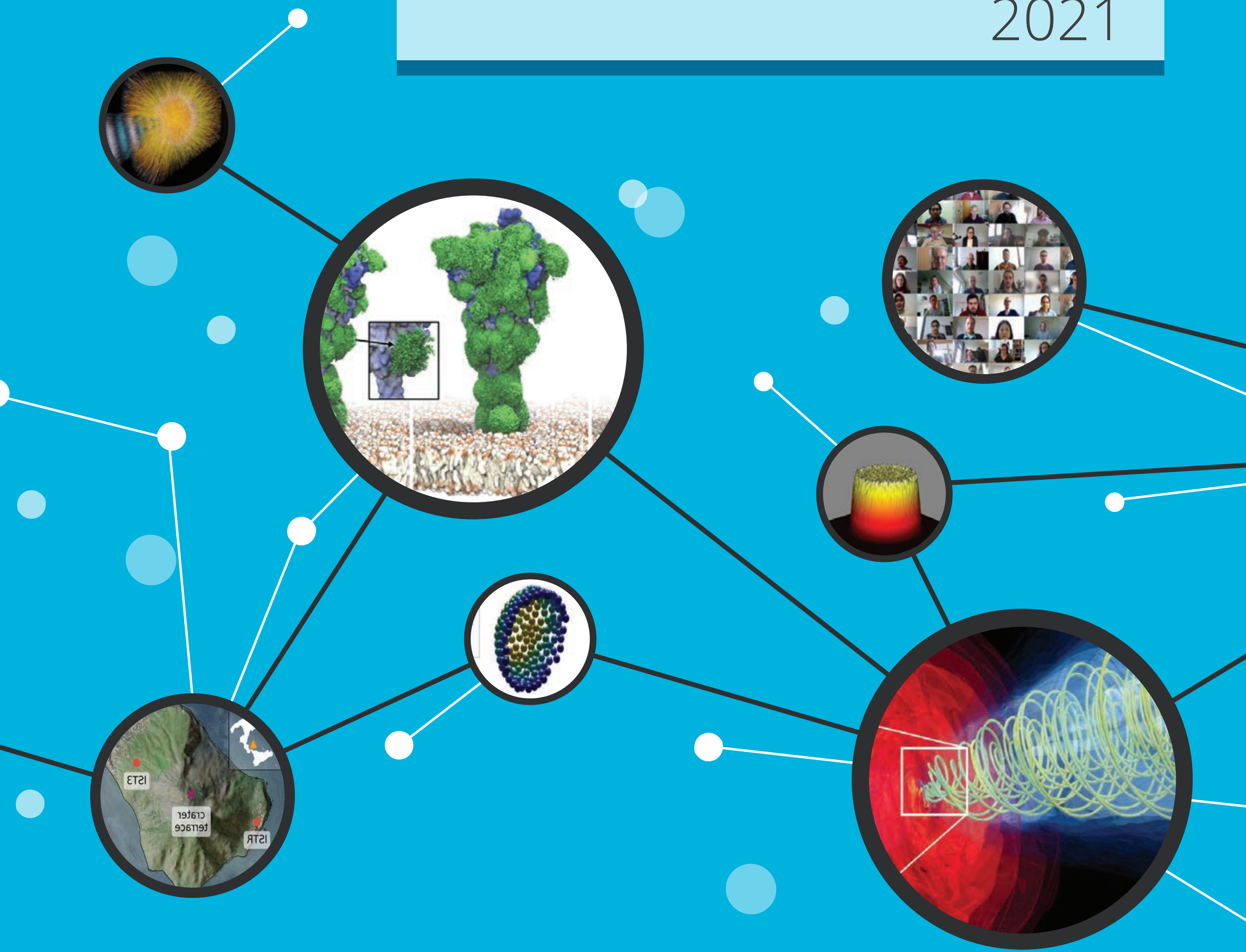
FIAS Frankfurt Institute for Advanced Studies

2021



Content

FIAS

science for the reality of tomorrow

Dear colleagues,
Dear friends and supporters of our science,
Dear knowledge seekers,

We have become accustomed to a new normality, but have not lost our focus on research. The newly founded research groups have established themselves. Our scientists spend their time in the home office planning successful collaborations and writing grant proposals.

Besides that, we organized several events, depending on the time of year and the number of participants, such as online, live, or hybrid events. The highlight was already in February: The Giersch International Summer School and Conference, brought over 250 participants from all over the world to FIAS digitally.

We could close the year with more good news. A newly signed cooperation agreement, between FIAS and Goethe University, allows us to structurally anchor our joint research activities. The new contract will allow for easier coordination of existing and new projects, which will be of great importance for a successful Frankfurt application in the next Excellence Initiative. We are already looking forward to tackling the implementation of these changes in 2022!

On behalf of all FIAS members

Prof. Dr. Volker Lindenstruth
Chairman of the Board

HIGHLIGHTS 2021

Volker Lindenstruth, Enrico Schleiff and Rolf Bernhardt (from left) signed the new cooperation agreement between FIAS and Goethe University on Nov. 11, 2021.

New cooperation agreement between FIAS and Goethe-University

Starting in 2022, Goethe University and the FIAS will intensify and expand joint research projects and the exchange of scientific knowledge. A new cooperation agreement has laid the legal foundations for this. The contract was signed on November 11th.

Interdisciplinary basic research in the natural sciences, life sciences, neurosciences, and computer sciences - in these areas Goethe University and FIAS have been collaborating since the research institute's foundation in 2003. The new contract will allow for easier coordination of existing projects and the start of new projects.

"The contract will give us the freedom to conduct even more interdisciplinary research and to design our projects complementary to the questions of the two partners," University President Prof. Dr. Enrico Schleiff said at the signing of the contract yesterday evening. "However, it is important for us that FIAS is now closely linked with the university's natural science departments. For example, a project at FIAS can now also be applied for through the university."

"Even though FIAS acts autonomously and independently, there have of course always been close ties between the two institutions. We are looking forward to strengthening and structurally anchoring this cooperation now," said Prof. Dr. Lindenstruth, Chairman of the Board of FIAS. He signed the cooperation agreement together with his board colleague Dr. Rolf Bernhardt.

For example, it is planned to jointly develop technical and content-related topics of high-performance computing in the natural and life sciences within the framework of the Center for Scientific Computing (CSC); only recently, Goethe University was accepted into the national network for high-performance computing. Another goal is to intensify cooperation in the life sciences: for example, researchers are already cooperating on the LOEWE focus on multi-scale modeling (CMMS), which aims to quantify complex biological systems, and the cluster project ENABLE, which is investigating the internal balance of cells (homeostasis), to help develop novel drugs for inflammation and infection diseases. Thus, FIAS will be involved in preparing the future Excellence Initiative of the Federal Government.

Awards:

Prof. Dr. Hannah Elfner has been a Fellow at FIAS and Professor at Goethe University since 2013. At the GSI Helmholtz Centre for Heavy Ion Research, she heads the theory column.

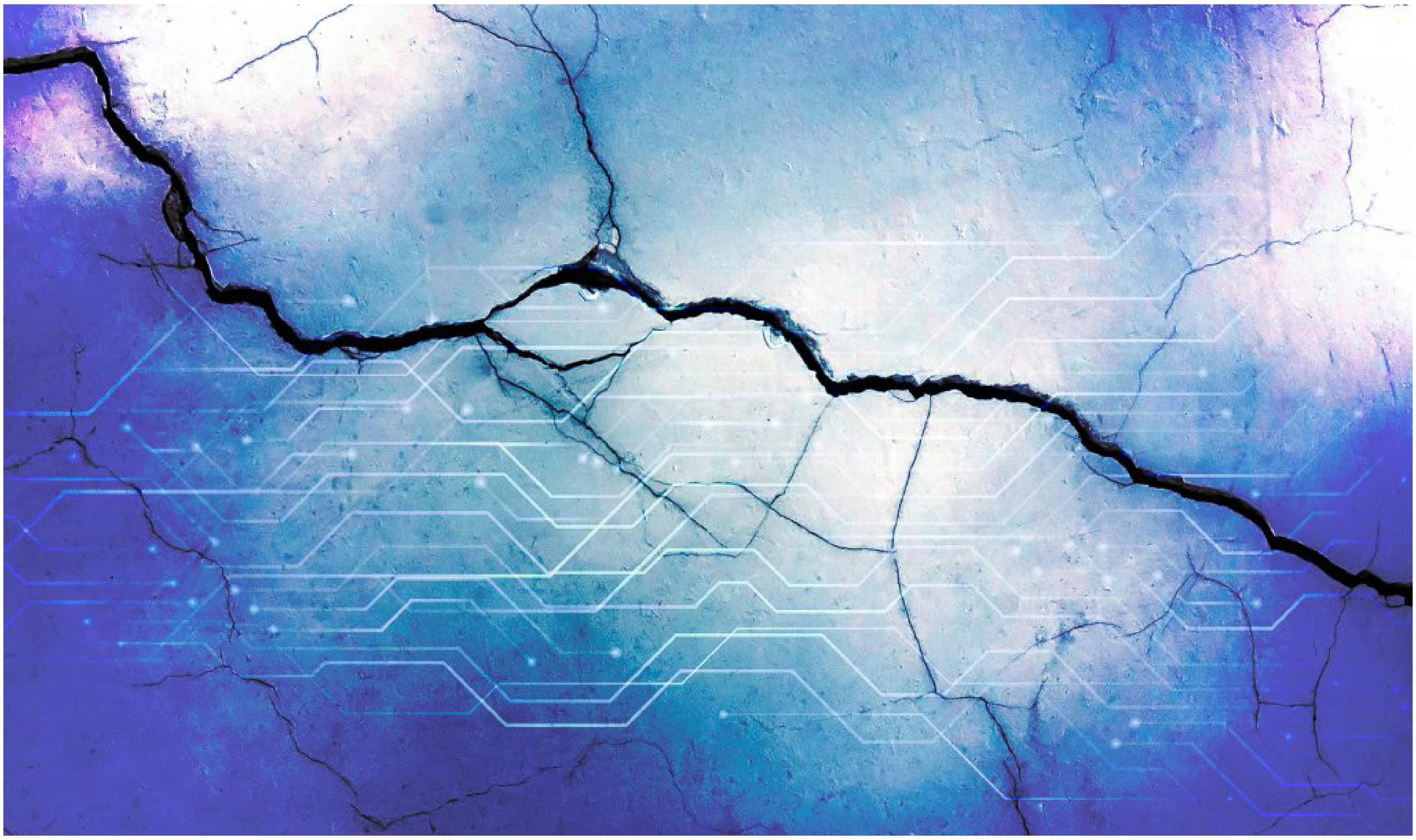
Hannah Elfner was named "Scientist of the Year" 2021

The Alfons and Gertrud Kassel Foundation awards the "Scientist of the Year" prize every second year to a scientist who, in addition to outstanding scientific achievements, is also committed to the work of young scientists. This year, FIAS Fellow Prof. Dr. Hannah Elfner receives the award, which is endowed with 25,000 euros.

In addition to her outstanding research, Hannah Elfner is always very committed to young scientists; despite her young age, she has already successfully guided nearly 30 young scientists to their scientific degrees. In addition to training students and doctoral candidates, she regularly provides insight into her research at lectures and events in public, showing quite incidentally that women can also be successful as physics professors. A point that is very close to her personal heart.

It is precisely this commitment that the Alfons and Gertrud Kassel Foundation honors with its "Scientist of the Year" award. Part of the prize money of 25,000 euros will therefore also be used to support young scientists.

Theoretical Sciences



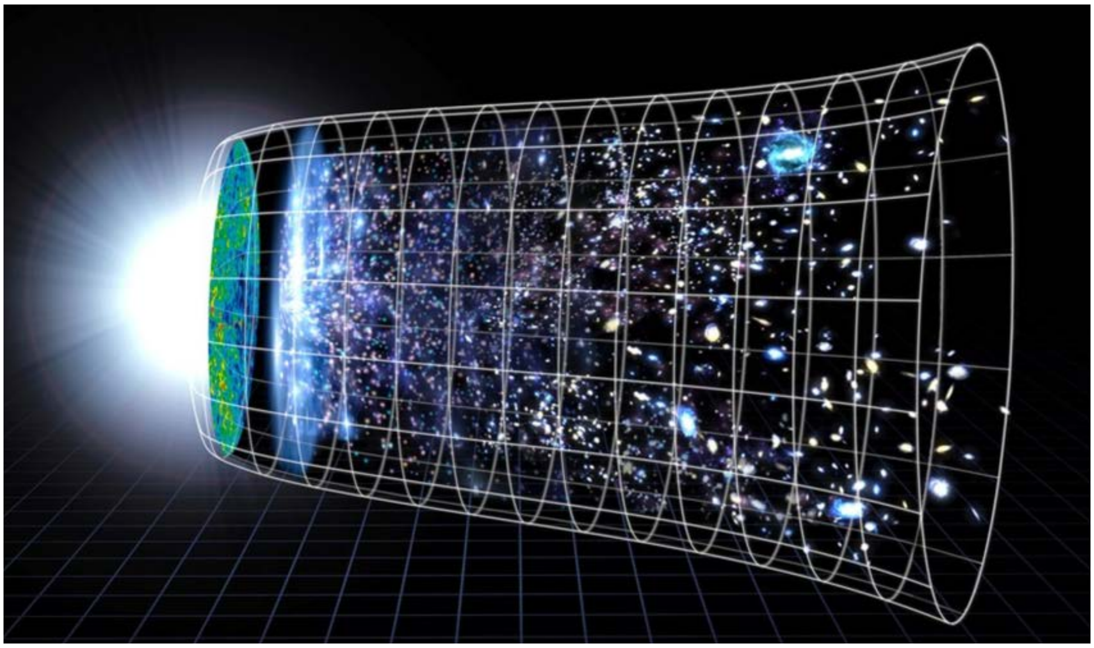
Methodological research in the field of AI is already proving groundbreaking in the area of theoretical natural sciences for the treatment of problems in theoretical physics. One focus is on high-energy and heavy-ion research and related astrophysical issues, such as the study of neutron star collisions and the phase structure of the hot, dense matter produced there, as well as field theory. AI methods developed at FIAS are also used to describe condensed matter properties, hydrodynamic and electro-dynamic flow fields in large networks, seismology, and sustainable energy research.

