FIAS Frankfurt Institute for Advanced Studies

2022

Content

FIAS

science for the reality of tomorrow

Dear colleagues,

Dear friends and supporters of our science,

Dear knowledge seekers,

what a change in everyday life and in scientific interactions at FIAS as the threat from the corona virus diminished and many of the precautions could be lifted during the course of 2022. Clearly the direct interaction in scientific communication is more beneficial than any “two-dimensional workaround” in a video conference.

There have been more changes at FIAS. Within the Goethe University cooperation FIAS assumes the role of an incubator for new research topics while the university provides continuity. The Board of Trustees followed suite by instituting a trimmed leadership at the helm while calling for scientific excellence from the FIAS Faculty, advising me as the newly installed chairman. I feel privileged to lead FIAS with a team of broad scientific excellence and a history that is legend.

What are the scientific topics? Complex systems such in heavy ion collisions are seen with new light in the gravitational merger of neutron stars; gravitation is a physics topic that has received tremendous support through experimental and theoretical advances. Machine Learning as a method appears everywhere and penetrates all aspects of society. FIAS scientists use the tool in many aspects among which are seismic studies, distributed energy networks and cell growth simulations in addition to molecular level simulations of the cell-membrane. This is only the start. Artificial intelligence is currently challenged for the ability of self-learning. Neuroscience tackles the brain, and while tremendous progress has been made in understanding certain aspects of recognition we are still far away from deeply understanding the holistic approach behind human recognition process. Quantum computers are at the verge of becoming a reality and hence their thematic application needs to be prepared.

The reorganisation of FIAS eases the internal structure and load and should allow the scientific agility that is adequate for an advanced institute. In that vein, FIAS has also begun to introduce lean administrative structures targeted to help the scientists while maintaining administrative and financial scrutiny. One political topic has been predominant: the Russian invasion of Ukraine, which causes utter grief at so many levels. FIAS has tried to help, and we were happy to welcome several Ukrainian scientists while the scientific exchange with the country continues. On a personal note, I am saddened to see even personal contacts to friends fall victim to the unjust regime. Let us hope for a peaceful ending of the year 2023.

On behalf of all FIAS members

Eckhard Elsen

HIGHLIGHTS 2022

Eckhard Elsen takes over

Prof. Dr. Eckhard Elsen is the new Scientific Director of FIAS as of May 1, 2022. He thus replaces the previous five-member board including the executive and an administrative director. The basis for this new structure is an amendment to the statutes. With a single executive director at the helm processes and decisions in the institute will be rendered more efficient and coordination simplified.

The FIAS Stiftungsrat elected the former director of research and computing at CERN as Scientific Director. "With his experience in the natural sciences and in the management of large scientific institutes, Elsen is the ideal choice and perfect fit for FIAS," agreed the previous executive scientific director Prof. Dr. Volker Lindenstruth and the previous administrative director Dr. Rolf Bernhardt. In Elsen's absence, his deputy, Lindenstruth, takes over his tasks. In the future, the important Senior Fellows will support the Scientific Director in fundamental questions of scientific orientation and the selection of Fellows.

The Board of Trustees (Stiftungsrat), which has a say in budgetary matters and the appointment of FIAS Fellows, was also reduced to five people. The president of Goethe University will remain a set member of the Stiftungsrat. Prof. Dr. Dr. h. c. Volker Mosbrugger was elected Chairman of the Stiftungsrat, succeeding Prof. Dr. Rudolf Steinberg. The paleontologist and professor at Goethe University was director general of the Senckenberg Gesellschaft für Naturforschung until 2020 and is president of the Frankfurt Polytechnic Society since 2019. Mosbrugger had conducted research on ecological and climatic changes in Earth history at the universities of Freiburg, Bonn, and Tübingen.

In the future, the FIAS committees will be supported by the Curatorship (Kuratorium), in which friends and sponsors of FIAS support the institute in joint consultation. With this new structure, FIAS will be able to act even faster administratively while optimally balancing the research orientation involving of all its experienced scientists.

In addition to Lindenstruth, Bernhardt and Prof. Dr. Luciano Rezzolla, the founding directors Prof. Dr. Dr. h. c. mult. Wolf Singer and Prof. Dr. Dr. h.c. mult. Horst Stöcker were also leaving the FIAS board in April. They founded the institute in 2003 and rendered outstanding services to FIAS with many years of commitment, as Steinberg emphasized as Chairman of the Stiftungsrat with a heartfelt thank-you. He held this office for 13 years and was also bid farewell with great thanks.

Welcome!
FIAS supports Ukrainian scientists

Seven scientists from Ukraine have found a temporary research position at FIAS. Personal commitment and the support of the Alexander von Humboldt Foundation and the Polytechnic Foundation of Frankfurt am Main ensure financial security, research opportunities, and a temporary home in Frankfurt for two professors, five (post)doctoral students and their families.

Roman Poberezhnyuk, a theoretical physicist with a doctorate from Kiev, was surprised by the war against his home country when he was on vacation in Spain. Since he had already spent several months as a visiting scientist at FIAS on several occasions, FIAS co-founder Horst Stöcker immediately invited him to Frankfurt. The FIAS administration helped find accommodation. "I am glad and happy about the help and the productive atmosphere here," says Poberezhnyuk. He initially received a temporary fellowship from the Polytechnic Foundation of Frankfurt am Main and was then supported for six months with a fellowship from the Alexander von Humboldt Foundation, followed by a scholarship by Philipp Schwartz Initiative (p. 30). Poberezhnyuk has been working with researchers at FIAS for years to understand the thermodynamic properties of dense elementary matter.

Oleh Savchuk previously also spent a year as a visiting student at FIAS. He now has a one-year fellowship at GSI Helmholtz Centre for Heavy Ion Research and is a PhD student at Mark Gorenstein´s lab. Prof. Gorenstein is chief scientific researcher at the Bogolyubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine, in Kiev. "We experienced the first bombardments in Kiev, practically moved into a bomb shelter, and finally decided to flee to Germany by car in March," says the Alexander von Humboldt Prize Winner in 2001. Thanks to a fellowship from the Alexander von Humboldt Foundation, Gorenstein is now able to live in Frankfurt with his wife, daughter, and granddaughter, conducting research at FIAS as well as experimentally investigating phase transitions and their signatures in cooperation with GSI.

Maria Khelashvili also reports on the bombings and frequent air alerts in Kiev. She was working on her PhD on ultralight dark matter at the Bogolyubov Institute. "I appreciate very much the opportunity to continue my research activities at FIAS," says the physicist. She can earn her living thanks to a grant from the Polytechnic Foundation. Khelashvili conducts research in general relativity and continues her work at FIAS on the statistical analysis of dark matter candidates.

Oleksandr Stashko, a PhD student from Kiev, is also working in the field of general relativity, gravitation and matter. In fall 2022, he went on to Princeton, USA, as a postdoctoral fellow. Until then, he was hosted as a visiting scientist at FIAS, financed by the Polytechnic Foundation. "I am incredibly grateful for the full support of my research stay here", says Stashko. In late summer, Dmitri Anchyshkin, also a professor at the Kiev Bogolyubov Institute of Theoretical Physics, arrived with his wife. Another graduate student, Zhanna Huranova, who completed her master's degree in physics and astronomy in Kiev two years ago, started working at FIAS as a doctoral student.

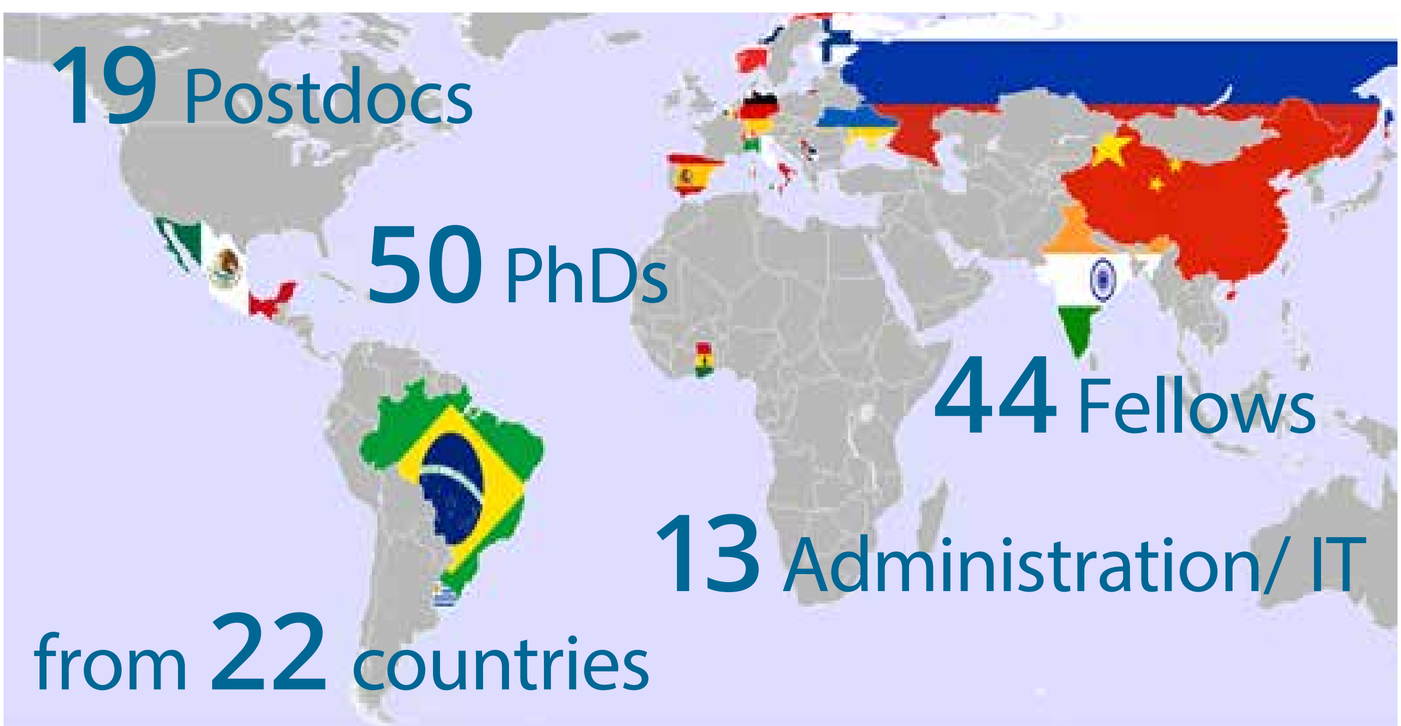
The Ukrainian scientists and their families were temporarily accommodated in guest houses of the Goethe University foundations and the Forschungskolleg Humanwissenschaften in Bad Homburg. The visiting scientists and FIAS owe thanks to Horst Stöcker and his great commitment. He says: "I was concerned with providing rapid transitional assistance to colleagues I knew personally, some of them quite hesitant and frightened."

Like the German Allianz der Wissenschaftsorganisationen, the FIAS Board strongly condemns the war of aggression on Ukraine. Even though science should be largely free of politics and has repeatedly built bridges across international conflicts, no one should stand idly by and watch these acts of war. Therefore, FIAS tries to offer help to Ukrainian scientists.

Guest scientists at FIAS: Maria Khelashvili, Oleh Savchuk, Oleksandr Stashko, Roman Poberezhnyuk, and Mark Gorenstein (from left to right). Photo: Störiko.

HIGHLIGHTS 2022

FIAS is an international team:



FIAS team contributed to black hole image

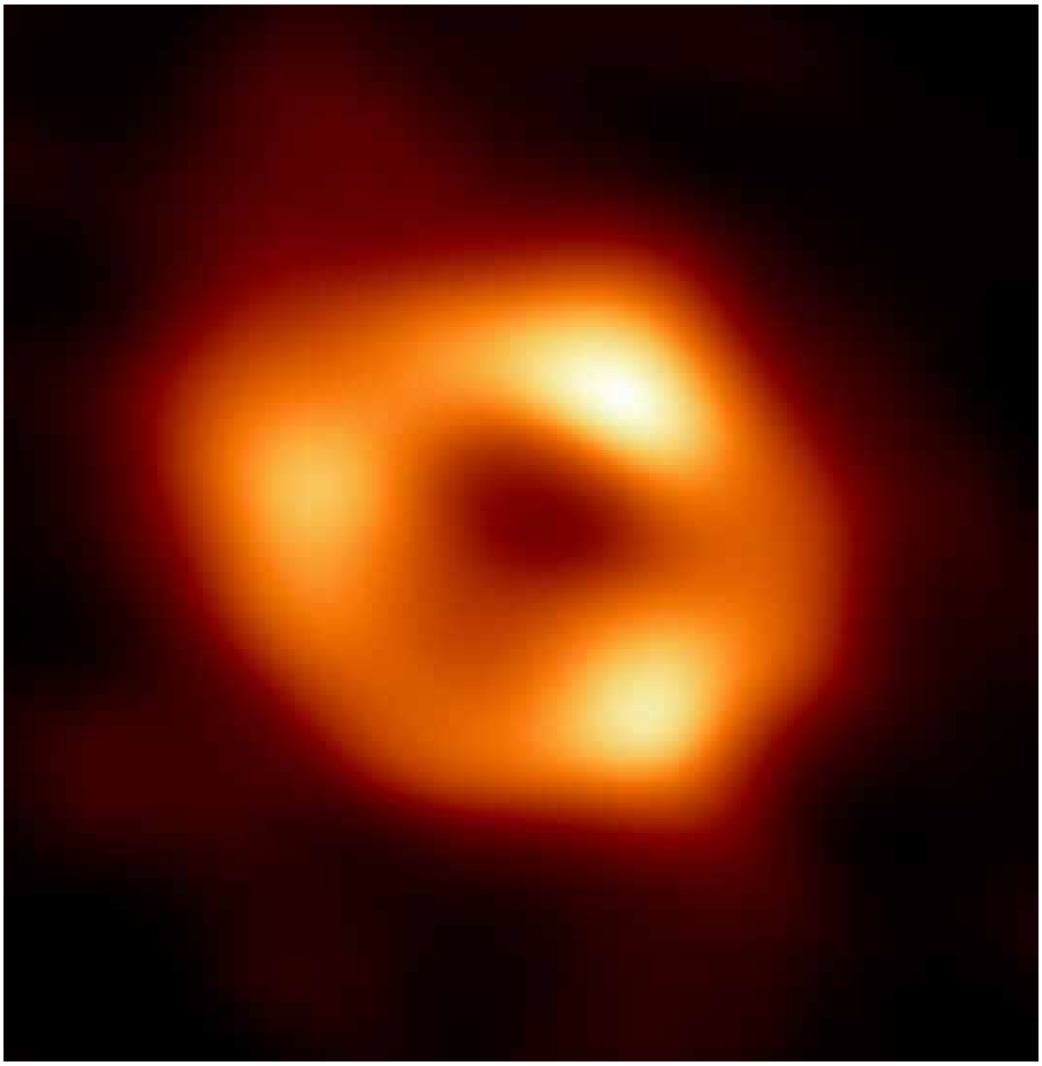
Eight super telescopes, many international working groups, and elaborate computer calculations over years led to the first image of the black hole at the center of our Milky Way.

The theoretical physicists led by FIAS Senior Scientist Luciano Rezzolla performed extensive calculations to determine the properties of the plasma being sucked up by the black hole. “We calculated three million synthetic images using different accretion and radiation emission models,” Rezzolla says. They also took into account variations caused by different viewing angles of the black hole.

Although the black hole itself is not visible - it is absolutely dark - the gas around it glows in a characteristic way: The image of Sagittarius A* shows a dark central region, the shadow of the black hole, surrounded by a bright, ring-like pattern. This is the light deflected by the black hole’s immense gravity - the black hole has four million times the mass of our Sun.

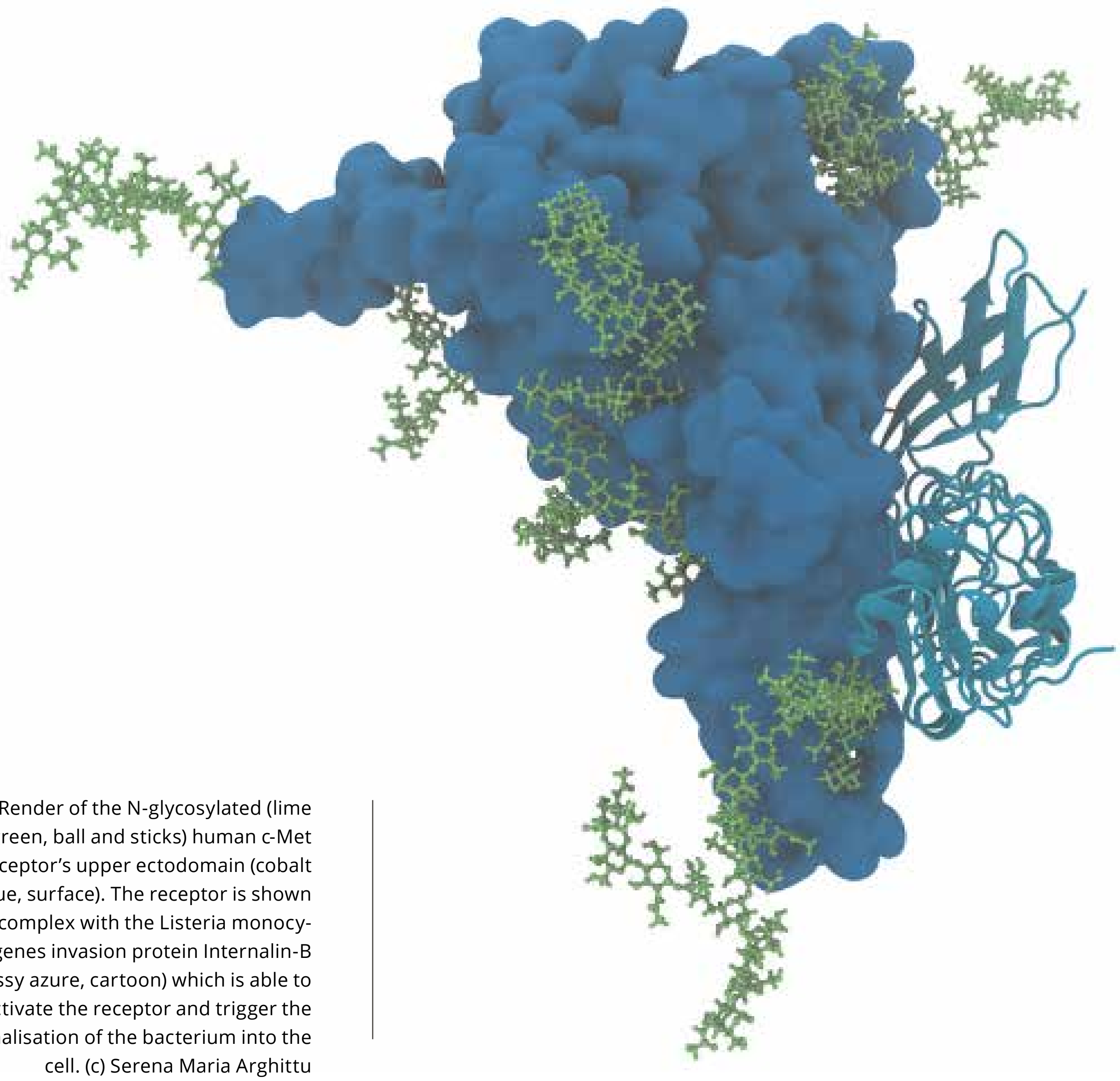
More telescopes joined together should soon allow more impressive images as well as movies of black holes.

Publication: First Sagittarius A* Event Horizon Telescope Results. I. The Shadow of the Supermassive Black Hole in the Center of the Milky Way. Astropysical Journal Letters (2022), DOI: 10.3847/2041-8213/ac6674 https://iopscience.iop.org/article/10.3847/2041-8213/ac6674



First image of a black hole. (Event Horizon Telescope)

HIGHLIGHTS 2022



Render of the N-glycosylated (lime green, ball and sticks) human c-Met receptor's upper ectodomain (cobalt blue, surface). The receptor is shown in complex with the Listeria monocytogenes invasion protein Internalin-B (glossy azure, cartoon) which is able to activate the receptor and trigger the internalisation of the bacterium into the cell. (c) Serena Maria Arghittu

SFB 1507: FIAS part of collaborative research centre on cell membranes

As part of the new collaborative research centre (CRC) 1507, Roberto Covino's group will contribute to understand the role of the cell membrane in regulating fundamental cellular programs. With modelling, calculations, and computer simulations, they want to elucidate the complex interactions between membrane proteins and lipids.

In SFB 1507 "Membrane-associated Protein Assemblies, Machineries, and Supercomplexes", the FIAS group, together with researchers from the universities of Frankfurt, Mainz, Jena, and the Max Planck Institute of Biophysics, is investigating the biological processes in cellular membranes. "There, protein complexes sense their environment," Covino explains. "Signals trigger regulatory programmes whose interplay and mechanism we still do not understand, despite their biological and biomedical importance."

Covino and his team use state-of-the-art modelling and simulations of molecular dynamics as well as innovative computational methods. For example, they plan to study the activation mechanism of the Unfolded Protein Response (UPR), a fundamental pathway central in health and disease. Computer simulations driven by artificial intelligence will, for example, help to understand the pairing (dimerisation) of transmembrane proteins. From this first step, more sophisticated protein assemblies in the membrane can be deduced.

