAS Fellows Horst Stöcker and Kai Zhou. Soma will use the skills learned at FIAS at a company to use deep learning algorithms for the development of demo systems.



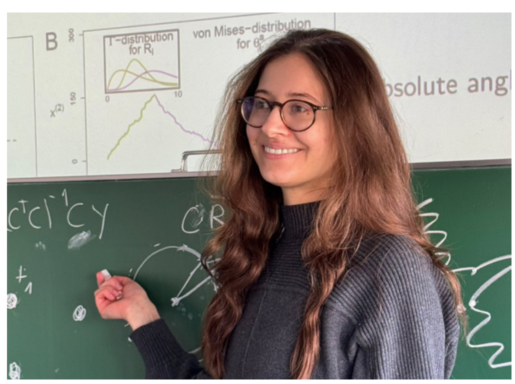
Pierre Ekelmans defended his PhD in theoretical neuroscience in April. As CMMS doctoral candidate he successfully completed his doctoral thesis in the field of computational biosciences. He conducted his research in the laboratory of former FIAS Fellow Tatjana Tchumatchenko, which focuses on the theoretical analysis of neuronal dynamics. He predicted the activity of excitatory-inhibitory networks.



Jan Hammelmann (right) finalized his PhD in June, working on fluctuations in the hadronic phase of heavy-ion collisions. He completed his doctorate in the group of FIAS Senior Fellow Hannah Elfner. For his studies he used a transport model developed in the group, called SMASH.

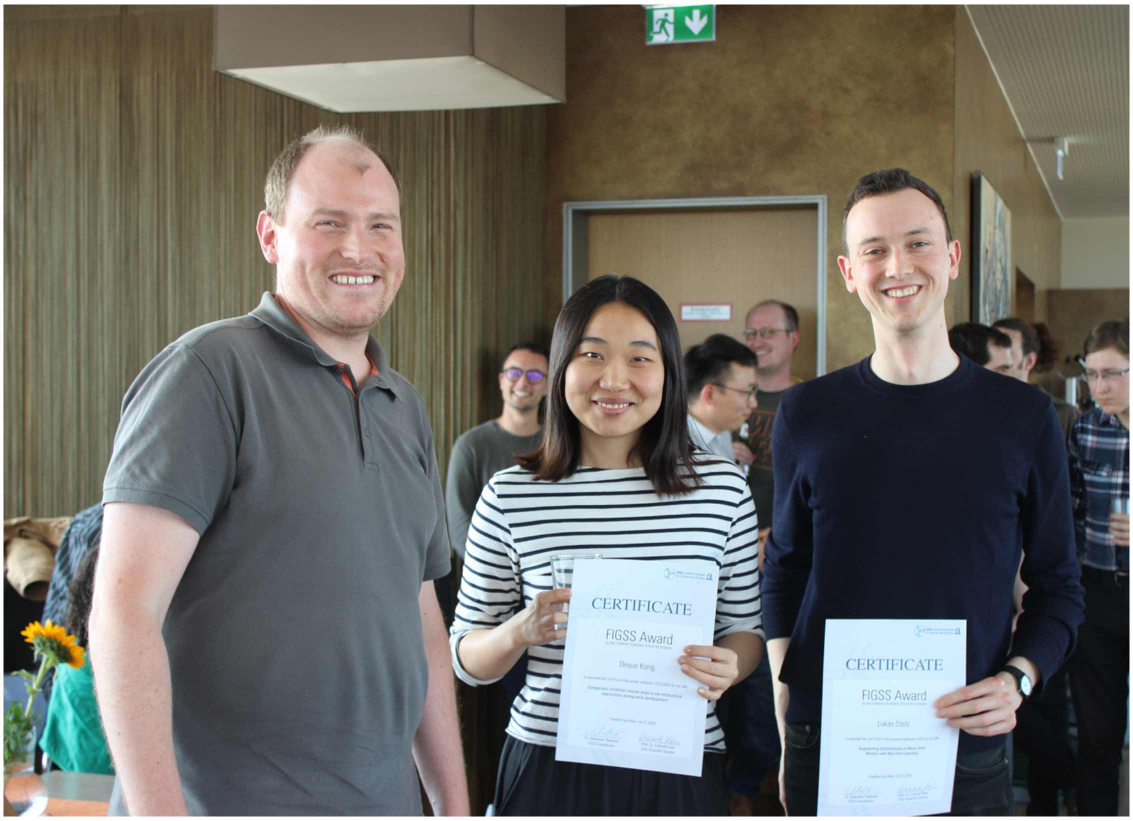
Johannes Lehrbach defended his PhD thesis in July. During his PhD, he was instrumental in building the computing infrastructure for the Event Processing Nodes (EPN) of the ALICE experiment at CERN. This cooperation is part of the research group of FIAS Senior Fellow Volker Lindenstruth.

Megha Chakraborty gained her doctorate on earthquake research in November. Her dissertation went beyond traditional seismology: She used deep learning as a tool to decode seismological data. Impressive publications and the award of the title „summa cum laude" reflect her successful research. She worked in the Seismology and Artificial Intelligence research group of FIAS Fellow Nishtha Srivastava, who supervised the dissertation together with FIAS Fellow Georg Rümpker.



Solveig Plomer defended her thesis in November. She developed a model to describe cell organelle movement. in the statistics group of Gaby Schneider (Goethe University). Within the LOEWE Schwerpunkt CMMS - Multiscale Modelling in Life Sciences she not only defined a new model for cell organelle movement but also developed a test and change point detection algorithm for changes in the model parameters.

Best FIGSS Talk prizes 2024: Lectures honoured



The best doctoral presentations were honored at the FIAS anniversary celebration in July. Prizewinners Deyue Kong (center) and Lukas Stelz (right) received a book voucher from FIGSS coordinator Sebastian Thallmair (Solveig Plomer and Jonas Köhler are missing from the picture).

For the second time, the Frankfurt International Graduate School for Science (FIGSS) at FIAS awarded the 'Best FIGSS Talk' for summer and winter semester 2023/24. The FIGSS was founded in 2004 and brings together FIAS doctoral candidates working on a wide range of research topics from nuclear physics to mathematical biology.

In the fortnightly FIGSS seminar, doctoral candidates present their research work to a broad scientific audience, including their doctoral colleagues at FIAS. In the summer semester 2023, seven doctoral candidates presented their work and current projects; in the winter semester 2023/24, there were six. A jury - consisting of the scientific coordinator of the FIGSS, Sebastian Thallmair, and the administrative coordinators of FIGSS, Doris Hardt and Patricia Vogel - evaluated the presentations.

The summer prize winner Solveig Plomer (Goethe University, CMMS) is working on mathematical models of changes in movement direction and speed in cell organelles. The second prize went to Lukas Stelz (FIAS). He presented epidemiological models, which he expanded using machine learning methods to increase their accuracy.

Winter prizewinner Deyue Kong (FIAS) uses neuronal networks to predict large-scale intracortical interactions during early embryonic development. The predictions were confirmed with the help of optogenetic methods. Jonas Köhler (FIAS) was awarded second prize for his update on analyzing earthquake sequences in Japan using deep learning.

In addition to a successful presentation of the research results, the prizewinners impressed the jury with clear introductions to their respective research topics, which provided the audience with a wide range of information.

Student representatives 2024

In February, the students at FIAS elected their new representatives for the year. 20 students voted in favor of Petros Vlachos and Santiago Galella, who were running for election.

“We are delighted and honored to take on the responsibility of student representatives,” said the two FIAS doctoral students. They thank everyone who participated in the elections, especially their predecessors, in particular Jonas Köhler (Megha Chakraborty had left FIAS during the election period), for their contribution to the community and their help and insights during the handover process.

Petros E. Vlachos is a theoretical neuroscience PhD student in the lab of Jochen Triesch. Originally from Greece, he studied artificial intelligence in the Netherlands and worked as a research assistant in the field of computational neuroscience. Currently, in his research, he is investigating the dynamics of learning and memory in brain networks.

Santiago Galella is a PhD student in the lab of Matthias Kaschube. He studied biomedical engineering and artificial intelligence in Barcelona, Spain. He is researching how cognitive maps of concepts and knowledge are formed and navigated both in the human brain and in artificial intelligence systems.

“Our goal is to foster a collaborative, inclusive environment and an active, more connected FIAS community,” said Petros and Santiago. The two planned to initiate events and meetings to enrich the academic and social aspects of our institute. “We welcome any ideas, feedback and participation!” said the FIAS student representatives.

A fresh start for IT and Finance

Beata Barta
Controlling

Ewelina Marusiak
Accounting

Eva Swoboda- Lorenz
Travel

FIAS re-organized its finance and IT teams in 2023/24. Beata Barta is in charge of the accounting department since July 2023. Since September 2024 she is supported by Ewelina Marusiak. They both are contact persons for all questions concerning finance, accounting, and controlling. The team is completed by Eva-Maria Swoboda-Lorenz, who is responsible for travel expenses since March 2024.

Thomas Holl
Head of IT
Data Protection

Sascha Reynolds
IT

The IT department at FIAS has also been reorganized. Since September, Thomas Holl and Sascha Reynolds are in charge of in-house IT services, network, and Slurm cluster. They take care of all IT issues, such as server and desktop hardware and licenses. Gabriel Grappasono is supporting them in user administration and access tokens.

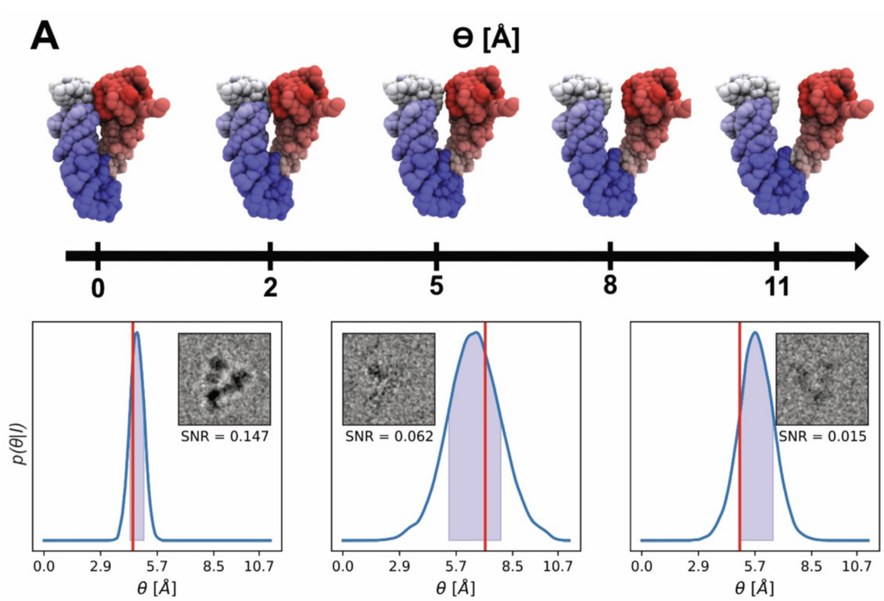
FIAS is happy to be up-to-date and agile again in both fields and warmly welcomes the new team members!

FELLOW REPORTS 2024

Machine learning makes sense of noisy experimental data

2024 was a crucial year for the group. Roberto Covino received a call to establish the "Computational Life Science" professorship at Goethe University. This fantastic achievement was made possible by the great work done by the group at the FIAS between 2020 and 2024 in the context of the CMMS project. It is a testament to the nurturing environment at FIAS that enabled establishing a young, dynamic, and productive group. The professorship was established thanks to a public-private partnership, with a generous contribution by Stefan Quandt, that helped to empower existing instruments by the Goethe University. At the same time, Roberto Covino was appointed Senior Fellow at the FIAS. This double affiliation demonstrates the ongoing intense cooperation between the FIAS and Goethe University, with the virtuous participation of local philanthropists like the Quandt family.

From a scientific point of view, this was a year in which we continued to work on a deep integration between computational physics approaches and machine learning. Our group developed a new, faster way to analyze cryo-electron microscopy (cryo-EM) images of biomolecules. Cryo-EM is a powerful tool for seeing the 3D structures of molecules, but analyzing the images to understand the different structures can be slow and difficult. This is because these images are extremely noisy. Our new method, called cryoSBI, uses simulations and machine learning to quickly and accurately determine the different structures present in a sample. It's much faster than previous methods and can handle large datasets, making it a significant advance in studying the dynamic nature of biomolecules.



A demonstration of how our new cryoSBI algorithm can identify specific molecular structures corresponding to noisy cryo-electron microscopy images.

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 2024 he was appointed W3 professor for Computational Life Science at Goethe University and Senior Fellow at FIAS.

Highlight

Roberto Covino became W3 professor for Computational Life Science at Goethe University and Senior Fellow at FIAS.