In 2021 FIAS and the Institute of Seismological Research (ISR) in Gandhinagar have now agreed on long-term research cooperation using novel artificial intelligence methods to understand the earthquake occurrence in the region of Gujarat, in northwest India.

The uneven universe

It is almost always assumed in cosmological calculations that there is an even distribution of matter in the universe. This is because the calculations would be much too complicated if the position of every single star were to be included. In reality, the universe is not uniform: in some places, there are stars and planets, in others, there is just a void. Physicists Michael te Vrugt and Prof. Raphael Wittkowski from the Institute of Theoretical Physics and the Center for Soft Nanoscience (SoN) at the University of Münster have, together with physicist Dr. Sabine Hossenfelder from the Frankfurt Institute for Advanced Studies (FIAS), developed a new model for this problem. Their starting point was the Mori-Zwanzig formalism, a method for describing systems consisting of a large number of particles with a small number of measurands. The results of the study have now been published in the journal "Physical Review Letters".

A representation of the evolution of the universe over 13.77 billion years. The far left depicts the earliest moment we can now probe, when a period of "inflation" produced a burst of exponential growth in the universe. (Size is depicted by the vertical extent of the grid in this graphic.) For the next several billion years, the expansion of the universe gradually slowed down. More recently, the expansion has begun to speed up again.



Background: The theory of general relativity developed by Albert Einstein is one of the most successful theories in modern physics. Two of the last five Nobel Prizes for Physics had associations with it: in 2017 for the measurement of gravitational waves, and in 2020 for the discovery of a black hole at the center of the Milky Way. One of the most important applications of the theory is in describing the cosmic expansion of the universe since the Big Bang. The speed of this expansion is determined by the amount of energy in the universe. In addition to the visible matter, it is above all the dark matter and dark energy which play a role here – at least, according to the Lambda-CDM model currently used in cosmology.

"Strictly speaking, it is mathematically wrong to include the mean value of the universe's energy density in the equations of general relativity", says Sabine Hossenfelder. The question is now how "bad" this mistake is. Some experts consider it to be irrelevant, others see in it the solution to the enigma of dark energy, whose physical nature is still unknown. An uneven distribution of the mass in the universe may have an effect on the speed of cosmic expansion.

"The Mori-Zwanzig formalism is already being successfully used in many fields of research, from biophysics to particle physics," says Raphael Wittkowski, "so it also offered a promising approach to this astrophysical problem." The team generalised this formalism so that it could be applied to general relativity and, in doing so, derived a model for cosmic expansion while taking into consideration the uneven distribution of matter in the universe.

The model makes a concrete prediction for the effect of these so-called inhomogeneities on the speed of the expansion of the universe. This prediction deviates slightly from that given by the Lambda-CDM model and thus provides an opportunity to test the new model experimentally. "At present, the astronomical data are not precise enough to measure this deviation," says Michael te Vrugt, "but the great progress made – for example, in the measurement of gravitational waves – gives us reason to hope that this will change. Also, the new variant of the Mori-Zwanzig formalism can also be applied to other astrophysical problems – so the work is relevant not only to cosmology."

Publication:

M. te Vrugt, S. Hossenfelder, R. Wittkowski (2021). Mori-Zwanzig formalism for general relativity: a new approach to the averaging problem. Physical Review Letters 127, 231101. DOI: 10.1103/PhysRevLett.127.231101

Picture:

NASA's Goddard Space Flight Center

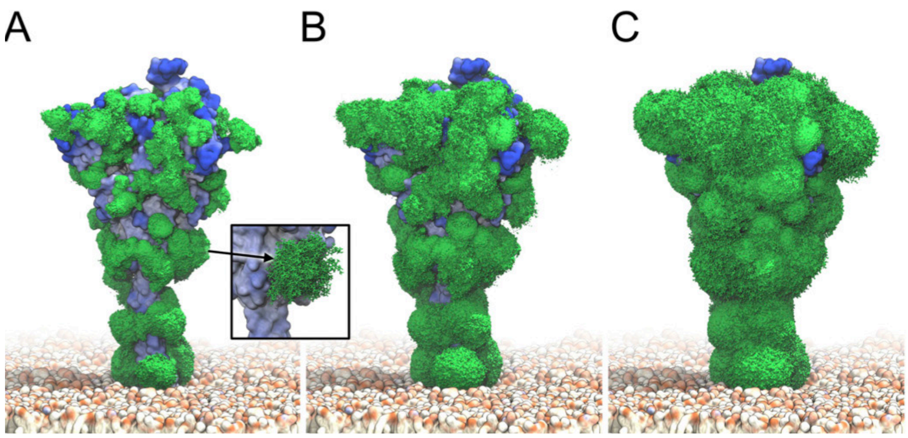
Theoretical Life- & Neuro Sciences

Biological and medical research depends on theoretical approaches to the analysis of complex data structures and the description of highly interconnected biological processes. In the field of theoretical life sciences, the FIAS develops methods taking into account the different scale levels for modeling biological systems and in the interdisciplinary theoretical neurosciences. The standardized integration of theoretical methods is also implemented in medical and pharmaceutical research, such as cancer research and drug development. In all fields, theoretical and experimental approaches and methods for the analysis of heterogeneous data sets are (further) developed - for the standardization of data acquisition and processing, for the development of detailed multi-scale models and their simulation using high-performance computing resources, and the application of AI methodologies. The FIAS follows the principle of integrative experiment design, which integrates experimental and theoretical competencies equally.

Goals for better vaccines: Computational identification of SARS-CoV-2 epitopes

The prominent spike protein of the SARS-CoV-2 virus exposed at its surface mediates viral entry into the host cell. It has been identified as primary antibody target; all vaccines aim at this protein. However, the spike – a chain of amino acids – is covered by sugars. These highly mobile glycan molecules shield the spike protein and can impair antibody binding.

A team including Roberto Covino, group leader and FIAS fellow, and Gerhard Hummer, director at the Max Planck Institute of Biophysics and senior fellow at FIAS, modelled the SARS-CoV-2 spike in atomic resolution. By sophisticated computer simulations, they obtained an accurate physical description of the protein embedded in a lipid membrane and of the highly dynamic glycans covering the spike. This physical model provides details on the shape and the movements of the spike and its components. The evolution of the system in time is crucial to understand how the glycan shields work: “Think of a car’s windshield wiper while it’s raining”, explains Covino: “At a single timepoint only a small part of the protein is shielded, but in the long term almost all of the protein is covered, since the glycans quickly “sweep” all over the spike.” (Figure)



Highly mobile sugars (glycans, green) cover most of the spike protein surface (blue), as shown by computer simulation of the interactions between atoms and molecules, called Molecular Dynamics (MD). While A shows the most typical positions of glycans, B and C reflect less probable positions. Over a longer timescale (measured in microseconds) most of the protein surface is hardly accessible, since the glycans shield the protein (C).

The high mobility of the glycans thus leads to a strong steric shielding of the spike protein. Using two different methods the team identified regions of high and low accessibility: One method simulates rays of light illuminating the surface of the protein; the other simulates an antibody fragment that tries to reach the spike’s surface.

Through this, the team not only found four known antibody binding sites but also identified five epitope candidates as targets for further vaccine development. The team focused on epitopes that are well conserved and thus provide an effective goal for vaccine development. Further selection criteria were accessibility to antibodies, low glycan shield, predicted immunogenicity, and rigidity. They combined the data obtained, i. e. accessibility, rigidity, conservation, and immunogenicity scores into a single consensus epitope score. Many interesting candidates were thus eliminated, mostly because accessibility and rigidity exclude one another. Four epitopes seem to be particularly promising as vaccination goals. The group showed that already light glycosylation sterically hinders the interaction between antibodies and spike protein significantly.

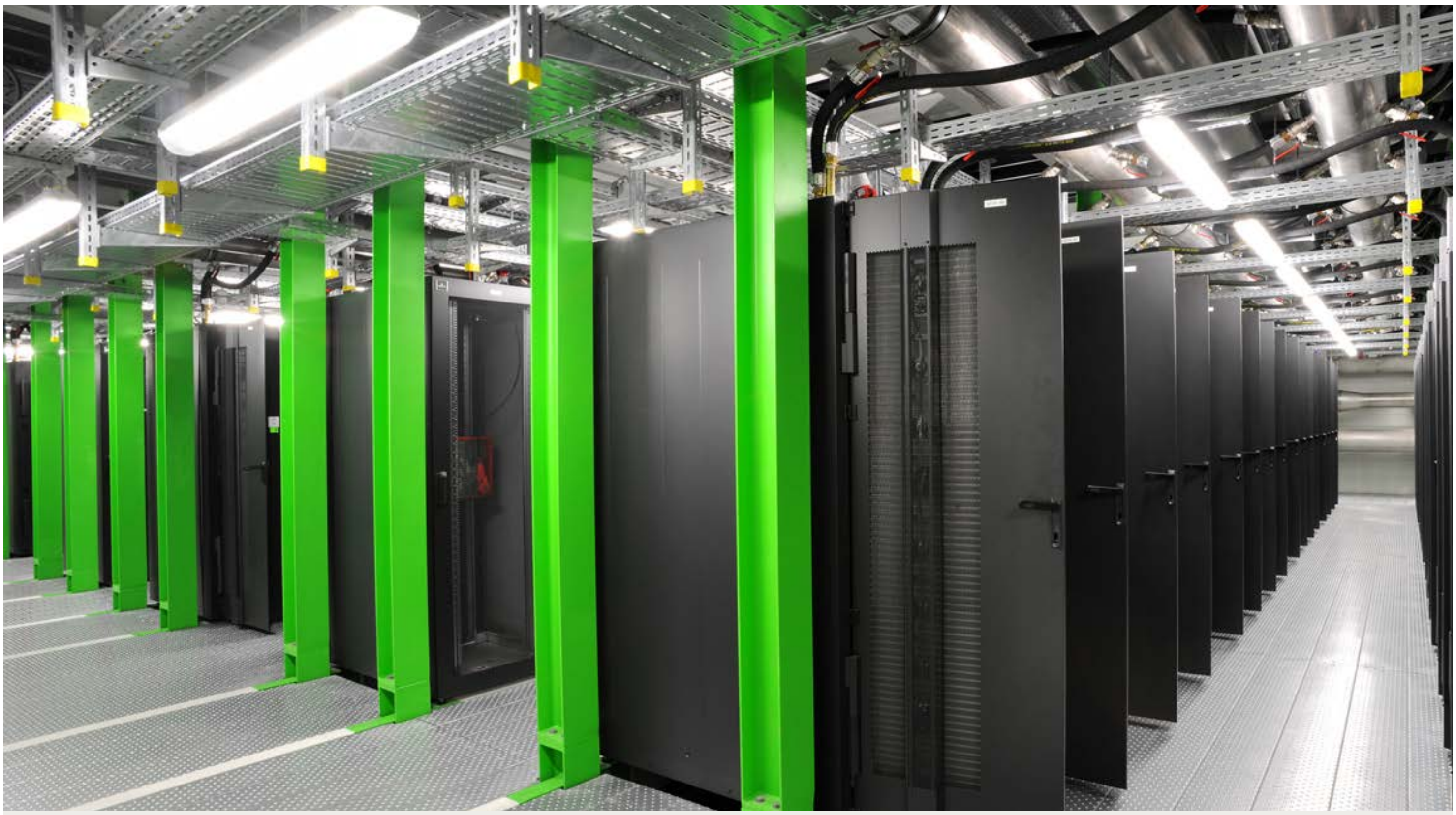
Covino, Hummer, and co-authors assume that the introduced epitope score can be generalized and extended to predict epitopes for other viral proteins. Their goal is to analyse diverse betacoronaviruses, with the aim to produce a vaccine that guarantees broad protection against multiple members of this virus family.

Publication:

Sikora M, von Bülow S, Blanc FEC, Gecht M, Covino R, Hummer G (2021) Computational epitope map of SARS-CoV-2 spike protein.

PLoS Comput Biol 17(4): e1008790. https://doi.org/10.1371/journal.pcbi.1008790

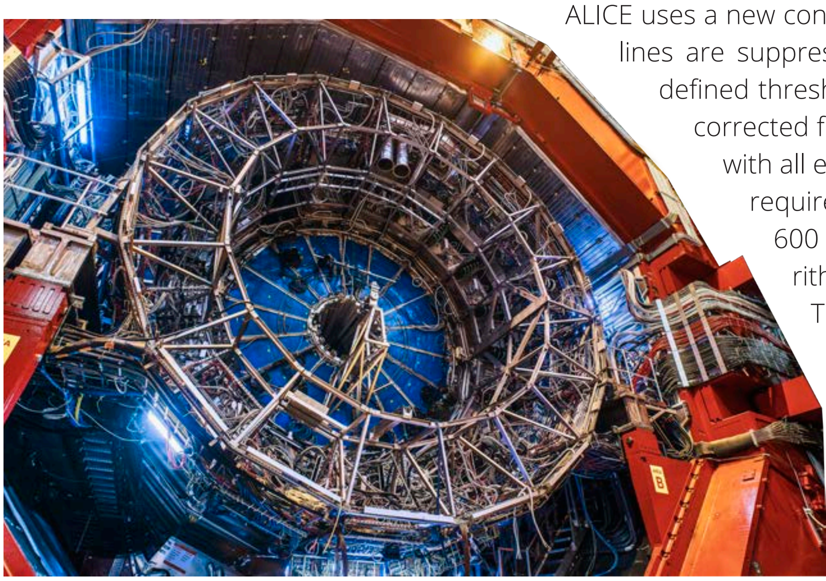
Computer Science & AI Systems



In the area of Computer Science & AI Systems, the already established work in the field of GREEN-IT is complemented by strategies of quantum computing and AI. Highly efficient computer architectures and program libraries are developed. In the past, computer architectures designed at FIAS achieved top positions in the worldwide ranking list for energy-efficient computers (Green500). The patented, highly efficient computer center architecture also allows a drastic reduction of construction costs. The use of GPU-based systems provides an ideal basis for the implementation of AI algorithms. The areas of application cover a very broad spectrum, ranging from tumor diagnostics to elementary particle physics and industrial problem-solving.