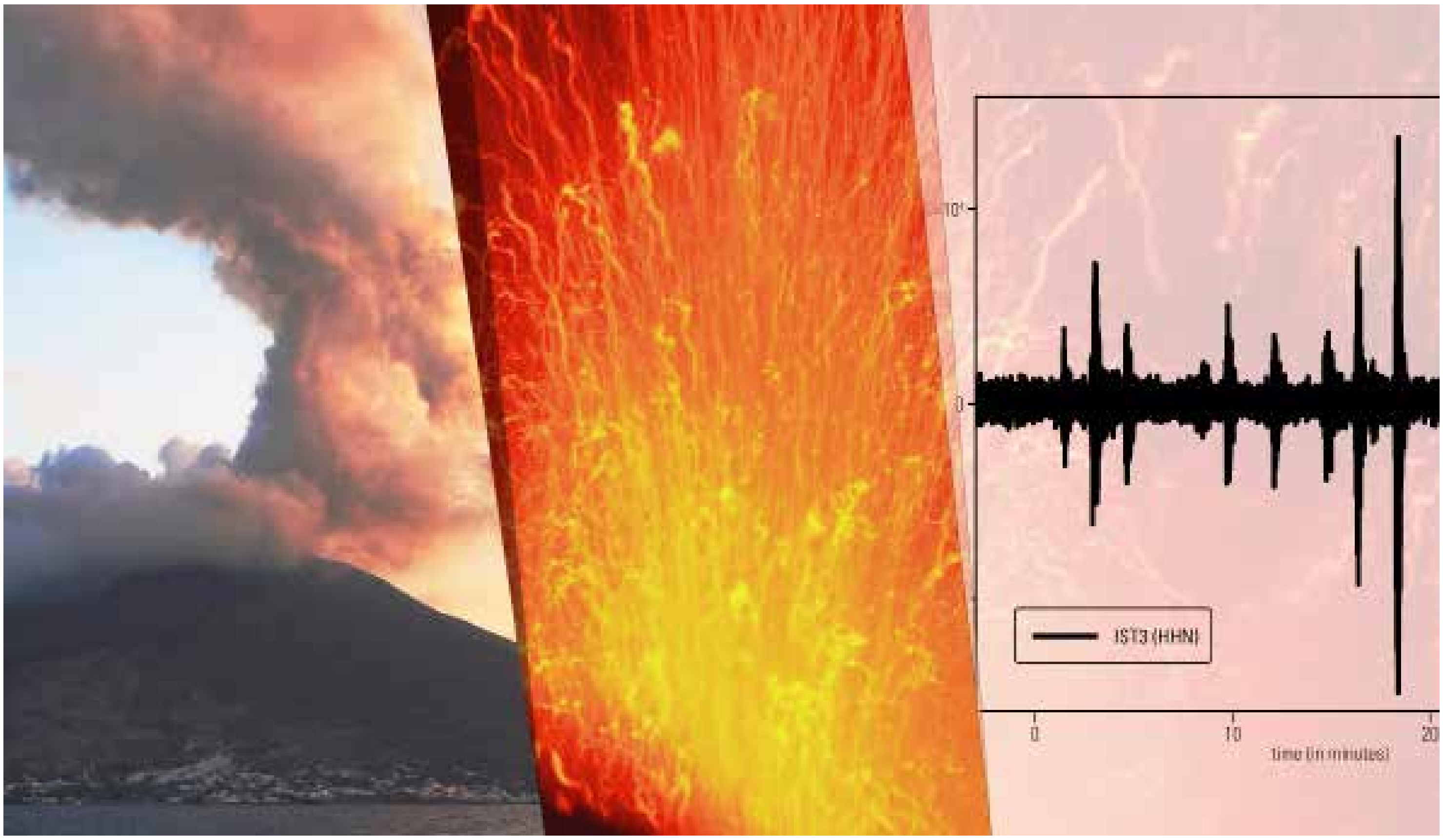
The group wants to develop an experimental-theoretical workflow to unravel the activation mechanism of certain (MET) receptors which control many cellular activities and are, for example, dysregulated in cancer.

To this end, a new PhD position is being created in Covino's research group. The German Research Foundation (DFG) will fund the SFB 1507 with 13.8 million euros over the next four years. Spokesperson Prof. Robert Tampé from the Institute of Biochemistry at Goethe University explains: "We want to understand the organisational and functional principles of large dynamic protein complexes, for example how they interact in cellular self-defence or in communication processes."

Christmas Lecture

With a wonderful lecture on the physics of snowflakes, Franziska Matthäus enchanted her audience at the public Christmas Lecture at FIAS - entirely in rhymes. Volker Lindenstruth added to the Christmas atmosphere by piano music on the theme of snow. The 80 internal and external guests were thrilled!

Theoretical Sciences

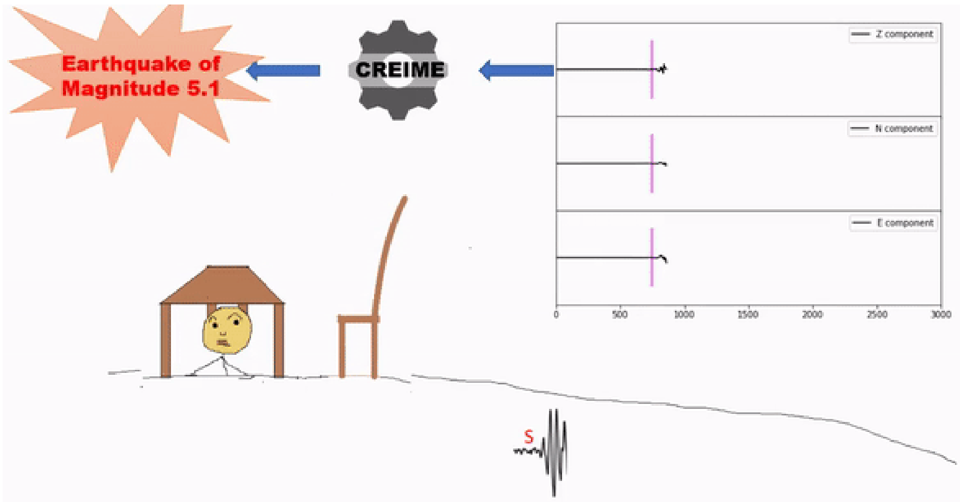


Methodological research in the field of AI is already proving groundbreaking in the area of theoretical natural sciences. The FIAS Seismology and Artificial Intelligence group used the Italian volcano Stromboli in the Mediterranean Sea as an example to develop a powerful module for immediately detecting seismo-volcanic events and creating a more complete event catalogs. These catalogs not only enable the evaluation of volcanic hazard but also the in-depth investigation of possible precursors based on the historic instrumental data.

Measuring volcanic activity

To understand and predict volcanic activity, data on its activities are collected worldwide. This is particularly complicated for Strombolian volcanoes, which are characterized by frequent mild eruptions. However, dangerous major eruptions can occur. For instance, Stromboli last erupted violently in 2019; resulting in a kilometer high ash-gas plume and one fatality.

Nishtha Srivastava's group also described a significantly improved model (CREIME) for early earthquake detection. Their model detects earthquakes more reliably and faster than previous studies, which can simplify advance warnings, especially in less developed regions of the world.



For the detailed analysis of these volcanoes, labeled datasets with information about seismo-volcanic events are required, especially for the application of deep learning methods. Therefore, volcanoes are monitored and analysed worldwide; nonetheless, this requires a lot of manual work.

To automatically analyse seismic data and identify events in this study, Darius Fenner (20) from Nishtha Srivastava's FIAS research team in collaboration with Georg Rümpker and Horst Stöcker developed the Adaptive-Window Volcanic Event Selection Analysis Module - AWESAM. This algorithm uses unlabeled raw seismic waveforms to extract time and amplitude information. A special filter allows to register both rare violent and regular small events. In a second step, these measurements are matched with another station to exclude local interfering factors. The strength of this method is the reliable detection of very small and frequent events as well as major explosions.

The scientists used publicly accessible continuous seismic recordings from two almost equidistant stations at Stromboli volcano in Italy as an example. The module allows for a straightforward generalization and application to other volcanoes with frequent Strombolian activity worldwide. Furthermore, this module can be implemented for volcanoes with rarer explosions.

This research was executed by Darius Fenner, a first-year Physics Bachelor student at Johannes Gutenberg University-Mainz (JGU), along with the 'Seismology and Artificial Intelligence (SAI)' research team. SAI research team lead by Nishtha Srivastava is funded by the German Federal Ministry of Education and Research (BmBF) with more than 1.6 million Euros as part of the "Promotion of female AI junior scientists" program. The SAI group seeks to apply Deep Learning and Machine Learning based algorithms on seismic signals to improve Earthquake Early Warning System (EEWs) and Seismic Signal Analysis. Additionally, they are also trying to better understand the pattern associated with Seismic stress release.

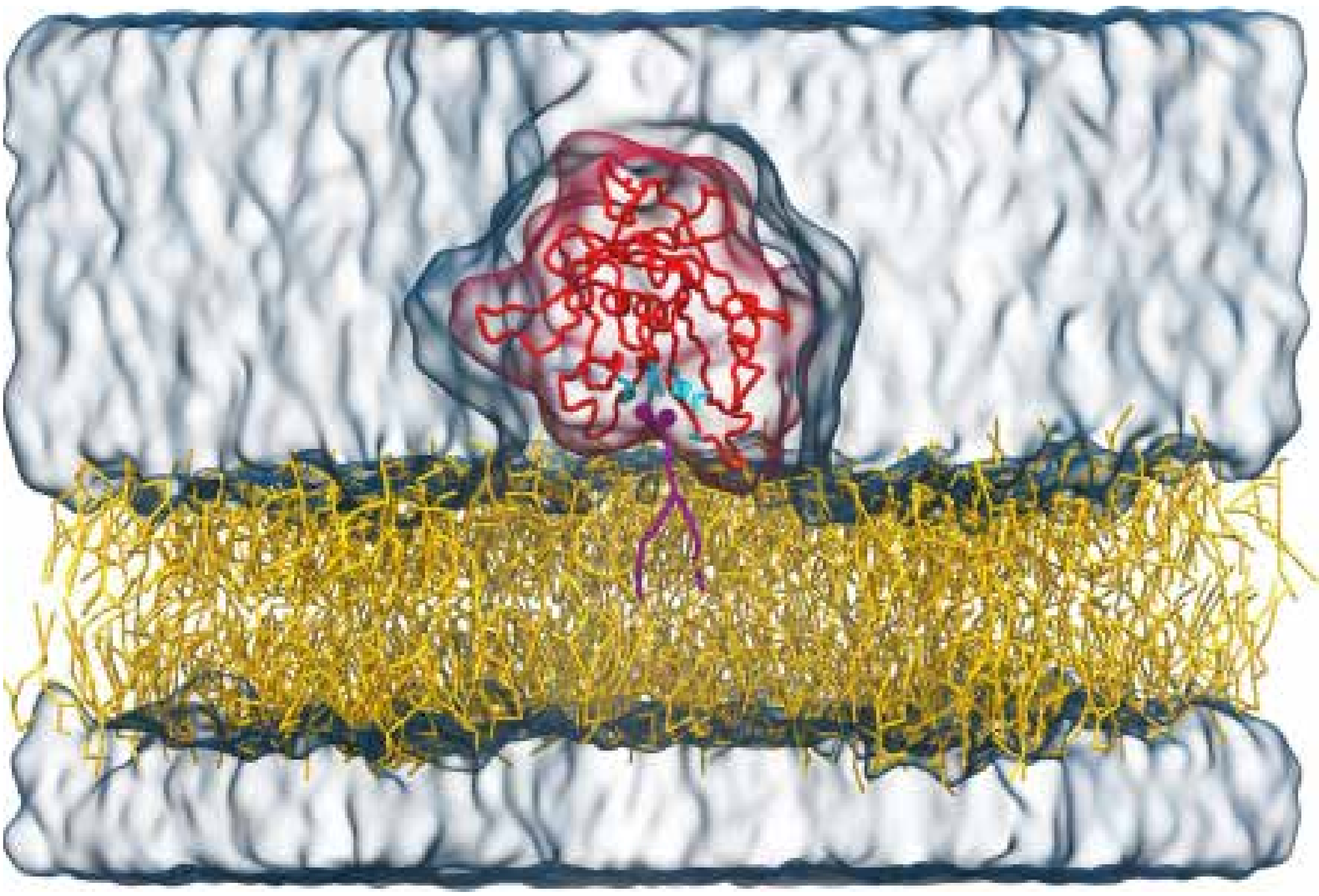
Publications:

Darius Fenner, Georg Rümpker, Wei Li, Megha Chakraborty, Johannes Faber, Jonas Köhler, Horst Stöcker and Nishtha Srivastava, Automated Seismo-Volcanic Event Detection Applied to Stromboli (Italy), Front. Earth Sci. 10:809037, doi: 10.3389/feart.2022.809037, https://www.frontiersin.org/articles/10.3389/feart.2022.809037/full

Megha Chakraborty, Darius Fenner, Wei Li, Johannes Faber, Kai Zhou, Georg Rümpker, et al. (2022). CREIME—A Convolutional Recurrent model for Earthquake Identification and Magnitude Estimation. Journal of Geophysical Research: Solid Earth, 127, e2022JB024595. https://doi.org/10.1029/2022JB024595

Megha Chakraborty, Claudia Quinteros Cartaya, Wei Li, Johannes Faber, Georg Rümpker, Horst Stoecker, Nishtha Srivastava, PolarCAP – A deep learning approach for first motion polarity classification of earthquake waveforms, Artificial Intelligence in Geosciences (2022) 3, 46-52, ISSN 2666-5441, https://doi.org/10.1016/j.aiig.2022.08.001

Life- & Neuro Sciences



Tubby protein (red) on top of a lipid membrane (yellow) with a PI(4,5)P2 signalling lipid (purple) in the known binding pocket. The amino acids of the binding pocket are displayed in cyan, water as transparent blue surface. Figure reproduced from V. Thallmair et al., Sci. Adv. 8, eabp9471 (2022).

A team led by Sebastian Thallmair at FIAS investigates the interactions of proteins and lipids (fats) in membranes by means of simulations. In the barrel-shaped Tubby protein, they identified a previously unknown binding site that could help to understand various diseases.

New binding site to cell membrane identified - Role in retinal and hearing disorders

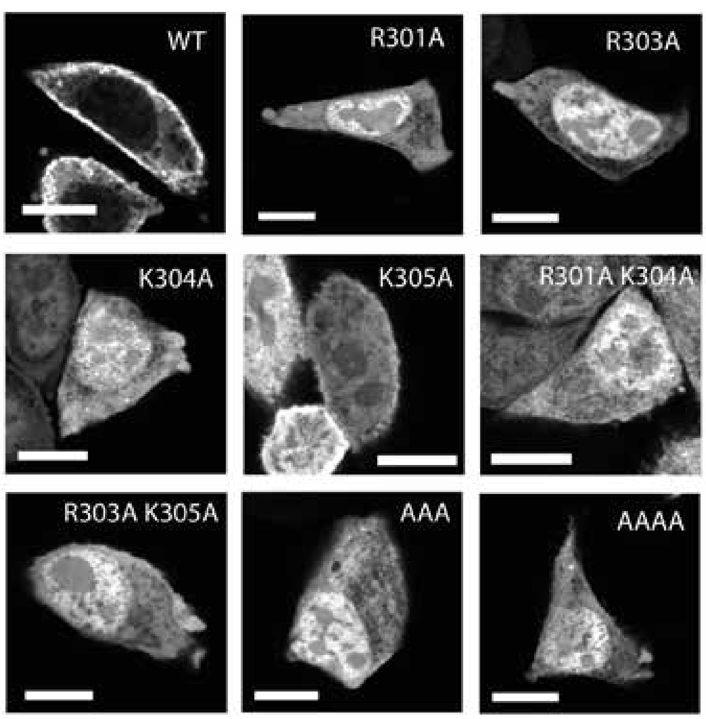
A team led by Sebastian Thallmair at FIAS investigates the interactions of proteins and lipids (fats) in membranes by means of simulations. In the barrel-shaped Tubby protein, they identified a previously unknown binding site that could help to understand various human diseases.

If the Tubby protein does not work, disturbances in the energy balance, obesity, degeneration of the retina, and hearing loss are observed. The exact background for these malfunctions is unclear, therefore insights in the functioning of Tubby are important. The Tubby protein family plays an important role in the transport of proteins within the cell membrane. They bind receptor proteins in a precisely fitting "pocket" and channel them into fine hairs, the primary cilia. These cilia act as antennae that recognise signals outside the cell and transmit them into the cell interior. If their function and thus signal transmission is disturbed, diseases can occur (ciliopathies).

For Tubby to function, it must dock to the inside of the membrane via a specific lipid ($PI(4,5)P_2$) that is found exclusively in the cell membrane. A team led by FIAS Fellow Dr. Sebastian Thallmair, Prof. Dr. Dominik Oliver (University of Marburg), and Prof. Dr. Siewert-Jan Marrink (University of Groningen, The Netherlands) investigated the binding mechanism of Tubby to this signalling lipid in more detail. In a recent publication, they describe a previously unknown binding site of the Tubby protein. "Using computational modelling, we identified a second binding pocket for the signalling lipid, in addition to the already known one," says Thallmair. The basis for these model calculations are the known protein structure as well as information on chemical and physical binding preferences or repulsion reactions of individual atom groups.

To validate the modelling results, the team placed mutations in the predicted binding site - which subsequently does not function properly anymore. This confirmed that the second binding pocket is essential for Tubby's function in living cells. It plays a key role in enabling Tubby to dock to the cell membrane. Furthermore, the team showed that both binding sites cooperate. "This means that, surprisingly, two bound signalling lipids act more than twice as strongly as just one bound signalling lipid," explains Thallmair.

Fluorescently labelled Tubby protein is also used as a marker to draw conclusions about the lipid concentration of different membrane areas. "For instance, we would like to understand how the signalling lipid is re-synthesised after it has been degraded," says Thallmair. "It is obviously only synthesised in certain, narrowly defined areas of the cell membrane." Tubby should help to identify these areas.

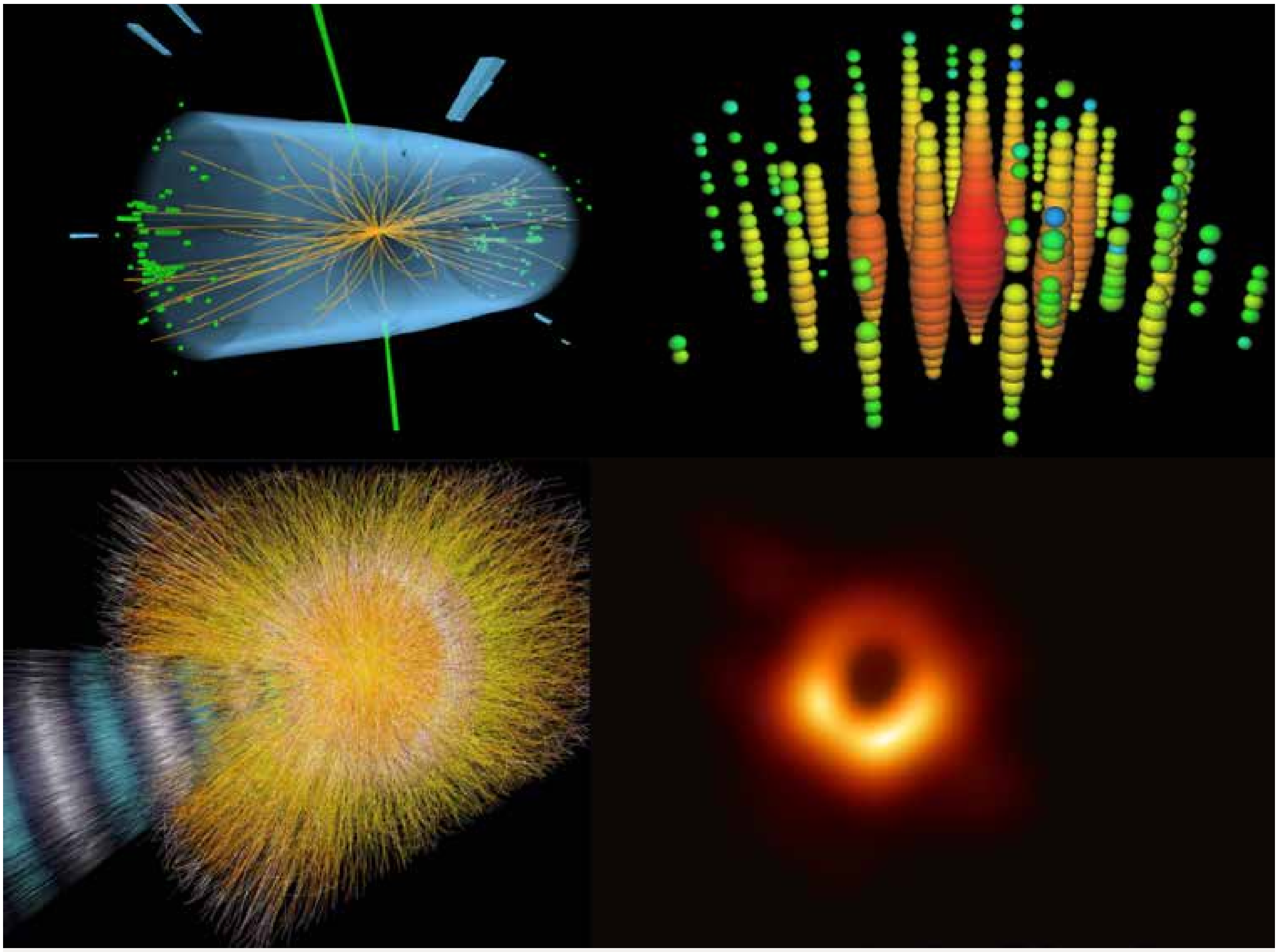


Representative confocal images of tubbyCT wildtype (WT) and mutants expressed in CHO cells show different degrees of membrane localization. While the WT (top left) is localized at the membrane, the mutants are mostly localized in the nucleus. Scale bars, 5 µm. Figure reproduced from V. Thallmair et al., Sci. Adv. 8, eabp9471 (2022).

Publication:

Veronika Thallmair, Lea Schultz, Wencai Zhao, Siewert Jan Marrink, Dominik Oliver, Sebastian Thallmair, Two cooperative binding sites sensitize $PI(4,5)P_2$ recognition by the tubby domain, Sci. Adv. 8, eabp9471 (2022). DOI: 10.1126/sciadv.abp9471

Computer Science & AI Systems



The achievements of PUNCH science range from the discovery of the Higgs boson (top left) over the installation of a 1 cubic kilometre particle detector for neutrino detection in the antarctic ice (top right) to the detection of the quark-gluon plasma in heavy-ion collisions (bottom left) and the first picture ever of the black hole at the heart of the Milky Way (bottom right). (picture: https://www.punch4nfdi.de)

How to use computer resources more effectively within experiments

Scientific experiments on the fundamental constituents of matter and their interactions generate an increasing amount of data that must be processed and analyzed. Scientists from particle, astroparticle, hadron, and nuclear physics have therefore joined forces to form a consortium. Its goal is to organize the huge data sets from many experiments in a “sustainable” way so that all data become easily findable, readily accessible, linkable as well as reusable. The participation of FIAS in the consortium PUNCH4NFDI (Particles, Universe, NuClei, and Hadrons for the NFDI) is funded within the framework of the National Research Data Infrastructure (NFDI) for an initial period of five years with a total of almost 280,000 Euros.

To obtain even more accurate results, many future scientific experiments from the PUNCH area will have to process a lot more data than before. At the same time, the technical requirements for processing at high data rates are growing. Scientists are faced with the challenge of making far more complex decisions on much shorter time scales than in the past, and they will have to make more effective use of the available computer resources.