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

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

Podcast at https://theoreticalneuroscience.no/thn25/

Projects at FIAS: 1

Collaborations

Peter Jedlicka, University Gießen
Gaia Tavosanis, Bonn
Ruth Benavides-Piccione, Madrid
Albert Gidon, Berlin
Karl Farrow, Leuven, NL

The biological complexity of single neurons

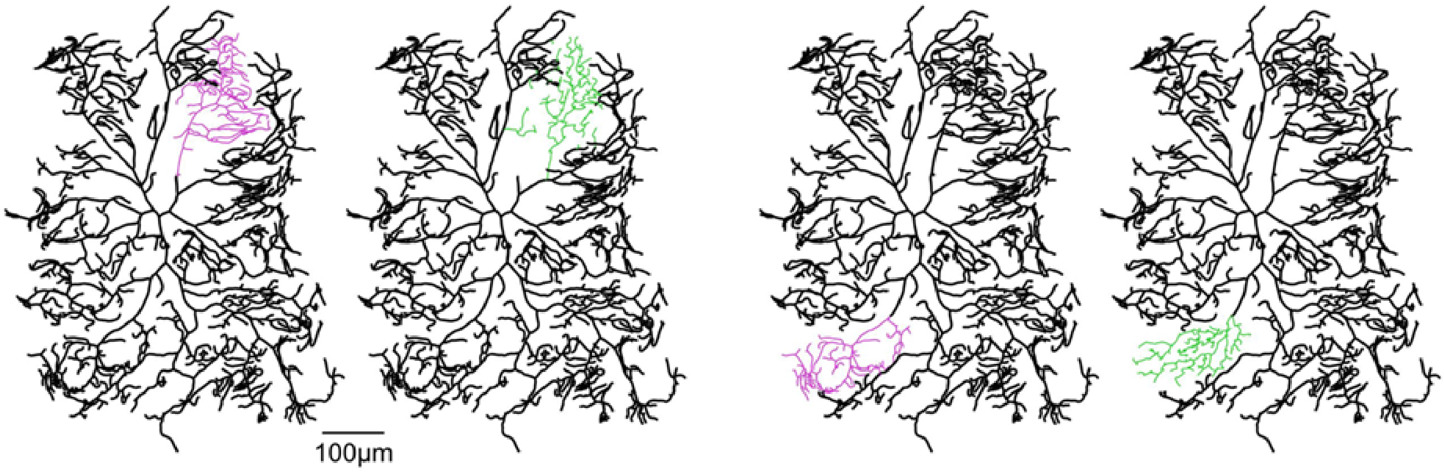
Dendrites are the beautifully branched input structures that shape a neuron's connectivity and the computations that it performs. We work with computer models that describe the morphology and electrophysiology of such dendrites. In the past, we found that dendritic morphology is well described by simple optimal wiring criteria, which can be used to generate synthetic arborizations in the computer. In this year's main work, we used our dendritic growth algorithms to repair cut dendrites (see Figure 1, for a fly larva neuron).

We found that our simplest growth model based on optimal wiring was able to recover the branches and the overall branching statistics of the original non-cut trees. Interestingly, the results reproduced a hallmark of biological regrowth: Regeneration either regrows the cut branch from the point where it was cut (Figure 1, example on the right) or fills in the available space by regrowing from neighboring branches (Figure 1, example on the left).

We then showed that one can use our biologically inspired repair algorithm on reconstructions of dendrites from human tissue. These are often incomplete because they are rare and human dendrites are large, which means they are unlikely to fit into one slice. Our repaired human dendrites are useful for predictions on the electrophysiology and they may help correct some of the assumptions currently made, e.g. for synaptic integration.

Publication: Groden M, Moessinger HM, Schaffran B, DeFelipe J, Benavides-Piccione R, Cuntz H+, Jedlicka P+. A biologically inspired repair mechanism for neuronal reconstructions with a focus on human dendrites. PLoS Computational Biology, 20(2):e1011267.

Modeling the repair of dendritic trees: Dendritic branches of Class IV dendritic arborisation neurons of the fly larva peripheral nervous system were cut (magenta) and regrown following optimal wiring constraints (green). Modified from Groden et al., 2024.



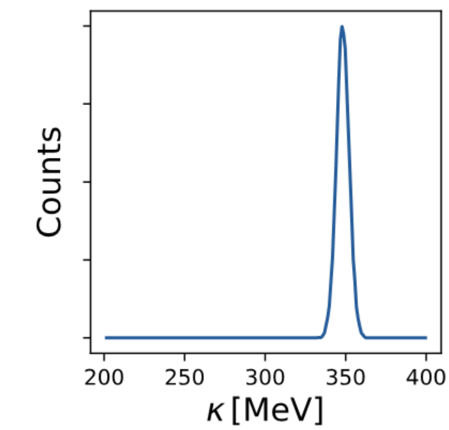
Equation of state of high density nuclear matter

The properties of nuclear matter at extreme densities are of high interest for the calculations of merging neutron stars. Similar conditions in terms of temperature and density can be explored in the laboratory with heavy-ion collisions at GSI. To extract information about the physics properties of interest, detailed microscopic modeling of the dynamics of such collisions is crucial. We have implemented the momentum dependence of the nuclear mean field in the hadronic transport approach SMASH (Simulating Many Accelerated Strongly-interacting Hadrons). The collective flow of matter produced in heavy-ion collisions is sensitive to the equation of state of nuclear matter at finite density.

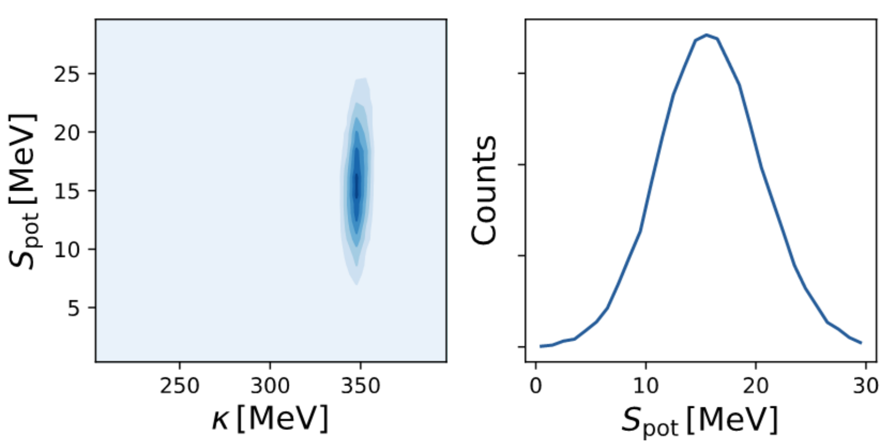
We have performed an extensive comparison of calculations to the available FOPI experimental data on Z=1 directed and elliptic flow measurements [1]. By carrying out a statistical analysis, it has been confirmed that at lower energies the soft equation of state fits very well, while higher energies, and in particular the elliptic flow requires a harder equation of state. A similar analysis has been done with respect to the highly differential HADES measurements of collective flow for protons and deuterons [2]. From this comparison, we have performed a parameter extraction with a Bayesian analysis and obtained a rather stiff equation of state, while the symmetry energy is in agreement with prior findings. This can be understood due to the large amount of resonances in the SMASH transport code that effectively softens the equation of state. The momentum dependence of the implemented nuclear force is crucial to get agreement with the data. This study contributes to understanding the equation of state of nuclear matter at high densities.

Associated publications: [1] Eur.Phys.J.A 60 (2024) 11, 232 e-Print: 2405.09889

[2] Justin Mohs et al., e-Print: 2409.16927



Posterior distribution for the parameters κ(incompressibility) and Spot (symmetry potential). The bottom left panel shows the posterior distribution as a function of both parameters and the upper and the right panel show the posterior as a function of only κ and SPot respectively with the other dependence integrated out. (from [2])



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 (GU) and a Fellow at FIAS since 2013, recently promoted to Senior Fellow. She obtained her PhD degree at GU in 2009 sponsored by a stipend of the 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 DFG and BMBF. In 2018, she was awarded the Zimanyi medal at the Quark matter conference. In 2021, she received the award "Scientist of the year" by the Gertrud and Alfons Kassel foundation at GU. In 2024, she took over the co-spokesperson role of CRC-TR-211.

Highlight

Strangeness in Quark Matter 2024 conference in Straßburg, attended as a member of the international advisory committee and visited the European parliament. Carl Rosenkvist presented first results in a poster.

Projects at FIAS: 2

Staff

Renan Hirayama (HFHF), Carl Rosenkvist (F&E), Alessandro Sciarra, Olga Soloveva, Justin Mohs, Niklas Götz, Nils Saß, Lucas Constantin, Martha Ege, Antonio Bozic, Joscha Egger, Robin Sattler, Olivia Kolandavelu

Collaborations

JETSCAPE collaboration, USA, MUSES collaboration, USA, Yuri Karpenko, Prague University, Czech Republic, Sören Schlichting, Bielefeld, Anton Andronic, Münster, Lucia Tarasovičová, Kosice, Slovakia

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

Publication of Die Pathologie special issue on 'Digital Pathology' in which the group participated as editors.

Projects at FIAS: 1

Staff

Robin Mayer
Ingvild Mathisen
Marina Kurtz
Fabian Fliedner

Collaborations

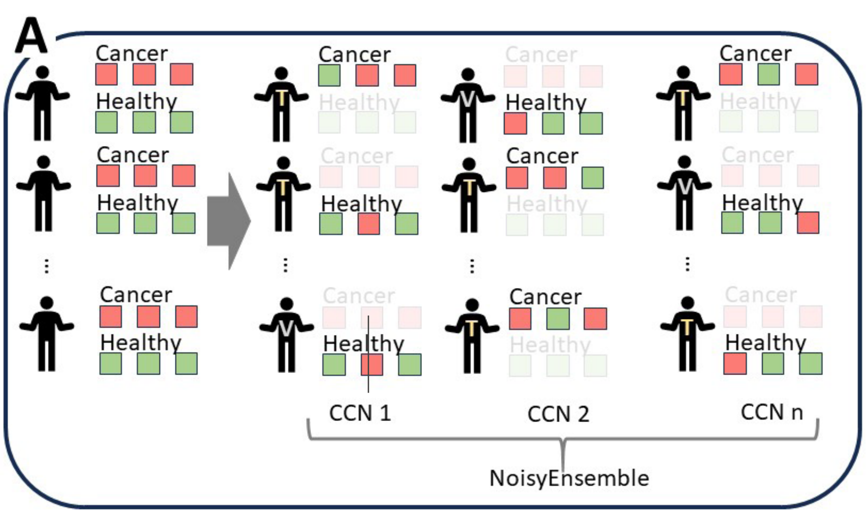
Peter Wild
Jochen Triesch
Henning Reis
Silke Kauferstein, GU

AI transferability in computational pathology

Two years ago, we introduced our NoisyEnsembles to overcome the problem of AI transferability in computational pathology, where a well-known problem is that trained models perform worse on data from hospitals, not included in the training and validation process, e.g. due to differences in tissue staining. Our NoisyEnseble is based on a bagging approach, where several convolutional neuronal networks (CNNs) were trained and patients were randomly re-sampled into the training and validation dataset for every CNN and a majority vote determines the final decision. In addition, we use only one class per patient and swap some of the labels during the training process to introduce label noise.

We have now tested our method extensively and were able to show that that it is not only working on ovarian cancer detection, but also on other tissues and tasks: Namely cancer detection in bladder tissue and the classification of morphological subtypes in intrahepatic cholangiocarcinoma. It is also important to mention that the method is not only improving transferability when models where trained with monocentric datasets, but also when stain-normalized multicentric datasets are used for AI training, which is the general approach to counteract the problem of transferability in the field. Other approaches to overcome the transferability problem, also known as domain shift, need information about the target domain during model training. However, these methods are not applicable because data from the target institute is not always available during training. And it is also important to ensure transferability for unforeseen domain shifts within one institute, e.g. caused by a slow wear of machines used for tissue preparation.

In addition, we have observed that also vision transformer (ViT) are able to improve model transferability compared to CNNs, however, our classical NoisyEnsemble (built from several CNNs) perform better compared to single ViTs and NoisyEnsembles built from ViTs.



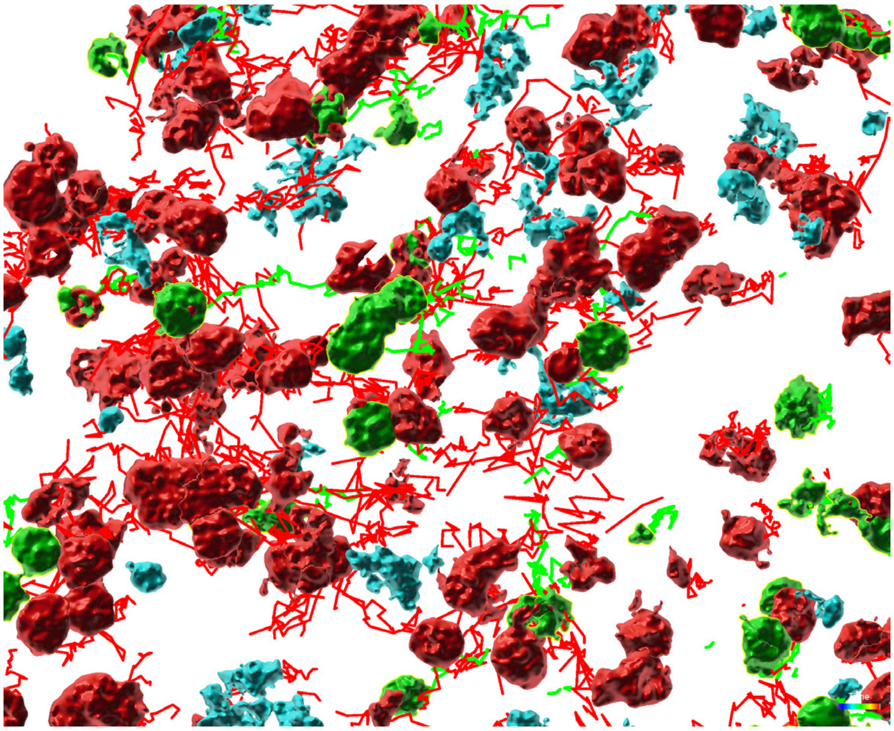
NoisyEnsembles improve AI performance on external datasets. Training procedure of the NoisyEnsemble. For each patient, several image patches are available for all classes (e.g. cancerous and non-cancerous). During training and validation, only one class is used and some tiles get a wrong label, patient and tile selection are different for every CNN in the ensemble. (Figure modified from: Mayer RS et al. Die Modelltransferierbarkeit von KI in der digitalen Pathologie : Potenzial und Realität. Pathologie. 2024; 45(2):124-132. doi: 10.1007/s00292-024-01299-5).