ALICE EPN Farm

The ALICE experiment at the CERN Large Hadron Collider (LHC) measures heavy-ion collisions. During those collisions, which happen 50.000 times per second, a quark-gluon plasma is created, which also existed during the first few microseconds after the big bang. ALICE measures almost all of the thousands of charged particles, which emerge from this plasma. To do that, ALICE consists of many subdetectors, including a GEM time projection chamber, a vertex detector, a transition radiation detector a muon calorimeter, and a calorimeter, to name a few. These detectors measure parts of the trajectory through the experiment and require specific, dedicated software to combine the many track segments into tracks and then reconstruct the particle from the track.



ALICE uses a new concept to read out all detectors at all times. Baselines are suppressed by comparing the measured signals with defined thresholds. Each of the millions of sensors has to be corrected for baseline, gain, etc. Then the individual events with all emerging particles are reconstructed online. This requires the processing of a data stream exceeding 600 GB/s. It is paramount to have efficient algorithms which find all particles with high precision. The work of Prof. Dr. Ivan Kisel, FIAS fellow, is of high importance here.

A strong effort was undertaken to have the reconstruction software run on GPUs which provide the best cost performance of available computing devices. However, FPGAs are also used for the first-level processing of the data entry of the online supercomputer.

These FPGA PCIe cards receive the 9000 fiber optic links from the detector and perform some first-level data handling. More than 95% of the entire reconstruction code is now running on GPUs and has been verified with simulated data, cosmic data, and data taken during the first pilot runs at CERN. The compute farm capable of processing the ALICE online data consists of 250 servers, implementing 64 AMD Rome physical cores, 8 AMD MI50 GPUs, and 512 GB of main memory. These servers are networked with a 100 Gb/s InfiniBand fat tree. The farm was deployed and has been running since April 2021. It should be noted that the compute farm would have cost 7-times the price of the existing farm if only CPUs had been used. ALICE is the only experiment utilizing GPUs at this level. The next step is to also have the offline physics analysis software equally use GPUs. This will change the entire particle physics computing scheme which currently is devoid of GPUs.

ALICE @FIAS:

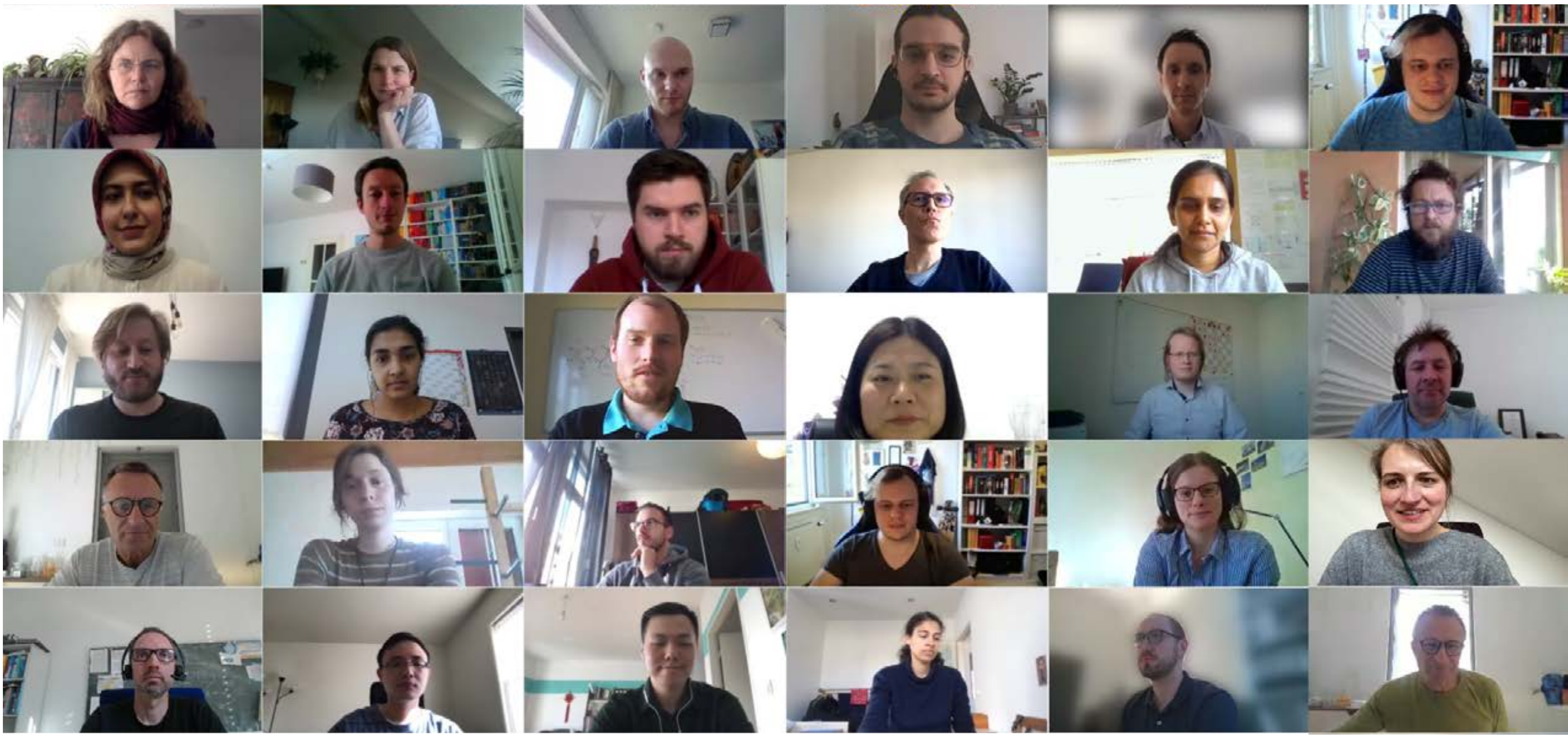
Prof. Dr. Lindenstruth and Prof Dr. Ivan Kisel are part of the ALICE collaboration. Therefore this work is conducted in close collaboration with Goethe University and CERN.

Pictures:

Top: The ALICE Detector; copyright CERN

Right: The ALICE compute farm, picture by Volker Lindenstuth

Events & Public Relations



In the second year of the pandemic, it was hardly possible to hold conferences and events on-site - for the protection of all involved. Thus, 2021 became the year of online conferences and workshops. A number of these events were held at FIAS. The highlight was certainly the continuation of our conference series "Giersch International Simposium" in February. Almost 260 international scientists attended the event.

The various research projects hosted most of their workshops and conferences virtually. A standout was the kick-off meeting of the SAI project. The meeting took place in September as a hybrid event. The Frankfurt scientists met on-site at FIAS, while the international partners were connected digitally.

In September, we were able to welcome our new Ph.D. students again with a live event. For many, this was the first opportunity to get in touch with other members of the graduate school. During a fun city rally through Frankfurt, the newcomers could get to know their new home.

In February, we hosted an international conference and summer school on theoretical and experimental quantitative cell biology. The event focused on theoretical aspects in life sciences and beyond. Due to the ongoing COVID-pandemic, it was held exclusively online.

The 8-day event combined a conference with the elements of a summer school, consisting of technical lectures by leading scientists, next-generation lectures, and laboratory demonstrations. Each day had a specific theme, ranging from Quantitative Imaging and Cell Biology; Modeling, BIG DATA, AI in Life Sciences to Medical and Neuroscience aspects.

The Giesch Symposia event series, held at FIAS since 2016 thanks to a generous donation from the STIFTUNG GIERSCH, has always excelled in integrating the interested public in the event. To ensure this in pandemic times, a public lecture was streamed over the internet each day. International greats from industry and research could be won as speakers here. As a treat, Nobel laureate Thomas Südhof from Stanford University, USA, spoke about "Molecular codes enabling brain function".

FIAS was able to attract as co-organizers the scientific networks DynaMem, CMMS, the 'Xidian-FIAS Joint Research Center' (XF-JRC), the Rhine-Main Universities, and the graduate program GRADE - iQbio. To give the international participants an insight into the work and the campus in Frankfurt - despite the online format - a short film series was produced. The participating laboratories and working groups from FIAS and Goethe University were thus able to provide an insight into their work and facilities.

Six impressive short films were produced, which will be available on the newly established FIAS YouTube channel even after the end of the conference.

The remaining public relations activities also largely took place online. For example, Frankfurt's neuroscience institutions joined forces with the non-profit Hertie Foundation and presented the "Frankfurt has ‚brain" website on the occasion of the international Brain Awareness Week 2021. Here, research results and fun facts are presented in an entertaining way.

Discovering new things in nature, making models, solving puzzles, or making estimates - all this was waiting for children and teens aged 10+ and their families during the 21 stages of the ProLOEWE science rally. It started on August 2 and almost all LOEWE Projects took part in the event. Therefore FIAS and the LOEWE focus CMMS produced a short film about fractals and modeling in modern biology.

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.

Our fellows are the foundation of FIAS.
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.

While Fellows are appointed for at least 5 years, many scientists are only in Frankfurt for a short time: Ph.D. students stay for 3-4 years, post-docs mostly for 1-2 years. In addition, we have about 10 visiting scientists a month who come to FIAS for a week or several months. This means that new people come to FIAS every month, and we do our best to make them feel at home as soon as possible.

Behind all this is a small but strong administrative team that organizes everything in the background.

Changes in the Boards:

Prof. Dr. Dr. h. c. Volker Mosbrugger is a new member of the Board of Trustees

Prof. Dr. Dr. h.c. Volker Mosbrugger

Volker Mosbrugger, the current president of the Polytechnic Society and former director of the Senckenberg Gesellschaft für Naturforschung (until December 2020), will support the work of the Foundation Board with immediate effect. The Foundation Board oversees the work of the Board of Directors and appoints its members. It decides on the FIAS budget and advises the Board on all matters of strategic importance. In recent years, for example, it has made a significant contribution to the successful restructuring of the research areas at FIAS and provided support in this process.

"Volker Mosbrugger respectively has been at the top of the major two Frankfurt civic societies, which have decisively shaped Frankfurt's research, cultural and educational landscape for more than 200 years." enthuses FIAS Chairman Volker Lindenstruth "Through his expertise in leadership, but also his great scientific background, Prof. Mosbrugger will be a great asset to our Board of Trustees."

Prof. Dr. Dr. h. c. Volker Mosbrugger studied and obtained his doctorate at the University of Freiburg. After his habilitation in Bonn, he was appointed to the Chair of General Paleontology at the Institute and Museum of Geology and Paleontology at the Eberhard Karls University of Tübingen. In 2005, Volker Mosbrugger came to Frankfurt, where he took over the directorship of the Senckenberg Gesellschaft für Naturforschung and in parallel accepted the call of the Goethe University as a Professor of Paleontology and Historical Geology.

As of this year, Mosbrugger retired officially, but continues to remain involved in Frankfurt science; in 2018, he succeeded Walther von Wietzlow as president of the Polytechnische Gesellschaft and also holds other important offices in the Polytechnische Gesellschaft's subsidiary institutes. He is also a member of various associations and scientific societies, such as the German Academy of Sciences, Leopoldina, and the German Academy of Science and Engineering, acatech.

"I have been following the activities of FIAS for a long time, as I am particularly interested in and fascinated by "complex systems" and the great challenges their analysis poses to the sciences." Volker Mosbrugger is pleased about his appointment to the FIAS Foundation Board.

"Perhaps over time, the problem areas of the Anthropocene that are particularly close to my heart can be focused on even more closely," he adds, as his personal research interests include the evolution of land plant form and function, as well as the evolution of terrestrial ecosystems and climate. Exploring the impacts of climate change and the associated loss of biodiversity for humans and the Earth system are central to his research interests.

Margarete Puschmann

We grieve for Margarete Puschmann

Magarete Puschmann was an indispensable member of the FIAS family for over 15. years. In addition to her generous donations, she participated in FIAS social activities, scientific lectures, award ceremonies, and summer parties, despite her advanced age, until the beginning of the pandemic. She has now passed away in Bad Homburg on the morning of June 8, 2021.

Fellow Reports 2021

**Dr.
Maria Barbarossa**

Dr. Maria Barbarossa studied mathematics at the University of Perugia, Italy and at the TU Munich. During her doctoral studies (PhD in Mathematics 2013, TU Munich) she started close collaboration with biologists and biochemists at Helmholtz Zentrum Munich. From 2013 to 2015 she was a postdoctoral fellow at the Bolyai Institute, University of Szeged, Hungary. In 2015 she returned to Germany as Margarete von Wrangell Fellow and joined Heidelberg University. Maria is a Fellow at FIAS since Spring 2020.

Public Relations Professional

In this year I have learned a lot about communication of scientific results to the media and the general public

Projects @ FIAS: 3

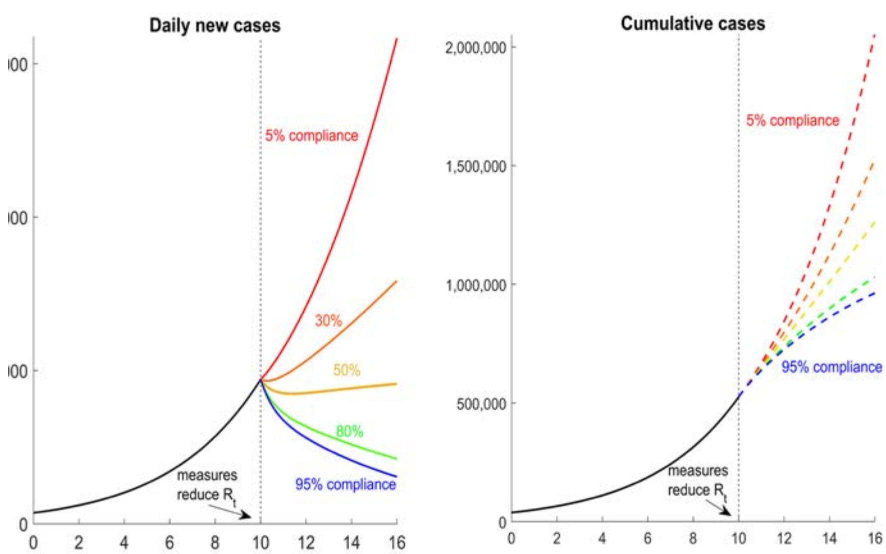
Collaborations

JSC Forschungszentrum Jülich
Heidelberg University
Karlsruhe Institute of Technology
TU Munich
University of Szeged

Mathematical models explaining COVID-19 nonpharmaceutical control

Almost one year after the beginning of the COVID-19 pandemic, Germany was in its third lockdown. Many wondered about the efficacy and duration of the imposed measures. In our group we used our skills in mathematical modeling and built a simple mathematical model, assuming that only part of the population adheres to specified contact restrictions.