In addition to the leading applicant DESY, FIAS is also one of the 18 other grant beneficiaries of the PUNCH4NFDI consortium. It includes 23 additional partners from the Helmholtz Association, the Max Planck Society, the Leibniz Association, and universities, such as Goethe University.

At FIAS, one focus of Prof. Dr. Volker Lindenstruth’s research group has long been to further develop parallel processor systems and computer clusters. Such systems are often subject to high real-time and reliability requirements. Now, this expertise will be part of the consortium’s task area 5 “Data Irreversibility”. Led by PD Dr. Andreas Redelbach, a scientist working at FIAS, and Prof. Dr. Michael Kramer from the Max Planck Institute for Radio Astronomy in Bonn, the aim is to recognize patterns in detector data under real-time requirements. Ideally, only data of “interest” will be stored permanently. The most efficient data selection possible under optimal hardware utilization implements forward-looking concepts of Green IT, developed among others at FIAS.

The expected solutions could also be relevant for other, data-intensive, research fields in optimizing signal search and facilitating future discoveries. An interdisciplinary application of the statistically complex simulation techniques from the PUNCH field has already emerged in the interpretation of epidemiological data.

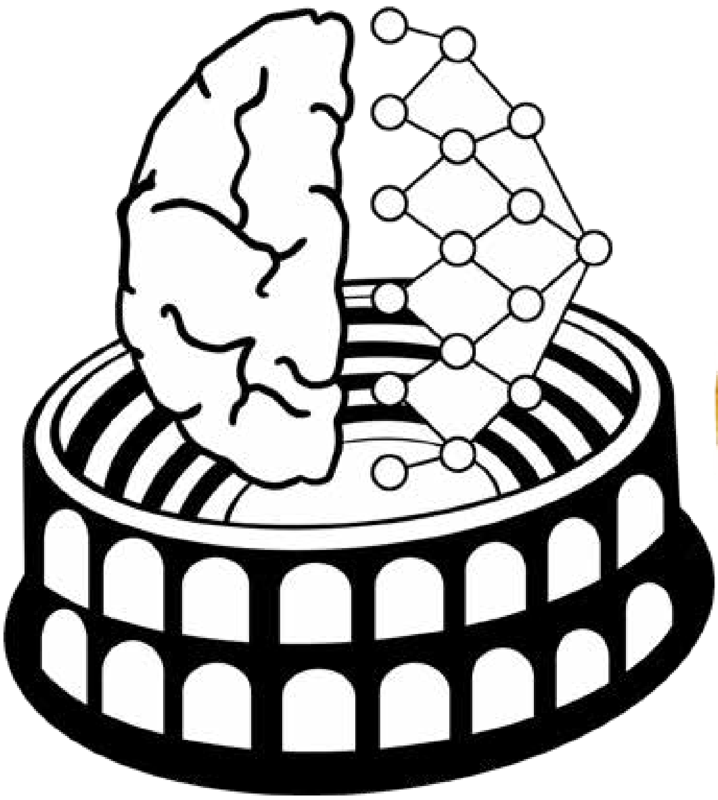
FIAS has also been a member since September 2021 of the non-profit association NFDI e.V. - Dedicated to promoting science through a National Research Data Infrastructure that establishes and develops overarching research data management in Germany.

At the end of the first funding period in fall 2026, there is the possibility of further funding for NFDI consortia to exploit the potential of as much research data as possible in the long term.

Homepage: https://www.punch4nfdi.de

Projects

How does the brain recognise an orange? An AI system developed for image recognition and speech recognition can link an image of an orange (input) with the word "orange" (output). The ARENA project investigates how abstract knowledge is stored in the brain.



Elected new Projects at FIAS 2022

Deep learning-based parameter estimation of high-resolution mathematical models for the analysis, prediction and control of COVID-19
DFG-Project, head Maria Barbarossa/Gordon Pipa
08/2022-07/2023. 95,900,00 €

Studies of compact stars with heavy baryons and quarks - second period
DFG-Project, head Armen Sedrakian
05/2022-04/2024. 191,500,00 €

SFB 1507 Membrane-Associated Protein Assemblies, Machineries and Supercomplexes
DFG-Project, head Roberto Covino
07/2022-06/2026. 249,124,00 €

Humboldt Research Fellowship for Postdocs
Alexander von Humboldt Foundation, holder Sahila Chopra
12/2022-11/2024

ARENA: DFG Research Group on Abstraction in the Brain and for Better AI Systems

How abstract knowledge is stored in the brain is being studied by psychologists and computer scientists in the new DFG research group ARENA. The findings should contribute to making artificially intelligent (AI) systems more efficient and flexible.

Since artificially intelligent systems have been able to reliably recognise objects and language, AI research has experienced a boom. However, the systems still have to be trained with a great deal of work and energy - and still store their knowledge about objects and words differently than the human brain: modern AI systems are usually neural network models. They consist of several layers of artificial nerve cells that are interconnected. That is why they are also called deep neural networks. An AI system developed for image recognition and speech recognition can link an image of an orange (input) with the word "orange" (output). However, such an AI system cannot generalise to other sensory impressions - which our brain, on the other hand, manages effortlessly.

This is because one of the most important properties of the human brain is the ability to abstract: our knowledge about an orange can be activated when we see, feel, taste or smell it. The brain thus abstractly represents our semantic knowledge about oranges - regardless of how we perceive oranges through the senses.

AI could learn this kind of abstract knowledge representation from the human brain. However, the 'format' in which our semantic knowledge is stored in the human brain is not yet well understood. Here again, brain research can benefit from the powerful AI models. The interdisciplinary research group ARENA (Abstract Representations in Neural Architectures) at the Frankfurt Institute for Advanced Studies (FIAS), Goethe University, and the Max Planck Institute for Software Systems in Saarbrücken, funded by the German Research Foundation (DFG), builds a bridge between computer science, psychology, and neuroscience to explore these questions. It will receive a total of around 3.7 million Euros over the next four years.

An important goal of the ARENA research group is to investigate whether AI systems that are trained with data of different formats - images, language or videos, i.e. multimodal data - develop more abstract forms of knowledge or at least forms of knowledge that are more similar to the human brain.

As part of the project, Prof. Dr. Jochen Triesch from FIAS will investigate how AI can independently learn abstract representations of objects. "In contrast to common AI approaches, it should achieve this autonomously and without outside help," says Triesch, "like a child learns to recognise objects and group them into abstract categories." His FIAS colleague Prof. Dr. Matthias Kaschube will investigate how both the brain and AIs can use "cognitive maps" to efficiently process abstract semantic information. Prof. Gemma Roig acts as a bridge professor between computer science and psychology in the research group.

The psychologists and neuroscientists involved are interested in how well AI systems can explain how the brain works when processing abstract meanings. To do this, they want to compare how an AI system and the human brain work when they solve the same tasks. To answer this question, AI models are used as a statistical tool to analyse brain activity measured with functional magnetic resonance imaging and magnetoencephalography methods at the Brain Imaging Center at Goethe University during the processing of language and object recognition tasks. The researchers expect that the same representations in the brain will be addressed at the highest level of abstraction.

A core part of this work will be the collection of a very large data set of test subjects who will work on a whole series of corresponding tasks in several study sessions while their brain activity is measured. "The planned data set is unique and will be shared with other scientists in the future, also in the spirit of open science," explains Prof. Christian Fiebach, the spokesperson of the ARENA research group.

But for the time being, the data collected will be used by the modellers in the ARENA research group to explore whether they can make AI systems more flexible and efficient, based on the biological model of the human brain. To this end, they are also incorporating findings from developmental psychology. Conversely, the experimenters would like to learn new analytical techniques from the modellers in order to make their models of the brain more precise. In other words, how can the neuronal image of the orange in the brain be better decoded, and how can this knowledge contribute to providing AI models with more human-like knowledge about the orange in the future?

Events

new: FIAS Mission Statement

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.

FIAS events 2022

After two years of homeoffice and no conferences social life is slowly coming back to FIAS. Many research projects still hosted their workshops and conferences virtually. But many events took place as live events again, finally.

FIAS Geoscience Seminar Series

Invited talks of international speakers of various topics in the field of geosciences in virtual format, hosted by Dr. Nishta Srivastava.

Astro Coffee Seminar Series

The long tradition of the Astro Coffee seminar has been revived on-site after the lockdowns due to the pandemic.

CMMS Talks Seminar Series

The new seminar series in the frame of CMMS started in April 2022 and takes place bi-weekly with a talk by internationally renowned guests at FIAS.

CMMS 2nd Molecular modelling and simulation workshop

The second Molecular modelling and simulation workshop within the project of CMMS took place in December 2022, including a keynote talk and four sessions containing interesting presentations.

IQbio Career Day

Within the scope of our graduate program, the IQbio Career Day took place in July 2022 to present possible fields of employment to doctoral students.

FIAS also hosted:

Ernst Strüngmann Forum: How Collaboration Arises and Why It Fails (May), Stigma Processes in the Context of Migration-Generated Diversity (June), Exploring and Exploiting Genetic Risk for Psychiatric Disorders (June/July), Digital Ethology: From Individuals to Communities and Back (July).

ELEMENTS Annual Conference: In May 90 guests to FIAS from the universities of Frankfurt, Darmstadt, and GSI came come together for the first ELEMENTS annual conference. They addressed fundamental questions of nuclear and particle physics and astrophysics, covering topics such as the nucleosynthesis of heavy elements in binary neutron star mergers and the Equation of State of dense nuclear matter. Early career researchers were encouraged to showcase their recent findings in presentations and a poster session, inspiring exchange across career stages.

EXPLORE summer school: In August the EXPeriential Learning Opportunity through Research and Exchange - an innovative international teaching project took place at FIAS. 13 students from Frankfurt's partner city Toronto and their 22 fellow students from Goethe University were meeting in person for the first time. Already in the winter semester, the young people worked in self-organised teams on very real physical data and questions related to the topic of dark matter. EXPLORE is based on the teaching format of "research-based learning". The aim is not only to provide students with specialist knowledge in physics, but also to give them a practical insight into modern international research work.

The EXPLORE Summer School opened at FIAS on the Riedberg campus together with Mayor Dr. Nargess Eskandari-Grünberg: "It is of special importance to me that Frankfurt will be further strengthened as a research location. In times where scientific findings are being questioned, it is particularly important that researchers communicate beyond borders". (Photo: Dettmar)

Events

Elena Spinetti from the group of Roberto Covino entering a cave during a retreat in Franconian Switzerland.
Photo: Martin Kaufmann

CMMS

The Frankfurt Center for Multiscale Modelling in the Life Sciences aims at a comprehensive understanding from molecular processes, such as the mode of action of an enzyme, to complex dynamics in tissues and organisms. This understanding is the basis for the adaptation of cell functions for biotechnological use, as well as for the development of biomedical, pharmacological or agricultural applications. Advances in the development of high-resolution microscopy methods for molecules, cells and cell systems, such as cryo-Electron Microscopy or Light Sheet Microscopy provide insights into structure and dynamics of biological components. By integrating quantitative data from experimental studies into models and simulations, basic mechanisms and causalities can be identified. This requires the further development of methods and techniques to overcome the scale constraint and the prediction of missing information in experimental data sets.

Center for Multiscale Modeling in the Life Sciences

The Loewe Research Program "Center for Multiscale Modeling in the Life Sciences" was established at FIAS in 2020, in the middle of the corona crisis. We experienced two years of work within the consortium under restricted contact options and very limited possibilities for interaction. As of 2022, the corona restrictions were slowly lifted, allowing us to engage in more interactive work. Since then, we have experienced a boost in communication and inspiration, largely resulting from the initiated seminar series and the joint retreat in late summer 2022.

The bi-weekly seminar series has now been running successfully for two consecutive semesters bi-weekly, every event composed of an invited talk and a small get-together with plenty of options to get in contact with our guests. Since the summer term 2022 we were able to welcome a large number of renowned scientists from the broad field of multiscale modeling, and are very thankful for their inspiring talks: Gašper Tkačik (IST Austria), Kerstin Hünninger and Thilo Figge (Jena), Antonio Scialdone (Munich), Anđela Šarić (IST Austria), Ahmad Reza Mehdipour (Ghent), Anna Marciniak-Czochra (Heidelberg), Rastko Sknepnek (Dundee), and Jan Hasenauer (Bonn). The seminar series will continue in the summer term of 2023.

The CMMS highlight of the year 2022, however, was our retreat in early September, for which we picked the location of Behringers Mühle in the romantic area of Franconian Switzerland. The one-week program involved crash courses to equip the PhD students with insight into methods and approaches used in other groups, presentations of the PhD students, an invited scientific talk by Ursula Klingmüller (Heidelberg), as well as project work. For the latter we defined a set of problems at the interface of the different skills, and assembled groups of PhD students with different backgrounds. One of the projects (rule-based simulation of processes on networks) was actually finalized during the retreat, in another project a new plausible mechanism for cell motility of mycoplasma bacteria was proposed, and at least one project is still ongoing! Our scientific work was balanced by social outdoor activities, such as hiking, kayaking, and a guided cave tour.

Our joint activities greatly contributed to a spirit of openness and collaborative research, we are looking forward to our next retreat in summer 2023.

CMMS PhD students from different groups discussing joint projects. Photo: Franziska Matthäus

Public Relations

The many activities at FIAS as well as the exciting research is reflected in many publications, on web-sites, in Social Media, and in public lectures. Newspapers such as Frankfurter Allgemeine Zeitung and other national and local publishers reported on FIAS events and scientific publications.


Frankfurter Allgemeine

Was Neutronensterne mit Pr

FRANKFURT Astrophysiker beschreiben durch Gleichungen das

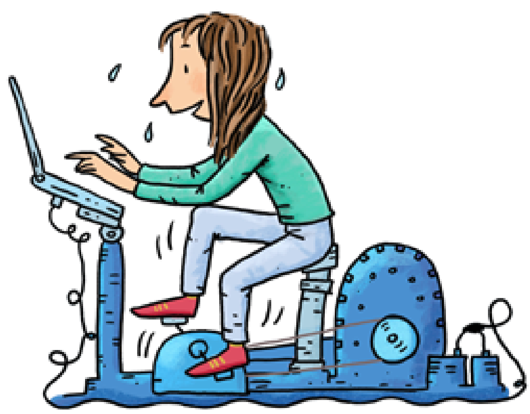

FRANKFURTER WOCHENBLATT

„Explore Summer School" am Frankfurt Institute for Advanced Studies auf dem C


Ophthalmologische Nachrichten

Tubby-Protein: Bisher unbekannte Bindestelle an Zellmembran identifiziert

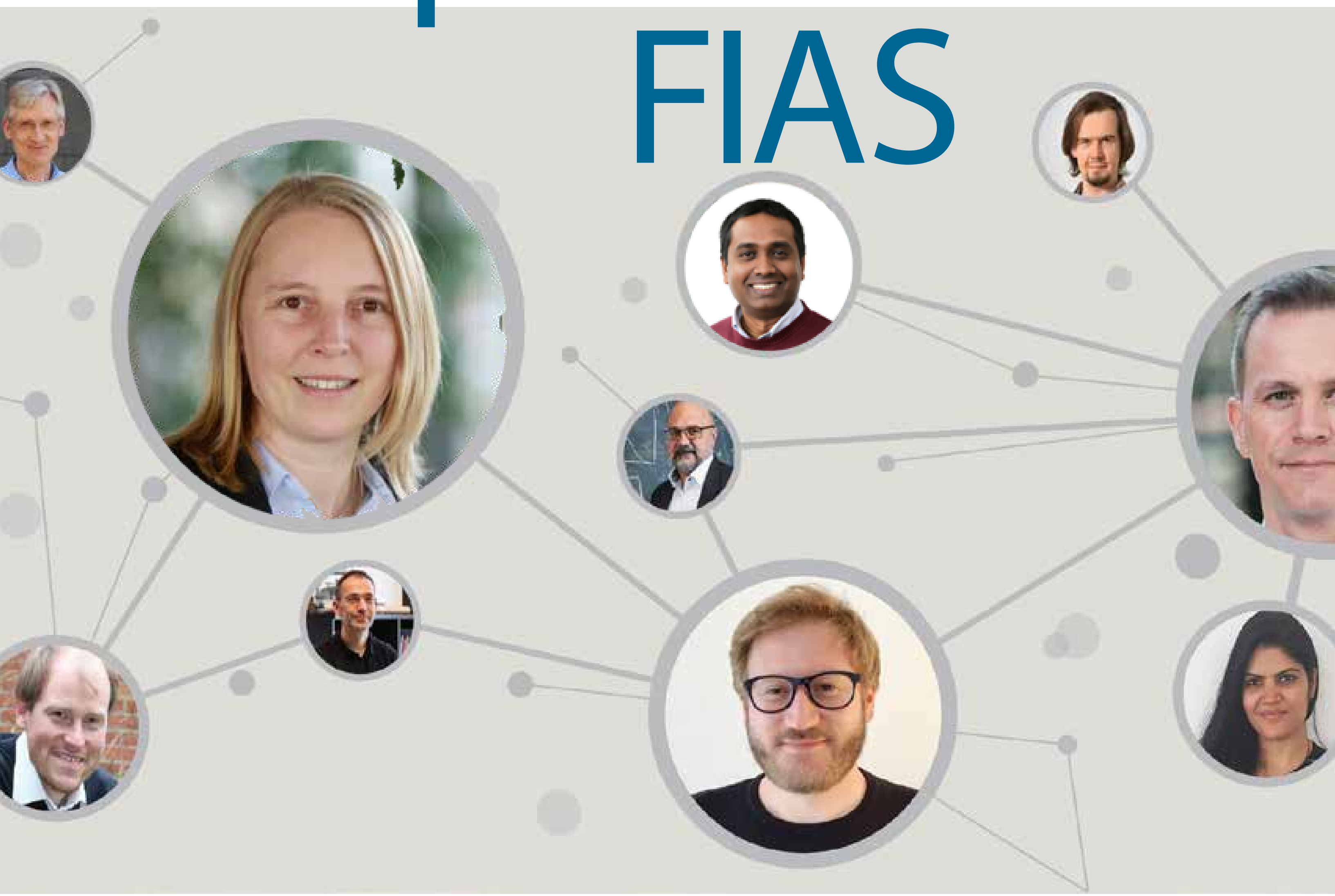
Children´s University 2022


(c) Tobias Borries

Smartphones, laptops or tablets: computers are used by every child nowadays. But after a few hours the battery is empty, and then only the power socket can help. What do computers actually need all that electricity for? Computer scientist Prof. Volker Lindenstruth and his team know. They took a look inside a large computer with interested children and explained how it could also save electricity. The lecture in the Audimax was part of the Goethe University's Children's University 2022, in the morning for school classes, in the afternoon for everyone.

In this lecture, children generated electricity themselves - and feel how much power is needed. They then took a look inside a computer and learned a lot about its inner workings and functions. The team explained in a lively and exciting a computer's power consumption and how it helps save electricity.

People at FIAS



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

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

Fellow Emeritus is a former (Senior) Fellow with a long-standing or particularly meritorious affiliation. An **Honorary Fellow** has rendered outstanding services to FIAS (e. g. benefactors, donors).

Goethe Plaque to FIAS Stiftungsrat Chairman Volker Mosbrugger

The city of Frankfurt honoured Prof. Dr. Dr. h.c. Volker Mosbrugger with the prestigious Goethe Plaque 2022, which is awarded annually to personalities of cultural life.

Mosbrugger, a palaeontologist, is chairman of the FIAS Stiftungsrat since June 2022 as well as president of the Frankfurt Polytechnic Society since 2019; he was director general of the Senckenberg Gesellschaft für Naturforschung in Frankfurt until 2020. Previously, the Constance native had conducted research on ecological and climatic changes in the Earth's history at the universities of Freiburg, Bonn, and Tübingen. The now 68-year-old promoted the hot topics of climate and environmental protection in research and at the Senckenberg Museum and brought biodiversity research into focus. Under his leadership, museum and research institute were rebuilt and expanded.

Mayor Eskandari-Grünberg presents Goethe plaque and certificate to Volker Mosbrugger. Photo: H. Menzel

Together with him the pianist, singer, and actress Sabine Fischmann was honoured with the award. "Sabine Fischmann and Prof. Dr. Volker Mosbrugger have done a lot for Frankfurt," said Ina Hartwig, Frankfurt's Head of the Department of Culture and Science. Mosbrugger had rendered outstanding services to the city's museum and science landscape since he came to Frankfurt in 2005: "He was and is remarkably committed to research around the topics of biodiversity and sustainability, as well as to the welfare as President of the Polytechnic Society." FIAS Director Eckhard Elsen praises his current commitment: "The Goethe Plaque stands for a long tradition of creative activities and especially of communicative exchange. As Chairman of the FIAS Stiftungsrat, Mosbrugger has taken on a task that also promotes this spirit."

Luciano Rezzolla receives Laureatus Professorship

The Walter-Greiner-Gesellschaft zur Förderung der physikalischen Grundlagenforschung (WGG) awarded two Laureatus professorships for outstanding achievements in research and teaching. As a part of the 24th academic summer ceremony of the physics department at Goethe-University, FIAS, and WGG several physicists were honoured. Prof. Dr. Luciano Rezzolla received the prestigious Carl Wilhelm Fueck Laureate Professorship for his work in the field of theoretical astrophysics. For many years he has conducted research as a Senior Fellow at FIAS.

Rezzolla sees the Laureatus Professorship not only as a scientific honour: "Being acknowledged by a society that explicitly supports research in Frankfurt makes me feel more welcome in the city than ever before." He emphasizes, "Scientific work is my greatest source of energy." On the same day he received another award: the International Society on General Relativity and Gravitation (ISGRG) appointed Rezzolla a fellow - the first fellow from a German institute. He is honoured for his "leading contributions to the development of robust numerical relativity simulations of astrophysical objects" – such as calculations that made the image of the black hole Sagittarius A* at the center of our Milky Way possible. As an ISGRG-Fellow he is joining the ranks of many famous scientists such as Stephen Hawking and noble price holder Roger Penrose.

The Walter Greiner Society is dedicated to the conceptual and financial support of fundamental research in physics at Goethe University and FIAS.

Prof. Dr. Luciano Rezzolla received the prestigious Carl Wilhelm Fueck Laureate Professorship for his work in the field of theoretical astrophysics. Photo: Fabian Feldmann

People at FIAS

Hannah Elfner (Photo: Dettmar, Goethe-Universität)

Hannah Elfner: Senior Fellow and Scientist of the Year

FIAS Fellow Hannah Elfner was nominated "Scientist of the Year 2021", receiving this prize in June 2022. Goethe University and the Alfons and Gertrud Kassel Foundation award this honour to researchers every two years. In addition to outstanding scientific work, the focus is also on promoting young researchers, for which part of the prize money of 25,000 Euros will be used.