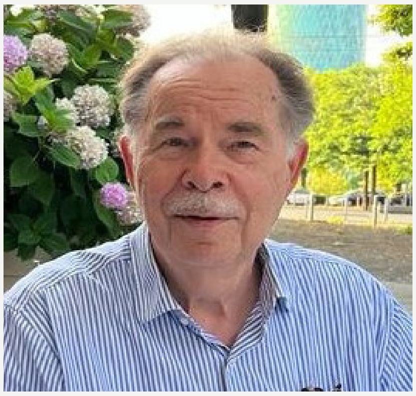
Visualization of human lymph nodes in space and time

In 2024 my group had a scientific focus on confocal laser visualization of human lymph nodes in space and time. Calculations of speeds and movements of T and B lymphocytes were performed and compared to other cell types by applying machine learning. Interestingly, cell contacts and contact duration times turned out to be informative. So we could demonstrate for the first time that checkpoint blockage in special lymphoma types can prolong the contact times between tumor cells and PD1 cells. Although the checkpoint drugs can be very successful in clinical applications and often induce a favorable outcome for the malignant disease, the molecular mechanisms are still poorly understood. Investigations using laser technologies in time and space are possibly able to revolutionize the biological understanding of immune cell interaction networks. Besides living tissue sections also capillaries were applied to measure cellular movements. With this technology, it could be shown that special molecular types of aggressive B cell lymphomas have differences in their movement speeds. Experiments using CART cells and NK cells were started (German French corporation funded by the DFG). The described scientific data were published. In addition, several scientific and educational lectures were given in Bonn, Frankfurt, Cologne, Erlangen, Bamberg, Hamburg, Wuppertal, Essen including the FIAS meeting on "digital twins". A public demonstration of scientific development of our group was given at the Mainufer Fest in Frankfurt and a special demonstration was performed at the planetarium in Halle in cooperation with the National Academy of Sciences- Leopoldina.

Publication: Hansmann ML et al.2024,Sherif M et al.2024, Yadigaruglu K et al.2024

Confocal laser visualization of human CD8 (green), PD1 T cells (red) and CD20 B cells in blue immunofluorescence showing movement tracks in a reactive lymphoid tissue.





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

Presentation of our scientific data to the public including children in Frankfurt (Mainuferfest) and Halle/Saale planetarium.

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 2024, the Hummer group used molecular dynamics simulations to capture ATP synthase and other key cellular machineries in action.

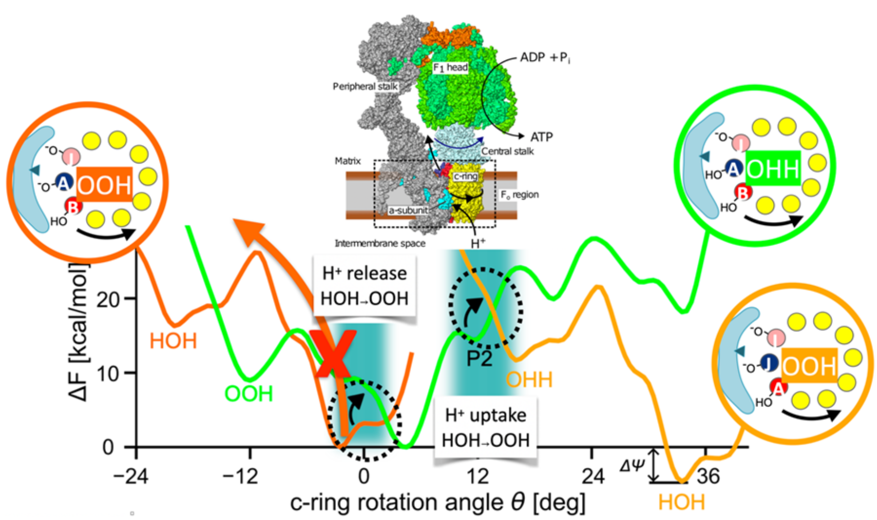
Projects at FIAS: 1

Collaborations

Roberto Covino
Sebastian Thallmair

Molecular simulations of cellular machinery

2024 was another exciting year for our group, with publications in Nature (2), Cell, Nature Communications (2), Science Advances (2), and Proc. Natl. Acad. Sci. USA (2), among others. As a highlight, Florian Blanc could quantify the force driving the synthesis of ATP in mitochondrial ATP synthase (Blanc, Hummer, Proc. Natl. Acad. Sci. USA 121, e2314199121, 2024). As power stations in our cells, mitochondria harness the energy from oxidizing food stuff to build up an electrochemical potential across their inner membrane. The potential is then used to drive protons across the membrane, coupled to the rotation of the Fo motor of ATP synthase. The Fo rotation in turn drives the rotation of the asymmetric central stalk (Okazaki, Hummer, Proc. Natl. Acad. Sci. USA, 2013; 2015), which deforms the three nucleotide binding sites of the F1 motor in such a way that ATP synthesis from ADP and inorganic phosphate Pi is kinetically favored. From extensive molecular dynamics simulations, Florian Blanc obtained the free energy profiles for the rotation of the barrel-shaped 10-fold symmetric c-ring forming the Fo rotor of an algal ATP synthase in all relevant protonation states. Free energy minima correspond to the experimental structures of the Fo rotor in states associated with proton uptake and release to opposite sides of the membrane. Florian Blanc showed that short water chains mediate these critical proton transfer reactions. And, most importantly, he demonstrated how a fully conserved arginine in the membrane-bound a subunit, with its positive charge, effectively imposes directionality on the driven rotation. In this way, Florian Blanc could capture and quantitatively characterize the fundamental symmetry-breaking event in all of life, which makes it possible to harness light and chemical energy for the synthesis of ATP to power the cellular machinery and the entire organism.



ATP synthase (top) combines two rotary molecular motors, Fo and F1. The curves show free energies for the rotation of the c10-ring of Fo in the relevant protonation states with 1 ("OHH") or 2 ("OOH") of the 10 glutamates deprotonated. The thick orange arrow indicates that back-rotation is kinetically blocked. The dashed circles indicate that the surfaces cross where protons are transferred onto and off the c10-ring. The 36o forward-and-down shift of the second "OOH" surface shows that the electrochemical potential ΔΨ≈200 mV biases the overall rotation in the forward direction.

Universality of neural representations

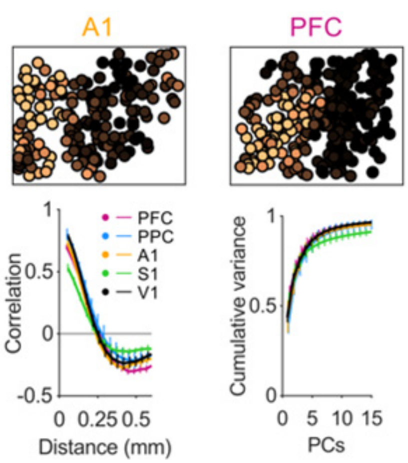
This year was particularly productive with articles published in PNAS and Nature Communications and in the top-tier computer vision conference ECCV. In addition, we have four more papers in press, including two in Nature Neuroscience, and three more are currently under review.

In our study published in PNAS, with our long-term collaborator Gordon Smith at the University of Minnesota, we showed that a distributed and modular functional architecture, known for many years to exist in the visual cortex, is in fact a universal feature of the entire 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.

Moreover, we provided direct evidence that this highly structured activity that is observed throughout the early developing cortex emerges via self-organization of neural activity. The process of dynamic pattern formation involves interactions in the form of local excitation and lateral inhibition akin to a Turing mechanism. This possibility was conjectured several decades ago, and our study in Nature Communications constitutes the first direct evidence in support of this long-standing hypothesis.

In addition to these research achievements, I brought the Bernstein Conference in 2024 to Frankfurt, hosting it now for three consecutive years. Being one of the top three annual meetings in computational neuroscience worldwide, attracting more than 500 international scientists, this meeting generates a lot of attention for Frankfurt within the scientific community. The PhD symposium took place at FIAS. Moreover, I organized the conference Bridging Fields in Creativity together with my collaborator Simon Rumpel in Mainz, in which we gathered a number of world experts working on the neural basis of creativity.

Finally, our group was also highly active in science communication. Insights into new developments in the research field of computational neuroscience were provided at the 20th anniversary's festivities and beyond, in venues such as Frankfurt hat Hirn, and the Night of Science, reaching the broader public. Outstanding are the Science-Slam activities by Jonas Elpelt, a PhD student in my group, who performed at six such public events in 2024 across Germany, including one in Frankfurt organized by the Physikalischer Verein with 1200 visitors.



Universal neural activity structure in the developing cortex. Top: Activity in auditory (A1) and higher association cortex (PFC). Bottom: Correlation function (left) and dimensionality (right) are highly similar across 5 cortical regions.

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 & Computational Vision in the Department of Computer Science and Mathematics at Goethe University and is Senior Fellow at FIAS.

Highlight

Diverse cortical representations (visual, auditory, planning, etc.) emerge in development from a universal functional organization.

Projects at FIAS: 5

Staff

Lorenzo Butti, Jonas Elpelt, Bastian Eppler, Santiago Galella, Deyue Kong, Thomas Lai, Maurycy Miekus, 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, UC Denver, USA, Gilles Laurent, Max Planck Institute for Brain Research
Mike Heilemann, Chemistry, GU
Amparo Acker-Palmer, Biology, GU
Christian Fiebach, Psychology, GU

High-level FPGA design, blockchain and applications of AI

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. Udo Kebschull retired in October 2024.

Highlight

In 2024, five Bachelor's and Master's theses were supervised in the working group.

Projects at FIAS: 6

Staff

Franca Speth
Felix Hofmann
Diar Takak
Thomas Janson
David Schledt

Collaborations

SVA-System Vertrieb Alexander GmbH and the German Aerospace Centre (DLR)
HZD Hessian Centre for Data Processingekom21 - KGRZ Hessen
BMBF (ALICE, CBM)

Thomas Janson has been working on the development of a C++ data flow template library for the implementation of algorithms on FPGA accelerator cards. This template library makes it possible to process complex algorithms, such as those needed for reading data from high-energy physics detectors, in real-time. This is achieved using a concept from data flow programming. Here, algorithms are described as data flow graphs, implemented as a deep pipeline structure on an FPGA, and executed in massive parallel.

The online feature extraction for the CBM-TRD is developed by David Schledt. CBM works in a trigger-less fee streaming mode. Therefore, online event selection is needed to filter and store the large amount of incoming data. A four-dimensional trace reconstruction is important for online event selection. To reduce the load on the computing cluster, David Schledt will bring the required feature extraction to the readout FPGA. Feature extraction means changing the data, reconstructing energy and time, and finding clusters. Methods from high-level FPGA design are used for this.

The signal delays of up to 22 minutes between Earth and Mars necessitate the use of an autonomous system supported by AI technology on Mars stations. In a project carried out by Franca Speth in Udo Kebschull's working group, AI components are being developed that analyzes system states and generate recommendations for action with a view to automating the operation of a Mars station. The experimental framework encompasses the utilization of data obtained from the Columbus module of the International Space Station to validate the system's functionality, paving the way for its potential application in future space missions.

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 complex data in the CBM project. This work was finalized in 2024.

Diyar Takak is currently researching the topic of digital identities in collaboration with ekom21 and the ONCE consortium. He is working intensively on blockchain-based protocol management of electronically archived hotel registration documents within the ONCE consortium. In addition, a blockchain-based protocol execution is being investigated that makes it possible to watch documents with confidential data stored on clouds in a sustainable and tamper-proof manner. The decentralized nature of the technology blockchain is being used. Within the ONCE consortium, there is also a need for a concept based on Self-Sovereign Identity for the authentication of digital identities in public administration. In addition, an Inter-Planetary File System is being added, which archives documents securely and in encrypted form via a distributed network and regulates access via a blockchain using digital identity. ISO 2700X standards are considered.

FPGA based embedded system and modern C++ code for a typical Peak Finder algorithm as it is often used for detection readout using the HLS Dataflow Template Library, for details see https://doi.org/10.1088/1748-0221/18/02/C02050. AI art generated with ChatGPT 4o (Feb. 2025).

On the feasibility of a QGP trigger in CBM based on ANN

In the CBM experiment at the FAIR accelerator, up to 10 million heavy-ion collisions per second are expected, making traditional data storage impossible. A real-time trigger algorithm is needed to detect rare events like Quark-Gluon Plasma (QGP) formation. Developing such a trigger is crucial for the experiment's success. Artificial Neural Networks (ANN) offer a promising solution, enabling fast and accurate selection of QGP events from vast background data.

The presented graph and table illustrate the sequence of data processing stages and the change in QGP classification efficiency at each stage. In the first stage, using a Convolutional Neural Network (CNN) trained on idealized PHQMD simulated data, a high classification efficiency of 95.1% is achieved. However, in real detector conditions, the efficiency decreases due to physical limitations. For example, at the CBM detector acceptance stage, the efficiency drops to 90.3% because some particles produced in the collision fall outside the detector's registration range. During track reconstruction using the Cellular Automaton (CA) Track Finder algorithm, the processing complexity increases due to the high density of tracks and their overlaps, reducing the efficiency to 85.8%. The final stage, the reconstruction of short-lived particles using the Kalman Filter (KF) Particle Finder, results in a final efficiency of 83.7%. This stage demonstrates the system's ability to identify rare and complex particles, which are key indicators for QGP analysis.

The table confirms the main sources of efficiency loss: detector acceptance limits, the complexity of trajectory reconstruction, and the challenges of identifying short-lived particles. Nevertheless, the overall efficiency loss is less than 12%, an impressive result for such a complex experiment. The need for a trigger in the CBM experiment arises from the requirement to process a massive data stream in real time. ANN, integrated with advanced reconstruction algorithms, shows high efficiency and reliability in performing this task. These results confirm that such a system can effectively isolate QGP events while maintaining high accuracy, even under the challenging physical conditions of the experiment.

Future research will focus on the development of a trigger system based on the Transformer architecture, which forms the basis of the foundation AI models. The Transformer has the unique ability to identify and recognize relationships, in this case between particles produced in the volume of the Quark-Gluon Plasma. This approach will improve the analysis of complex interactions in high-density events and open up new possibilities for experimental heavy-ion physics.

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.