The simulations reported below show a fictitious situation, which, however, comes very close to the situation in Germany in early fall 2020. We follow an ongoing COVID-19 wave under mild control measures for 10 weeks. The reproduction number for these mild control measures is 1.5. Simulated restrictions are de facto reducing contacts so that from week 10 the dynamic should proceed under lower reproduction number. If everyone in the population adhered to these restrictions, they would in a reproduction number of 0.75, hence in exponentially decreasing cases. We split the total population into a compliant group, which attains to the prescribed contact restrictions and a non-compliant population that keeps the same behavior as before contact reduction. We show how the number of cases would develop if 5%, 30%, 50%, 80% or even 95% of the population adhered to the contact restrictions. The simulations show that in the case of 50% compliance, the introduction of the measures leads to a plateau, which was actually seen in the reported data from November 2020 in Germany. Very similar images can be generated under different assumptions, e.g. different detection and stricter / milder measures with a lower / higher proportion of the population adhering to the measures. In reality, different people most probably adhere to individual rules to different degrees rather than being either fully compliant or not compliant at all. Our simulations were shown in the media to illustrate that the more people reduced their contacts, the faster the outbreak could be controlled.



Daily new cases and cumulative cases vs. number of weeks, before and after interventions. From week 10 on, control measures reduce the reproduction number from 1.5 to a lowest possible value of 0.75, assuming contacts are uniformly reduced in the population. If only a certain percentage of the population complies with contact reduction, the control measures might fail to contain the epidemic. When control measures begin to reduce the reproduction number Rt we assume about 20,000 detected cases per day and about 520,000 cumulative cases detected since the beginning of the epidemic, a situation which mimics the German data in October 2020.

Dr. Roberto Covino
Roberto Covino 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.

Interdisciplinary Group

Students have usually either a background in physics or in biochemistry, and they have fun teaching each other their core expertise.

Projects @ FIAS: 1

Collaborations

Mike Heilemann, Goethe University
Robert Ernst, University of Saarland
Pietro Faccioli and Philippe Hauke, Trento University
Taki Nishimura and Sharon Tooze, Crick Institute London
Elif Karazöz, Max Perutz Labs Vienna

Simulation of biological systems

2021 was an intense year for the CovinoLab! After a long work, we co-authored a pre-print presenting an autonomous artificial intelligence that adaptively runs simulations to discover interesting molecular mechanisms. One of the lab's focuses is to further develop this framework and apply it to exciting biological questions.

In 2021 many young enthusiast scientists joined the group. Gianmarco Lazzeri and Elena Spinetti, both graduated with a master's in "Quantitative and computational biology" from Trento University, joined as Ph.D. students. Jan Stuke, Senere Arghittu, Joan Nigorra, Margherita Mele, and Lars Dingeldein joined as master's students. Their projects ranged from developing new statistical analyses of complex data to simulation-based statistical inference and the study of exciting molecular systems. Five of them successfully graduated during the year, often with the highest honors.

Our lab became one of the founding members of the newly established "International Max Plank research School in Cellular Biophysics ."The school recruited the first cohort of Ph.D. students from many international applications. After a competitive selection, we were thrilled to obtain funding to recruit Serena Arghittu as a Ph.D. student. Serena officially started her Ph.D. in the lab at the beginning of 2022.

The lab was also a member of the new CRC1507: "Membrane-associated Protein Assemblies, Machineries, and Supercomplexes ."We defended the proposal in December and passed with flying colors.

Finally, but probably most importantly, we could get back to a more normal group life. Students worked together in the same rooms and reclaimed fundamental aspects of the scientific activity: discussing, explaining their projects, and supporting each other. Despite the horrible weather, the CMMS outing on the Tuanuns was great fun. We climbed the Großer Feldberg and walked from there to the Saalburg.

The CovinoLab is now bustling with activity and new ideas, and we are excited to have an even more eventful 2022!

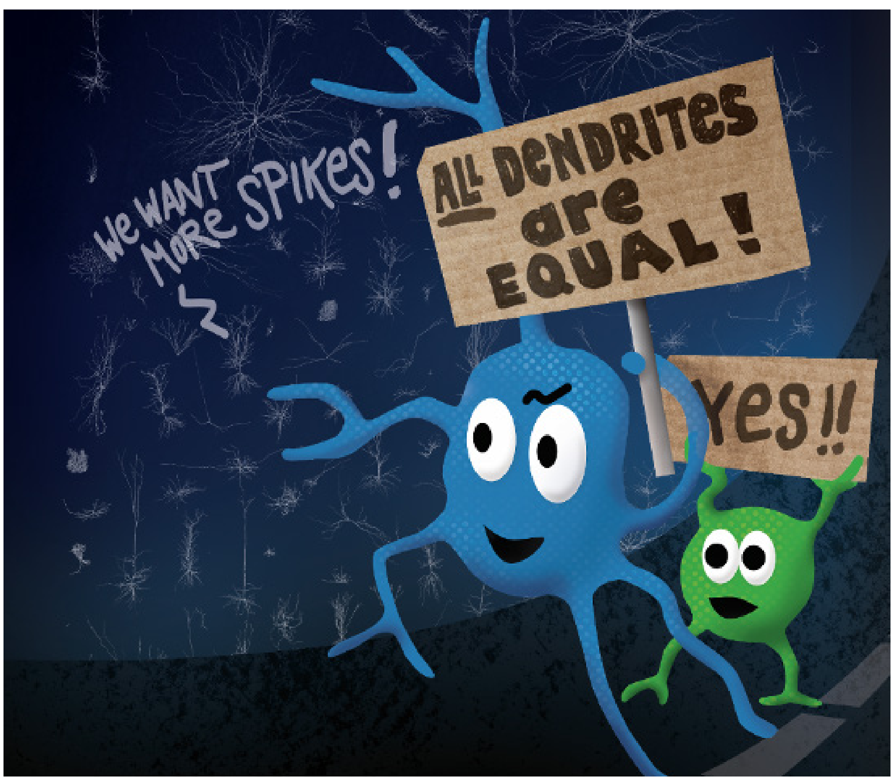
The Covino Lab at Feldberg on Jul 11th 2021

Dendritic constancy

In the 1960s, Wilfrid Rall successfully applied equations from cable theory to neurons. It meant that he could calculate the propagation of currents in dendritic trees, the input structures of neurons. Until then, the contribution of dendrites to neuronal function had been largely ignored. But Rall could show that electrical signals from individual inputs across the dendrites attenuated dramatically and could interact in sophisticated ways – a turning point for our understanding of neural computation.

We explored a feature of cable theory that seems to generalise across diverse dendritic trees: instead of following the impact of single inputs, we considered synaptic activity when it distributes across the whole or parts of the dendritic tree. Interestingly, the cable then tends to collapse to a single point, making the neuron's responses independent of the dendrite's shape or size. This means that the input-output function of neurons may conveniently not change during development or in the context of neurological diseases when dendrites undergo massive structural changes.

So in a way, neurons are more equal than one may think. Importantly, however, dendritic constancy does not diminish the importance of the large palette of synaptic learning rules and local computations in dendrites that make neurons unique and are sure to keep neuroscientists on their toes for times to come. Nevertheless, we believe that seeing how dendrites can behave equally across scales will contribute to a better understanding of general principles in neuronal function. Intriguingly, in a recent follow-up study we have shown that the normalisation of synaptic input weights based on the dendritic constancy mechanism improves the learning performance in artificial neuronal networks. Thus, dendritic constancy may be of interest not only for neuroscience but also for the machine learning community.



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.

Science meets Music

Watch this beautiful visualisation of classical music by pianist Jimin Oh-Havenith with our dendrites https://www.youtube.com/watch?v=uksJ0VZL050

Projects @ FIAS: 1

Collaborations

Peter Jedlicka
Gaia Tavosanis
Thomas Deller
Jonathon Howard

The call for equal rights affects one of the smallest components of the brain, too: the dendrites
© Ernst Strüngmann Institute

Prof. Dr.
Hannah Elfner

Hannah Elfner is groupleader at GSI, professor for Theoretical Physics at Goethe University and a fellow at FIAS since 2013. She obtained her PhD degree at Goethe University in 2009 and spent 3 years as a Humboldt fellow and visiting assistant professor at Duke University. In 2016, she received the most prestigious award for young scientists in Germany, 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.

Christmas tresure hunt

Instead of a traditional Christmas party that was prevented by the COVID pandemic, the group went on a treasure hunt through Frankfurt – enjoying Glühwein and cookies outside.

Projects @ FIAS: 2

Collaborations

JETSCAPE collaboration, USA

MUSES collaboration, USA

Charles Gale, McGill University, CA

Yuri Karpenko, Prague University, Czech Republic

Dmytro Oliinychenko, INT, Seattle, USA

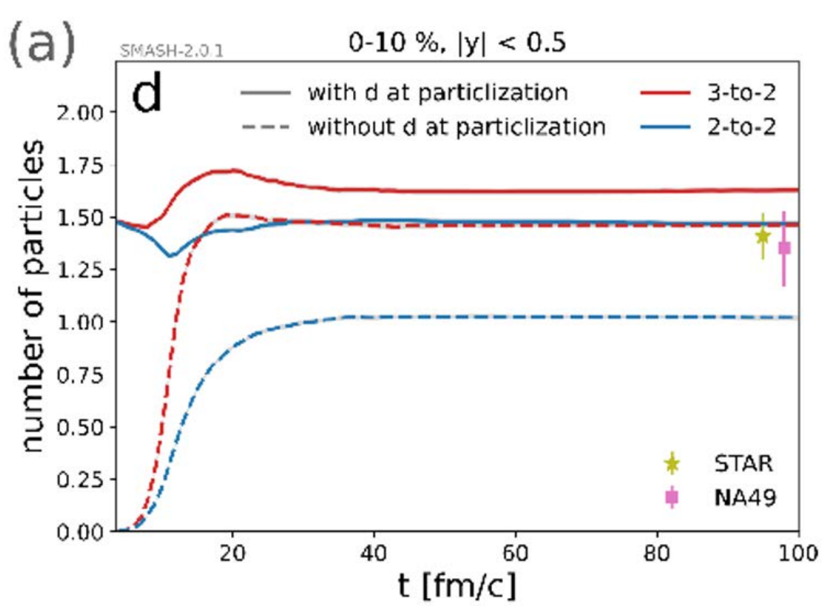
Multi-particle collisions in hadronic transport approach

Hadronic transport approaches are the tool to describe the microscopic non-equilibrium dynamics of heavy-ion collisions at low beam energies and in the late stages of high energy collisions, when the hot and dense fireball has cooled down. At that point, the quark-gluon plasma has been converted back to hadrons. Most approaches rely on binary scatterings, since they can be treated with a simple geometric collision criterion. Within SMASH (Simulating Many Accelerated Strongly-interacting Hadrons) it is now possible to collide any number of hadrons M and produce any number of hadrons N in the final state. This has been made possible by the implementation of stochastic rates.

The new functionality has been applied to two different physics cases. One shown below in the figure concerns the production of deuterons on the hypersurface of a hydrodynamic evolution in AuAu collisions at sqrts=7.7 GeV corresponding to collisions as they have been studied at the Relativistic Heavy-Ion Collider (RHIC) and the CERN-SPS. It has been shown that explicit 3<->2 reactions allow for a faster thermalization and regeneration of the deuteron yield during the hadronic phase. The second application concerns the first study taking into account the backreaction for proton-antiproton annihilation processes at LHC energies. The 5 pions <-> ppbar process is important and leads to a regeneration of 50% of the proton yield. The fraction of 15-20 % of the reactions that are reversed by the backreaction does surprisingly not depend on the beam energy or the centrality of the collision. The details of the proton yield are crucial for all future studies aiming at extracting quantitative information from heavy-ion measurements.

Associated publication:

Phys.Rev.C 104 (2021) 3, 034908 and arXiv: 2107.08812



Evolution of mid-rapidity deuteron yields in Au+Au afterburner stage. (a): 0-10% centrality class and experimental data from STAR collaboration at RHIC and NA49 collaboration at CERN.

Computational Pathology

Our aim is to infer molecular properties based on tissue and cell morphology depicted in so-called whole slide images (WSI). These WSI's are prepared in the routine diagnostics of pathology for each patient and the developed methods can be used e.g. to determine molecular heterogeneity within a tumor easily and without further testing.

We have developed a complete pipeline for processing WSI's and predicting molecular subtypes using gastric cancer as an example. For prediction, bagging ensemble cNN's (convolutional neural network) were trained, which decreased the error rate from ~47% to ~33% compared to individual cNN's on an independent test set from a different clinic. Random guessing for that problem would result in error rates on 75%, as four molecular subclasses exist. Using these predictions, we demonstrated that there is intra tumor heterogeneity of molecular subclasses in up to ~50% of gastric carcinomas and that classical laboratory in situ methods are not suitable to determine these subtypes, which was subsequently confirmed using OncoScan arrays.

To further improve this pipeline, we are currently investigating the impact of image quality. In particular, we are looking at the influence of color differences, where stain normalization of WSI's can improve cNN generalization, and other factors such as overall tissue quality/origin.

Reference: Flinner N, Gretser S*, Quaas A, Bankov K, Stoll A, Heckmann LE, Mayer RS, Doering C, Demes MC, Buettner R, Rueschoff J, Wild PJ. Deep Learning based on hematoxylin-eosin staining outperforms immunohistochemistry in predicting molecular subtypes of gastric adenocarcinoma. J. Pathol. (in press).*

Dr. Nadine Flinner

Nadine Flinner 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.