Prof. Dr. Hannah Elfner has been a Fellow at FIAS since 2013 and is a professor at Goethe University and the GSI Helmholtz Centre for Heavy Ion Research. In October she was appointed as FIAS Senior Fellow. She is the first woman to make it into this highest category at FIAS - comparable to a W3 professorship at the university. "We appoint experienced and outstanding researchers - and Hannah Elfner is absolutely one of them, as now the youngest member," says FIAS Director Eckhard Elsen.

Elfner is working on a state of matter that existed in the early universe only microseconds after the Big Bang. "I am fascinated by how the smallest building blocks of our world work – that is what I want to understand," she says. "Afterwards, the smallest and free components of matter, the quark-gluon plasma, transformed into today's building blocks of matter, the protons and neutrons". This can be simulated in energy-intensive particle accelerators by accelerating atomic nuclei made of lead or gold to almost the speed of light, so that when they collide with each other, temperatures and densities are created that existed shortly after the Big Bang. Elfner describes these processes in mathematical models: She calculates the temporal development of the microscopic heavy ion collisions and compares various assumptions for the properties of matter with experimental data.

Currently, 16 scientists in her group are conducting research in seven national and international collaborations. For example, in the ELEMENTS cluster project with colleagues from Darmstadt, they are trying to understand how the properties of matter at high densities can be determined from heavy ion collisions in order to elucidate the astrophysical processes involved in the fusion of neutron stars. In the JETSCAPE collaboration, they are working with ten US groups to develop a comprehensive computer model to describe the processes in heavy ion collisions.

Regular activities and excursions keep the team together. Elfner is very committed to young scientists; despite her young age, she has already successfully guided almost 40 young scientists to their scientific degrees. In addition to educating students and doctoral candidates, she regularly gives the public an insight into her research in lectures and at events - in the process, she demonstrates how successful women can be in physics.

FIAS has now underlined her exceptional performance and high level of commitment by appointing her a Senior Fellow. The Stiftungsrat (Board of Trustees) unanimously appointed her to the ranks of the FIAS Faculty. "I am delighted about the appointment," says the Frankfurt native - "and that I can continue to contribute to FIAS and its shaping". FIAS Director Elsen adds: "With this appointment, the theoretical description of the interaction of nuclear matter will continue to be competently and prominently represented at FIAS in the future".

The exploration of the world in miniature will not let go of Hannah Elfner in the future: "A better understanding of the transition from protons/neutrons to the quark-gluon plasma at high densities would be great". Now her focus is also on a small human: the junior life of her daughter began right after the senior award.

People at FIAS

Funding for Roman Poberezhnyuk

The Philipp Schwartz Initiative for Researchers at Risk is supporting the FIAS visiting scientist Dr. Roman Poberezhnyuk with an 18-month scholarship.

The theoretical physicist from Kiev, who holds a doctorate, was caught unprepared by the war against his home country while on holiday in Spain. As he had already spent several months as a visiting scholar at the Frankfurt Institute for Advanced Studies (FIAS), he immediately found support and accommodation here. He initially received temporary fellowships from the Stiftung Polytechnische Gesellschaft and the Alexander von Humboldt Foundation. The funding now granted as a Schwartz Fellow is also a recognition of his research achievements. Poberezhnyuk has been working for years with researchers from Prof. Horst Stöcker's group at FIAS to understand the thermodynamic properties of dense elementary matter.

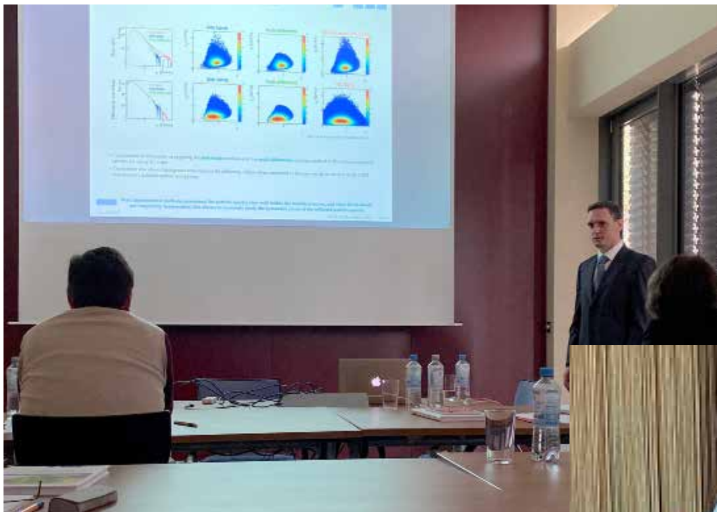
FIAS has been cooperating with Ukrainian scientists for many years, as documented by several joint publications. Horst Stöcker was recently awarded an honorary doctorate from the Bogolyubov Institute of the National Academy of Sciences of Ukraine in Kiev for this longstanding, productive collaboration.

The Philipp Schwartz Initiative goes back to the Austrian pathologist Philipp Schwartz, who lost his professorship in Frankfurt in 1933 due to his Jewish faith. He emigrated to Switzerland and founded the "Emergency Society of German Scholars Abroad". Under his name, the Alexander von Humboldt Foundation and the German Federal Foreign Office continue this work by enabling academics in danger in their home countries to work at German institutes.

Poberezhnyuk receives a fixed sum for the sponsorship period; in addition, the host institution is supported with 20,000 EUR. An extension to 24 months is possible. "We are very pleased that this dedicated scientist - also thanks to the active support of Goethe University - can continue to work at FIAS and that his research, as well as FIAS's commitment to now seven Ukrainian researchers, is thus recognised," says FIAS Director Eckhard Elsen.

Seven new doctorates at FIAS

Bastian Eppler (bottom picture, left), Pavel Kisel (right picture), Grigory Kozlov, Diyuan Lu, Tobias Mistele, Anna Schäfer and Charles Wilmot (left picture, standing) sucessfully ended their doctoral thesis at FIAS. Congratulations to all new PhDs - and their supervisors!



Honorary doctorate to Horst Stöcker

The National Academy of Sciences of Ukraine, the Bogolyubov Institute of Theoretical Physics has awarded an honorary doctorate to Prof. Horst Stöcker.

The Bogolyubov Institute awarded the FIAS Fellow for his distinguished contributions to theoretical physics, in recognition of the good cooperation and support of Ukrainian science.


DIPLOMA

Хорста Штокера

Horst Stöcker

Doctor Philosophiae Honoris Causa

Farewells in the administration

Three deserving employees ended their service in 2022: The highly appreciated administrative director Dr. Rolf Bernhardt (left) left in summer. Walburga Bergmann (middle) began her well-deserved retirement. IT Manager Alexander Achenbach left FIAS at the end of the year. A big thank you for their great commitment and all best wishes for their future!

FELLOW REPORTS 2022

From high-performance computing to machine learning

2022 was an exciting year for our lab! Various research projects gained momentum, and some produced exciting publications. Our group was part of a prestigious Collaborative Research Center supported by the German Science Foundation.

We engaged in exciting interdisciplinary collaborations with international experimental groups, ranging from the UK to Austria, Canada, the USA, and Japan. We investigated the mechanism of action of proteins that are key in two essential cellular phenomena: the unfolded protein response (UPR) and autophagy. The UPR is a global cellular regulation mechanism that takes action to counteract the detrimental effect of cellular stress. Autophagy is the cellular housekeeping mechanism. Both processes are fundamental to maintaining health in humans. Our models and computer simulations integrated our collaborator's cutting-edge experiments. We elucidated fundamental aspects of how the UPR and autophagy are activated and regulated at the molecular level. We are currently putting the finishing touches on the manuscripts reporting on these two studies.

In collaboration with scientists from the University of Trento, we published two exciting papers building bridges between theoretical disciplines. We built on concepts from information theory to better extract useful information from complex high-dimensional data produced in modern computer simulations. In another fun paper, we integrated machine learning, quantum field theory, and quantum computer algorithms to create one of the first-ever simulations of a molecular reorganization on a quantum computer.

Finally, we created an innovative method building on deep probabilistic learning to extract quantitative information from experiments that manipulate and measure molecular properties, one single molecule at a time. We concluded the year with a fantastic workshop organized by the young CMMS group leaders that saw our PhD students presenting their research in a day full of scientific talks and discussions.

I voluntarily took part in teaching activities at Goethe Uni in Membrane Biology ans Modern Statistical Data Analysis for Practitioners.

The Covino Lab (with family and friends) on a hike along the Rhein (Niederwalddenkmal).

Dr. Roberto Covino

He studied physics and theoretical physics at the University of Bologna, graduating with a master's thesis on black hole evaporation. He then moved to Trento University for his PhD. Afterwards he joined the newly founded Department of Theoretical Biophysics at the MPI of Biophysics in Frankfurt. During his postdoc, he studied the mechanism of sensing in cellular membranes and developed novel computational methods integrating physics-based models and machine learning. He joined FIAS in April 2020.

Highlight

End of year workshop where all the PhD students presented their research.

Projects at FIAS: 4

Staff

Gianmarco Lazzeri
Elena Spinetti
Lars Dingeldein
Serena Arghittu
Magnus Petersen

Collaborations

Sebastian Thallmair, FIAS
Mike Heilemann, Achilleas Frangakis, Michaela Müller-McNicoll, Volker Dötsch, Christoph Welsch, Goethe University
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

Download Cajal's dream at https://sidequestvr.com/app/7951/cajals-dream and fly through a forest of virtual dendrites.

Projects at FIAS: 1

Staff

Bassem Hermila

Collaborations

Peter Jedlicka, ICAR3R – Interdisciplinary Centre for 3Rs in Animal Research, Justus Liebig University Gießen
Gaia Tavosanis, Center for Neurodegenerative Diseases (DZNE), Bonn
Jonathon Howard, Department of Molecular Biophysics & Biochemistry, Yale University

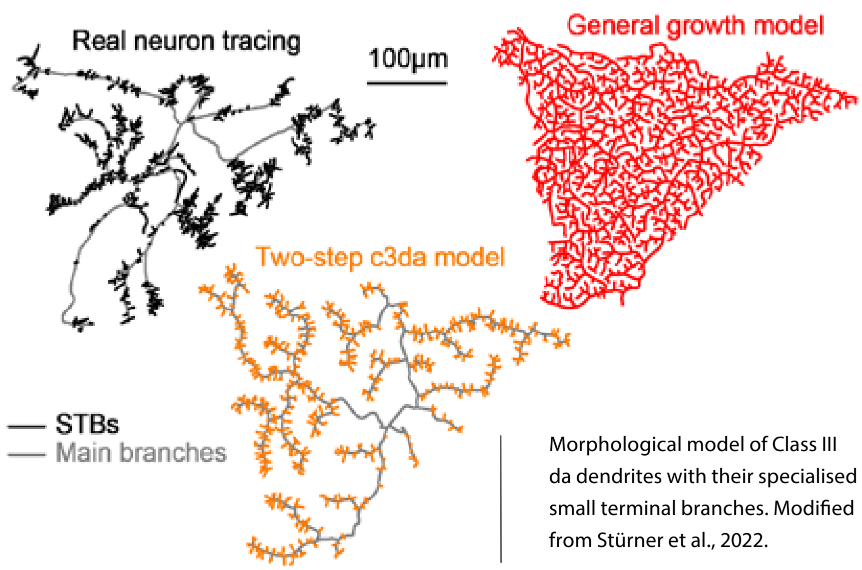
A branching code for neuronal dendrites

Dendrites of neurons are the beautifully branched input structures that shape a neuron's connectivity and the underlying computation on its inputs. We are working with computer models that describe the morphology from simple optimal wiring criteria: The dendrite collects inputs from other neurons in a way to minimise the required material and the conduction delays in the circuit. One question is whether this type of optimisation should also lead to space-filling trees and which developmental growth program might be responsible for this.

Recently, we introduced a regularity index R, based on average nearest neighbour distances to vary the input organisation in our models. Interestingly, the input regularity RInput, which could be measured and modelled during dendritic maturation and in EM-based connectomes, could be read out in the regularity of a dendrite's branching points distribution but not in the value for termination points that were more randomly spread. Most importantly, RInput in different cell types could be fundamentally different such as in fly dendritic arborisation (da) neurons or rather similar such as in fly lobula plate tangential cells.

In response to these insights and efforts, we formulated a novel theory of dendrite growth based on detailed developmental experimental data in Class IV da neurons in the fly. These dendrites optimise wiring and space filling. Synthetic dendrites generated from scratch using growth rules based on optimisation principles followed the dendritic development observed in these cells.

Having identified the Class III da neuron for its irregular space filling because of its specialised branches (STBs, Figure 1, black) we found that for these cells the general space filling growth model obtained in Class IV da neurons (Figure 1, Red), did not perform well. Modelling Class III da neurons interestingly required a second step that confined STBs in a close range to the main branches (Figure 1, Orange). A more regular space filling was partly recovered in actin regulatory protein mutants indicating the importance of these proteins in a secondary growth program step for STB formation. Overall, computer modelling helps us dissect the precisely timed growth programs that seem to lead to the diversity of dendritic trees that we observe in the brain.



Morphological model of Class III da dendrites with their specialised small terminal branches. Modified from Stürner et al., 2022.

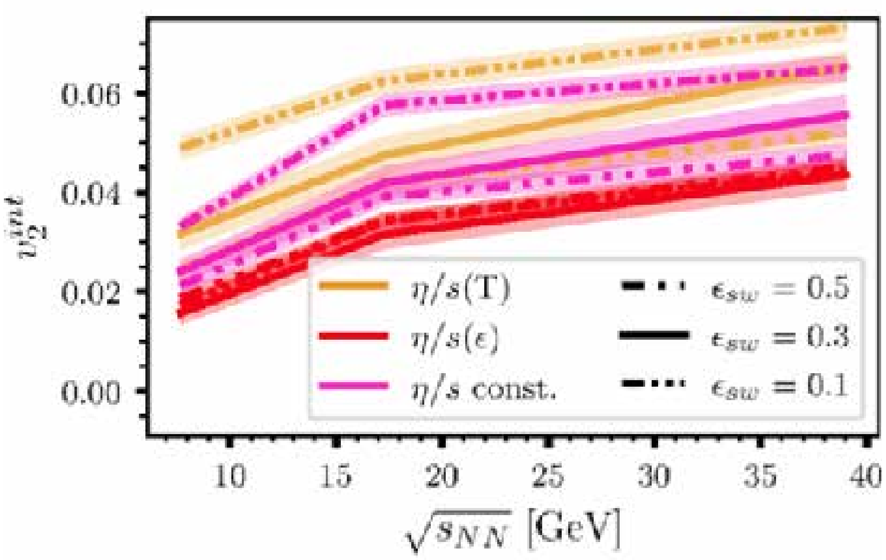
Density dependence of shear viscosity of quark-gluon plasma

Hybrid approaches based on relativistic fluid dynamics for the hot and dense stage and hadronic transport for the dilute regime are well suited to describe the dynamical evolution of the collision of two ions at very high beam energies. Such collisions are experimentally investigated at the Relativistic Heavy Ion Collider on Long Island and the Large Hadron Collider at CERN. We have established a new hybrid approach employing the SMASH (Simulating Many Accelerated Strongly-interacting Hadrons) transport approach for the initial and final stage and the vHLLE code for the viscous hydrodynamic evolution. The advantage is that in such an approach the phase transition to the quark-gluon plasma can be treated by a change of the equation of state.

In the particle multiplicities and spectra of the most abundant particle species have been investigated and all necessary parameters have been adjusted.

The approach has subsequently been applied to investigate the density dependence of the shear viscosity of strongly interacting matter. Therefore, an energy density and net baryon density dependent parametrization has been formulated. A very nice result is shown in the figure below. The elliptic flow that is generated does not depend on the switching transition between fluid dynamics and hadronic transport in case of the newly parametrized form for the shear viscosity over entropy density ratio. In turn, this finding points to the fact that this viscosity is close to the one of the hadron gas in the non-equilibrium evolution.

Simulations of the elliptic flow as a function of the collision energy for different switching criteria and different forms of the shear viscosity over entropy density. (from Phys. Rev. C 106 (2022) 5)



Prof. Dr. Hannah Elfner

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

Highlight

The ceremony for the Scientist of the year 2021 award, finally allowed in June 2022, and the retreat with my working group in May, which helped to reconnect after the pandemic.

Projects at FIAS: 3

Staff

Jan Hammelmann (DFG SinoGerman), Renan Hirayama (HFHF), Alessandro Sciarra, Gabriele Inghirami, Hendrik Roch, Justin Mohs, Niklas Götz, Nils Saß, Antonio Bozic, Timo Füle, Branislav Balinovic, Julia Gröbel, Lucas Constantin

Collaborations

JETSCAPE collaboration, USA
MUSES collaboration, USA
TMEP collaboration, international
Yuri Karpenko, Prague University, CZ

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.

Highlight

First last authorship paper!

Projects at FIAS: 1

Staff

Robin Mayer
Dilan Savran

Collaborations

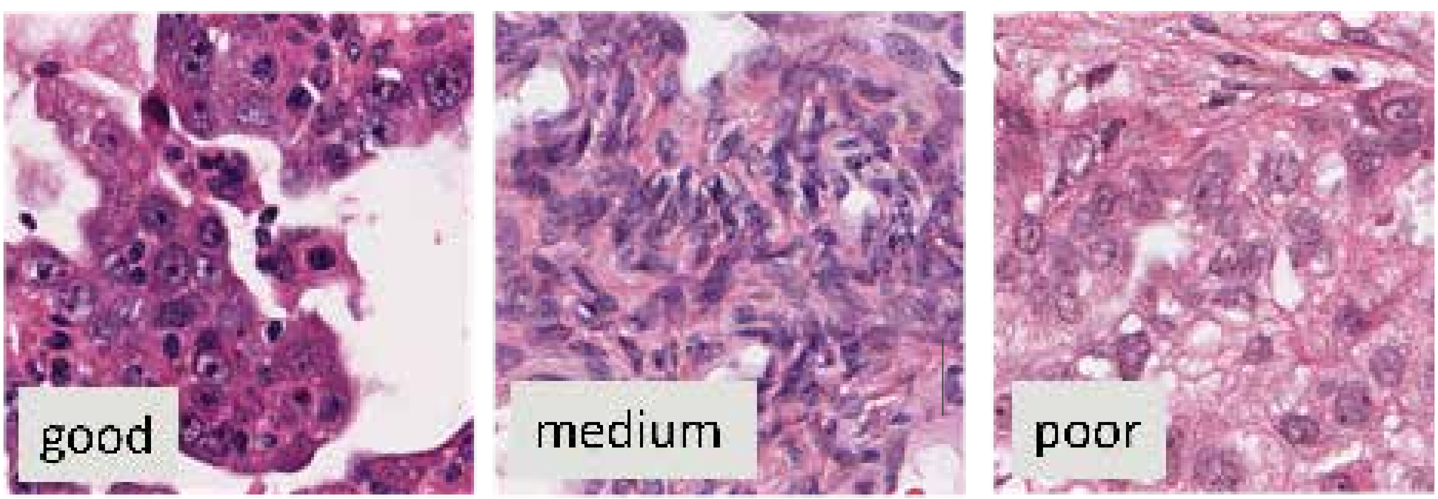
Peter Wild, Sotirios Fragkostefanakis, FIAS
Henning Reis, Sylvia Hartmann, GU

Tissue Quality in Computational Pathology

After successfully predicting cancerous and healthy areas for different cancers (e.g. stomach or ovary) together with some molecular properties in histopathological tissue sections we have focused in 2022 on the influence of the tissue itself. We showed that convolutional neuronal networks (CNN's) which were trained on high quality data were only poorly transferable to low quality data. But vice versa CNN's trained with low quality data also performed well with data of high quality. This finding indicates that it is pretty important to use tissue sections of a high quality in clinical routine in case CNN's should be included into the medical workflow. But slides of lower quality should be definitely included in CNN training to enlarge the dataset size and to improve CNN transferability to other datasets. Interestingly the use of actual quality control tools did not improve our prediction results on cleaned data, indicating that also these tools are barely transferable at the moment.

In general transferability between different datasets is a well described problem in computational pathology, which is not always caused by different quality levels. Also different workflows, protocols, staining solutions or scanner devices can cause similar problems. To now overcome these transferability problems and to improve prediction results for tissue slides with low quality we have introduced Noisy Ensembles: Individual CNN's where trained via a bagging approach with some label noise (intentionally 15% mislabeled data) introduced into the training dataset and a simple majority vote was implemented. Using this approach the accuracy of the individual CNN was decreasing but on high quality data the performance of the complete ensemble is nearly unchanged, while for low quality data it even improved.

Exemplary tiles of tissue sections with good, medium and poor quality. Classification was performed by a pathologist based on different criteria like image sharpness or contrast (from: Mayer RS, Gretser S, Heckmann LE, Ziegler PK, Walter B, Reis H, Bankov K, Becker S, Triesch J, Wild PJ, Flinner N. How to learn with intentional mistakes: NoisyEnsembles to overcome poor tissue quality for deep learning in computational pathology. Front Med. 2022;9:959068. doi:10.3389/fmed.2022.959068.



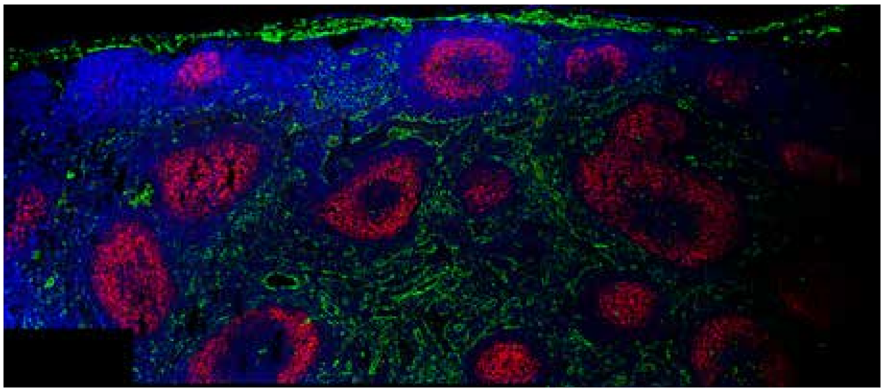
4D demonstrates interactions in the human immune system

A major focus of the research activities of my working group in 2022 was the further development of the 3D and 4D technologies we had established in the human immune system. These are representations of lymphatic tissue in space and time. With the help of confocal lasers and suitable cell markers, we are able to visualise the different cell types in the lymph node as well as in other tissues. Tracking data is thus generated, which is then analysed with the help of bioinformatics and machine learning methods.