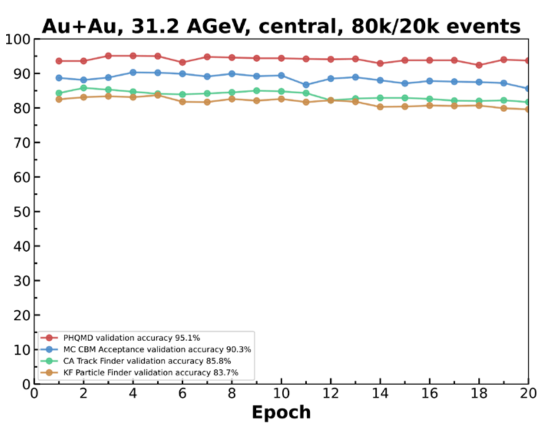
Projects at FIAS: 3

Staff

Artemiy Belousov
Aizat Daribayeva
Robin Lakos
Akhil Mithran
Oddharak Tyagi

Collaborations

CBM
ALICE
STAR



	Stage	Efficiency	Drop
1	CNN on PHQMD	95.1%	
2	CBM Acceptance	90.3%	- 4.8%
3	CA Track Finder	85.8%	- 4.5%
4	KF Particle Finder	83.7%	- 2.1%

Application of CNN to the CBM experiment.

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

CERNCOURIER article on ALICE EPN farm: https://cerncourier.com/a/alice-ups-its-game-for-sustainable-computing/

Projects at FIAS: 4

Staff

Johannes Lehrbach
Felix Weiglhofer
Andreas Redelbach
Grigory Kozlov
Alexander Schröter

Collaborations

CERN
GSI

Fast data processing at large-scale research

The consortium PUNCH4NFDI (Particles, Universe, NuClei, and Hadrons for the NFDI) is funded based on the DFG and National Research Data Infrastructure (German acronym: NFDI) in order to organize data from many experiments in particle, astroparticle, hadron, and nuclear physics in a "sustainable" way in many aspects. Many future experiments will have to make more complex decisions on much shorter time scales and use computing resources more effectively. Volker Lindenstruth's group is contributing to the consortium's task area 5 "Data Irreversibility". Co-led by Andreas Redelbach, one goal is to recognize patterns in detector data under real-time requirements. Ideally, only data of "interest" will be stored permanently.

Metadata describing measurements should not only describe a dataset and its relevant parameters, but should also contain information about the experimental conditions and, in particular, also any relevant information about how and why certain information was selected. A number of specific challenges arise in this context, caused by the huge data streams and the need for heavy online processing. In the document https://doi.org/10.5281/zenodo.10692169, A. Redelbach et al., a general data processing graph for particle and astrophysics experiments has been developed, also summarizing representative use cases for data reduction in all PUNCH communities. Some limitations for existing data processing have been identified that will require extended layers or branches due to more complex workflows in the future.

Processing and analyzing of PUNCH4NFDI data are mainly done on the federated infrastructure Compute4PUNCH for which a prototype exists. The work of Gautam Dange has enabled the integration of interactive analyses using JupyterNotebooks in the Compute4PUNCH system. The first focus of this integration has been the pipeline for machine learning based pulsar analysis (https://gitlab-p4n.aip.de/punch_public/ml-ppa) and further use cases will also leverage this integration for interactive workspaces of analysis.

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

Quantum Computing Breakthroughs

Frankfurt has solidified its position as a leader in quantum and high-performance computing with major developments in 2024. The inauguration of Hessen's first quantum computer, "Baby Diamond", at Goethe University marked a milestone, with leading scientists and government officials attending the commissioning event. This five-qubit quantum computer operates at room temperature, representing a breakthrough in practical quantum computing applications.

FIAS and Goethe University expanded its collaborative reach by joining the John von Neumann Institute for Computing (NIC), alongside Forschungszentrum Jülich, DESY, and GSI Helmholtzzentrum. This partnership aims to advance research in high-performance computing, AI methods, and energy-efficient technologies while providing resources and training for the next generation of scientists. Additionally, MSQC played a prominent role at global events like the Supercomputing Conference SC24 in Atlanta and the International Supercomputing Conference in Hamburg. The Digital-Gipfel Frankfurt showcased Goethe University's expertise in quantum technology, featuring live demonstrations of NV-Center-based quantum computing. Meanwhile, efforts to integrate a 10+ qubit superconducting system into Jülich's supercomputing infrastructure reached a crucial milestone through the collaborative CQC project. The group continues to expand and is focusing on developing multi-hybrid algorithms that combine the use of different types of quantum computers within one algorithm as well as developing access infrastructure for the Baby Diamond.

FIAS and Goethe University through MSQC continue to drive innovation in quantum research, fostering global collaborations, and advancing the future of computing.

Baby Diamond, the first quantum computer in Hesse, is located in Frankfurt-Bockenheim. The computer itself is isolated behind the glass door, while the control electronics are housed in the black box on the right. The manufacturer of the system is XeedQ GmbH. Photo: Manpreet Jattana.

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 Forschungszentrum 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

In May, the group welcomed Rutian Zhou as a new PhD student funded by the research training group iMol (Interfacing image analysis and molecular life science). Tim Liebisch left for a postdoc at sunny Barcelona.

Projects at FIAS: 2

Staff

Zoë Lange
Marc Pereyra
Rutian Zhou

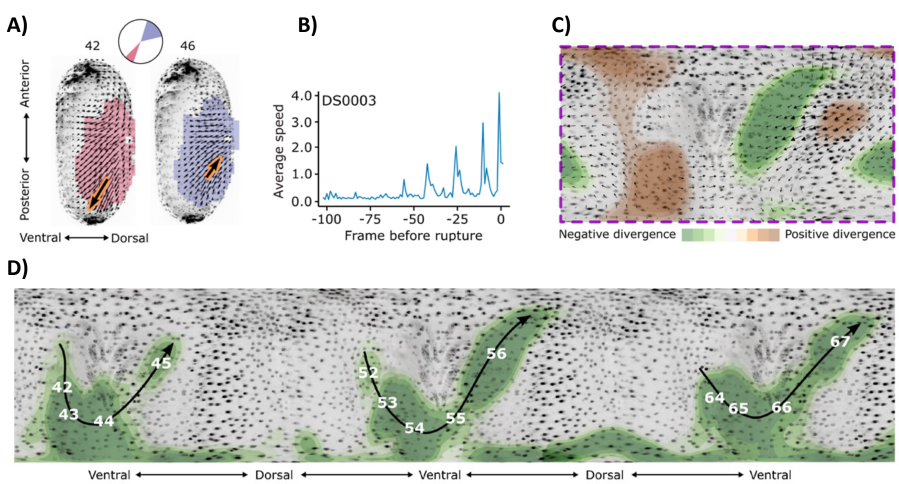
Collaborations

AK Stelzer (GU)
Thomas Sokolowski (FIAS)
Alf Gerisch (TU Darmstadt)
Kevin Painter (Politecnico di Torino, Italy)
Denis Headon and Jon Riddell (Roslin Institute, Edinburgh, UK)
Mingfeng Qiu (University of Canterbury, Christchurch, New Zealand)

Quantification of contraction waves in Tribolium castaneum

In collaboration with the group of Ernst Stelzer, we investigated developmental processes in the red flour beetle Tribolium castaneum. During development, the beetle embryo is enveloped by extra-embryonal membranes. These membranes exhibit repeated contraction waves, which were discovered only recently by Mariia Golden, PhD student in the group of Ernst Stelzer. These contraction waves are a novel observation of which neither origin nor function are yet known. In a collaborative effort, we developed an analysis pipeline last year, which relies on movement-based segmentation to detect and localize the contractile areas. For this, we used quickPIV, a correlation-based movement analysis approach for 2D and 3D time-lapse videos. Furthermore, we incorporated tissue cartography to map the curved 3D tissue layer into 2D. With this approach we were able to automatically detect and quantify the contraction waves in beetles with nuclear or membrane label. The contraction waves show characteristic dorsoventral movement components. This movement signature was used for the movement-based segmentation algorithm. The workflow will be used in the future to investigate the variability of the spatiotemporal dynamics of the contraction waves in a larger number of beetles and under various conditions. However, already in the smaller set of embryos investigated so far, we have learned that the contraction waves occur repeatedly with a roughly constant frequency, continue after rupture and during the retraction phase with a similar frequency but different angle, exhibit a characteristic local velocity signature, a short ventral and extended dorsal phase, as well as symmetry between the two lateral sides. In addition, the divergence minima (areas of cell aggregation) exhibit an interesting U-shaped flow (see Figure), that needs to be investigated further in future work. A paper describing the analysis pipeline is currently in revision in BMC Bioinformatics and is available under https://www.biorxiv.org/content/10.1101/2024.08.23.609389v1.

Contraction waves in the extraembryonic membranes of the red flour beetle Tribolium castaneum. A) Segmentation of the contractile area: ventral phase of contraction (red) and dorsal phase (blue). B) Average speed of the entire tissue area of one sample beetle showing repeated contraction waves as velocity peaks, here with increasing amplitude. C) Divergence map showing areas of contraction (green) and expansion (orange). D) The positions of contractions follow a characteristic U-shaped path, which repeats for consecutive contractions. The figure is composed of panels from https://www.biorxiv.org/content/10.1101/2024.08.23.609389v1.



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 2024, together with FIAS postdoc Dr. Hung Tran and some other colleagues, we came up with a generator for networks that includes negative edge weights but disallows cycles of negative length. Networks of this kind serve, e.g., as a testbed for routing algorithms of electric vehicles, where some energy recovery takes place when driving downhill but, of course, endless descent routes are not possible in practice: Lukas Geis, Daniel Allendorf, Thomas Bläsius, Alexander Leonhardt, Ulrich Meyer, Manuel Penschuck, Hung Tran: Uniform Sampling of Negative Edge Weights in Shortest Path Networks. CoRR abs/2410.22717.

In another publication we considered efficient methods to check whether generated graphs contain certain substructures: Ulrich Meyer, Hung Tran, Konstantinos Tsakalidis: Certifying Induced Subgraphs in Large Graphs. J. Graph Algorithms Appl. 28(3): 49-68.

Finally, Hung Tran was contributing to a FIAS collaboration in the area of population biology: Brouard, V., Pokalyuk, C., Seiler, M., Tran, H.Spatial Invasion of Cooperative Parasites Theoretical Population Biology,159, pp 35-58.

Further research cooperations at FIAS in 2024 include CMMS (Project "Construction, analysis and dimensional reduction for binary networks", together with 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

We co-organized a successful Dagstuhl Seminar on Machine Learning Augmented Algorithms for Combinatorial Optimization Problems (Oct 27-31, 2024). Further pieces of information are available under https://www.dagstuhl.de/seminars/seminar-calendar/seminar-details/24441

Projects at FIAS: 2

Staff

Yannick Gerstorfer
Hung Tran

Cooperations

CMMS
DFG FOR 2975

Dagstuhl Seminar on Machine Learning Augmented Algorithms for Combinatorial Optimization Problems in October 2024; (c) Dagstuhl.

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 is conducting research in the field of theoretical subatomic physics and astrophysics.

Highlight

Fruitful scientific collaborations with several Ukranian postdocs.

Projects at FIAS: 2

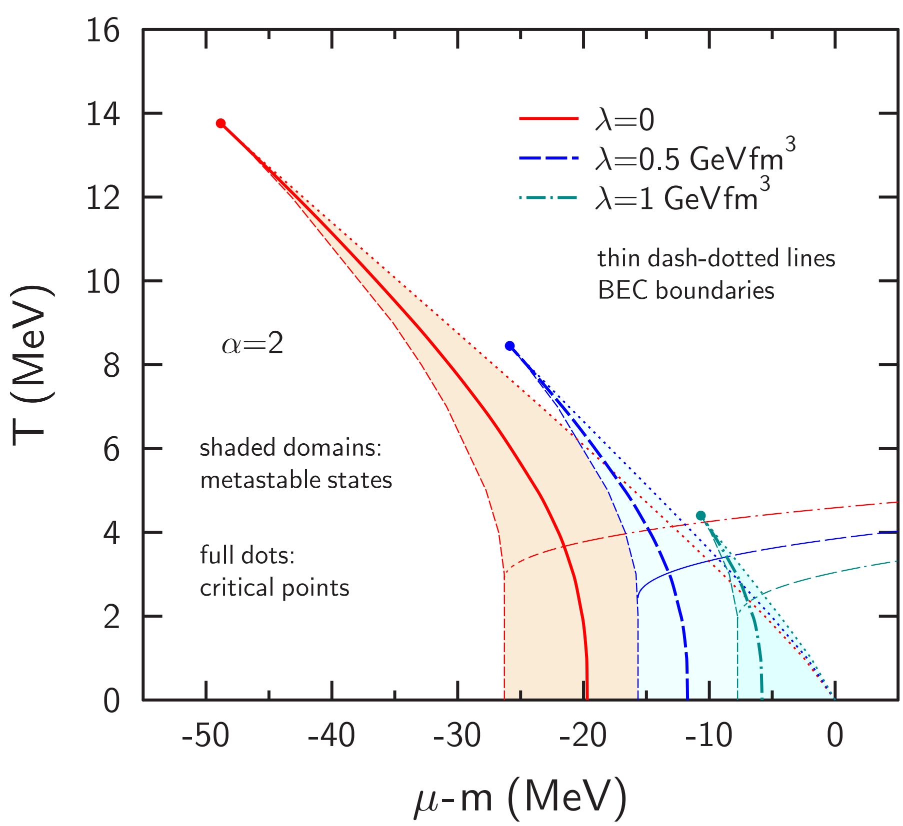
Collaborations

Horst Stoecker
Mark Gorenstein
Leonid Satarov

Large phase diagram of interacting α-bosonic matter

We have investigated the phase diagram and Bose-Einstein and repulsive condensation (BEC) of bosonic matter (BM) with attractive self-interaction. As compared to previous studies, we take into account the derivative interaction (DI) proportional to the gradient of the bosonic field squared. Our calculations have been done in the mean-field approximation for the case of matter composed of alpha particles. We have discovered that the phase diagram of BM is strongly sensitive to the strength of DI λ. With raising λ, the critical point of the first-order phase transition moves to the region of smaller temperatures and larger chemical potentials.