Group Leader at the KGU

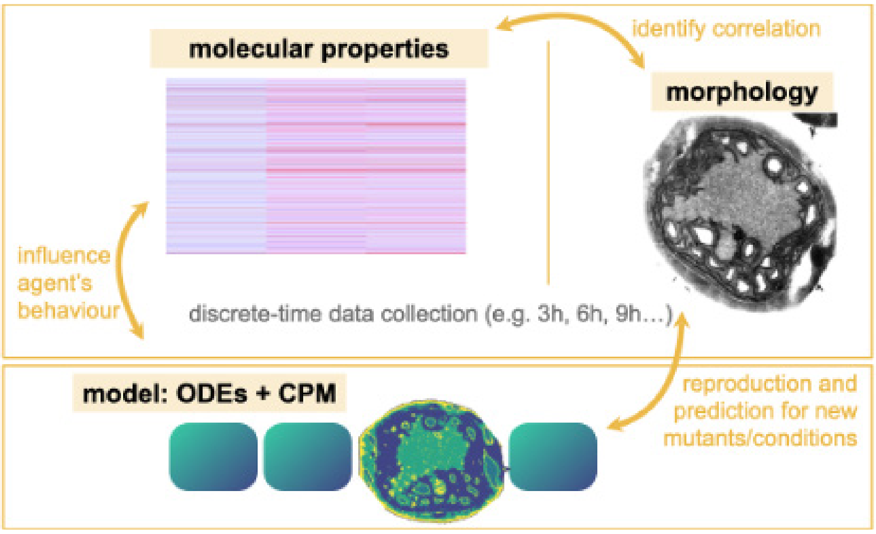
Since 2020, Nadine is the Mildred Scheel group leader (MSNZ) at the Dr. Senckenberg Institute of Pathology (SIP), University Hospital Frankfurt

Collaborations

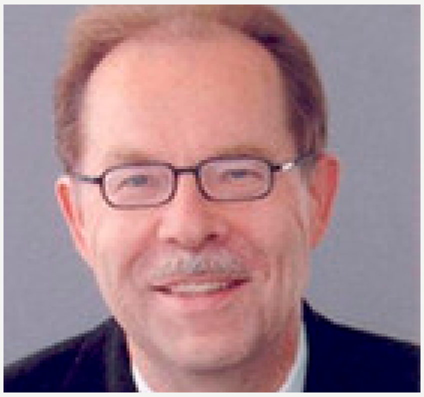
Peter Wild, Goethe University

Olga Goncharova, Dr. Senckenberg Institute of Pathology

1a



General Overview over the CMMS project on modelling heterocyst differentiation



Prof. Dr.
Martin-Leo Hansmann

Martin-Leo Hansmann 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

In 2001 he was awarded the German Cancer Aid Prize.

Projects @ FIAS: 1

Collaborations

Dr. Wojciech Samek (Frauenhofer HHI), Prof. Dr. Frederick Klauschen (Charite‘ Berlin), Prof. Dr. Klaus-Robert Müller (TU Berlin)

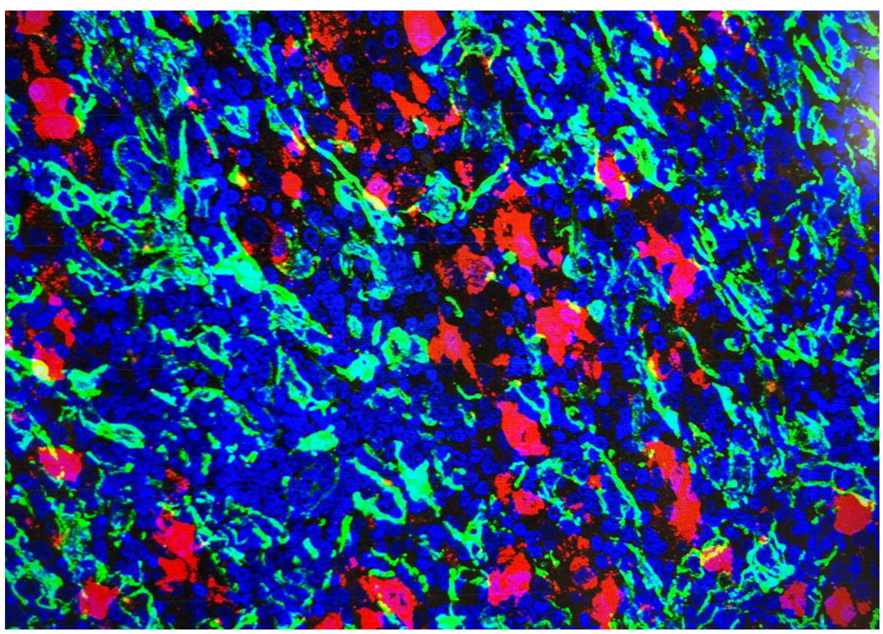
Computational life science on deep learning Biomedicinie

The BMBF funded project made considerable progress, in that we could show, that cell movement is an independent and important factor for classification of different populations of lymphocytes and non lymphoid cells in the immune system. These are quite new findings that have not been reported in humans up to now.

The first paper on cell movement in human lymphoid tissue was published (Donnadieu et al.2020).We could show that PD1 cells, which are a special cell population, needed for germinal center cell reactions, have different speeds in defined compartments of germinal centers. PD1 cells with high speed are found in the periphery and those with low-speed in the centre of germinal centers. So we were able, for the first time, to define movement landscapes of human lymphoid tissue. We started to investigate these phenomena applying bioinformatic and machine learning technologies.

Our group published 17 papers in 2020. Besides movement evaluations, our scientific work was concentrated on 3-D studies in immuno reactions . Laser scanning technologies enabled us to visualize networks in between reticulum cells, as well as T cells and their neoplastic variants, to give new insights in the development of malignant lymphomas. Usually tumours are diagnosed by histology. Our approaches started to construct a new network situation as a basis of lymphoma classification.

The aim for most of our studies is to establish the so called virtuel lymph node. We could visualize lymph node structures in 3D and 4D using laser scanning and include the data in a mathematical model. This model will enable in the near future to calculate qualitative and quantitatively the immuno reactions in a synthetic lymph node setting.



Distribution of macrophages (red) in a lymph node network (green).

A new perspective on dark matter

Galaxies rotate faster than Einstein's theory of General Relativity predicts. This is also true for our own galaxy, the Milky Way. But just exactly why the predictions of General Relativity do not fit with the observations is presently unclear. Most astrophysicists believe that 80% of the matter in our universe is an invisible type of "dark matter". If true, the Milky Way is embedded into a huge cloud of this dark matter, and planet Earth flies through it. Another, alternative, explanation – called "modified gravity" – is that General Relativity isn't quite correct.

One of the projects I have worked on last year with PhD candidate Tobias Mistele is whether the rotation of our Milky Way can be explained by a hybrid theory, that is a combination of dark matter and modified gravity. It is a type of matter which can form a superfluid, and in this superfluid phase it mediates an additional force that mimics gravity. This hybrid theory combines the benefits of both, dark matter and modified gravity, without the disadvantages of either. It was previously shown to work well for other galaxies.

The data from the Milky Way is both better and worse than that of other galaxies. Better because we have more data and it's from nearby. Worse, because we are embedded in the galaxy and move through it. However, our new work shows that the superfluid dark matter can well explain the rotation of the Milky Way.

Dr.
Sabine Hossenfelder

Sabine graduated from Frankfurt in 2003 and was a postdoctoral fellow, among others, at UC Santa Barbara, and the Perimeter Institute in Canada. Before returning to Frankfurt, she held a position as assistant professor at Nordita, in Stockholm, Sweden. Sabine's research is broadly in the foundations of physics, and is presently supported by the German Research Foundation and the Franklin Fetzer Fund. Besides her research, Sabine is also active in science communication.

YouTube Star

Sabine hosts a poupular YouTube Channel, with currently more than 400.000 subscribors.

Projects @ FIAS: 4

Collaborations

University of Bristol, UK
Maynooth University, Ireland
University of Münster, Germany
University of Oxford, UK

An example of a spiral galaxy, the Pinwheel Galaxy (also known as Messier 101 or NGC 5457)
Image Credit: ESA/Hubble

Prof. Dr.
Matthias Kaschube

Matthias Kaschube studied Physics and Philosophy in Frankfurt and Göttingen and obtained his doctoral degree in theoretical physics working with Fred Wolf and Theo Geisel at the Max Planck Institute for Dynamics and Self-Organization. From 2006-2011 he was Lewis-Sigler Theory Fellow at Princeton University, working on theoretical neuroscience and developmental biology. In 2011 he joined FIAS and became Professor for Computational Neuroscience at Goethe University.

Vice-Dean

From 2017-2019 he served as Vice-Dean of the Goethe Universitys Department of Informatics and Mathematics.

Projects @ FIAS: 5

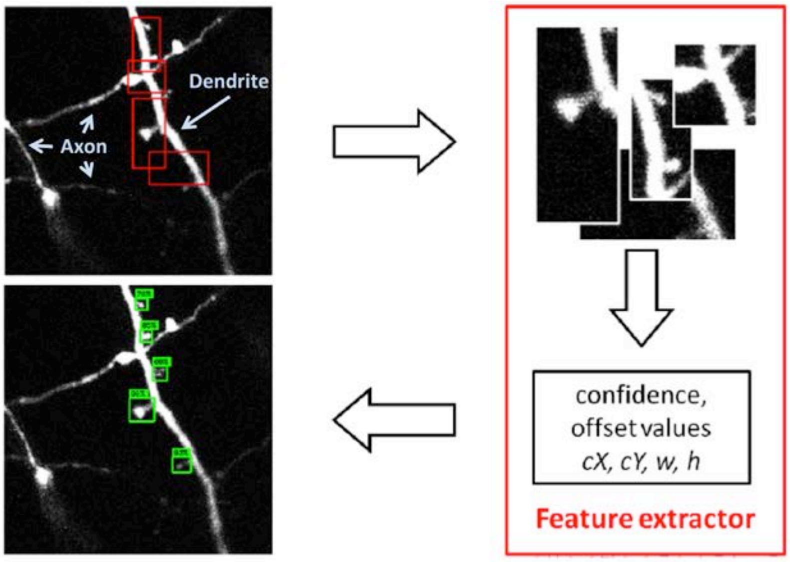
Collaborations

David Fitzpatrick (Max Planck Florida Institute), Simon Rumpel (Univ. Mainz), Gilles Laurent (Max Planck Institute for Brain Research), Kenichi Ohki (Univ. of Tokyo)

Deep learning-based detection of synaptic connections

The functionality of neural circuits in the brain depends significantly on the strengths of synaptic connections between neurons. Recent developments of deep tissue live imaging techniques enable to visualize large numbers of synapses and to monitor them over extended periods of time, from hours up to several weeks. Extracting the strengths of synaptic connections and analysing how they change across time, for instance while an animal acquires the skills necessary to perform a given task, could shed important light on the neural underpinnings of learning. However, measuring the strengths of individual synaptic connections from live imaging data has been a daunting task relying largely on visual inspection and manual annotation and so difficulties in scaling this up to simultaneous measurements of large numbers of synapses has been the bottleneck in such analyses. In collaboration with neurobiologist Simon Rumpel at the University of Mainz, we have made significant improvements towards developing a scalable image analysis pipeline, enabling to automatically detect large numbers of spines (proxies for synapses) in fluorescence imaging stacks and to track them across several days (Figure; Vogel et al., manuscript in preparation). For spine detection we exploited transfer learning, adopting a deep convolutional neural network (CNN) that was pretrained to detect and classify objects in natural images. We combined a Faster R-CNN to generate and refine region proposals of candidate spines with an Inception-ResNet for the recognition step of spines. The detection outperforms previous methods and achieves a near human level performance (F1 score of 0.90 tested on data sets labeled by n=5 experts; for experts, F1=0.94).

The work arose from an excellent bachelor thesis by Fabian Vogel, previously recognized as Hessen's youngest student entering the computer science program at Goethe-University at the age of 16.



Deep learning-based detection of synaptic connections (so-called spines are used as a proxy for synaptic connections): First, using pre-trained convolutional neural networks a large number of candidate regions (proposals of spine locations) are automatically generated (red boxes; only a small subset is shown). Then, each region is evaluated for the presence of a spine and refined in size and position (green boxes). For illustration, only a small dendritic branch is shown. The method can reliably distinguish dendritic spines from axonal structures

Block chain technologies in public administrations

Blockchain technology continues to be a controversial topic. In particular, the possible applications and the energy requirements. If the Blockchain architecture is specifically built on its projects, other consensus methods are possible in addition to the Proof of Work known from Bitcoin, so that the energy and hardware requirements can be significantly reduced. Especially since consensus is an essential part of this technology, we are happy to announce the addition of PhD student Felix Hoffmann to the research team, who will be working on consensus methods in his thesis, posing the question of whether meaningful computational tasks could be performed instead of hash value computation. One example of this could be the calculations of Alice experiments, in which computational tasks are currently already being distributed and performed.

In addition, the team has grown to include another PhD student. Mr. Diyar Takak is trying to use blockchain technology as a distribution and management hub to increase transparency in read as well as write accesses to data with changing cryptographic keys. The collaboration will be carried out with ecom21, which participates as a cooperation partner of FIAS in the research project of the Digital Showcase Projects announced by BMWi.

Negotiations for a continuation of the cooperation with the HZD (Hessische Zentrale für Datenverarbeitung) have been positive for the previous PhD student Philipp Lang, so we are happy to be able to continue his research. He is trying to apply the RADIUS protocol to blockchain technology in order to perform a realization of single sign-on also on a physical level.

In addition to the research projects, the seminar and lecture continued to take place, so that knowledge could be transferred to the students, but also interested parties for bachelor and master theses could be found.

Prof Dr.
Udo Kebschull

Professor Udo Kebschull 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.

New FIAS Fellow

His research focuses on the low-latency processing of large amounts of data, such as those generated by experiments in high-energy physics

Projects @ FIAS: 1

Collaborations

Hessische Zentrale für Datenverarbeitung (Hessian center for data processing)

co author
Philipp Lang

New methods for energy system planning and operation

Dr. Alexander Kies

Alexander Kies, born 1986 in Bremen, heads the research group FIAS Renewable Energy Systems and Artificial Intelligence (FRESNA) at the Frankfurt Institute for Advanced Studies (FIAS). He obtained his B.Sc. (2007-2010) and M.Sc Physics (2010-2012) at the University of Bremen with a focus on theoretical semiconductor physics. Afterwards, he obtained his PhD in physics at the University of Oldenburg with a cumulative thesis on energy system analysis. He has been employed at the FIAS since 2016 and performs research on energy system modelling, energy markets and artificial intelligence.

Featuerd Project

You will find more about his work in the featured article on page 13 within this issue.