We published a paper that uses 4D technology to analyse malignant lymphoma, Hodgkin's lymphoma, and non-Hodgkin's lymphoma. Surprisingly, we found that the length of cell contacts between B and T cells is typical for different types of lymphoma. Based on these data, decisive improvements in diagnostics as well as completely new approaches in therapy and probably also in predicting the effectiveness of cell therapies are possible. Based on these data, we have used machine learning methods for the first time to characterise cells of the immune system on the basis of cell speeds and cell movements, combined with cell morphologies. We found that the combination of the appearance of a B or T cell with its movement is highly informative. It is comparable to an immunohistochemical characterisation of a cell type. The new strategies also allow us to define new cell types and subtypes. Finally, we were able to produce movement maps based on cell movements in the tissue, which give us information about cellular interactions between different immune compartments.

In addition to the scientific focus programme described above, we worked on individual malignant diseases of the immune system. We defined new biological and diagnostic properties in certain malignant tumour types. These investigations also point to steps that should lead to greater diagnostic precision and further patient-tailored diagnostics and therapy.

Publications: Wagner P et al. New definitions of human lymphoid and follicular cell entities in lymphatic tissue by machine learning. Sci Rep. doi: 10.1038/s41598-022-18097-9.
Bein J et al. T-cell-derived Hodgkin lymphoma has motility characteristics intermediate between Hodgkin and anaplastic large cell lymphoma. J Cell Mol Med. doi: 10.1111/jcmm.17389.
Sadeghi Shoreh Deli A et al. 3D analyses reveal T cells with activated nuclear features in T-cell/histiocyte-rich large B-cell lymphoma. Mod Pathol. doi: 10.1038/s41379-022-01016-8.
Hartmann S et al. Tumour cell characteristics and microenvironment composition correspond to clinical presentation in newly diagnosed nodular lymphocyte-predominant Hodgkin lymphoma. Br J Haematol. doi: 10.1111/bjh.18376.
Ballhausen A et al. Immune phenotypes and checkpoint molecule expression of clonally expanded lymph node-infiltrating T cells in classical Hodgkin lymphoma. Cancer Immunol Immunother. doi: 10.1007/s00262-022-03264-8.



Confocal laser visualisation of a part of a human lymph node. B (red) and T cell (green) areas are shown (blue, DAPI). (AG Hansmann)

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

First characterisation of malignant human lymphatic diseases in tissue in space and time.

Projects at FIAS: 1

Staff

Hendrik Schäfer
Patrick Wurzel
Sonja Scharf

Collaborations

TU Berlin
Fraunhofer Institute, Berlin
Molecular Informatics, Goethe-Uni

Prof. Dr. Gerhard Hummer

He studied physics and received his PhD at the University of Vienna, Austria, and 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) as 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 2022, the Hummer group performed the first molecular dynamics simulations of a full nuclear pore complex.

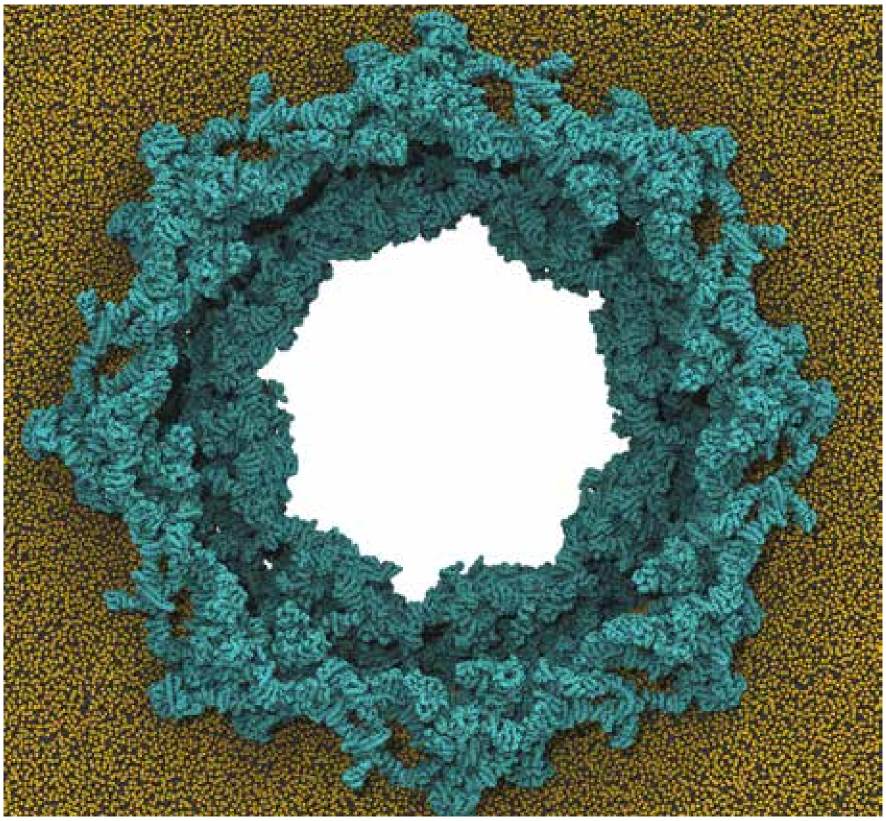
Projects at FIAS: 1

Collaborations

Roberto Covino
Sebastian Thallmair

Molecular simulations of the nuclear pore complex

2022 was a truly exciting year for our group with publications in Science, Cell, Science Advances, PNAS, Nature Communications (2x), EMBO J (2x), JACS Au, and Molecular Cell, to name but some. This output is a reflection of the growing relevance of molecular simulations in the biosciences and beyond. Our most exciting result in 2022 has been the first molecular dynamics simulations of a nuclear pore complex. We conducted this study as part of an amazing collaboration with the group of Martin Beck at the MPI of Biophysics and with Jan Kosinski at EMBL. The human nuclear pore complex is a massive assembly of about 1000 proteins that together form what is arguably the most complex structure in human cells: a ring with eight-fold symmetry that sits in the half-toroidal pores of the double-membrane nuclear envelope. Its function is to gate the molecular traffic between the cytosol of the cell and its nucleus. In particular, it ensures that gene regulatory molecules such as transcription factors are allowed in, messenger RNA (mRNA) is shuttled out, and pathogenic factors such as viral RNA are blocked. This makes the nuclear pore complex not only a defining feature of eukaryotic cells, but also critical to their function. With our molecular simulations, we could show that the membrane of the nuclear envelope exerts significant mechanical tension on the nuclear pore complex. We could also show that mechanical tension in the nuclear envelope can counterbalance the ring tension. Together, we could show in molecular dynamics simulations that mechanical tension can reversibly drive the nuclear pore between a constricted and a dilated state, and thus provide the lever to open and close the pore for the nucleocytoplasmic traffic. Our study was published as (Mosalaganti, Obarska-Kosinska, Siggel et al., Science 376, eabm9506 2022, DOI: 10.1126/science.abm9506) and featured in news outlets around the world, from Der Spiegel to Time Magazine.



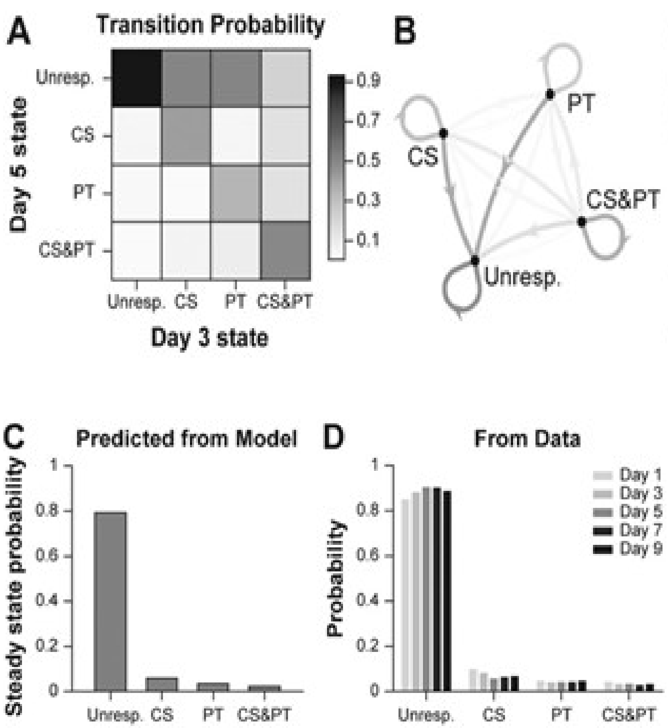
The human nuclear pore complex, as the gate-keeper guarding the human genome and ensuring the safe transfer of mRNA of the cell nucleus, has been studied in molecular dynamics simulations (Mosalaganti et al., Science 376, eabm9506, 2022; Image: Marc Siggel).

The stable unstable brain

The classical view holds that the brain's representations of the external world are fairly stable, and updated only during learning. In 2022 we published two articles together with neurobiologist Simon Rumpel (University of Mainz) that challenge this view by showing that the representations of sounds in the auditory cortex change considerably even in a familiar, unchanged environment. These results are consistent with several recent studies in other brain regions.

In our first article (Aschauer et al., Cell reports, 2022) we found that after only two days 30% of the stimuli that had evoked a response in a local population of neurons were replaced by different stimuli (previously mapped to different local populations). Thus, from the perspective of a local network, there is an ongoing, and balanced, influx and outflux of stimuli mapped to this network. How does learning interact with these ongoing dynamics? We showed that it alters the relative rates of these fluxes, resulting in a co-mapping of certain stimuli, which the experiments suggest can be interpreted as newly formed associations.

In the second article (Chambers et al., Cerebral Cortex, 2022) we 'zoomed out' and studied the effect of these ongoing dynamics at the larger level of extended, millimeter-wide networks in auditory cortex. We found that while individual cells changed their responsiveness to sound stimuli, the global structure in the mapping of frequencies to the cortical surface (the 'tonotopic map') remained stable across all imaging time points, reflecting a statistical equilibrium. The gain and loss of responsiveness in individual neurons was well approximated by a first order Markov model, hinting at a duty cycle governing these transitions in individual neurons. Interestingly, these dynamics are reminiscent of 'drop-out' in machine learning, a strategy to prevent overfitting by transiently excluding random subsets of neurons during network training.



Neurons transition between four states: Unresponsive, responsive to complex sounds (CS), to pure tones (PT), or to both (CS&PT). A first order Markov model captures these transition dynamics. A) Transition matrix. B) Diagram of matrix in (A). C) Steady state predicted from (A). D) State distribution in experimental data.

Prof. Dr. Matthias Kaschube

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

Highlight

The DFG DIP-grant "The Neurobiology of forgetting" has started, and funded Jonas Elpelt and Sigrid Trägenap, both doctoral students in my group.

Projects at FIAS: 5

Staff

Lorenzo Butti, Jonas Elpelt, Bastian Eppler, Deyue Kong, Thomas Lai, Pamela Osuna, Sigrid Trägenap

Collaborations

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

Prof. Dr. Udo Kebschull

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

Highlight

Work with ekom21 on blockchain-based logging of electronically archived hotel registration forms.

Projects at FIAS: 3

Staff

Philipp Lang
Diyar Takak
Felix Hoffmann

Collaborations

Hessische Zentrale für Datenverarbeitung (Hessian center for data processing)
ekom21 – KGRZ Hessen

Applications of blockchain technology

Blockchain technology continues to be a controversial topic. Special features are the possible uses and energy requirements. The team with Philipp Lang, Diyar Takak, and Felix Hoffmann conducts targeted research in the blockchain cryptography specialization in order to identify and improve upon weaknesses of blockchain technology and to use desirable properties to advantage.

Under Philipp Lang, there is cooperation with the Hessische Zentrale für Datenverarbeitung (HZD) with authentication via the RADIUS protocol using the blockchain that can be used in the Eduroam network. The single sign-on should also be implemented on a physical level so that students can authenticate themselves at any university within the Eduroam network. In addition, Lang continues to cooperate intensively with the Bloxberg consortium, which has grown into an association with many university cooperations. Future blockchain-based applications are to be tested here.

Diyar Takak is also very interested in working with the Bloxberg association and is benefiting from Lang's preliminary work in order to test future applications on the blockchain. Diyar Takak is working with ekom21 on blockchain-based logging of electronically archived hotel registration forms within the ONCE consortium. In addition, Tayak is on a blockchain-based protocol execution that makes it possible to track documents stored on clouds with confidential/private data in a sustainable and tamper-proof manner due to the decentralized nature of blockchain technology. In this project, Takak is supported by Philipp Lang.

Within the framework of the ONCE, there is also a need for an SSI-based concept for the authentication of digital identities in public administration. This is also being tackled in cooperation of Lang and Takak. Felix Hoffmann researches blockchain consensus algorithms and distributed computing approaches. He explores the idea of a Proof-of-Useful-Work consensus algorithm which in contrast to hash-based Proof-of-Work creates value outside of the blockchain network by supporting real-world scientific experiments with data. He also explores alternative distributed computing approaches such as BOINC projects which enable volunteer computing without an underlying blockchain. Hoffmann is part of HFHF from which he was granted a scholarship. In HEP there is a need for large amounts of computing power, for instance the High-Luminosity Era of LHC will require more accurate Monte Carlo simulations than ever before. The trend of increasing luminosity and simulation accuracy also affects other HEP experiments such as CBM at FAIR, which would greatly benefit from a novel Proof-of-Useful-work consensus in the future.

Finally, the blockchain seminar was conducted under the direction of Kebschull with the help of Takak and Hoffmann. This will be offered again along with lectures in computer security and mainframe computing. Additionally, all three candidates actively supervise Bachelor and Master theses. In 2022, a total of 19 theses were supervised and one promotion was successfully completed.

Search for hypernuclei in the STAR experiment

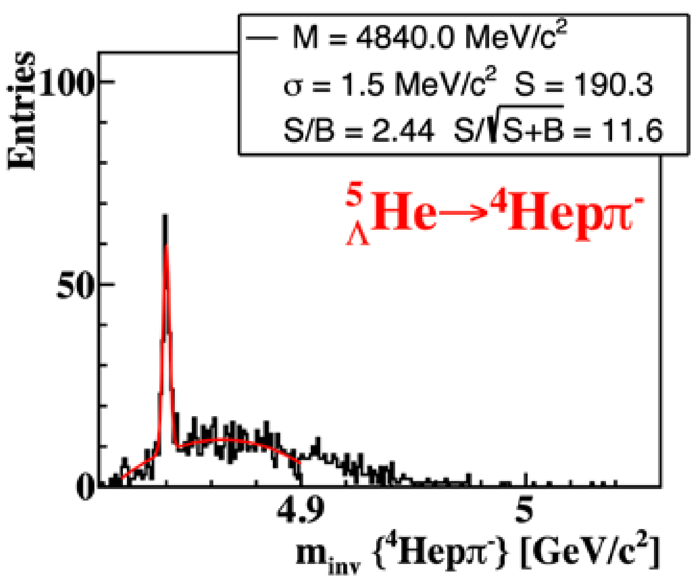
Hypernuclei search in the STAR experiment at Brookhaven National Laboratory (BNL) in the USA is an ongoing research effort aimed at studying the properties of nuclei that contain strange quarks.

The STAR experiment is a large-scale collaboration in heavy-ion physics that utilizes the Relativistic Heavy Ion Collider (RHIC) at BNL to study the properties of matter at extreme conditions, including the behavior of strange quarks in nuclei. The experiment uses high-energy collisions of heavy ions to create new forms of matter, including hypernuclei, which are then detected and analyzed. The study of hypernuclei provides valuable information on the behavior of strange quarks in the nuclei and can shed light on our understanding of the strong interaction, the force that holds the nucleus together.

In recent years, the STAR experiment has made significant contributions to the field of hypernuclear physics, including the observation of new hypernuclei and the measurement of their properties. The results of these studies have helped to improve our understanding of the strange quark sector and the behavior of baryons in extreme conditions. The study of hypernuclei continues to be an active area of research in the STAR experiment, and new developments and advancements are expected in the future.

Moreover, the study of hypernuclei also has potential implications for several other areas of physics, including the study of neutron stars, the properties of dense matter, and the behavior of strange quarks in a nuclear environment. In addition to the STAR experiment, there are several other ongoing efforts to study hypernuclei, both at accelerator facilities and through theoretical calculations. These efforts complement each other and provide a comprehensive understanding of the strange quark sector.

Recently, as part of the Beam Energy Scan (BES-II) research program in the STAR experiment, our FIAS group, together with scientists from the CBM (FAIR/GSI) and STAR (BNL) groups, using the CBM FLES reconstruction algorithms, has detected in real time 37916 $_{\Lambda}^{3}$H, 37819 $_{\Lambda}^{4}$H, 978 $_{\Lambda}^{4}$He, and 190 $_{\Lambda}^{5}$He hypernuclei. The detection of such a significant number of hypernuclei will allow us to study in detail the behavior of strange quarks in the hypernuclei.



In the STAR experiment within the Beam Energy Scan (BES-II, 2019-2021) research program, our FIAS group, together with scientists from the CBM (FAIR/GSI) and STAR (BNL) groups, using the CBM FLES reconstruction algorithms, has detected 190 $_{\Lambda}^{5}$He hypernuclei at a significance level of 11.6, which means that the signal level exceeds the background fluctuations by a factor of 11.6.

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

We detected 76.903 hypernuclei in real time in the STAR experiment (BNL, USA) using the FLES reconstruction algorithms of the CBM experiment (FAIR/GSI).

Projects at FIAS: 3

Staff

Artemiy Belousov
Akhil Mithran
Oddharak Tyagi
Robin Lakos
Gianna Zischka

Collaborations

CBM
ALICE
STAR

Prof. Dr. Volker Lindenstruth

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

Highlight

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

Projects at FIAS: 4

Staff

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

Collaborations

CERN
GSI

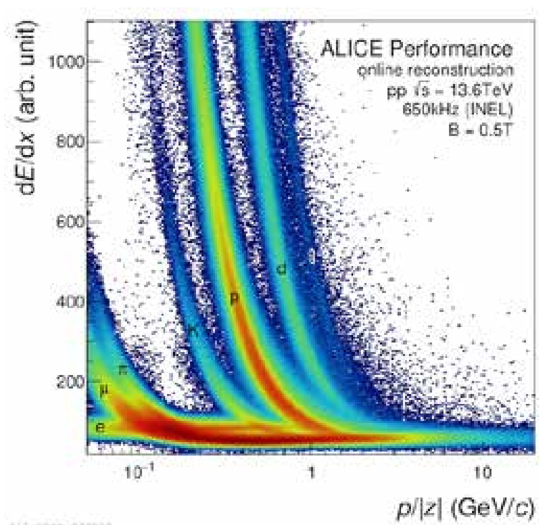
Fast data processing at large scale research

On July 5, 2022, the newly upgraded Large Hadron Collider (LHC) returned to full operation, providing proton-proton (pp) collisions at a record energy, commencing the higher luminosity Run 3. For ALICE, the dedicated experiment to study the strongly interacting matter produced in heavy-ion collisions at the LHC, many upgrades were necessary to prepare for the increased number of collisions. These included an upgrade to the compute farms, necessary for handling the higher data rates and the more intense data processing. ALICE can now collect a continuous stream of data as opposed to the old trigger-based readout. Consequently, in Run 3 and 4, ALICE will collect nearly 10x more data than in all previous LHC data taking periods and will thus deliver higher precision measurements.

The new compute farm comprises the First Level Processors (FLP) and the Event Processing Nodes (EPN). The former receives detector data and performs local processing. For the TPC detector (the largest data source) zero suppression is performed here as well, reducing the 50 kHz lead-lead (Pb-Pb) data rates from an unmanageable 3.5 TB/s to 900 GB/s. The data are then sent the EPN farm, using Infiniband network, via data-distribution software. The EPN farm contributes the most compute power and is composed of 280 servers, each equipped with eight AMD MI50 GPUs, two 32-core Rome CPUs, and 512 GB of memory: totaling to 2240 GPUs. The farm provides the fastest possible TPC track reconstruction, which is the largest contributor to the online processing, with 90% of the compute being provided by the GPUs.

At FIAS, our group has spearheaded the use of GPUs for the processing and compression of ALICE data. In previous LHC runs, since 2010, the High-Level Trigger compute farm was crucial for data compression of the Pb-Pb events. Today fast processing and compression are even more crucial as we must, in real time, keep up with the massive increase of data volumes and fit them on the available storage space. This is only possible with GPUs, as they are extremely efficient processors relative to CPUs and are faster with parallelized tasks. The ALICE EPN farm design decision provided significant cost savings as well, e.g., a GPU-less farm would require 8x as many servers.

The online data processing was successful in 2022: ALICE processed pp collisions up to a 2.6 MHz inelastic interaction rate. There was no large-scale Pb-Pb run in 2022, however a day of low intensity was provided by the LHC for testing our data-processing systems, and the data collection went smoothly.



TPC energy loss (dE/dx) as a function of momentum from the on-line processing on the EPN farm.

Modular Supercomputing and Quantum Computing

In 2022, the MSQC group has substantially intensified its research and development activities in the area of the novel architecture and programming paradigm of modular supercomputing. This includes communication networks for optimized interaction and scheduling of disaggregated resources, but also the integration of future non-von Neumann architectures, in particular quantum computers to enable performing the most promising application of future quantum computers, so-called hybrid quantum HPC computations. MSQC supports the Goethe University in its further development into a national center for high performance computing within the NHR-SüdWest in the German NHR network, in particular in the efforts to include quantum computing. We closely collaborate with the Jülich Supercomputing Centre (JSC), in particular with its quantum computing platform JUNIQ, in order to create a broad extension of the offer in quantum computing at the CSC.

In Modular Supercomputing, we explore novel architectures and programming paradigms to enable this innovative technology. This includes simulation and analysis of heterogeneous network and storage infrastructures, monitoring and analysis of system utilization and workload behavior, I/O and memory optimization of new application workloads or container standard. We have launched a number of projects. One illustrative example for our work is MAWA-HPC, a comprehensive system for modular and automated workload analysis for HPC. MAWA will be a generic workflow and tool suite that can be applied to different use cases in different domains and supports different community tools through its modular design. Furthermore, we are member of the EUPEX Project, the European Pilot for Exascale, with more than ten European partners, and we are contributing to the NHR Project Container Standards in HPC.