Phase diagrams of bosonic matter on the (μ,T) plane for different values of the derivative strength λ. Thick lines correspond to mixed-phase states of the liquid-gas phase transition. Shading show regions of metastable states. Dots represent positions of critical points. The dash-dotted lines show the boundaries of BEC states.



Exploring the collisions of black-holes and neutron stars

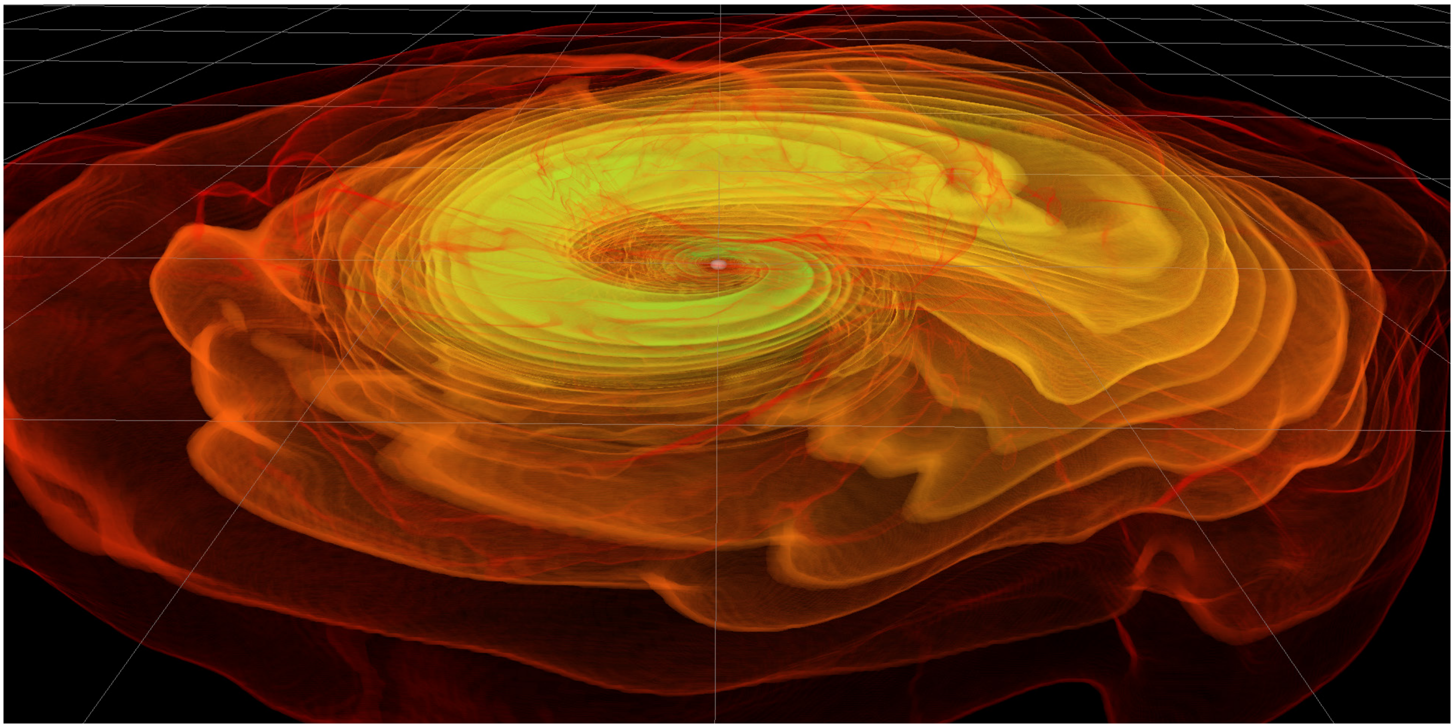
Prof. Dr. Luciano Rezzolla

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

The group of Luciano Rezzolla explored black hole-neutron star (BHNS) mergers, which are also considered as a promising target of current gravitational-wave and electromagnetic searches, being the putative origin of ultra-relativistic jets, gamma-ray emission, and r-process nucleosynthesis. Since the possibility of any electromagnetic emission accompanying a gravitational-wave detection crucially depends on the amount of baryonic mass left after the coalescence, i.e., whether the neutron star (NS) undergoes a "tidal disruption" or "plunges" into the black hole (BH) while remaining essentially intact, it is important to determine what physical conditions lead either to a disruption or to a plunge. To this scope, we have carried out the most systematic investigation to date of quasi-equilibrium sequences of initial data across a range of stellar compactnesses, mass ratios, BH spins, and equations of state was carried out, computing more than 1000 individual configurations. In this way, it was possible to determine for the first time the separatrix between the "tidal disruption" or "plunge" scenarios as a function of the fundamental parameters of these systems. Using these results we have performed simulations exploring the possible space of binary parameters in terms of the mass ratio and BH spin so as to construct a complete description of the dynamical processes accompanying a BHNS binary merger. The dynamical simulations have thus allowed not only to verify the reliability of stringent predictions about the occurrence or not of a plunge but also to measure the "strength" of the tidal disruption when it takes place. Finally, using the results of the simulations, it was possible to perform a careful investigation of the evolution of the BH mass and spin as a result of the merger, the total remnant rest-mass of the resulting accretion disk and its properties, and of the corresponding post-merger gravitational-wave emission.

The 3D density distribution of a neutron star that is disrupted as it orbits around a rotating black hole (credit: Will, Topolski, Rezzolla).



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

First detection and characterization of volcano-seismic signals from submarine Kavachi volcano (Solomon Islands) by a land-based seismic array.
Five-year research grant (BMWK) for developing advanced seismic monitoring of deep geothermal reservoirs.

Projects at FIAS: 1

Cooperations

Department of Geology, Ministry of Mines, Honiara, Solomon Islands
Institute of Seismological Research, Gandhinagar, India

Seismic Anisotropy and Shear-Wave Splitting

Shear-wave splitting occurs when seismic waves travel through elastically anisotropic regions within the Earth's upper mantle (about 35 to 670 km depth), causing one shear wave to travel faster than the other. Anisotropy often arises from the preferred alignment of minerals, such as olivine, due to long-lasting mantle flow and deformation processes. By measuring the polarization direction of the fast shear wave and the delay time between the two split shear waves, we can infer the orientation and intensity of mantle flow. Analyzing these parameters across a region reveals patterns in mantle deformation and helps to map flow fields associated with geodynamic processes such as subduction and continental collision.

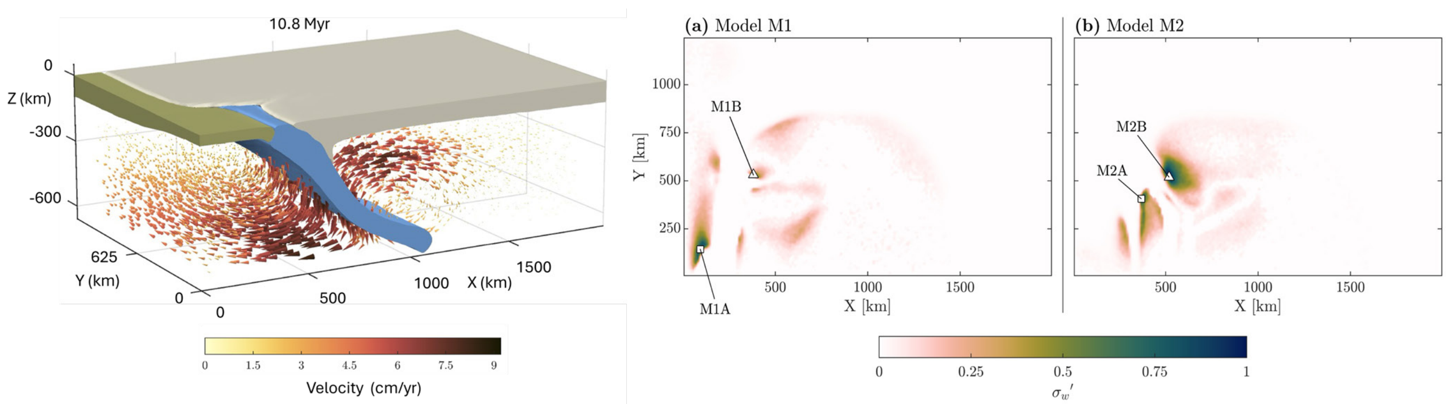
Geodynamic modeling allows us to simulate the large-scale flow fields in the Earth's mantle. From these simulations, we can estimate how mineral fabrics (and thus seismic anisotropy) develop in response to the flow. The predicted anisotropic properties can then be used to generate synthetic seismic wavefields. By comparing the synthetic wavefields with those observed by seismometers, we can test the ability of shear-wave splitting analysis to accurately resolve the true mantle flow field. Iterating between geodynamic modeling, seismic simulations, and shear-wave splitting analyses enables us to refine both models and observational strategies to improve our understanding of processes in the Earth's mantle.

In a recent study (see below) we considered cases of double subduction, a scenario in which two adjacent oceanic plates simultaneously sink into the Earth's mantle. The modeling indicates regions in the mantle where complex anisotropy develops. Detecting and analyzing these regions can provide important constraints to better evaluate and distinguish between currently discussed hypotheses regarding the role of double subduction in Earth's tectonic evolution.

Reference

Kruse, J.P., Rümpker, G., Link, F., Duretz, T., Schmeling, H., 2024. Anisotropy and XKS-splitting from geodynamic models of double subduction: Testing the limits of interpretation, Geophysical Journal International, ggae328, https://doi.org/10.1093/gji/ggae328

Left: Snapshot of a subduction-zone model at 10.8 Myr. Colored cones represent the magnitude and direction of mantle flow velocity. Right: Lateral variations of the anisotropy factor σ_w' for two different subduction-zone models. Large values indicate regions with strong anisotropy variations as a function of depth within the Earth's mantle.



Clinical and translational informatics

My research focuses on applying information technology solutions, data science and bio-medical informatics towards the 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 federated data management, federated data analysis, and 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/sensor data from different clinical cohorts and EHRs by applying sophisticated bio-medical informatics, statistical and advanced Machine Learning (ML) for unraveling 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.

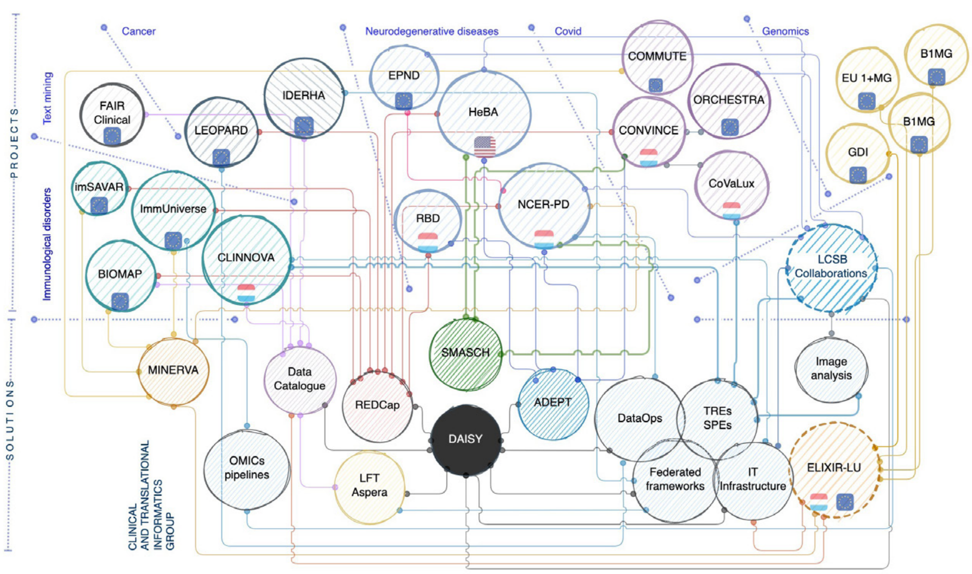
Dr. Venkata Satagopam

He is FIAS Fellow, Group Leader of Clinical and translational Informatics Group and Deputy Head of Bioinformatics core facility, LCSB, University of Luxembourg; Technical Coordinator (TeC) of ELIXIR Luxembourg Node and CTO & Cofounder 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 his Masters degree 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 organization of several conferences, workshops, code/data hackathons.

Highlight

The team embarked on a journey to build sophisticated Federated data management and AI/ML analysis infrastructure in IHI-IDERHA project .

Projects at FIAS: 1



The interaction between various funded research projects and tools, solutions from clinical and translational informatics group.

Probing Fundamental Physics through City-Size Stellar Objects

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.

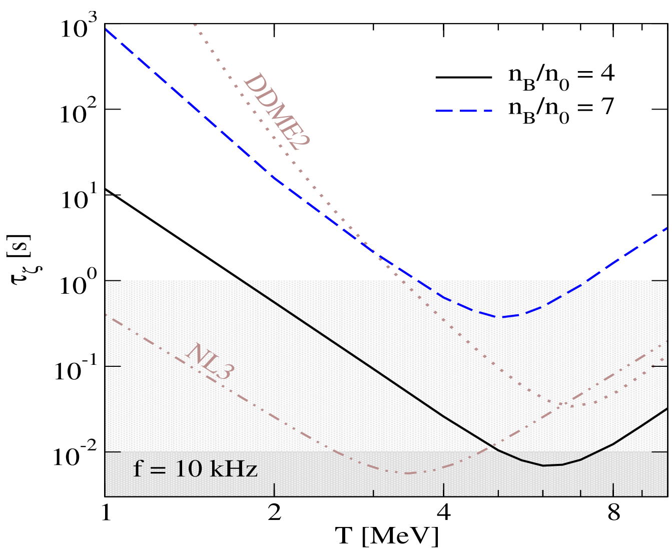
Projects at FIAS: 1

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)

We have worked on a range of topics related to neutron star physics, including (a) equations of state for astrophysical simulations, which were exported to CompOSE database; (b) structure and properties of stars featuring phase transition to quark matter; (c) bulk viscosity of dense hot baryonic and quark matter in neutron star binary mergers; (d) effects of short-range correlations on the Urca processes in neutron stars.