Projects @ FIAS: 3

Collaborations

Jakub Jurasz (AGH Krakow),
Bruno Schyska (DLR)

Energy systems are transitioning under the challenge of climate change. Climate change is one of the greatest challenges today's society faces. Tackling it requires the reorganisation of the infrastructure supplying our energy needs. Planning of this infrastructure requires sophisticated tools, models and algorithms. The FIAS Renewable Energy Systems and Artificial Intelligence (FRESNA) group has published several high-impact papers on novel methodologies and algorithms. These introduce new methods to quantify and deal with uncertainty and study the uncertainty and relevance of meteorological input to energy system models.

The methods will be used in the future to study the use of AI-generated meteorological data for energy system models.

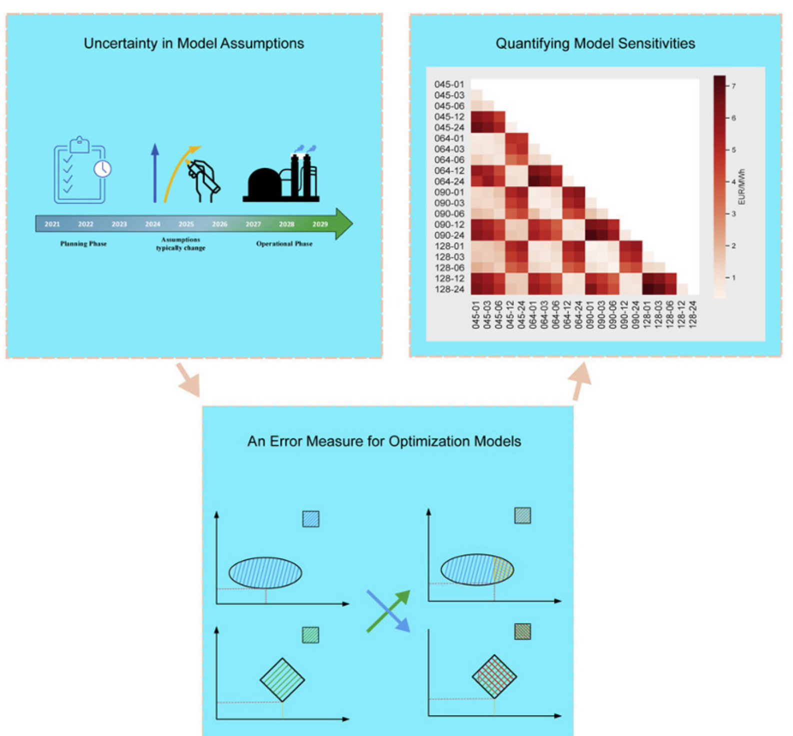
All models and data will be made publicly available under appropriate licensing.

Associated publications:

Schyska, B., et al. "The sensitivity of power system expansion models." Joule 5.10 (2021): 2606-2624.

Kies, A., et al. "Critical review of renewable generation datasets and their implications for European power system models." Renewable and Sustainable Energy Reviews 152 (2021): 111614.

Hofmann, F., et al. "Atlite: a lightweight Python package for calculating renewable power potentials and time series." Journal of Open Source Software 6.62 (2021): 3294.



Algorithms for heavy ion collisions

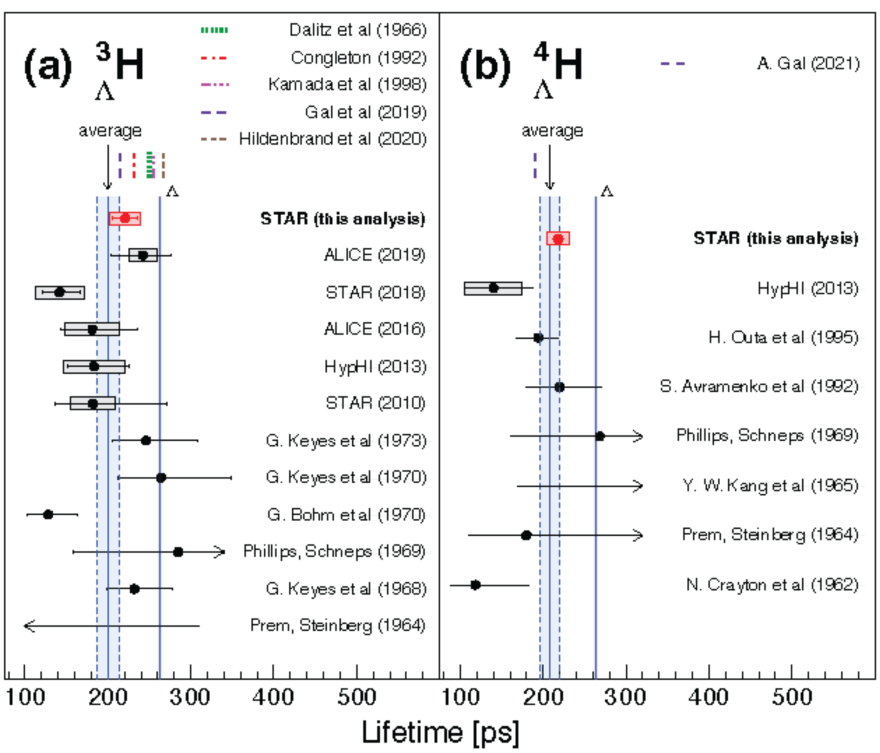
The work of the group was focused on investigating the efficiency and reliability of the algorithms for reconstruction and analysis of heavy-ion collisions developed as the FLES (First Level Event Selection) package for the heavy-ion experiment CBM (FAIR/GSI). Within FAIR Phase-0, the FLES package was adapted for the STAR experiment (BNL, USA) and applied to physics research in the beam energy scan program (BES-II).

Our algorithms were used in real time on the High-Level Trigger (HLT) computer cluster for express processing and analysis of STAR data. During the acquisition of the BES-II data, a complete data processing chain was run, including pre-calibration of detectors, reconstruction of particle trajectories, search for short-lived particles, and physics analysis of the decays of interest. Of particular interest to our group is the search for and study of the properties of hypernuclei.

Hypernuclei are nuclei containing at least one hyperon. Hypernuclei provide an opportunity to study the hyperon-nucleon (Y-N) interaction, which is an important ingredient in the equation of state for high-density nuclear matter, such as the core of neutron stars or the hadronic phase of heavy-ion collisions.

Traditionally, hypernuclei have been studied using emulsion methods, for example. The first observations of hypernuclei and antihypernuclei from heavy-ion collisions are from E864 in 2004 and STAR in 2009 respectively.

The hypertriton 3ΛH is a weakly bound object, leading to small overlap between the Λ and the deuteron core. This leads to the theoretical expectation that the lifetime of 3ΛH is close to τΛ of free Λ. However, STAR and HypHI have reported lifetimes 30-40% shorter than τΛ. This is commonly known as the hypertriton lifetime puzzle.



The figure shows 3ΛH (a) and 4ΛH (b) measured lifetime, compared to previous measurements, theoretical calculations and the free-Λ lifetime. Horizontal lines represent statistical uncertainties, while boxes represent systematic uncertainties. The experimental average lifetimes and the corresponding uncertainty of 3ΛH and 4ΛH are also shown as vertical blue shaded bands.

**Prof. Dr.
Ivan Kisel**

Ivan Kisel 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.

Featuerd Project

You will find more about his work in the featured article on page 13 within this issue.

Projects @ FIAS: 2

Collaborations

CBM
PANDA
ALICE
STAR

Prof. Dr.
Volker Lindenstruth

Professor Volker Lindenstruth studied physics at TU Darmstadt and received his doctorate in 1993 at Goethe University. He spent his Postgraduate years at the UC Space Science Laboratory. In 1998, he returned to Germany as a Professor and department head at the University of Heidelberg. In addition, he has been the head of the ALICE HLT project at the LHC since 2000. In 2007 he joined Goethe University as professor and at FIAS he held the position of Fellow but became a Senior Fellow soon thereafter.

Patentet Technology

The energy-saving high-performance data centers he co-developed were successfully patented.

Projects @ FIAS: 4

Collaborations

CBM
ALICE
PUNCH4NFDI

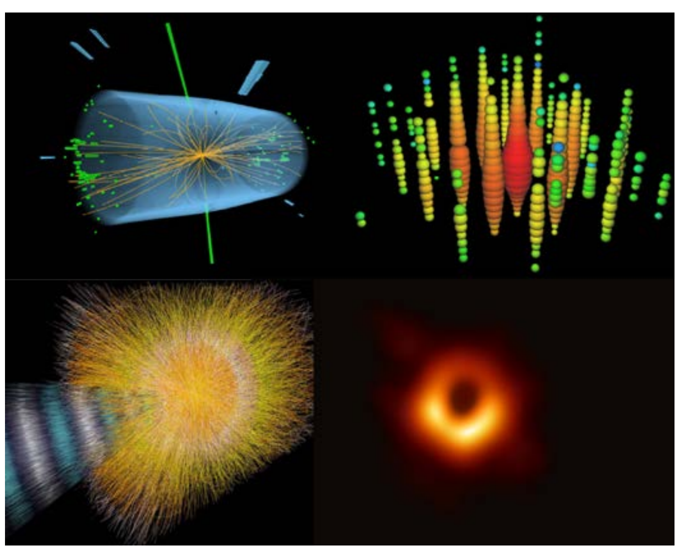
How to use computer resources more effectively within experiments

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 €.

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 our 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 FIAS scientist PD Dr. Andreas Redelbach, and Prof. Dr. Michael Kramer from the MPI 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 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 antartctic 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)

Modular Supercomputing and Quantum Computing

With the end of "Dennard Scaling" and the beginning of the phase-out of Moore's Law, the fac-tor of scalability in supercomputing became more important in order to maintain the desired growth rates in applicable computing power, especially in data rates. This was promoted by the increasing number of cores per processor, communication channels and SERDES elements as a result of increasing miniaturization, and by the increasing number of processors per system. Exascale – the next performance level – will take us into a completely new area of system paral-lelization, code scalability, reliability requirements for supercomputer technology, energy and processing power requirements and the effective allocation of resources.

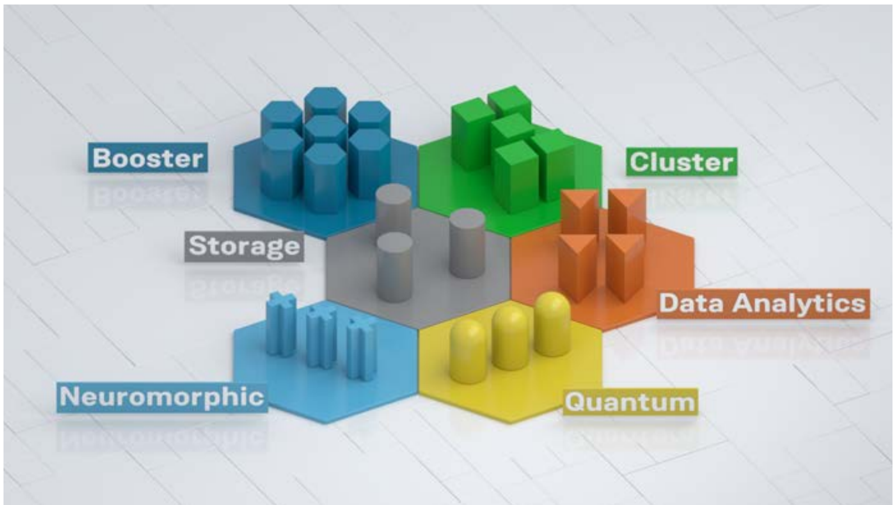
I have been pursuing the Modular Supercomputing Architecture (MSA) since 2000. In 2010 I filed a patent, which has since been granted worldwide. Starting in 2012, I have been co-designing MSA with the DEEP projects, funded by the European Commission. In 2017, a first production system was implemented at the Jülich Supercomputing Centre, JURECA – ranked 29th in the TOP500 list. In 2020, JUWELS, Europe´s most powerful supercomputer, went into operation, based on MSA.

MSA has evolved into a broad concept, capable of integrating future computing systems like quantum computers/annealers and neuromorphic systems into the modular network. At FIAS I do basic research on MSA – involving interaction and optimization of the use of disaggregated computing resources, MSA optimization of fast connection networks, integration of parallel file systems and cloud/high-performance computing mechanisms.

I intend to work closely with users in theoretical astrophysics, nuclear/elementary particle phys-ics, neuroscience and biology. It is my concern that HPC returns to a high application efficiency on the way to Exascale. I plan to integrate the first practical quantum computing devices for hy-brid HPC-QC calculations into a MSA network with the Frankfurt HPC systems, especially for use in first applications for industry and finance.

Prof. Dr.
Thomas Lippert

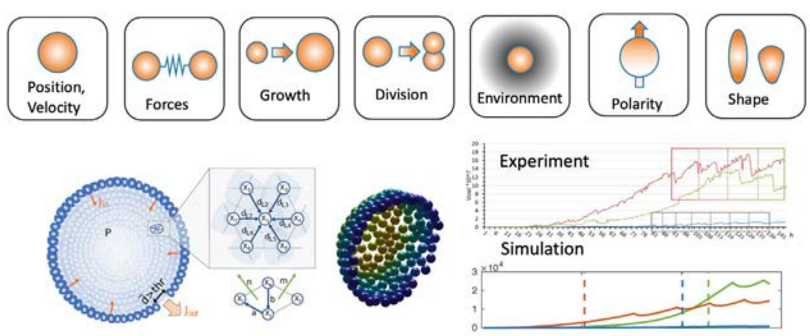
Prof. Dr. Dr. Thomas Lippert received his diploma in Theoretical Physics in 1987 from the University of Würzburg. He completed Ph.D. theses in theoretical physics at Wuppertal University on simulations of lattice quantum chromodynamics and in the field of parallel computing with systolic algorithms at Groningen University. He is director of the Jülich Supercomputing Centre at Forschungzentrum Jülich, member of the board of directors of the John von Neumann Institute for Computing (NIC) and the Gauss Centre for Supercomputing (GCS). Since August 2020 he holds the chair for Modular Supercomputing and Quantum computing at Goethe University Frankfurt and was appointed Senior Fellow at FIAS in March 2020.