In our research area Quantum Computing, we conduct research and development on several levels: First, we are leveraging the group's extensive experience in modular supercomputing to create the technical requirements for the technical coupling of HPC-QC systems and their use: This ranges from high-level programming for quantum computers to the compile-time toolchain, run-time toolchain, and hybrid HPC-QC programming. We are also heavily involved in fundamental research on quantum computing, where we are working on tools to study the quality of qubits and qubit gates, tools to measure the crosstalk properties of qubit registers, and determining the limits of the quantum theoretical description of QCs. We are also currently in procurement discussions to purchase a first small pilot quantum computer system for Goethe University in 2023, to be expanded to more than 20 qubits by the end of 2024. An exemplary project here is the integration of quantum processors into the Modular Supercomputing Architecture, where we show that quantum processors fit naturally into the MSA concept. We achieve the integration by extending the OmpSs-2 programming model, which has already been used in the MSA context for other accelerators. Furthermore, we entered into a close cooperation with the companies Quantum Machines (Israel) and ParTec (Munich) within the framework of the new project CQC (cryo-quantum computing). A first software prototype developed by us will be ready for use in mid-2023.

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 the Chair 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.

MAWA-HPC
MODULAR AND AUTOMATED WORKLOAD ANALYSIS

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 GU.

Highlight

At the European Conference for Mathematical and Theoretical Biology (ECMTB) in Heidelberg this year with about 600 participants, PhD students of the AK Matthäus were successful, winning 3 out of 12 poster prizes, including the Lewis-Wolpert prize for Marc Pereyra.

Projects at FIAS: 3

Staff

Zoë Lange, Camile Kunz, Tim Liebisch, Marc Rereyra

Collaborations

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

A new PDE model coupling pattern formation processes

Pattern formation is an important mechanism exploited in living systems, for instance during development. Embryonal skin patterning in mammals and birds results in regularly placed cell clusters which form the precursors for hair follicles and feather buds. Regular spatial patterns can emerge based on different mechanisms. Diffusion-driven instability arises in reaction-diffusion systems of chemical compounds, such as growth factors. Hereby, diffusion and interaction lead to a spatial instability of the system and the appearance of periodic pattern. Another mechanism is the interaction of motile cells interacting with chemical compounds, called chemotaxis. In mouse skin patterning both mechanisms interact. The upper, epithelial cell layer, secretes growth factors, which, through diffusion-driven instability generate a spatial patterning which serves as a map for moving cells of the dermal layer performing chemotaxis. Camile Kunz of the AK Matthäus developed in the past years a coupled system of PDE's to model the interaction between the two patterning mechanisms. Linear stability analysis as well as numerical simulations show, that the combination of both patterning mechanisms enlarge, in most cases, the parameter space for patterning, and thus make the patterning process more robust. We find that the patterns emerge faster when chemotaxis is dominant, however, on the cost of pattern regularity. Analysis of the model also helped to find a new condition for patterning, which is not present in the two individual mechanisms. Further, for some parameter settings, the combination of the two processes can lead to a destabilization and extinction of the pattern, instead of providing enhanced robustness. This mathematical model thus provides further understanding of embryonal development and can be used to guide further experimental studies. An article on the results of this project is currently in preparation.

Members of AK Matthäus presenting their poster prizes obtained at the ECMTB 2022 in Heidelberg.

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 2022 we extended our work on preferential attachment graphs: While traditionally the probability for new nodes to link to previous ones is linearly proportional to the current degrees of the existing nodes our new generators manage to handle non-linear linking probabilities (ALENEX 2023).

Similar generators also played an important role in the practical evaluation of our new results on certifying induced subgraphs in large networks (WALCOM 2023). In addition, we published two survey book chapters on recent advances in scalable network generation: the first one considers the field in general whereas the the second one reviews the works obtained in DFG priority programme SPP 1736 (Algorithms for Big Data, https://www.big-data-spp.de), which was coordinated by our group and ended in 2022. Altogether SPP 1736 produced about 300 publications with by now more than 9500 citations.

Prof. Dr. Ulrich Meyer

He joined FIAS in January 2020. He is a full professor at Goethe University Frankfurt since 2007. From 2014 to 2022 he was also the spokesperson of the DFG priority program "Algorithms for Big Data" (https://www.big-data-spp.de/, SPP 1736). He 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

In 2022, we celebrated the final meeting of our SPP 1736 Big Data priority programme in Frankfurt with many members of both funding phases and and various invited talks. Our open access book (LNCS 13201, link https://link.springer.com/book/10.1007/978-3-031-21534-6) surveys selected research results.

Projects at FIAS: 2

Staff

Yannick Gerstorfer
Hung Tran

Cooperations

within CMMS
DFG FOR 2975

Group meeting of the DFG priority programme SPP 1736 (Algorithms for Big Data).

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 long-term stays in the Niels Bohr Institute (Denmark) and the University of Minnesota (USA), he joined the newly-established Frankfurt Institute for Advanced Studies, in 2004. Here he leads the group of theoretical subatomic physics and astrophysics.

Highlight

Established cooperation with NAPLIFE collaboration in the field of laser-generated dense plasma.

Projects at FIAS: 2

Collaborations

Horst Stoecker
Mark Gorenstein
Leonid Satarov

Nuclear reactions induced by laser beams in polymer targets

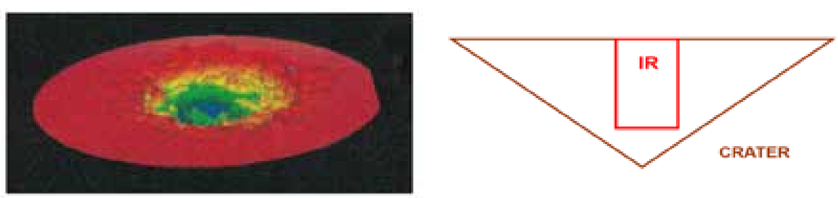
We have analysed the results of NAPLIFE experiments on laser irradiation of UDMA-foils, with implanted gold nano-particles. The left figure below shows a typical snapshot of a crater formed in such target. These experiments have shown a significant formation of deuteron atoms at high enough laser intensities, although initially the target contained no deuterium. Moreover, the deuterium yield increases with the concentration of implanted nano-particles.

To explain this interesting result, we have proposed a simple model assuming that deuterons are produced in the nuclear transmutation reactions. We assume that free protons are liberated from UDMA molecules under the action of the laser beam. Initially, these protons occupy the narrow cylindrical channel made by the laser beam, see right figure. At later times these protons propagate through the UDMA material and may induce nuclear reactions in the whole crater volume.

Our analysis has been focused on the possibility of nuclear transmutation reactions of fast protons on carbon isotopes, 12C and 13C, both present in the UDMA molecules. We have demonstrated that proton energies achievable in the laser-target interaction are sufficient for deuteron formation in such reactions, especially for targets with implanted golden nano-particles.

Additional investigations are necessary for verifying these results. It would be interesting to perform experiments with higher laser intensities e. g. at GSI/FAIR PHELIX and future ELI-ALPS facilities. Additional diagnostics tools would be desirable, including measurements of X-rays, neutrons, α-particles, etc.

On the theoretical side, the numerical modeling of target plasma evolution is necessary to estimate yields of secondary particles and their momentum distributions. Special investigation should be made to study the origin of hot-spots created by nano-particles, and their role in the nuclear transmutation.



Left panel: typical configuration of the crater, created in the UDMA target by laser beam. Right panel: schematic cross section of the crater and the laser irradiation region (IR). The energy and momentum of the laser beam (propagating from above) is initially absorbed in the IR.

Size limits of neutron stars and image of black hole

How large is a neutron star? Previous estimates varied from eight to sixteen kilometres. Astrophysicists around Rezzolla have now succeeded in determining the size of neutron stars to within 1.5 kilometres by using an elaborate statistical approach supported by data from the measurement of gravitational waves.

Neutron stars are the densest objects in our universe, with a mass larger than that of our sun compacted into a relatively small sphere whose diameter is comparable to that of the city of Frankfurt. This is actually just a rough estimate, however. For more than 40 years, the determination of the size of neutron stars has been a holy grail in nuclear physics whose solution would provide important information on the fundamental behaviour of matter at nuclear densities.

The data from the detection of gravitational waves from merging neutron stars (GW170817) make an important contribution toward solving this puzzle. At the end of 2017, Rezzolla and his students Elias Most and Lukas Weih already exploited this data to answer a long-standing question about the maximum mass that neutron stars can support before collapsing to a black hole - a result that was also confirmed by various other groups around the world. The team now worked to set tighter constraints on the size of neutron stars.

The crux of the matter is that the equation of state which describes the matter inside neutron stars is not known. The physicists therefore decided to pursue another path: they selected statistical methods to determine the size of neutron stars within narrow limits. In order to set the new limits, they computed more than two billion theoretical models of neutron stars by solving the Einstein equations describing the equilibrium of these relativistic stars and combined this large dataset with the constraints coming from the GW170817 gravitational wave detection.

The researchers were able to determine the radius of a typical neutron star within a range of only 1.5 km: it lies between 12 and 13.5 kilometres, a result that can be further refined by future gravitational wave detections.

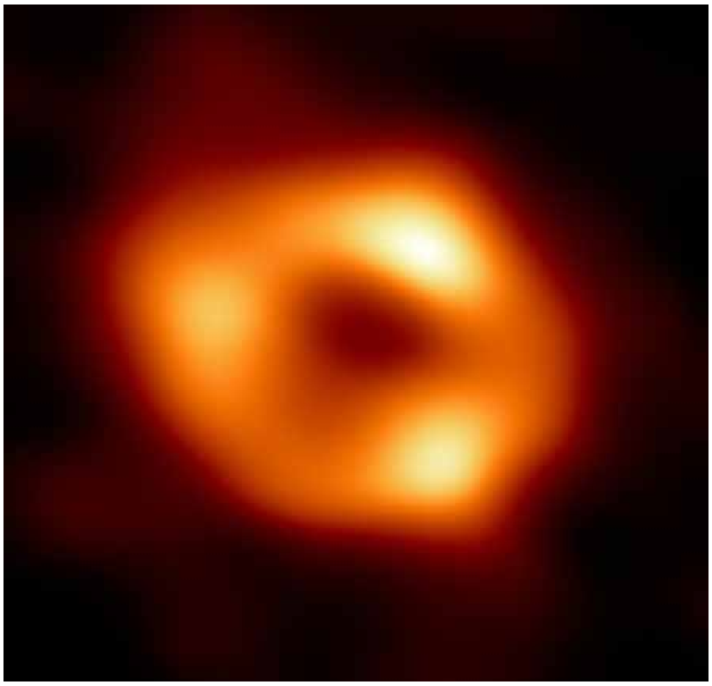
Prof. Dr. Luciano Rezzolla

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.

Highlight

Fueck Laureatus professorship for outstanding achievements in research and teaching by Walter-Greiner-Gesellschaft.

Projects at FIAS: 1



Eight super telescopes, many international working groups, and elaborate computer calculations over years led to the first image of the black hole at the center of our Milky Way. The group of Luciano Rezzolla performed extensive calculations to determine the properties of the plasma being sucked up by the black hole. They calculated three million synthetic images using different accretion and radiation emission models, also taking into account variations caused by different viewing angles of the black hole. Although the black hole itself is not visible - it is absolutely dark - the gas around it glows in a characteristic way: The image of Sgr A* shows a dark central region, the shadow of the black hole, surrounded by a bright, ring-like pattern. This is the light deflected by the black hole's immense gravity - the black hole has four million times the mass of our Sun.

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

Research visit to the Institute of Seismological Research (ISR) in Gandhinagar, India.

Projects at FIAS: 1

Cooperations

Department of Geology, Ministry of Mines, Honiara, Solomon Islands
Department of Geospatial Sciences and Technology, Ardhi University, Dar es Salaam, Tanzania
Institute of Seismological Research, Gandhinagar, India

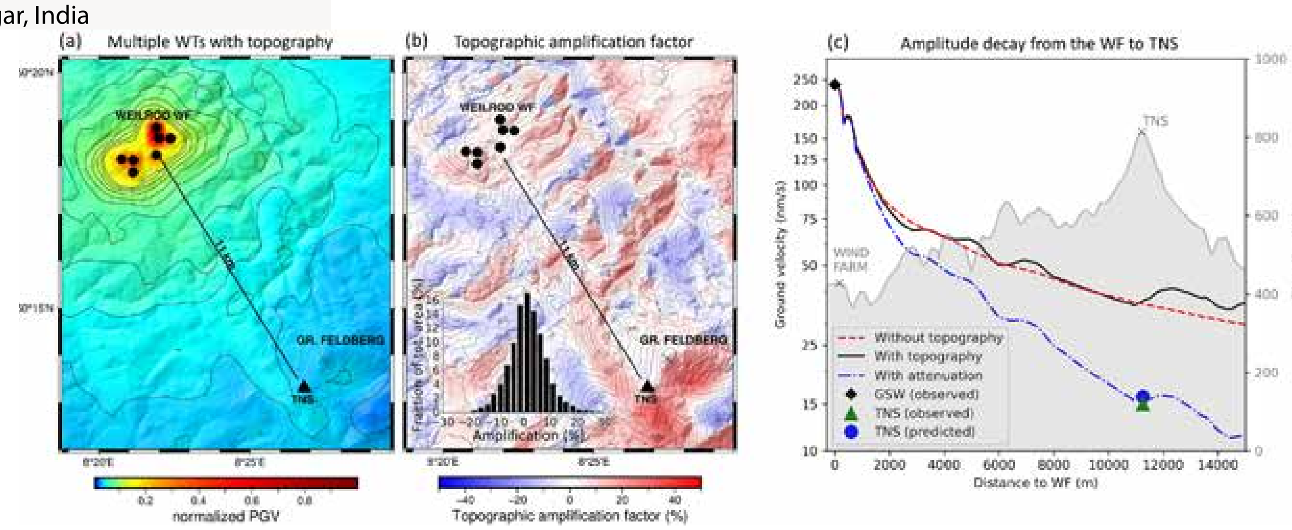
Modelling to predict seismic signals from wind farms

In an effort to reduce greenhouse gas emissions, renewable energies are increasingly being used to generate electricity. In particular, the number of wind turbines (WT) has risen sharply in recent years and continues to grow rapidly. To leverage negative effects on the surrounding environment, WTs are often erected in remote (and windy) areas. Similarly, seismic stations are typically located in remote areas to minimize the noise effects resulting from industries, railways, and traffic. Being mechanically coupled to the earth, WT also generate ground vibrations, which can have adverse effects on the capability of seismic observatories to detect and analyze earthquakes. However, the distances at which these signals modulate seismic records are disputed between the operators of wind farms (WFs) and seismic observatories.

To quantify the noise signal amplitudes at distant seismometers, we developed the first numerical model to predict the seismic wavefield emitted by WFs that simulates the complex interplay of wavefield interferences (due to multiple WT), surface topography and subsurface attenuation. This modelling approach can reliably quantify the influences of WFs on ground-motion recordings and thus provide necessary information to aid decision-making in advance of WF installations.

In a first case study (Limberger et al., 2022), we consider the 3D seismic wavefield generated by seven WTs comprising the Weilrod WF, situated northwest of Frankfurt (Germany). Considering the interference of the seismic signals generated by all seven WTs and including complex topographic effects, we compare the modelling results with observations from the permanent seismic station at the Taunus Observatory (TNS) located 11 km from the WF. By including wave-attenuation effects, we are able to precisely predict the noise signal amplitude at TNS based on additional near-field measurements. This novel approach is currently applied to a number of additional case studies.

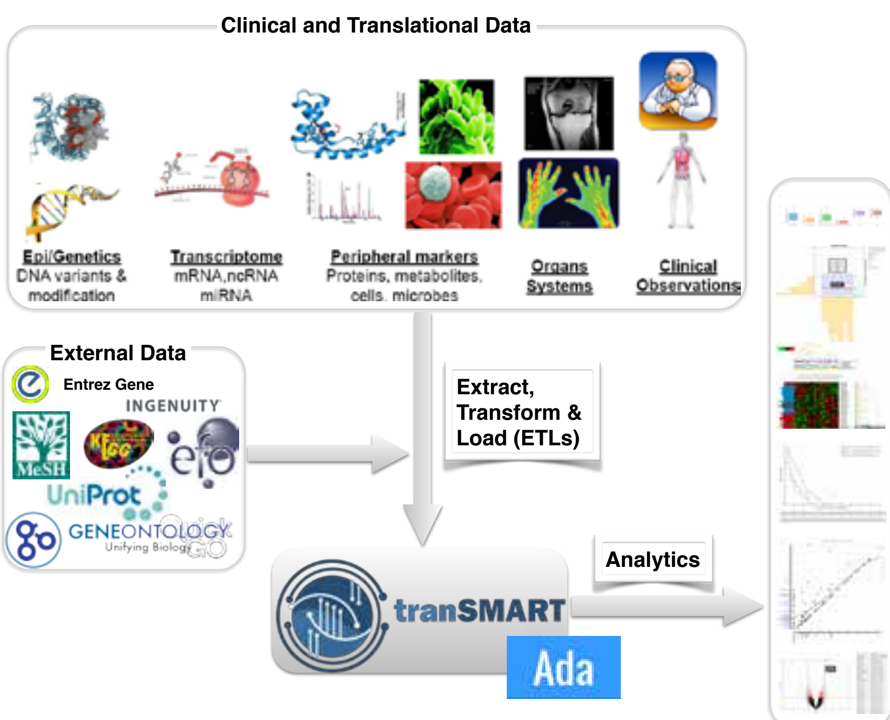
Maps of the average peak ground velocity (PGV) with topography (a) and the amplification factor due to topography (b) for all seven WTs in the Weilrod WF. The measured amplitude at TNS (distance 11 km) is finally predicted by including attenuation in the model (c).



Clinical and translational medicine informatics

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

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



Dr. Venkata Satagopam

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

Highlight

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

Projects at FIAS: 1

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

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)

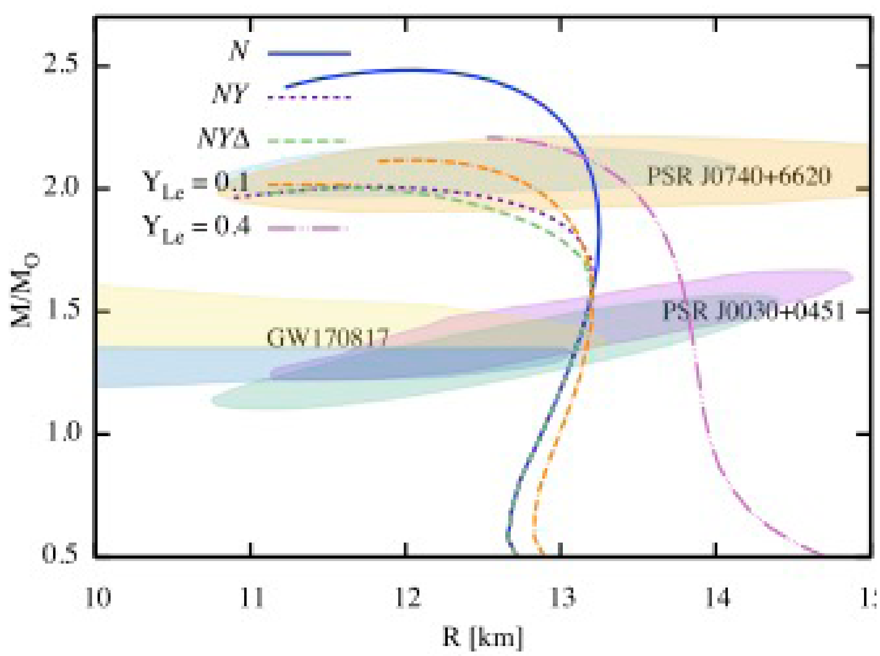
Studying densest forms of matter in the Universe

We have continued the studies of relativistic density functionals for hyperonic and Delta-resonance matter and compact stars. The equation of state of such matter was extended to finite temperatures and stars were studied at constant entropy per baryon (see the figure). Tables of equations of state were created which can be used for simulations of binary neutron star mergers and supernova explosions.

We have continued the studies of hybrid stars composed of quark cores and a hadronic envelope. It was shown that ultracompact stars can be formed with radii in the range of 6-8 km and small masses of the order of 1 solar mass. This surprising result indicates an alternative to the strange star hypothesis scenario for very small size compact stars.

The group also worked on the computations of bulk viscosity of dense matter as it occurs in binary neutron star mergers. The regime in which matter is transparent to neutrinos was studied in detail. This regime is shown to be relevant for the simulations of neutron star mergers.

Gravitational mass versus radius for non-rotating spherically-symmetric hot stars. Three sequences are shown for beta-equilibrated, neutrino-transparent stars with nucleonic (N), hypernuclear (NY), and Delta-admixed hypernuclear composition at zero temperature. In addition, we show sequences of fixed entropy per baryon equal to unity neutrino-trapped, isentropic stars composed of hypernuclear-Delta matter in two cases of constant lepton fractions. The ellipses show astrophysical constraints.



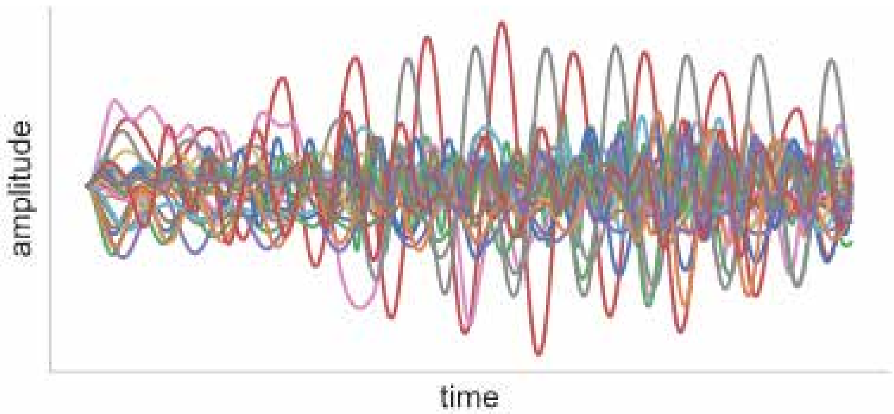
Simulation of recurrent cortical networks

The brain is an incredibly complex and sophisticated organ, responsible for a vast array of cognitive and perceptual processes. At the heart of these processes lies the cerebral cortex, a highly interconnected, modular recurrent network of neurons responsible for a wide range of functions, including sensory processing, motor control, and higher cognitive processes such as attention, memory, and decision-making.

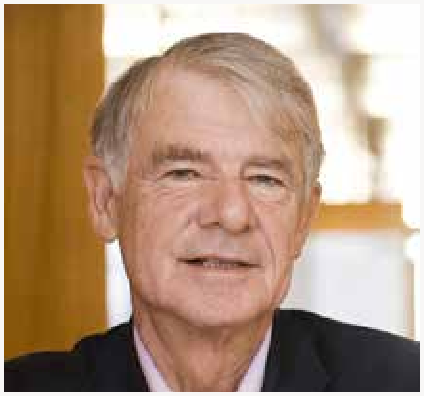
One of the striking features of the cerebral cortex is the vastness of its computational state space. This space is characterized by complex oscillatory dynamics resulting from neurons and subnetworks connected to one another in a highly recurrent and modular fashion. Moreover, the transmission of signals between neurons in the cortex is precisely timed, with delays that are carefully tuned to optimize the computational capabilities of the network. It is widely believed that these anatomical properties are fundamental to the brain's remarkable ability to quickly process time-varying sensory inputs using relatively slow units, bind multimodal percepts, and make difficult decisions in dynamic and unknown environments.