A key new result concerns the Urca processes, published in Phys. Rev. Lett. 133, 171401 (2024), where we showed that the short-range correlations smooth out the threshold behavior of these processes, which in turn have a strong impact on compact star thermal evolution.



Timescales of damping of oscillations in binary neutron star mergers in the case where the postmerger object contains quark matter. This timescale is shown as a function of temperature and at different fixed densities indicated in the plot. The timescales due to quark matter are shown by solid and dashed lines and that of nuclear matter by grey lines. From: Mark Alford, Arus Harutyunyan, Armen Sedrakian, Stefanos Tsiopelas, Bulk viscosity of two-color superconducting quark matter in neutron star mergers, Phys. Rev. D 110, L061303 (2024).

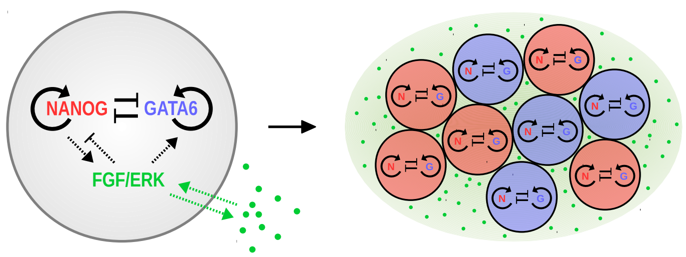
New research paths

Living organisms are able to process information reliably and efficiently, both inside their cells and at the tissue and organism levels. Though relying on fundamentally stochastic biochemical processes, cellular information processing can attain astonishingly high precision and reproducibility, particularly 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 constraints 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 more recently AI-aided inference for reducing the computational cost associated with realistic biophysical models.

In 2024 we finalized a long-year effort (PhD project of Michael Ramírez Sierra) that elucidated crucial regulatory and signaling mechanisms in the early mouse embryo development, using a model that combines event-driven spatial-stochastic simulations with simulation-based inference (SBI), a recent inference technique based on machine learning. Moreover, we completed an international collaborative project that quantifies the temporal stability of self-maintaining gene expression patterns, using both spatial-stochastic simulations and analytical modeling, finding remarkable agreement between the predictions obtained by the two approaches. Finally, and strikingly, we concluded our work that predicts the structure and necessary evolved features of the gap-gene network in early fly development by a purely theoretical ab initio optimization of a spatial-stochastic model of this system, without any fitting to data. This work is now published in PNAS.

In 2024 we intensified our collaboration with the group of Kai Zhou, for combining machine-learning approaches in epidemiology with our spatial-stochastic modeling techniques.



Schematic of the Nanog/GATA6 gene regulatory network in early mouse embryogenesis: Nanog and GATA6 mutually repress each other inside the cells of the growing tissue, allowing for creation of exclusive cell fates. Spatial signaling via protein Fgf4 implements a tissue-level biochemical feedback mechanism that regulates the cell fate ratio and buffers against noise.

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 of a long-year project in which a gene-regulatory network crucial to fly embryogenesis could be derived ab-initio by optimizing its information throughput.

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, Ulrich Meyer, Kai Zhou (FIAS)

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

Procured a EuroHPC grant for the GANANA project - a pioneering EU-India collaboration advancing HPC applications in biomedical sciences, weather modeling, and geohazards.

Projects at FIAS: 2

Staff

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

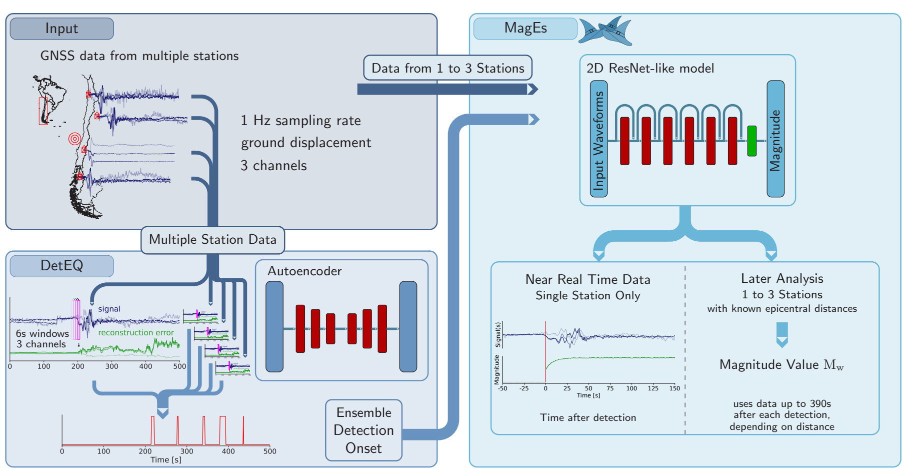
Collaborations

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

Monitoring Big Quakes: SAIPy detects & estimates magnitude

Over recent years, Global Navigation Satellite System (GNSS) data has gained increasing recognition in seismology for its ability to capture the ground displacements directly caused by large earthquakes, which is crucial for both earthquake source characterization and early warning systems. With this in mind, an additional pipeline in SAIPy for analyzing high-rate Global Navigation Satellite System (HR-GNSS) data was introduced. This branch integrates two powerful models: DetEQ for earthquake detection and MagEs for magnitude estimation. DetEQ is trained using the noise data recordings from nine stations located in Chile. The detection pipeline encompasses: (i) the generation of an anomaly score using the ground truth and reconstructed output from the autoencoder, (ii) the detection of relevant seismic events through an appropriate threshold, and (iii) the filtering of local events, which would lead to false positives. MagEs is a deep learning model inspired by the ResNet architecture, featuring custom modifications tailored to HR-GNSS displacement data analysis. It captures complex patterns in multistation time series and handles variable time window lengths and different numbers of stations. The pipeline begins with DetEQ, which processes three-channel data from multiple GNSS stations to identify the initial seismic onset at each station. These onset times serve as reference points for subsequent analysis. By leveraging detection times from multiple stations, the pipeline can pinpoint the earliest onset while filtering out local disturbances. These reference times are then fed into MagEs for magnitude estimation. This work was conducted in close collaboration with the scientists from University of Sinaloa, Mexico.

Workflow of DetEQ and MagEs models integrated within the SAIPy package. DetEQ performs large earthquake detection using HR-GNSS data from multiple stations, identifying the onset of ground displacements, and considering at least 3 stations. Following detection, MagEs estimate the earthquake magnitude, processing data from one to three stations.



Fluctuations and nuclei production at QCD phase transition

This year our group made significant progress in the study of the properties of dense and hot matter as it can be found in collisions of heavy nuclei at accelerators (e.g. at GSI, RHIC, and the LHC). Together with our partners at the Suranaree University of Technology in Thailand, we simulated, for the first time, the clustering arising from a phase transition in dense QCD matter within a non-equilibrium transport approach. The paper showed the time evolution of the third-order cumulant of the net baryon number distribution in central Gold-Gold collisions as expected at the CBM experiment at FIAR.

For the first time, we calculated quantitatively an enhancement of the double ratio of light nuclei in the presence of a conjectured QCD phase transition as shown as the strong enhancement in the observable presented here.

In addition to the scientific progress, our group organized a school and workshop on "AI4science as well as science communication" together with our partners at the XIDIAN international Joint Research Centre. Here, several lecturers gave 2 weeks of classes on these topics. The program of the school also included a diverse cultural aspect.

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 papers.

"School on AI4Science and Science communication" at FIAS in August 2024.

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 Fellow in 2017. Since 2024 he is a permanent staff scientist at the Helmholtzzentrum für Schwerionenforschung GSI in Darmstadt.

Highlight

Organized a successful "School on AI4Science and Science communication" at FIAS in August 2024.

Projects at FIAS: 1

Staff

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

Collaborations

HADES collaboration, GSI Darmstadt
Benjamin Dönigus, IKF Goethe Universität
Prof. Bleicher, Goethe Universität.
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

**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

Megha Chakraborty gained her doctorate with impressive publications and „summa cum laude".

Projects at FIAS: 8

Staff

Omar El Sayed
Shriya Soma
Megha Chakraborty
Manjunath Omana Kuttan
Markus Schlott
Marcelo Netz-Marola
Sahila Chopra

Deep Learning as a tool to decode seismological data

Megha Chakraborty submitted her doctoral thesis in May and defended it in November 2024. Her research focussed on the use of deep learning as a tool to decode seismological data. Her cumulative thesis comprised five research papers across two subfields of seismology: earthquake monitoring and characterization, and shear wave splitting analysis. Rapid and reliable characterization of parameters such as time of occurrence, magnitude, and source properties from continuous recordings is used for early earthquake warning. Shear wave splitting analyses the underlying seismic structures and provides valuable insights into the dynamic processes in the Earth's mantle; this area is still relatively unexplored by deep learning. The thesis was very well-received and was awarded a Summa cum laude grade.

Out of the five research papers, two were published last year:

W. Li, M. Chakraborty, C. Q. Cartaya, J. Köhler, J. Faber, M. A. Meier, G. Rümpker, N. Srivastava, SAIPy: A Python package for single-station earthquake monitoring using deep learning, Computers & Geosciences, Volume 192, 2024, 105686, https://doi.org/10.1016/j.cageo.2024.105686: SAIPy is one of the most significant outcomes of Charkaborty research; it is an open-source Python package that she co-created along with her former colleague Wei Li. SAIPy provides a simple interface for the application of deep learning models directly to seismological waveforms. To the best of our knowledge, this is the first paper to introduce a deep-learning based automated pipeline to continuous seismic data. The pipeline is capable of identifying earthquakes against the background noise with an accuracy of 99.8% and estimating their strength, which can be very useful for early warning. The library also allows seismologists to retrain individual models on new data enriching its applicability. SAIPy is already in use in the seismological community.

M. Chakraborty, G. Rümpker, W. Li, J. Faber, N. Srivastava, and F. Link, "Feasibility of Deep Learning in Shear Wave Splitting analysis using Synthetic-Data Training and Waveform Deconvolution", Seismica, vol. 3, no. 1, 2024: This publication describes a deep learning model (trained on theoretical waveforms) that calculates shear wave splitting parameters from waveforms which is a crucial step in the study of the internal structure and dynamic of the earth's interior. This novel method shows good agreement with previously published studies when applied to real data from USArray seismological network and provides a significant baseline for the application of deep learning to decipher splitting parameters from waveforms.

Megha Chakraborty

Covariant canonical gauge theory of gravitation (CCGG)

In the year 2024, the group was focusing on further investigating the role of torsion of spacetime in gravity and cosmology, resulting in the following publications:

The paper by David Vasak et al. provides an overview of the covariant canonical gauge gravity (CCGG). New insights: 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.

Armin van de Venn et al. extended the singularity theorem first proposed by the Nobel laureate Roger Penrose by including the influence of different modes of torsion. A “deviation equation” was derived that offers an alternative pathway to the Raychaudhuri equation with torsion. Only a totally antisymmetric torsion tensor is proven to not influence the congruence of timelike curves. Corresponding conditions for the vector torsion is derived and the critical requirement of non-autoparallel curves is highlighted.

The work by Vladimir Denk et al. led to a novel view of the propagation of torsion waves in vacuum. In the weak torsion limit, axial torsion obeys a wave equation with an effective mass that depends on scalar curvature. Its source is the net fermionic spin density of the system. Possible measurable effects and approaches to experimental analysis are addressed.

Jürgen Struckmeier et al. prove that the Pauli interaction emerges when the minimal coupling recipe is applied to the non-degenerate version of the Dirac Lagrangian. A “Pauli-type” coupling of gravity and matter arises if fermions are embedded in curved spacetime leading to an anomalous spin-torsion interaction and a curvature-dependent mass correction. Possible implications for an effective non-zero rest masses of neutrinos and the impact of mass correction on the physics of “Big Bang” cosmology, black holes, and of neutron stars are addressed. An upper limit for the “strength” of the torsion consistent with causality is discussed.

The work by David Bensity et al. analyzed the role of Dark Energy (and its simplest model, the Cosmological Constant or Λ) as a repulsive force that opposes gravitational attraction within galactic structures to derive an upper limit of Λ that is independent of cosmological models. Implications for future measurements on the upper limit and the condition for detecting the impact of Λ on galactic scales are addressed.

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

Publication of the “World Scientific” textbook “Extended Lagrange and Hamilton Formalism for Point Mechanics and Covariant Hamilton Field Theory” authored by J. Struckmeier and W. Greiner.

Projects at FIAS: 3

Staff

David Benisty (now Leibniz-Institute for Astrophysics Potsdam)
Vladimir Denk (PhD student)
Matthias Hanauske
Johannes Kirsch
Marcelo Netz-Marzola (PhD student)
Horst Stöcker
Armin van de Venn (PhD student)
David Vasak

Collaborations

Eduardo Guendelman, Ben-Gurion University of the Negev, Israel
Peter Hess, Universidad Nacional Autonoma de Mexico, Mexico City
Friedrich Wilhelm Hehl, Köln
Frank Antonsen, Copenhagen Univ.
Andreas Redelbach, Goethe Uni
Tomoi Koide, University Rio de Janeiro (sabbatical visit 2024 at 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

Sebastian Thallmair was invited to give a lecture to the public entitled "Wie Lichtschalter in Medikamenten der Zukunft eingesetzt werden können" in the Lecture Series FIAS Forum.