Modular Supercomputing Architecture – MSA (Credits: Forschungszentrum Jülich/TRICKLABOR)

Modeling and analysis of pancreas organoid dynamics

Organoids are powerful experimental model systems that mimic features of organ development and function. In 2021 we teamed up with the group of E. Stelzer to analyze and simulate the dynamics of pancreas organoid cell cultures. These organoids grow from murine pancreas cells to form spherical multicellular systems exhibiting size oscillations and rotations. The origin of the size oscillations was unclear and attributed to either leakage in positions of cell division events or rupture due to osmotic pressure. Using formal mathematical arguments and an agent-based model for pancreas organoid dynamics we could show that the size oscillations originate from rupture in response to increasing osmotic pressure. The mathematical analyses, based on the geometry of the system forming hollow spheres and simple assumptions on the generation of the osmotic pressure, yield a scaling law coupling the occurrence of size oscillations to the cell division dynamics. We showed that a constant cell division rate can balance the osmotic pressure. In fact, we showed that if the cell count increases at least quadratically in time, no ruptures or size oscillations are expected. For some organoids exhibiting linear cell count dynamics the derived scaling law predicts size oscillations. To confirm the results, we developed an agent-based model accounting for cell-cell adhesion and repulsion, cell division, production of osmotic substances and pressure. A bending potential preserved the local structure during rupture events. Both, simulations and the experimental data confirmed the derived scaling law, which speaks in favor of the mechanical rupture hypothesis and against leakage during cell division. This interdisciplinary research project featuring organoid handling, light sheet and bright field microscopy, theory, modeling and simulation was published in BMC Biology 2021 (Hof et al., Long-term live imaging and multiscale analysis identify heterogeneity and core principles of epithelial organoid morphogenesis, BMC Biology 19(37), 2021.)



We extended our agent-based modeling toolkit which now incorporates a description of the cell position, velocity and intercellular forces, as well as (pressure-dependent) growth and division, interaction with the environment, cell polarity and cell shape. Bottom left: The toolkit is used to build an agent-based model of pancreas organoids by adding the secretion of osmotically active substances and osmotic pressure. Bottom right: Simulations based on the model recapture size oscillation characteristics observed in experiments and confirm the derived scaling law predicting organoid rupture and pressure release for cell division dynamics scaling as 1/t.

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.

We currently host the fastest 3D PIV package worldwide

M. Pereyra, A. Drusko, F. Strobl, F. Krämer, E. Stelzer, F. Matthäus, QuickPIV: Efficient 3D particle image velocimetry software applied to quantifying cellular migration during embryogenesis, BMC Bioinformatics 22: Art. no. 579, 2021, https://github.com/Marc-3d/PIV3D.

Projects @ FIAS: 1

Collaborations

M. Kaschube, E. Stelzer, M. Windbergs, A. Frangakis (GU)

A. Gerisch (TU Darmstadt)

K. Painter (Politecnico di Torino, IT)

D. Headon, J. Rainger (Roslin Inst. Edinburgh)

Network models

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. To this end, we kept on developing practically efficient sampling algorithms for a number of established random graph models including preferential attachment networks, graphs with prescribed degree sequences, and models based on geometric embeddings. All models are applicable, but not limited, to social networks. The PhD-thesis of group member Dr. Manuel Penschuck (defended in early 2021, https://d-nb.info/1239730012/34) provides a nice overview of our work till 2020. His input generator software also played a crucial role in our recent experimental study of external-memory algorithms for connected components (SEA 2021). New generator results submitted and accepted in 2021 concern engineering aspects (ALENEX 2022) and parallel global edge switching for the uniform sampling of simple graphs with prescribed degrees (IPDPS 2022).

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

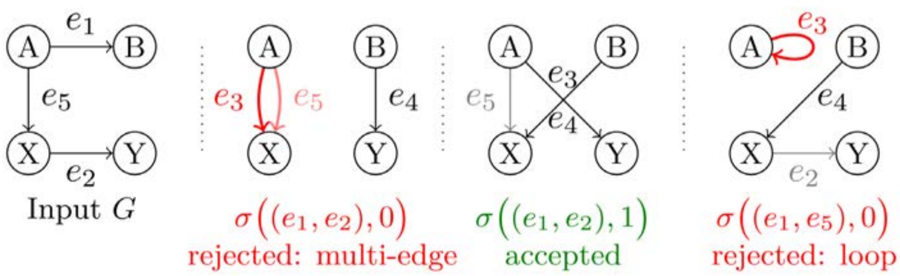
Prof. Dr. Ulrich Meyer

Prof. Dr. Ulrich Meyer joined FIAS in January 2020. He is at full professor at Goethe University Frankfurt since 2007. Since 2014 he is also the spokesperson of the DFG priority program "Algorithms for Big Data" (SPP 1736, www.big-data-spp.de) which spans more than 15 sites allover Germany, Austria, and Switzerland. He received his Ph.D. 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.

Got a call to TU Hamburg

Received a call in 2021 for the Fujitsu Endowed Professorship "Hardware-aware Combinatorial Optimization", but stayed in Frankfurt because of the good conditions offerd.

Projects @ FIAS: 1



Edge switching is an important basic operation in randomized network generation.

Prof. Dr.
Igor Mishustin

Igor Mishustin 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.

Medicine Physics

In addition to his work in subatomic and astrophysics, he has done important research on cancer therapy with ion beams.

Projects @ FIAS: 1

Collaborations

Abdel Nasser Tawfik

L.M. Satarov

M.I. Gorenstein

L.P. Csernai

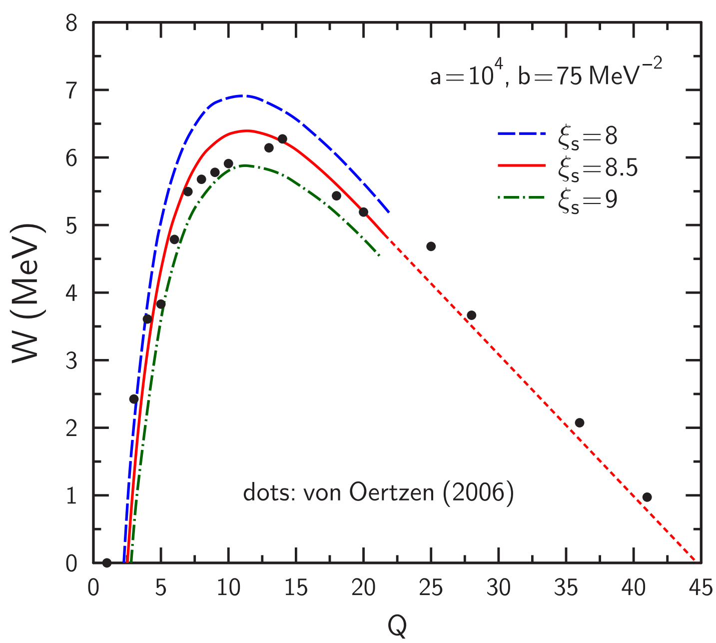
Bose-Einstein condensation in finite drops of alpha particles

Ground-state properties of finite drops of α particles (Q-balls) are studied within a field-theoretical approach in the mean-field approximation. The strong interaction of α's is described by the scalar field with a sextic Skyrme-like potential. The radial profiles of scalar- and Coulomb fields are found by solving the coupled system of Klein-Gordon and Poisson equations. A general- ized condition for Bose-Einstein condensation in a finite system of charged bosons is formulated in terms of particle effective mass. The formation of shell-like nuclei, with vanishing density around the centre, is predicted at high enough attractive strength of Skyrme potential. The equilibrium values of energy and baryon number of Q-balls and Q-shells are calculated for different sets of interaction parameters.

Empirical binding energies of α-conjugate nuclei are reproduced only if the gradient term in the Lagrangian is strongly enhanced. It is demonstrated that this enhancement can be explained by nonzero range of strong αα interaction.

Publication:

L.M. satarov, I.N. Mishustin and H. Stoecker; "Bose-Einstein condensation in finite drops of alpha particles", submitted to Phys. Rev. C (arXiv:2112.12539v1);



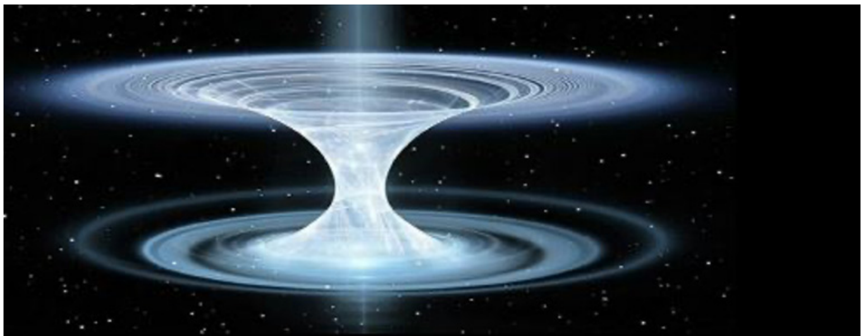
Binding energy of Q-balls as the function of alpha-particle number Q. Short-dashed line is obtained by linear extrapolation of the solid curve to the region Q >21.5, which is the particle number corresponding to chemical potential equal to alpha-particle mass. Dots show binding energies of alpha-conjugate nuclei compiled by W. von Oertzen, Eur. Phys. J. A29, 133 (2006).

Classical and Quantum Gravity

In 2021, Prof. Dr. Nicolini has been the recipient of a research grant from the Limiteless Space Institute of the A&M University System Houston TX to study the creation of a wormhole in a laboratory. Such a work is a hot topic within the current research about the possibility of interstellar travels. In his research, Professor Nicolini employed quantum gravity methods, like the Wheeler-de Witt equation and showed how a wormhole can be sustained by the fluctuations of the graviton or of a quantized matter field. On the research side, Professor Nicolini's associate Dr. Tzikas has published on Physics Letters B a single authored paper in the framework of black hole thermodynamics. Specifically, Dr. Tzikas determined the phase transition of a regular black hole in an isothermal cavity. The related phase structure could offer crucial theoretical insights in nuclear physics, by means of the conjectured duality between gravity and gauge theories.

On the side of the honors, we recall the following facts. Nicolini has been inducted in the world's top 2% of scientists for citation impact both for list of the year 2020 and of the whole career. He has also been elected Executive Editorial Board Member of the IOP Scinotes, Institute of Physics Publishing (IOP), Editor for the European Physical Journal Plus (EPJP), Springer-Nature and Peer Review Ambassador of the whole IOP group.

In September 2021, Nicolini has been appointed visiting associate professor at the Center for Astro, Particle and Planetary Physics of the New York University Abu Dhabi. In addition to his appointment, he obtained a research fund award to study the formation of primordial black holes.



Man-made wormholes might become realistic intestellar propulsion Systems in the near future. Image Credit: Echa & Science.

**Prof. Dr.
Piero Nicolini**

Piero Nicolini received his PhD from the University of Bologna in 2002 and his habilitation from the Goethe University in 2013. After postdoctoral positions in Marseille and in Trieste, he is currently a Research Fellow at FIAS, an Apl. Professor at the Goethe University and a visiting associate professor at the New York University, Abu Dhabi. His research interests cover quantum gravity, quantum field theory, and theoretical particle physics. Professor Nicolini is worldwide well known for having first proposed noncommutative geometry as a tool for studying evaporating black holes beyond the semiclassical limit.

Top Editor

Piero Nicolini is in the editorial board for 3 international journals and is serving as editor for 8 journals.

Projects @ FIAS: 1

Collaborations

Prof. Dr. Bernard Carr (Queen Mary University London)

Prof. Dr. Patricio Gaete (University of Valparaiso)

Prof. Dr. Remo Garattini (University of Bergamo)

Prof. Dr. Jonas Mureika (Loyola Ma¬rymount University & Kavli Institute, UC Santa Barbara)

Prof. Dr.
Luciano Rezzolla
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.

New board member

Luciano Rezzolla is the newest member of the board of directors at FIAS.

Projects @ FIAS: 1

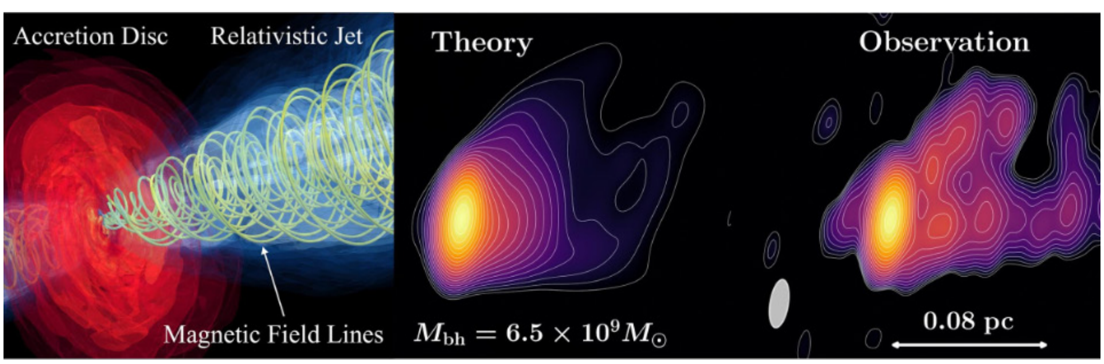
Relativistic Jet from M87: Unprecedented match between theory and observations

In April 2019, the Event Horizon Telescope (EHT) Collaboration captured the first image of a supermassive black hole at the center of the giant galaxy Messier 87 (M87), 55 million light-years away from Earth. The image has since become iconic and provided evidence of the existence of supermassive black holes at the center of massive galaxies. Importantly, it has also represented a fundamental confirmation of Einstein's theory of general relativity.

The black hole in M87 (M87*) has an enormous mass of six and a half billion solar masses and is among the most massive black holes known. However, M87 also offers another astounding feature: a jet of plasma that is shot from the center of the galaxy and that propagates at near the speed of light on a scale of 6000 light years, a good portion of our whole galaxy. What powers this jet and provides its stability over these enormous length-scales is still unknown and the subject of intense research of the scientists around the globe and Goethe University.

Using highly sophisticated three-dimensional supercomputer simulations of the plasma accreting onto a rotating black hole, scientists in Frankfurt and Würzburg, Germany, and Shanghai, China, have obtained a realistic and physically consistent description of the temperatures and densities near the launching site of the jet. Using then radiative-transfer calculations to track the complex motion of radiation in the curved spacetime has then provided the radio images of the innermost region of the jet which can be directly compared with the radio astronomical observations carried out over decades.

In this way, the scientists were able to show a remarkably good match between the theory and the observations, not only in terms of the jet morphology, but also of the energy spectrum of the radiation emitted from the jet, which has been collected over the last three decades with numerous telescopes and satellites. This very positive accord between theory and observations provides another important confirmation that Einstein's theory of general relativity offers the most accurate and natural explanation for the existence of supermassive black holes at the center of galaxies.