Despite its fundamental importance, our understanding of the dynamics of recurrent neuronal networks in the brain is still incomplete. In particular, the role of oscillatory dynamics and how biologically plausible unsupervised Hebbian learning could work in such networks remains elusive. Moreover, their architecture and dynamics are in stark contrast to the feed-forward neural networks that dominate modern machine learning, which are largely incompatible with the brain's anatomical evidence and commonly trained using supervised learning rules.

In my research group, we combine experimental and theoretical approaches to better understand the principles that govern neural computation in the brain. Our work aims to uncover the fundamental mechanisms that enable the brain to efficiently perform computations on time-varying signals, and to develop new approaches for computation that are more closely aligned with the brain's biological architecture. Implementing features of the cerebral cortex in artificial neuronal networks led to systems that proved extremely efficient in classical benchmark tests on pattern recognition with respect to learning speed, noise tolerance and sparsity of required parameters.



Example of harmonic oscillator recurrent neural network (HORN) dynamics resulting from stimulation with a hand-written digit. F. Effenberger, P. Carvalho, I. Dubinin, W. Singer. A biology-inspired recurrent oscillator network for computations in high-dimensional state space, bioRxiv, 2022.11.29.518360.



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

He studied Medicine in Munich and Paris, received his PhD from the LMU Munich and his habilitation at the TU Munich. He was one of the directors of the MPI for Brain Research, as well as founding director of FIAS and the Ernst Strüngmann Institute for Neuroscience. His research is devoted to the exploration of neuronal foundations of cognitive functions. Central to his research is the question over how many brain areas processes are connected to allow for coherent perception.

Highlight

The most exciting discovery in the last year was, that the brain uses computational strategies that closely resemble at the algorithmic level the strategies realized in quantum computers.

Projects at FIAS: 1

Staff

Felix Effenberger
Igor Dubinin

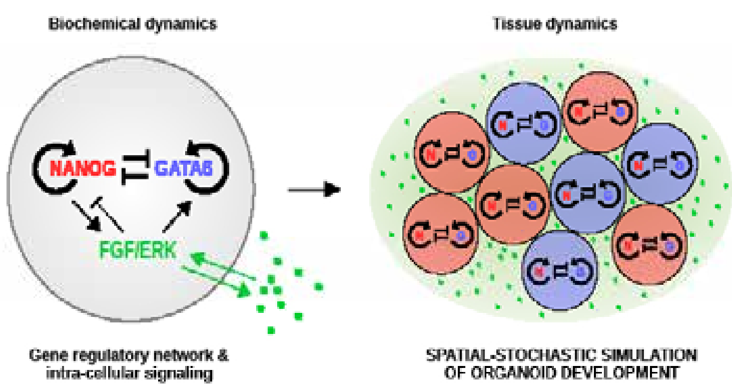
Event-driven multiscale biochemical simulations

Living organisms have the capability to process information reliably and efficiently, both inside their cells and at the tissue level. However, to this end they employ biophysical and biochemical processes that are fundamentally stochastic, and therefore limit the reliability of biological information transmission and processing. Nonetheless, cellular information processing can attain astonishingly high precision and reproducibility, in particular in the field of early embryo development. Here, reliable early 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 emerging group at FIAS aims at unraveling such mechanisms via numerical and analytical models that accurately incorporate the biophysical and resource contraints faced by the cells. Such models chiefly rely on realistic modeling of the fundamental intracellular stochastic processes determining biological noise, which quickly can become intractable both mathematically and numerically. A hallmark of our approach therefore is to employ event-driven simulations, smart mathematical approximations, problem-specific numerical optimization techniques, and recently also deep-learning based inference approaches for reducing the computational cost associated with realistic biophysical models.

In 2022 we adopted a novel deep-learning-based inference technique, simulation-based inference (SBI), and combined it with our event-driven spatial-stochastic simulator for developing tissue. This allowed us to efficiently infer predictions for more than a dozen of relevant of biophysical parameters governing tissue patterning in several scenarios of early mouse embryo development. Our results further elucidate the structure of the core network driving cell fate specification in the preimplantation mouse embryo, and in particular also highlight the role of spatial coupling via signaling molecules in the intercellular space of the developing tissue. In 2023, we will develop our model further such that it will incorporate cell growth and division, in order to characterize the early developmental mechanisms in a fully dynamical spatial-stochastic model of the mouse embryo.

In summer 2022 we intensified our collaboration with the Zagórski group at Jagiellonian University in Cracow, which culminated in joint research on the stability of competing morphogen expression boundaries, currently being prepared for publication.



Schematic of the Nanog/GATA6 gene regulatory network driving early mouse embryo development: Nanog and GATA6 mutually repress each other inside the cells of the growing tissue, allowing for creation of exclusive cell fates. Nanog activates signaling protein Fgf4, which is exchanged between cells and adjusts the required cell fate ratio via feedback on the core network.

Dr. Thomas Sokolowski

He studied physics and mathematics at Saarland University. But soon took the path towards theoretical biophysics he completed his P.h.D. in 2013 from Vrije Universitet Amsterdam (VU). Afterwards he stayed as a postdoc at IST Austria from 2014 until 2020, where he focused on optimizing complex 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

In early 2022 we started a new project that will assess how the detailed spatial arrangement of transcription factor binding sites affects their overall binding affinity.

Projects at FIAS: 1

Staff

Michael Ramírez Sierra
Mirjam Schulz
Niklas Heuser

Collaborations

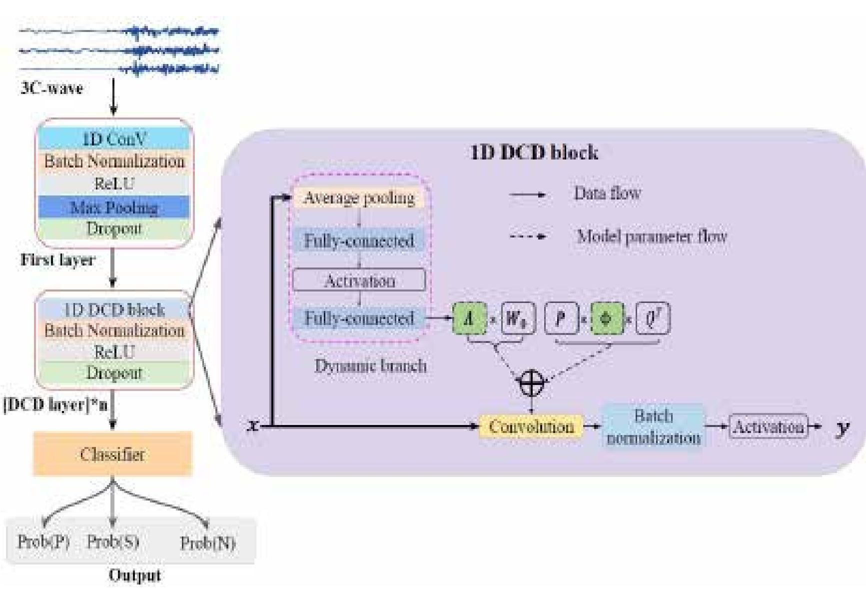
William Bialek, Princeton
Thomas Gregor, Princeton/ Institut Pasteur (Paris)
Gašper Tkačik, IST Austria
Sabine Fischer, Uni Würzburg
Marcin Zagórski & Dr. Maciej Majka, Jagiellonian University (Cracow)
Pieter Rein ten Wolde, AMOLF (Amsterdam)

DynaPicker: Dynamic CNN for Earthquake detection

Earthquake detection and seismic phase picking play a crucial role in the travel-time estimation of Primary (P-) and Secondary (S-) waves, which is an important step in locating the hypocenter of an event. The accuracy of traditional automatic pickers, when applied to real-time seismic data, may not be satisfactory, especially in the case of a poor signal-to-noise ratio. Additionally, the increasing number of seismic sensors deployed for earthquake monitoring produces a huge amount of seismic data, making data flow and processing along with defining the manual features for traditional automated methods more difficult and time-consuming.

Advanced technologies, such as convolutional neural networks, have been widely introduced to detect seismic events and create earthquake catalogs from continuous waveforms produced using conventional methods. However, their performance is restricted by the static convolution kernels. To cope with this challenge, we propose a dynamic convolutional neural network-based framework, termed DynaPicker, to detect seismic body wave phases that allows a dynamic inference with the deep learning architecture. Our model takes a window of the normalized three-channel seismic waveform as input and predicts its label as P-phase, S-phase, or noise. Then, the pre-trained model is employed to automatically pick the arrival time of real-time continuous seismic data.

Dynamic convolution achieves a significant performance improvement over convolutional neural networks (CNNs) by adaptively aggregating K static convolution kernels. Figure 1 schematically visualizes the proposed model architecture which consists of convolutional layers, batch normalization, dropout, DCD-based layers, and a 1D dynamic classifier adapted from the work. The results of our experiments show that DynaPicker can yield a testing accuracy of 98.82% in seismic phase identification. We demonstrate the robustness of this method's ability in classifying seismic phases, even when the low-magnitude seismic data is polluted by noise. Moreover, DynaPicker can be extended to deal with input data of varying lengths for seismic phase detection. Given continuous seismic data, DynaPicker can correctly identify more seismic events and produce a lower arrival time picking error compared to the baseline methods.



Schematic diagram for the proposed Dynamic Convolution Decomposition (DCD) based model. The model architecture represented on the left side includes a convolutional layer, 1D-DCD layers, and the classifier. The 1D-DCD block displayed on the right side is the backbone of the 1D-DCD layer, which is adapted from the work of Y. Li et al. (2021) and converted into the 1D case in this study.

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

My project proposal EQUATE has been selected for the 2023 edition of the Partenariat Hubert Curien (PHC) Procope program, a collaborative project between Laboratoire de Mécanique Paris-Saclay and FIAS on hybrid strategies to enhance Earthquake Early Warning systems in Europe.

Projects at FIAS: 2

Staff

Wei Li, Claudia Quinteros Cartaya, Megha Chakraborty, Jonas Köhler, Patrick Laumann, Darius Fenner

Collaborations

Institute of Seismological Research Gandhinagar, India
Laboratoire de Mécanique Paris-Saclay

Dr. Jan Steinheimer-Froschauer

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

Highlight

Affiliate with Lawrence Berkeley Laboratory and member of the DIG-UM Digitization board for the ErUM community (Research focus of the BMBF: Erforschung des Universums und der Materie).

Projects at FIAS: 2

Collaborations

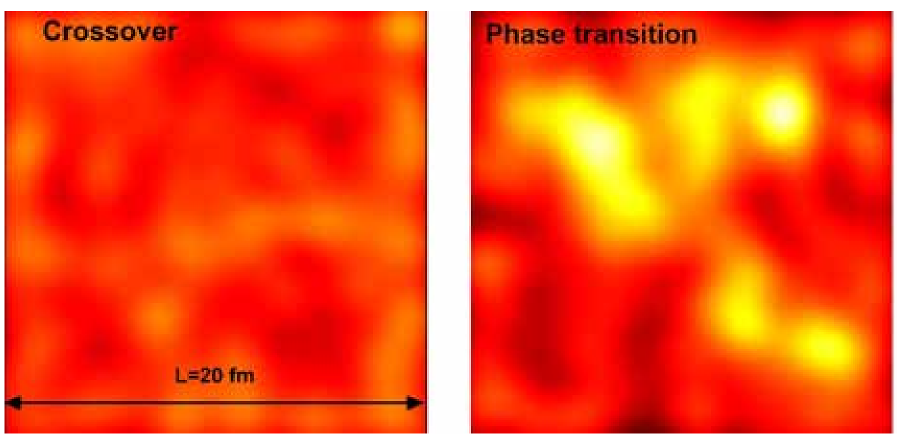
HADES collaboration, GSI Darmstadt
Benjamin Dönigus, IKF Goethe Universität
Marcus Bleicher and Elena Bratkovskaya, Goethe Universität
Abhijit Bhattacharyya, Calcutta University, Kolkata, India
Christoph Herold, Suranaree University, Nakhon Ratchasima, Thailand
Volker Koch, LBNL Berkeley, USA
Yasushi Nara, Akita International University, Akita, Japan
Qingfeng Li, Huzhou Universität, China
Jörg Aichelin, SUBATECH, Nantes, Frankreich

The high density QCD Equation of state in a transport descrip-

A major remaining challenge in the study of the strong interaction is to map out the phase diagram of QCD in terms of temperature and net baryon density. While theoretical guidance from lattice QCD simulations exists for almost vanishing net densities, concluding a smooth crossover from a hadronic system to deconfined quarks and gluons, the phase structure of QCD at large net baryon densities is still mostly unknown. Here, we can still speculate about a possible phase transition or even exotic phases of matter which could exist in the interior of compact stars as well as in the fireball created by relativistic heavy ion collisions.

While the study of the equation of state (EoS) of QCD at the highest beam energies relies on fluid dynamic simulations, compared to experimental data from RHIC and the LHC, a consistent dynamical treatment of heavy ion collisions in the high density regime, including a realistic EoS, was still missing.

Our group at FIAS was successful in implementing a flexible high density equation of state, including also a phase transition with unstable region, in a Quantum Molecular Dynamics (QMD) framework. Such an approach has several advantages compared to the current state-of-the-art as it allows for a fully non-equilibrium description of the fireball evolution of a heavy ion collisions within a single integrated approach. This model was then used to simulate various observables in heavy ion collisions at FAIR and show the sensitivity on the equation of state. In addition, a feasibility study for using statistical methods, like a Bayesian inference of the equation of state, using our new model was successfully completed. We now possess the tools necessary to directly connect observables from the FAIR and RHIC experiments to the QCD phase structure. The results of our research have been published in a number of papers.



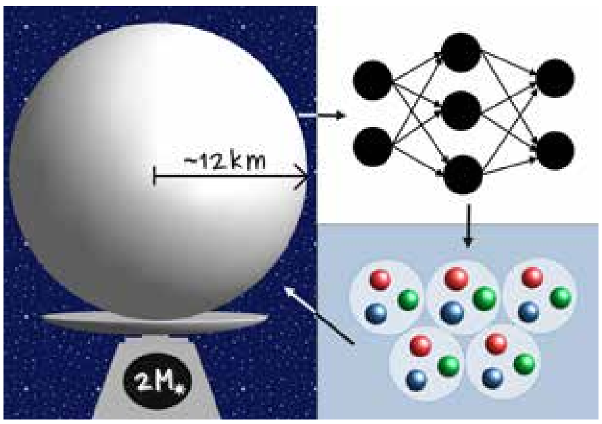
Density distributions in a box of 20fm length. Bright colors indicate high net baryon density. The left figure was simulated using UrQMD with a crossover in density while the right hand side included a first order phase transition. It can be clearly seen how the dynamical description of the phase transition leads to phase separation and density clumping.

MAGIC and AI for Science

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

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

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



Neutron stars encompass the densest form of matter: twice the mass of the sun in a spherical volume with a radius of a few kilometers (left). Using neural networks (top right), the group developed an algorithm that uses the macroscopic properties of neutron stars (specifically, the masses and radii) to obtain the corresponding microscopic quantities, i. e. the underlying equation of state (bottom right). Image: Shriya Soma

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

He studied physics at Goethe University, where he 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 Stöcker 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, in this capacity, founded the Helmholtz Institutes in Mainz and Jena, as well as, adjacent to GSI, the international research facility FAIR in Europe. He has more than 600 publications and graduated more than 60 early career scientists to doctorates. He holds several patents. In 2004, he was the founding director and CEO of FIAS, and still is one of the Senior Fellows.

Highlight

The support of 20 Ukrainians over 7-10 months, 10 of them scientists.

Projects at FIAS: 6

Staff

Mariia Bilousova
Omar El Sayed
Shriya Soma
Omana Kuttan Manjunath
Zhengyang Yu
Anton Motornenko
Leonid Satarov
Markus Schlott
Filippo Guidi

Prof. Dr. Jürgen Struckmeier

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

Highlight

Gauge-theoretical derivation of the spin-torsion coupling for fermions and interpretation of Dark Energy from propagating torsion of space-time.

Projects at FIAS: 1

Staff

Vladimir Denk (PhD student)
Johannes Kirsch
David Vasak
Armin van de Venn (PhD student)

Collaborations

David Benisty, Ben-Gurion University of the Negev, Beer-Sheva, Israel (now postdoc at Cambridge University, UK)
Matthias Hanauske
Eduardo Guendelman, Ben-Gurion University of the Negev
Peter Hess, Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico, Mexico City
Friedrich Wilhelm Hehl, University Cologne
Frank Antonsen, Copenhagen
Andreas Redelbach, Goethe University and Member of the FIAS Computer Science Group

Covariant Canonical Gauge Theory of Gravitation (CCGG)

The gauge theory of gravitation shows that spin particle fields necessarily act as a source of spacetime torsion. This extends the classical Einstein approach of General Relativity (GR) in which matter without internal degrees of freedom give rise to a torsion-free curvature of spacetime. Moreover, our canonical gauge theory also imposes Lagrangians of the free gravitational field that contain a quadratic Riemann-Cartan tensor term in addition to the usual Ricci scalar of the Einstein-Hilbert Lagrangian. As a consequence, the generalized theory of gravity is necessarily associated with additional coupling constants that require both well-grounded physical interpretations and careful justification based on cosmological observations. These modifications of GR entail various consequences for developing cosmological models.

The dynamics of torsion invoked by the quadratic kinetic term could be identified as "dark energy". Moreover, the quadratic torsion term represents a stiff fluid that leads to a bouncing cosmology solution. A constraint on the bouncing solution is calculated using cosmological data from different epochs.

We showed that the cosmological constant represents the energy of the space-time continuum when the latter is deformed from its (A)dS ground state to a flat geometry. Our CCGG framework predicts a total energy-momentum of the system of space-time and matter to vanish, in line with the conjecture of a "Zero-Energy-Universe" (Lorentz/Levi-Civita). Consequently a flat geometry can only exist in presence of matter where the bulk vacuum energy of matter, regardless of its value, is eliminated by the vacuum energy of space-time. The observed cosmological constant of 10^{-52} m^{-2} is found to be merely a small correction attributable to deviations from a flat geometry and effects of the dynamical geometry of space-time, namely torsion and possibly also vacuum fluctuations of matter and space-time. That quadratic extension of General Relativity thus provides a significant and natural contribution to resolving the 120 orders of magnitude miss-estimate called the "cosmological constant problem".

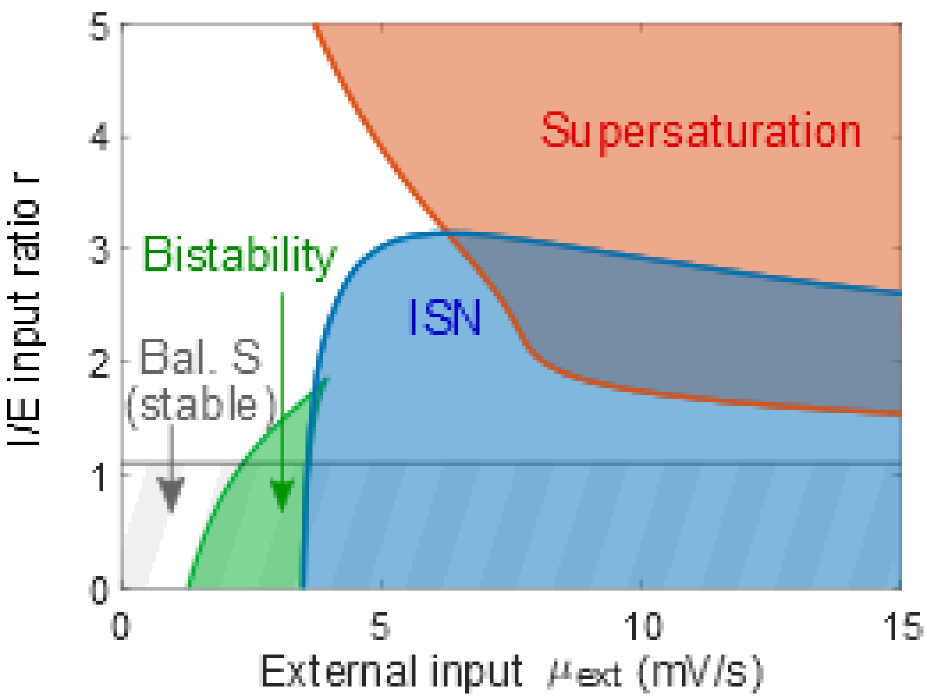
We continued our analytical investigation of the CCGG framework in a cosmological setting. We derive modified Friedmann equations in which torsion is able to explain the accelerated expansion of the Universe as a geometric effect without resorting to a cosmological constant. Simultaneously, a numerical analysis thereof has been worked on. It extends our study and allows for more freedom in the exploration of the universe's history. In order to compare theory with data, we are planning a Markov Chain Monte Carlo (MCMC) analysis in collaboration with Goethe University. The natural next step will then be to utilise Machine Learning methods for our statistical analyses. This is going to be arranged in collaboration with one of the Deep Learning groups at FIAS.

A theorem on scalar-valued functions of tensors was derived, which can be regarded as the tensor analogue of the identity following from Euler's theorem on homogeneous functions. The identity has been applied for analyzing the relation of metric and canonical energy-momentum tensors of matter and gravity. It allows to formulate an equivalent representation of the generalized Einstein field equation for arbitrary version of vacuum space-time dynamics - including torsion and non-metricity.

Johannes Kirsch, Jürgen Struckmeier, Armin van de Venn, David Vasak, Vladimir Denk (from left) give new insights into space and time.

Deciphering neural algorithms

In 2022, the Tchumatchenko group has shed light on neural network activity and synaptic plasticity. We have studied the role of dopamine and serotonin for valence encoding, looked at how biological insights regarding synaptic dynamics etc can be used in the design of artificial neural networks and have uncovered synaptic symmetry rules underlying cortical activity in the visual cortex.



| Possible activity regimes in binary networks (source: Tchumatchenko group)

Prof. Dr. Tatjana Tchumatchenko

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

Highlight

The Tchumatchenko group has shown that activity in spiking networks can have distinct phases that can be predicted mathematically.

Projects at FIAS: 1

Staff

Pierre Ekelmans

Collaborations

Ulrich Meyer, FIAS

Dr. Sebastian Thallmair

He studied chemistry and biochemistry at the LMU Munich, where he completed his PhD in theoretical chemistry in 2015. After a short period as postdoctoral researcher in Munich, he joined the University of Groningen (The 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.