Group Members

Cristina Gil Herrero (PhD student)
Saara Lautala (Postdoc)
Thilo Duve (Master & PhD student)
Francesco Carnovale (visiting PhD student)

Projects at FIAS: 3

Collaborations

Roberto Covino (FIAS)
Stefan Knapp, Clemens Glaubitz, Jens Bredenbeck, Irene Burghardt (GU)
Balázs Fábián, Gerhard Hummer, Florian Wilfling (MPI Biophysics Ffm)
Dominik Oliver (Marburg)
Nadja Simeth-Crespi (Göttingen)
Wiktor Szymanski (Groningen)
Paulo C. T. Souza (Lyon)
Pablo Rivera-Fuentes (Zürich)
Ana C. Migliorini Figueira (Campinas)
Rickey Yada (Alberta)

Understanding, controlling, and inhibiting protein function

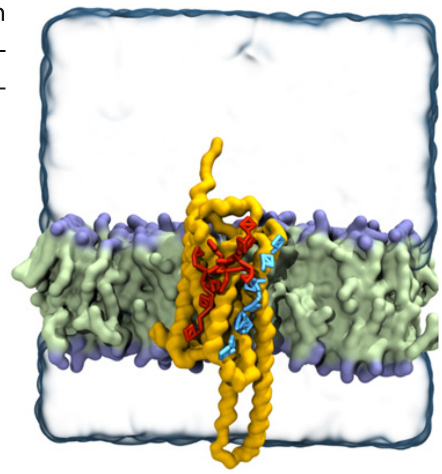
In 2024, we continued our research on light-switchable molecules and their application in biology. We optimized atomistic and coarse-grained models for lipid molecules with tails that can be switched between a straight and a bent conformation. In doing so, light can be used to modify the properties of lipid membranes. This could be used to control the release of drugs locally and spatially or as a starting point to develop novel antibiotics. We also 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 (Marburg), we investigated the membrane binding behavior of Extended Synaptotagmins. They are key to maintaining contact sites between endoplasmic reticulum and plasma membrane. Moreover, they transport lipids from the endoplasmatic reticulum to the plasma membrane. This research was performed in the context of the initiative "Subcellular Architecture of Life" (SCALE) by the Goethe University in close collaboration with Florian Wilfling (MPI for Biophysics) and Dominik Oliver. Sebastian Thallmair was also strongly involved in preparing the SCALE full application for the Exzellenzstrategie funding scheme together with numerous members of the initiative.

Together with researchers from the University of Zurich, we extended our characterization of fluorescence sensors. We applied atomistic molecular dynamics simulations to understand differences in the behavior of fluorescence sensors. Moreover, our paper on facilitated membrane permeation of drug molecules by G-protein coupled receptors was published (see Figure).

Thilo Duve completed his Master thesis in September and joined us in October for his PhD thesis. He will continue working on modeling photoswitchable molecules in biological environments. In November, Francesco Carnovale from Trento University joined our group as a visiting PhD student to work on a coarse-grained model for $Si(OH)_4$ polymerization. Sadly, we had to say goodbye to Saara Lautala, because her postdoctoral stay in our group ended in December – how time flies!

Thallmair was invited for a lecture at the "CECAM flagship workshop on frontiers of coarse-grained models" in Lyon and the Indo-German "International Conference on Engineered Chemical and Biochemical Systems" in Amritsar. He presented the work of the group among others in seminars at the University of Strasbourg and the MPI for Polymer Research in Mainz. Sebastian also gave three public talks on the potential of light-switchable molecules in future drugs.

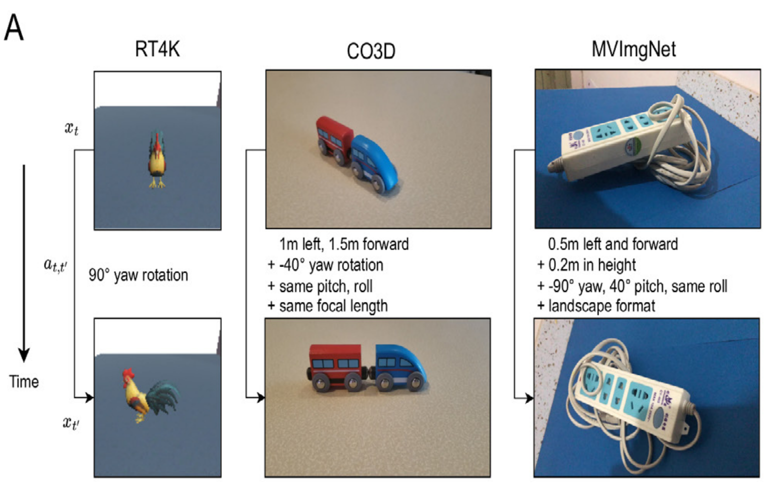


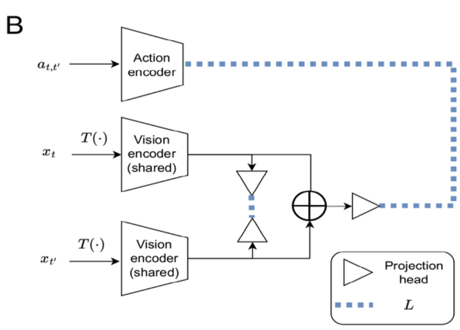
Active substances can penetrate the water-repellent fat layer in the center of the membrane (green) more easily with the help of the β2-adrenoceptor (yellow). The excerpt from the computer simulation shows this for two drugs for lung diseases - salmeterol (red) and salbutamol (light blue). from C. Gil Herrero, S. Thallmair, J. Phys. Chem. Lett. 15, 12643 (2024).

Making AIs learn like children

Current AI systems still learn quite differently from humans. Most artificial vision systems, for example, learn from passively absorbing large image or video databases and identifying structure in these data. In contrast, humans actively explore the visual world around them. Can we mimic this much more active style of learning in AI systems and is this beneficial? Much of the group's research revolves around this question. In one exemplary project, we have developed a new learning approach that learns about objects during interactions with these objects and is „aware" of the learner's actions.

Conventional self-supervised learning (SSL) has revolutionized visual representation learning but has not achieved the robustness of human vision. A reason for this could be that SSL does not leverage all the data available to humans during learning. Specifically, when learning about an object, humans often purposefully turn or move around objects and research suggests that these interactions can substantially enhance their learning. We therefore explored whether such object-related actions can boost SSL. For this, we extracted the actions performed to change from one ego-centric view of an object to another in four video datasets. We have introduced a new loss function to learn visual and action embeddings by aligning the performed action with the representations of two images extracted from the same video clip. This permits the performed actions to structure the latent visual representation. Our experiments showed that our method consistently outperformed previous methods on downstream category recognition. In our analysis, we found that the observed improvement was associated with a better viewpoint-wise alignment of different objects from the same category. Overall, our work has demonstrated that embodied interactions with objects can improve SSL of object categories.





A: Actions transforming views of an object into new views. B: New architecture aligning action representations with their visual effects during object viewing. Quelle: Aubret, A., Teulière, C., & Triesch, J. (2025). Self-supervised visual learning from interactions with objects. In European Conference on Computer Vision (pp. 54-71). Springer, Cham. , https://link.springer.com/chapter/10.1007/978-3-031-73226-3_4

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

At the International Conference on Development and Learning in Austin, Texas, USA, our group showed a very strong presence: five talks and organizing a workshop.

Projects at FIAS: 6

Staff

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

Collaborations

Roland Fleming (Gießen), Nadine Flinner (FIAS), Mohammad Ganjtabesh (Iran), Ileana Hanganu-Opatz (Hamburg), Matthias Kaschube (FIAS), Lucia Melloni (Frankfurt), Alexander Ororbia (Rochester, USA), Rajesh Rao (Seattle, USA), Gemma Roig (Frankfurt), Felix Rosenow (Frankfurt), Simon Rumpel (Mainz), Gudrun Schwarzer (Gießen), Bert E. Shi (Hong Kong, China), Yee Lee Shing (Frankfurt), Céline Teulière (Clermont-Ferrand, F), Peter Wild (FIAS), Chen Yu (Austin, USA), Fleur Zeldenrust (Nijmegen, NL)

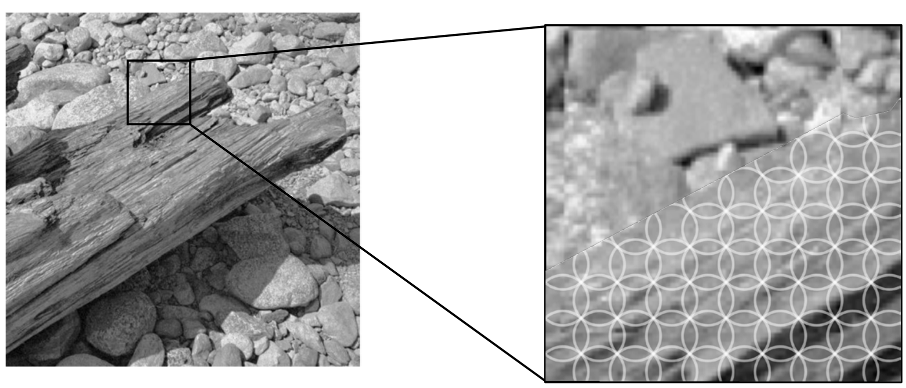
Beyond the Paradigm of Deep Learning-based AI

The present technology of artificial intelligence (AI), apart from revolutionizing economic and social processes, is currently boasting to be the pathway to artificial minds. Academia, with its age-old traditions of studying the mind, has so far failed to respond. For decades, my work has been dedicated to grappling with understanding the function of the brain, and one focus of my work was trying to overcome the fundamental limits of the mechanisms that have been recognized this year as the basis of the current version of AI with the Physics Nobel Award.

A fundamental issue addressed by the acknowledged work is the question of how coherent structure is represented in neural terms. According to John Hopfield, one of the awardees, patterns are represented by large sets of neurons (Hebb's 1949 `assemblies') that are tied together by mutual connections into monolithic wholes. As large patterns are once-in-a-lifetime affairs, these are nearly useless. According to Geoffrey Hinton, the other awardee, (and to the long tradition of multi-layer perceptrons) large patterns are to be represented by single neurons. For them to be wired up to cover all variant patterns that refer to the same object, these need enormous masses of training data and training time.

In 2023 and 2024 I have made progress with concretely modelling an alternative to these two problematic ways of neural representation. This has the form of compositional networks (`nets'), formed out of net fragments, each of which represents a sub-pattern frequently encountered in the environment. Nets on the one hand are arrays of low-level feature neurons and as such represent pattern structure explicitly (in distinction to current AI's single neurons), and on the other hand they have, as composites, the flexibility to cover variants (in distinction to Hopfield's monolithic assemblies) while being as structurally stable as assemblies. For a model realizing nets see http://arxiv.org/abs/2407.05650.

This Figure, taken from http://arxiv.org/abs/2407.05650 and adapted from Olshausen and Field (2005), illustrates the difficulty of finding object contours in images in spite of frequent absence of local contrast (see cut-out, right). Our explanation is that contours are mostly detected as borders to coherent texture, represented by nets composed of local net fragments (schematically suggested as overlapping circles).



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

Preprint: P.J. Sager, J.M. Deriu, B.F. Grewe, Th. Stadelmann and C. von der Malsburg. The Cooperative Network Architecture: Learning Structured Networks as Representation of Sensory Patterns", https://arxiv.org/abs/2407.05650

Projects at FIAS: 1

Collaborations

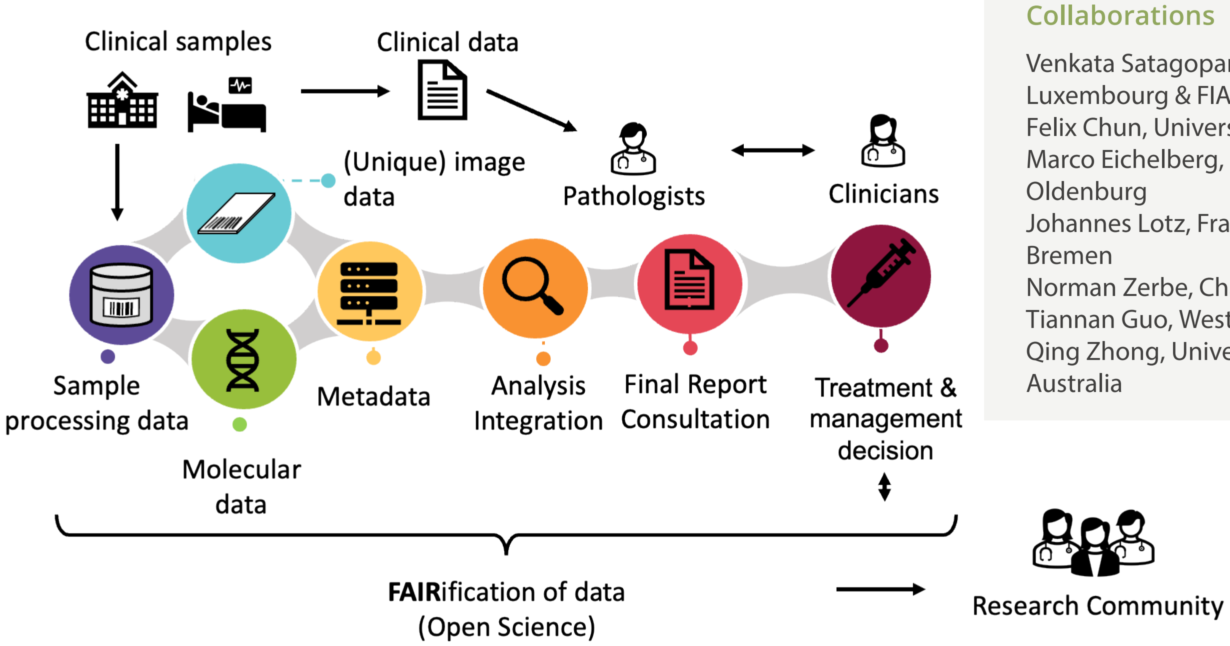
Benjamin Grewe and Rodney Douglas (Institute for Neuroinformatics, University Zurich, ETH Zurich)
Thilo Stadelmann (Zurich Hochschule für Angewandte Wissenschaften)
Joachim Triesch (FIAS) and the INAC (Initiative for Natural and Artificial Consciousness) team

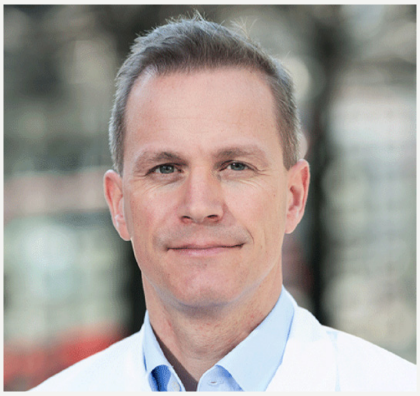
Advancing Diagnostic Strategies in Metastatic Prostate Cancer

The Wild research group aims to improve diagnostic precision through liquid biopsy, digital pathology, and the FAIRification of data.

Liquid Biopsy for Metastatic Prostate Cancer Patients: We investigated next-generation sequencing (NGS) in liquid biopsy (LB) and tumor tissue (TT) for detecting BRCA1/2 and homologous recombination repair gene alterations in metastatic prostate cancer (mPC). With PARP inhibitors approved and ongoing trials, identifying these alterations is crucial for treatment selection. In a study of 50 mPC patients, TT NGS identified BRCA1/2 alterations in 9%, while LB NGS detected them in 20%. Despite a negative percentage agreement of 85% and a positive percentage agreement of 50%, LB NGS showed a higher detection rate. These findings support an integrated approach to optimize patient stratification for PARP inhibitor therapy (Mandel et al., Eur Urol Focus 2024).

Advancing Digital Pathology through Biobank-Based Analyses: We also focused on integrating digital pathology and biobank-based analyses to enhance diagnostic precision and biomarker discovery. High-throughput image analysis, AI-driven algorithms, and multiplex tissue analysis improve tumor heterogeneity assessment and genetic profiling. Whole-slide imaging and computational pathology enable standardized, reproducible evaluations, supporting precision medicine and personalized treatment strategies. Additionally, we emphasize the FAIRification of whole slide image data and clinicopathological data—ensuring that research data is Findable, Accessible, Interoperable, and Reusable—to enhance data sharing, reproducibility, and collaboration in precision oncology (www.prosurvival.org; funded by the Federal Ministry of Education and Research).





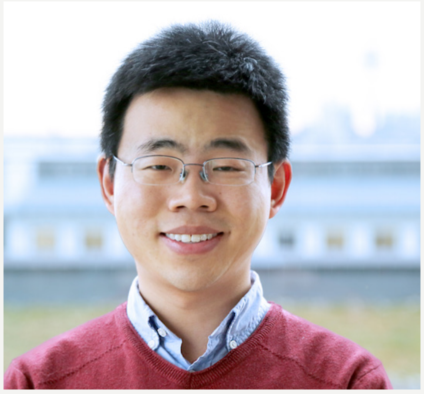
Prof. Dr. Peter Wild

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.

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



Prof. 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. Professorship at Shenzhen University since 2024.

Highlight

Kai Zhou attended the summer school from XF-IJRC and taught generative AI.

Projects at FIAS: 1

Staff

Manjunath Omana Kuttan
Mingjun Xiang
Shuai Han
Lukas Stelz
Chen Li

Collaborations

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

Integrating renewable energy sources by machine learning

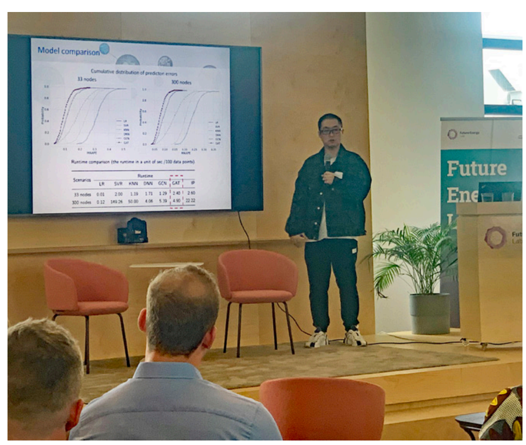
In 2024, we further advanced the usage of machine learning to tackle one of the biggest challenges in renewable energy: ensuring a stable power supply despite the high variability of solar and wind sources. To address this issue, we developed a state-of-the-art AI system that compensates for weather-dependent fluctuations, enabling efficient and reliable distribution of electricity. By dynamically adjusting to changes in solar and wind conditions, our approach not only meets energy demands but also minimizes costs.

We achieved a significant milestone in this endeavor through a breakthrough study led by our PhD student, Chen Li. Integrating renewable energy sources such as wind and solar power into the grid is complex, as weather changes can rapidly affect power generation and demand constant grid adjustments. For instance, a single cloud passing over a photovoltaic system can trigger major fluctuations in electricity output within a short timeframe. Traditional methods often struggle with this level of variability, especially in large power systems.

To overcome these challenges, we developed a cutting-edge, physics-informed machine learning method that adapts quickly to changing conditions, making it ideal for real-time applications. By leveraging electricity demand data and weather patterns, our approach delivers immediate solutions to equalize fluctuations. At the core of this innovation are graph attention networks, which analyze graphical data on weather and power demand. These networks identify critical nodes in the power grid that significantly influence power dispatch patterns, enhancing the efficiency and transparency of our AI-driven decisions.

Our recent publication demonstrates how this new method outperforms existing data-driven techniques in two different scenarios involving renewable energy systems. We have shown that our approach not only provides rapid and feasible solutions but also maintains interpretability—an essential factor for building trust in AI-based systems.

Currently, this technology is in its early stages and has been tested primarily on small and medium-sized power grids. However, we are confident that it has the potential to transform modern energy systems. "As we continue to explore and refine this technology," says our team member, physicist Chen Li, "we move closer to a cleaner, greener, and more sustainable future." Looking ahead, we plan to expand our research by integrating AI-based energy storage solutions, further strengthening the reliability of renewable power grids.



FIAS PhD student Chen Li spoke as an invited speaker at the 'Strommarkttreffen' (Electricity Market Meeting) in Berlin. He presented his works on optimising power dispatch using machine learning.

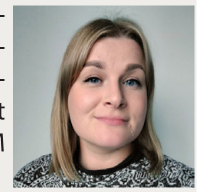
FIAS Postdocs

Nika Jurov studies the processes of active auditory attention and is currently simulating it with neural networks as an active efficient coding mechanism in echolocating bats.

Tom Reichert is developing and employing advanced numerical transport simulations that describe the collisions of atomic nuclei at nearly the speed of light. These extreme conditions lead to the formation of a new state of matter - the Quark-Gluon-Plasma.

Manjunath Omana Kuttan develops AI methods for ultra-fast simulations of high energy, heavy nuclei collisions for experiments to study the strong nuclear force at high density/ temperature.

Saara Lauatala uses molecular dynamics simulations in all-atom and coarse-grained resolution to investigate the interactions between proteins and lipids at cellular membranes, specifically ER-PM contact sites.

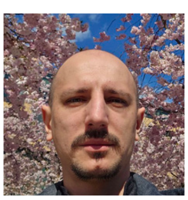


Michael Ramirez-Sierra applies simulation-based inference to uncover mechanistic insights into plasma membrane receptor dynamics.

Gautam Ravindra Dange specializes in high-performance computing. His expertise spans system configuration, simulation, parallel processing, digital twins, and machine learning. He is involved in advancing research and development initiatives within PUNCH4NFDI and ALICE.

Claudia Quinteros Cartaya focusses on the applicability of deep learning frameworks for rapid earthquake analysis using seismograms and GPS data, and integrating deep learning models in the open-source package SAIPy.

Arthur Aubret develops and applies bio-inspired machine learning models to study the fundamental principles underpinning the development of high-level visual representations in humans and machines.

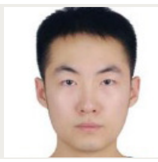


Grigory Kozlov is engaged in research on charged particle trajectory reconstruction in heavy-ion physics experiments, the porting of tracking algorithms for GPUs, and the study of energy efficiency in high-performance computing.

FIAS PhD students

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

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

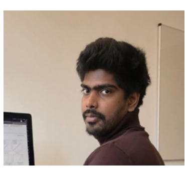


Blending artificial intelligence and thermodynamics to investigate biomolecular systems with computer simulations. Physics, chemistry, biology, informatics: **Gianmarco Lazzeri** combines them.

Serena Arghittu describes self-regulatory mechanisms of plasma membrane proteins (lipid transport, glyco-receptors) and develops computer vision methods for cryo-electron-tomography.

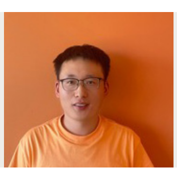
Mingjun Xiang is using deep learning methods to process Terahertz imaging and optimize imaging system.

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.



Akhil Mithran`s field of research is utilizing transformers, Graph neural networks and reinforcement learning.

Shuai Han researches integrating deep learning with physical models to investigate the spatiotemporal dynamics of epidemic spread, focusing on leveraging mathematical models.



Cristina Gil Herrero studies molecular interactions of pharmaceutical-like compounds and proteins, as well as photoswitchable lipids using molecular dynamics simulations.

Virginia Boretti biophysically characterizes mixed radiation fields with a particular focus on space applications.

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

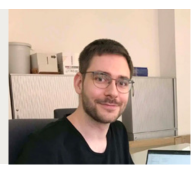
Lars Dingeldein uses simulation-based inference to solve inverse problems in molecular biophysics.

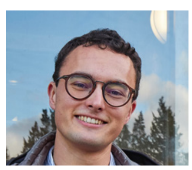
Zoë Lange studies how organs and organisms take shape during development by statistically inferring cell forces from microscopy images.

Magnus Petersen develops deep learning approaches that help optimize physics simulations for better performance and broader scope.

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

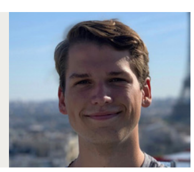
Robin Lakos is working on a neural-network-based 4-dimensional track finding and event-building approach for the future heavy-ion experiment "Compressed Baryonic Matter" at GSI/FAI, Darmstadt.

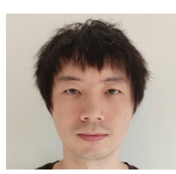




Philip Sommer investigates the effects of energy deprivation on neural information processing.

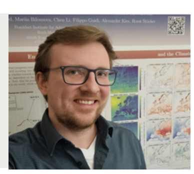
Nicolas Strangmann studies proton-proton collisions at ALICE/CERN, using photon-jet correlations to investigate whether a Quark-Gluon Plasma can form in small collision systems.





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.

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.

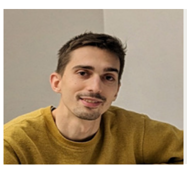
Jonas Köhler is creating millions of real looking earthquake catalogs (using the ETAS model) and training a deep-learning model in differentiating earthquake mainshocks from their aftershocks.

Lukas Stelz uses a combination of machine learning and mechanistic models to study the spread of infectious diseases and how these models perform with limited amounts of data.

Carl Rosenkvist studies how heavy ion collisions produce strange particles, which helps us understand matter under extreme conditions like those in neutron star cores and the early universe.

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.

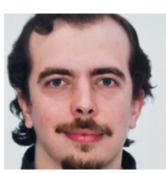
Luca Lunati is working on the design and implementation of the Galactic Cosmic Ray (GCR) Simulator up to 10 GeV/n at the GSI-FAIR facility.



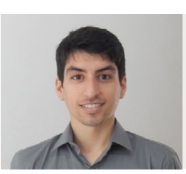
Santiago Gallela studies the nature of abstract representations and cognitive maps in the brain and in artificial neural networks.

Ahmed Alramly applies deep learning to neuroimaging data to advance our understanding of psychiatric disorders.

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



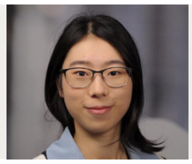
Marcelo Netz-Marzola is studying how anomalous Pauli-type couplings (predicted by generalized field theories) alter fermion behavior in both electromagnetic and gravitational strong-field regimes.



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

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

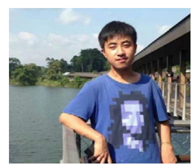
Adrian William Romero Jorge explores how hypothetical particles (dark photons) might be detected by analyzing dilepton production in heavy-ion collisions using a transport model.



Rutian Zhou analyzes multicellular systems by using advanced computational image analysis methods to process and interpret microscopic images.

Felix Hoffmann designs and implements a novel Proof-of-Useful-Work blockchain architecture in Golang.

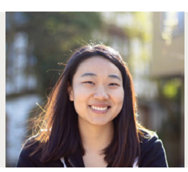
Lorenzo Butti investigates neural activity in the early developing cortex. His research focuses on how neural activity is shaped by the underlying circuitry, using network and inference models.



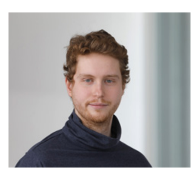
Zhengyang Yu is dedicated to developing bio-inspired self-supervised learning models, drawing inspiration from infant visual development and their first-person videos.

Johannes Pöplau explores the phase structure of matter at extreme densities with the functional renormalization group.

Renan Hirayama studies electromagnetic and hard probes of a heavy-ion collision in a framework combining hadronic transport and hydrodynamics.



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



Thilo Duve uses Molecular Dynamics simulations to study how molecular photoswitches can be used to control protein-ligand interactions using light.

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The Frankfurt Institute for Advanced Studies (FIAS) is an interdisciplinary research institution. Internationally renowned scientists conduct research at the highest level on complex scientific future topics with a focus on simulations and theories as a basis for meeting the challenges of our time.

As a non-profit foundation under civil law, we are committed to society and handle the funds we use with care. We are committed to the Sustainable Development Goals that guide our research activities. Our thoughts and actions are based on openness and diversity in scientific discourse.

At FIAS we practice interdisciplinarity, and we offer a framework for creativity and the development of innovative ideas. The promotion of young scientists is our particular concern. We are committed to internationality and diversity and live equal treatment and mutual support. Our attitude towards each other is respectful and appreciative.

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FIAS is dedicated to fundamental research using theoretical methods in the natural and life sciences, as well as related fields. Through interdisciplinary collaboration and innovation across disciplines, it expands scientific knowledge and inspires solutions to the diverse global challenges of our time.

FIAS trains doctoral candidates to conduct independent scientific research, enabling them to shape the future with responsibility and initiative. The institute cultivates the next generation of leaders who have learned to think in broader contexts.

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