Highlight

Cristina Gil Herrero won a poster prize at the "BioExcel School on Biomolecular Simulations" and therefore was invited to present her results in a BioExcel Webinar.

Group Members

Cristina Gil Herrero
Marieli Gonalves Dias

Projects at FIAS: 1

Collaborations

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

Understanding, controlling, and inhibiting protein function

In 2022, we continued our research on light-switchable pharmaceuticals and, together with collaborators, we presented a design and optimization strategy for light-switchable inhibitors of bacterial dihydrofolate reductase. Computational testing of potential substituents and the optimization of their position was a key part in the rational design protocol. In addition, we characterized photo-crosslinkers which can be attached to proteins to alter and control the protein conformation. The experiments were performed in Groningen (NL).

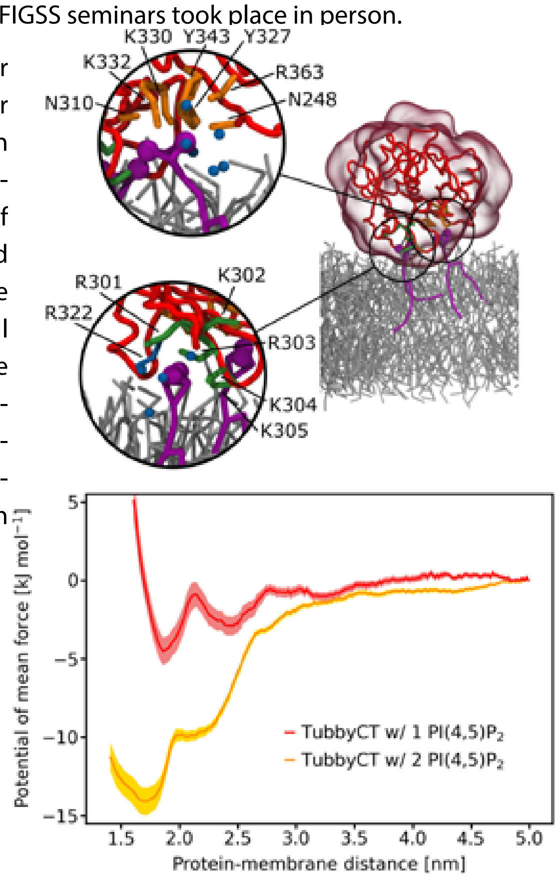
In another joint experimental and computational study, we investigated the membrane binding of the Tubby protein. Tubby is involved in ciliary trafficking and its malfunction can lead to for instance retina degeneration and hearing loss. We discovered a previously unknown second binding site for a specific lipid, PI(4,5)P2. This second binding site is crucial for the membrane binding of Tubby, as demonstrated in life cell experiments performed in Marburg.

In 2022, the Thallmair Group became part of the initiative "Subcellular Architecture of Life" (SCALE) by the Goethe University. Together with Florian Wilfling (MPI for Biophysics), we successfully applied for a postdoc position to investigate the role of the Tubby protein in membrane contact sites.

In November 2022, we welcomed Marieli Goncalves Dias for a one-year research visit. Marieli is PhD student at the University of Campinas (Brazil) and will perform molecular dynamics simulations of nuclear receptors and coregulators.

With the beginning of the summer semester 2022, Sebastian Thallmair took over the position as scientific coordinator of the Frankfurt International Graduate School for Science (FIGSS), the graduate school at FIAS. We are very happy that many of the biweekly FIGSS seminars took place in person.

We concluded the year with the "2nd Molecular Modelling and Simulation Workshop" at FIAS, organized in the framework of CMMS. The great talks and lively discussions made the workshop a wonderful event and emphasized the need for in person meetings. Our PhD students Cristina and Marieli successfully presented their research projects.

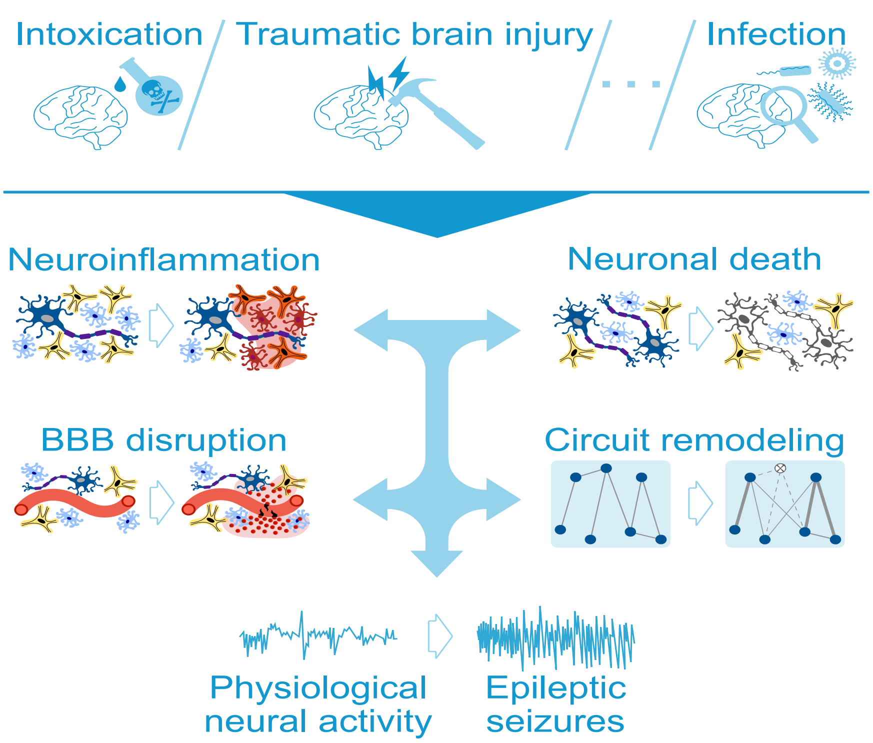


Representative snapshot showing the binding mode of two PI(4,5)P2 lipids in the binding pockets of tubbyCT (top). The magnified details show the binding mode in the crystal structure binding site (upper zoom) and the previously unknown second binding site (lower zoom). The bottom graph depicts the potential of mean force for the binding of tubbyCT to a membrane with one PI(4,5)P2 lipid (red) and two PI(4,5)P2 lipids (orange), respectively.

Modeling neuroimmune interactions in epilepsy

The development of epilepsy (epileptogenesis) involves a complex interplay of neuronal and immune processes. In one of our projects together with collaborators from the US and Italy we have presented a first-of-its-kind mathematical model to better understand the relationships among these processes (see figure). Our model describes the interaction between neuroinflammation, blood-brain barrier disruption, neuronal loss, circuit remodeling, and seizures and aims to disentangle the contribution of each for the development of epilepsy. Formulated as a system of nonlinear differential equations, the model reproduces the available data from three animal models, where epilepsy is induced through very different perturbations of the intact brain. The model successfully describes characteristic features of epileptogenesis such as its paradoxically long timescales (up to decades) despite short and transient injuries or the existence of qualitatively different outcomes for varying injury intensity. In line with the concept of degeneracy, our simulations have revealed multiple routes toward epilepsy with neuronal loss as a sufficient but non-necessary component. Interestingly, we have also shown that our model allows for in silico predictions of therapeutic strategies, revealing injury-specific therapeutic targets and optimal time windows for intervention. These findings may have important implications for treating patients with brain injuries, who have an increased risk of developing epilepsy.

Mathematical model of neuroimmune interactions during the development of epilepsy. Different triggers (top) can start the development of epilepsy (epileptogenesis). Sometimes it takes many years until the epilepsy manifests itself. Different interdependent mechanisms (middle) contribute to epileptogenesis and can ultimately result in healthy brain circuits becoming prone to generating epileptic seizures (bottom).



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 already during his graduate education.

Highlight

Jochen Triesch enjoyed a visiting professorship at the Université Clermont-Auvergne (France) financed by the French Tech Chair program.

Projects at FIAS: 6

Staff

Arthur Aubret, Tristan Stöber, Thomas Barbier, Samuel Eckmann, Francisco López, Diyuan Lu, lex Stoll, Petros-Evgenios Vlachos, Charles Wilmot, Xia Xu, Zhengyang Yu, Markus Ernst, Marius Vieth

Collaborations

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

Dr. Esteban A. Hernandez Vargas

He obtained a PhD in Mathematics at the National University of Ireland. Then he held a three-year postdoc position at the Helmholtz Centre for Infection Research, Braunschweig. In the same place, he established the Systems Medicine of Infectious Diseases research group. Since March 2017, he is a Research Fellow funded by the Alfons und Gertrud Kassel-Stiftung at FIAS Frankfurt.

Highlight

Machine learning approaches for tracking respiratory influenza infection in the lungs.

Projects at FIAS: 1

Staff

Josephine Naa Ayeley Tetteh
Suneet Singh Jhutty

Collaborations

Dunja Bruder (HZI, Germany)
Franklin Toapanta (Maryland University, USA)
Alejandro Hernan Gonzalez (CONICET, Argentine)
Sorin Olaru (CentraleSupelec, France)
Xin Du (Shanghai University, China)

Machine Learning against Infectious Diseases

Throughout history, we have witnessed alarming high death tolls derived from infectious diseases around the globe. The novel coronavirus SARS-CoV-2 has uncovered one of the biggest pandemics in recent history. While China did a large effort to shrink the outbreak, COVID-19 developed into a pandemic in more than 210 countries moving the epicentre from China to Europe and consequently to America.

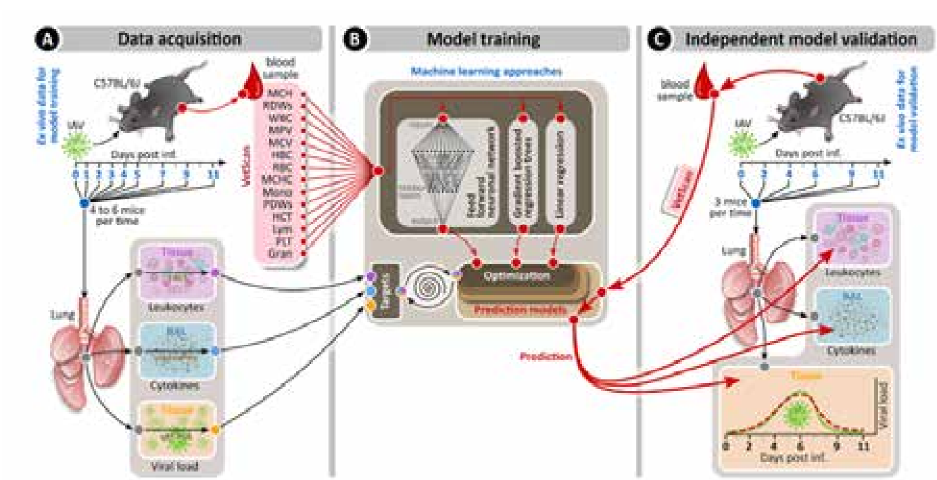
The spread of viruses between infectious and susceptible hosts can be orchestrated via close physical interactions. Understanding disease transmission remains a central vexation for science as it involves several complex and dynamic processes. The link between the infection dynamics within an infected host and the susceptible population-level transmission is widely acknowledged. However, several technical aspects of the interface of within- and between-host are still in their infancy. Fusing interdisciplinary activities, the groundbreaking ambition of our research is to apply mathematical modeling and computational simulations to in vivo experiments to

1. dissect host immune-regulatory mechanisms during acute and chronic infections, and their respective shift in the elderly;

2. develop mathematical models for decision making to influence the use of vaccines and drugs; and

3. develop multiscale epidemiological models in SARS-CoV-2 as a virtual disease tool to evaluate therapies and public health policies.

Our research group has a special interest in viral infections. Our collaborators are testing our simulation predictions in laboratory experiments. With the aid of the established models, it will be possible to predict rational combinations of antivirals as well as immune modulators and test them specifically. Thus, it is also conceivable that the insights gained from our research could result in therapeutic alternatives in the coming years.

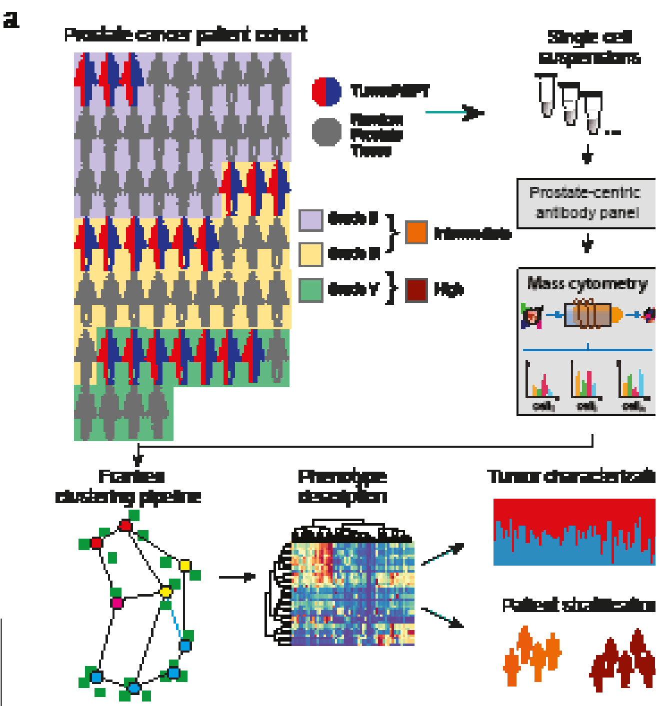


Machine learning approaches for tracking respiratory influenza infection in the lungs. Mice were intranasally infected with a sublethal dose of IAV PR/8/34 on day 0 and sacrificed on the indicated days. Blood was collected for hematology analyses, bronchoalveolar lavage was performed to analyze lung cytokines, and lung tissue samples were used to monitor either viral load or pulmonary leukocyte subsets (A). The hematological data from this initial set of experiments were used to build and train different machine-learning models (B). Data from a separate experiment were used to test and evaluate machine learning algorithms (C).

Single-cell proteomics defines heterogeneity of prostate cancer

Localized prostate cancer exhibits multiple genomic alterations and heterogeneity at the proteomic level. Single-cell technologies capture important cell-to-cell variability responsible for heterogeneity in biomarker expression that may be overlooked when molecular alterations are based on bulk tissue samples. A study from the Wild research lab aimed to identify prognostic biomarkers and describe the heterogeneity of prostate cancer and the associated microenvironment by simultaneously quantifying 36 proteins using single-cell mass cytometry analysis of over 1.6 million cells from 58 men with localized prostate cancer. We performed this task, using a high-dimensional clustering pipeline named Franken to describe subpopulations of immune, stromal, and prostate cells, including changes occurring in tumor tissues and high-grade disease that provide insights into the coordinated progression of prostate cancer. Our results further indicate that men with localized disease already harbor rare subpopulations that typically occur in castration-resistant and metastatic disease.

Main projects in 2023 will be BMBF PROSurvival (www.prosurvival.org), Federated Machine Learning and Computational Pathology of Prostate Cancer and KHZG DigPath Hub Frankfurt.



b

Antibody	Description
Immune context	
CD45	Leukocytes
CD15	Granulocytes
CD20	B cells
CD68	Macrophages
CD3	T cells
Stroma	
S100A4	Fibroblasts
Vimentin	Mesenchimally-derived
SMA	Motility and invasion
Proliferation/Viability	
Ki-67	Proliferation marker
pH3	Proliferation marker
cl.PARP	Apoptosis marker
cl.Caspase	Apoptosis marker
Transcription factor	
AR	Prostate nuclear receptor
EZH2	Histone methylation
NKX3.1	Prostate tumor suppressor
GCR	Prostate nuclear receptor
PR	Tumor suppressor
p53	Tumor suppressor

Antibody	Description
Epithelial cells	
EpCAM	Pan epithelial
panCK	Pan epithelial
E-Cadherin	Pan epithelial
CK18	Luminal cells
CK8	Luminal cells
CK5	Basal cells
CK14	Basal cells
CK7	Transitional epithelial cells
CK19	Transitional epithelial cells
Prostate cells	
PSA	Prostate epithelium
Prostein	Prostate epithelium
PSMA	Prostate epithelium
AMACR	Prostate cancer
Other	
PTEN	Tumor Suppressor
CA9	Hypoxia
CD31	Endothelial cells
CD24	Stem cells
Synaptophysin	Neuroendocrine cells

Schematic of method for characterization of primary prostate cancer tissue using mass cytometry. (a) The patient cohort consisted of 58 primary prostate cancer cases. For 16 patients, tumor and adjacent benign prostatic tissue (ABPT) samples were available, (b) Markers used to categorize prostate epithelial cells as luminal, basal, or transitional, and markers used to identify tumor cells, cells from the microenvironment and proliferation. De Vargas Roditi et al., Cell Rep. Med. 2022; 3(4):100604.

Prof. Dr. Peter Wild

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

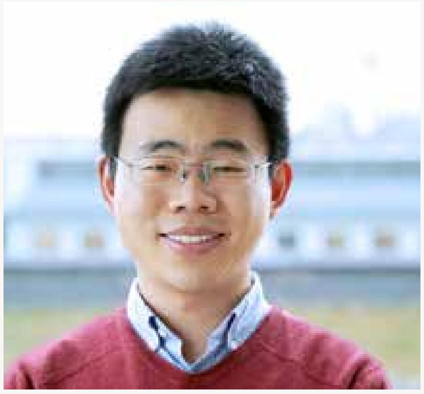
Highlight

Completion of the world's largest proteomics project in prostate cancer.

Projects at FIAS: 1

Collaborations

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



Dr. Kai Zhou

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

Highlight

Detecting Chiral Magnetic Effect in heavy ion collision via Deep Learning.

Projects at FIAS: 3

Staff

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

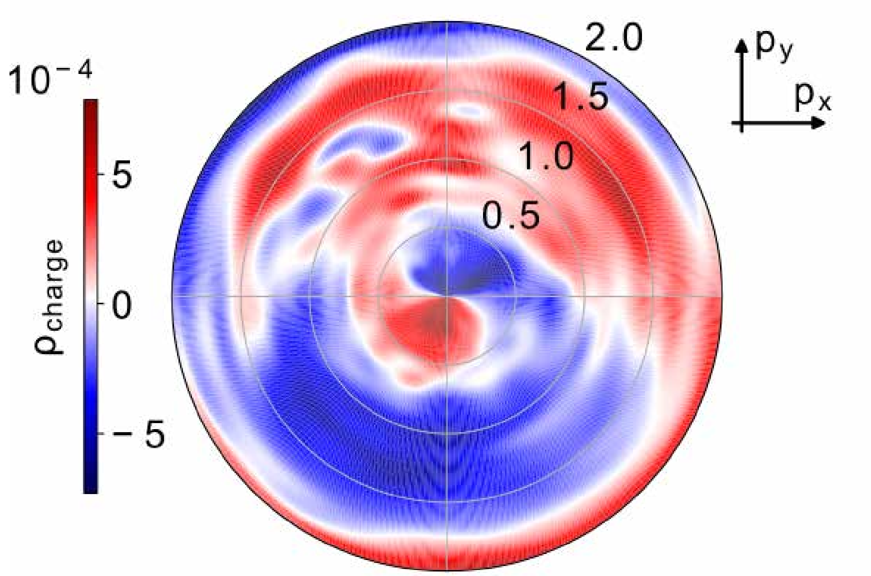
Collaborations

XinNian Wang, Berkeley & Wuhan
Long-Gang Pang, Berkeley,
Carsten Greiner, GU
Moritz Greif, GU
Gergely Endrődi, GU
Bao-yi Chen, GU and Ti'jin
Zhe Xu, Tsinghua, Beijing
Pengfei Zhuang, Tsinghua, Beijing

AI for Science study

During 2022, we deployed a broad range of AI for Science projects across several different research fields, including mainly high energy nuclear physics, neutron star astrophysics, statistical physics, Terahertz Holography Imaging, Seismology Earthquake investigation, Virus infection dynamics, Lightning phenomenon, Smart Valve with anomaly detection, etc. Specifically, in the context of high energy nuclear physics, the search for chiral magnetic effect (CME) in heavy ion collisions (HIC) has attracted long-term attention which is fundamentally important to reveal the vacuum structure of QCD and its induced emergent topological fluctuations of gluon fields. However, due to the large background noises being associated in experiment the identification of CME from HIC is really challenging for long while. We for the first time propose to analyze the final-state hadronic spectrum measurements from HIC in the sense of big data to pin down fingerprints of CME that may happened during the collisions. Accordingly, a deep learning model with convolutional layers is introduced to detect the CME signals, and supervised training is performed based upon simulation events from the string melting a multiphase transport (AMPT) as training data. The model gives accurate recognition to CME signal with robustness against different collision scenarios or even different physics model, thus we achieved a powerful meter to quantify the CME for QCD study within HIC. Very interestingly, the DeepDream analysis was deployed to visualize the patterns captured by the trained deep learning model, as shown in Fig:1, which paves the way to drill physical knowledge hidden in the learning algorithm after confronting the big data. Another highlight for our group is that, we devised a Regional-local adversarially learned one-class classifier anomalous sound detection, which works for global long term interactions in frequency domain space and this novel approach shows superior results on four real-world industrial anomaly detection task dataset including our collected acoustic data from SAMSON AG. The work got accepted by KDD'2022.

DeepDream map for the trained CME-meter-network, which reproduces well the underlying physics as well (from: Yuan-Sheng Zhao et al, Physical Review C (Letter) 106(5).



Donors and Sponsors

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

Endowed Professorships:

2016: Giersch Stiftungsprofessur Prof. Dr. Franszika Matthäus
2014: Helmut-Maucher-Stiftungsprofessur Prof. Dr. Nils Bertschinger
2007: Johanna-Quandt-Stiftungsprofessur Prof. Dr. Jochen Triesch

Endowed Fellowships:

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

We are FIAS

An adhoc snapshot in June 2022 of the administrative team that supports the FIAS scientists in all aspects of their research including computing. Our FIAS team thrives on people and change: As every year some staff set off for new shores, and new faces joined us in 2022.

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Gabriel Grappasonno - Student Assistant
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Prof. Dr. Peter Wild

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Prof. Dr. Henner Büsching
Prof. Dr. Laslo Csernai
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Prof. Dr. Thomas Haberer
Prof. Dr. Peter Hess
Dr. Alexander Kies
Prof. Dr. Thomas Metzinger
Dr. Piero Nicolini
Prof. Dr. Constantin Rothkopf
Dr. Laura Tolos

Emeritus Fellows

Prof. Dr. Christoph von der Malsburg
Prof. Dr. Igor Mishustin

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