Using Einstein's theory of general relativity and simulations of plasma accreting onto a black hole, scientists at Goethe University in Frankfurt, Germany, have been able to model the morphology of the jet emerging from the giant galaxy M87 and to reproduce its multi-frequency energy emission. The unprecedented good match between theory and observation provides yet another confirmation of Einstein's theory of gravity
Credit: Cruz-Osorio/Fromm/Mizuno/Rezzolla (Frankfurt).

Rapid analysis of large seismological data sets

My research focuses on the field of seismology and my current research activities fall into five major areas:

(1) understanding of tectonic processes such as rifting and mountain building, subduction of oceanic plates, and mantle-plume upwellings through the seismological analysis of deformation and flow fields within the Earth's crust and mantle;

(2) studying seismic wave propagation in anisotropic elastic media through waveform modeling and inversion of seismograms;

(3) innovative monitoring of earthquake activity based on temporary deployments of networks and arrays of seismic stations at scales ranging from 10^2 to 10^6 m;

(4) detection, analysis and understanding of seismic and infrasound signals in response to volcanic and magmatic activities;

(5) improvement of seismic recording conditions by removal of noise effects.

In the last 15 to 20 years I have been involved in developing and coordinating seismological research activities in the Middle East, East Africa, and the Indian ocean region. More recently my group has participated in a large-scale European effort to study the Alpine region and related tectonic processes. The vast amounts of seismological data that have and will become available through these and similar research activities conducted by the seismological community require innovative and highly-automized processing and analysis tools to fully exploit the seismic recordings. The new developments in machine and deep learning (ML, DL) based on neural networks over recent years provide a promising base for such automized approaches of data processing.

Through the collaboration with scientists at FIAS and their expertise in applications of ML- and DL-concepts to tackle physical problems, I aim to develop novel tools required for the rapid analysis of large seismological data sets. The ability to utilize the information contained in seismic recordings more completely will significantly improve the imaging and understanding of processes within the earth, which are hidden from direct observations. The new methods also provide opportunities to search for previously undetected patterns that may link subtle waveform changes and earthquake rupturing. As an application for these tools, we are currently developing a proposal for a new AI-based "traffic-light" system to better control the release of induced seismic activity in deep geothermal reservoirs used for electric power generation.

**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, Germany. He joined FIAS in May 2020.

Taunus Observatory

The seismic station at the Taunus Observatory is maintained by the departement of Geophysics at the Institut of Geosciences at Goethe University in Frankfurt together with the BGR (Bundesanstalt für Geowissenschaften und Rohstoffe).

Projects @ FIAS: 1

Prof. Dr. Armen Sedrakian

Prof. Dr. Armen Sedrakian 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).

Academy of Science

Sedrakian is a foreign member of the National Academy of Science of Armenia.

Projects @ FIAS: 1

Collaborations

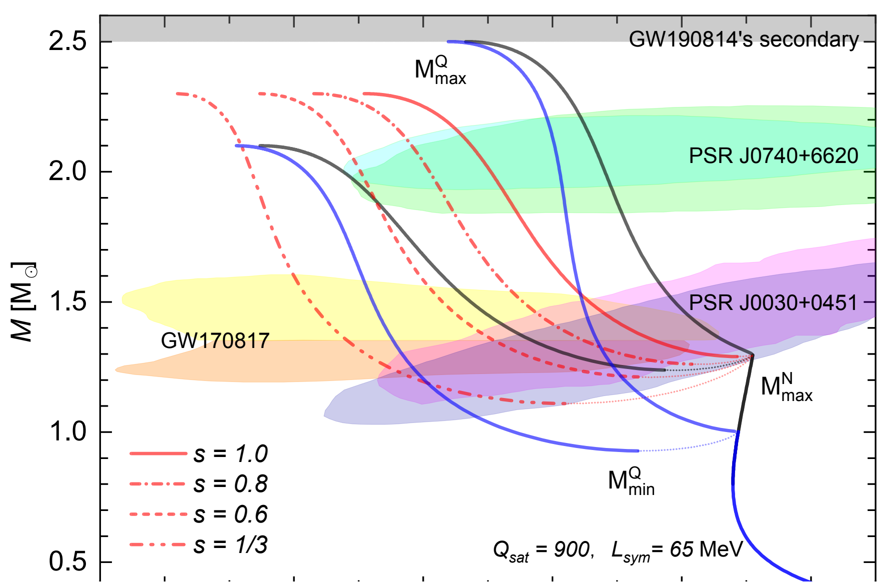
Prof. M. Alford (Washington U., St. Louis), Prof. Fridolin Weber (San-Diego State U.), Arus Dr. Harutyunyan (Byurakan Astro. Observatory), Peter Rau (Cornell University), Dr. Adraian Raduta (Phys. Eng. Institute, Bucharest), Dr. Micaela Oertel (LUTH, Meudon)

Equation of state of superdense matter

Our group have been working on relativistic density functionals for hypernuclear systems including delta-resonances. We also studied the implications of the transition to quark matter phase on the properties of the compact stars. The constraints from multi messenger astrophysics are an important ingredient of our studies and we have analyzed in detail the consistency of our density functional with the currently available astrophysical data.

We have completed a study of second order hydrodynamics of strongly correlated fluids within the non-equilibrium statistical operator formalism which allows to study hydrodynamical phenomena in the non-perturbative regime. Kubo formulae have been obtained for the new transport coefficients which arise in this new formulation of hydrodynamics.

Furthermore, we have studied the oscillations of neutron-star merger remnant and found out that they might become unstable to gravitational wave emission instability, as is the case in ordinary stars.



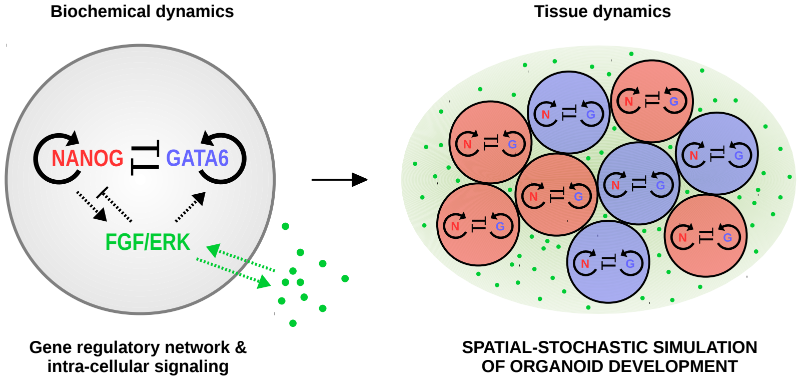
Illustrative mass-radius relation for hybrid EoS models. The dotted thin lines indicate unstable configurations. All the solid curves correspond to speed of sound squared equal unity (maximally stiff equation of state). For the remaining curves, the value of this quantity, dented by s, is indicated in the plot.

Event-driven multiscale bio-chemical 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 fun-da-mentally stochastic, and therefore limit the reliability of biological in-for-mation 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 nu-merical 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 causing biological noise, which quickly can become intractable both math-ematically and numerically. A hallmark of our approach therefore is to employ event-driven simulations, smart mathematical approximations, and problem-specific numerical optimization techniques for reducing the computational cost associated with realistic bio-stochastic models.

In 2021 we made significant progress in developing an event-driven stochastic simulator for developing tissue. First implemented for the single-cell setting, we carried out biophysically realistic simulations of the Nanog/GATA6 cell fate specification network in early mouse embryogenesis, gaining important insights into the role of mutual interactions and feedbacks in that system. Simulations additionally accounting for cell growth and division allowed us to identify additional requirements for the timely proceeding of early cell specification. We then extended the simulator to incorporate spatial coupling of neighbouring developing cells via biochemical signals and now study its impact on patterning robustness. These efforts are continued in 2022 and will open up the way towards a comprehensive understanding of how the interplay of tissue growth and spatio-temporal gene regulatory feedbacks can guarantee fast and robust cell fate specification in preimplantation mouse embryos.



Dr.
Thomas Sokolowski

Thomas 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.

New research paths

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. This project will be taken on by guest scientist Mirjam Schulz.

Projects @ FIAS: 1

Collaborations

Prof. Dr. William Bialek, Princeton

Prof. Dr. Thomas Gregor, Princeton / Institut Pasteur (Paris)

Prof. Dr. Gašper Tkačik, IST Austria

Prof. Dr. Sabine Fischer, Uni Würzburg

Prof. Dr. Sebastian Maerkl, EPFL (Lausanne)

Prof. Dr. Pieter Rein ten Wolde, AMOLF (Amsterdam)

**Dr.
Nishtha Srivastava**

Nishtha Srivastava 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 September 2020.

Promoting Women in AI

Her research is funded by a BMBF program to promote women in AI, and she is also personaly involved in promoting young women in AI.

Projects @ FIAS: 1

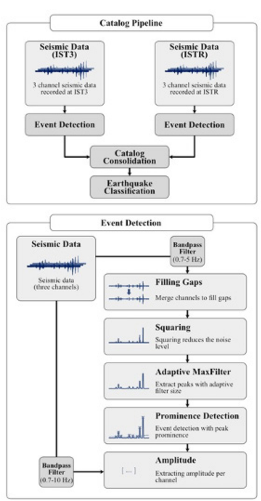
A Python Module for Automated Volcanic Event Detection Applied to Stromboli

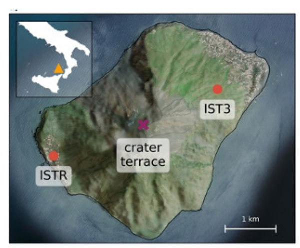
Many active volcanoes exhibit Strombolian activity, which is typically characterized by relatively frequent mild volcanic explosions and also by rare and much more destructive major explosions and paroxysms. The analyses of major and minor events can help to understand the eruptive behavior of the volcano and the underlying physical and chemical processes. Catalogs of volcanic eruptions and, specifically, seismo-volcanic events may be established using continuous seismic recordings at stations in the proximity of volcanoes. However, this could be a labor-intensive and time-consuming process. Here, we introduce a detection algorithm for identifying small and large seismic events due to volcanic activity at Stromboli: the Adaptive Window Volcanic Event Selection Analysis Module (AWESAM). This strategy of creating seismo-volcanic event catalogs consists of three main steps: (i) identification of potential volcanic events based on squared ground-velocity amplitudes, an adaptive MaxFilter, and a prominence threshold. (ii) catalog consolidation by comparing and verification of the initial detections based on recordings from two different seismic stations. (iii) identification and exclusion of signals from regional tectonic earthquakes.

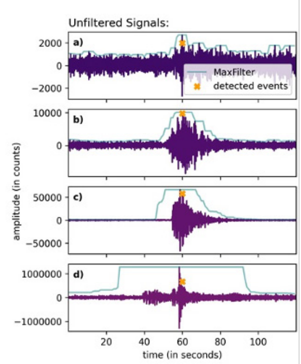
The python package is applied to publicly accessible continuous seismic recordings from two almost equidistant stations at Stromboli volcano in Italy to generate a seismo-volcanic event catalog. We compared this AWESAM generated catalog with a hand-picked catalog and found that around 95% of the seismo-volcanic events with a signal-to-noise ratio above three are detected. As a first example for the application of the information provided by the catalog, the temporal evolution of the amplitude-frequency relationship for the years 2019-2020 is studied by using over 290,000 seismo-volcanic events at Stromboli. The module allows for a straightforward generalization and application to other volcanoes worldwide, as it does not require an extensive seismic network.

Reference:

Fenner, D., Ruempker, G., Li, W., Chakraborty, M., Faber, J., Koehler, J., Stoecker, H. and Srivastava, N., 2021. AWESAM: A Python Module for Automated Volcanic Event Detection Applied to Stromboli. arXiv preprint arXiv:2111.01513. (Accepted in Frontiers in Earth Sciences).







Superficial layers of the cerebral cortex: A delay coupled, anisotropic, recurrent oscillator network
Columns coding for related features are coupled preferentially.

The QCD phase transition in (Ur)QMD

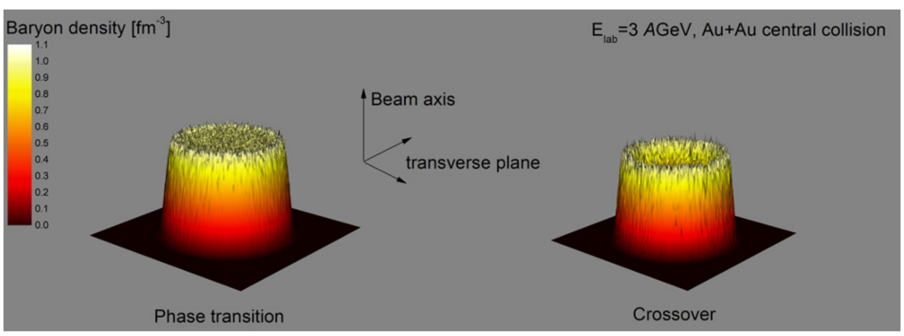
A microscopic description for a phase transition in CBM@FAIR

The Quark Gluon Plasma (QGP) is a state of matter that existed in the early universe and can only be created in relativistic collisions of heavy nuclei and possibly in the interior of neutron stars and their mergers. Current research on the QGP, at the GSI/FAIR, BNL/RHIC, CERN/LHC, NICA and HIAF facilities, focusses on its thermodynamic properties as well as fundamental features like deconfinement and chiral symmetry restoration. There are still many open questions regarding the properties and especially phase structure of the QGP at large baryon densities in the context of recent astrophysical observations of neutron star mergers, which may probe yet unknown properties of the QGP.

In our group at FIAS a method was developed to include any realistic (relativistic mean field) equation of state for QCD matter in a Quantum Molecular approach for relativistic heavy ion collisions. This enables us, for the first time, to simulate non-equilibrium, heavy ion collisions microscopically, in the presence of a first order phase transition. The figure below shows the result of an ensemble of such simulations, where the baryon density in central Au+Au collisions was extracted in the transverse plane at the time of highest compression. We can observe a clear difference when a phase transition is used or a crossover QCD transition is assumed.

Importance of the new model for data interpretation:

Our results enable us to investigate and predict a multitude of possible observables which are sensitive to the existence of the QCG phase transition and for the first time draw clear conclusions on the existence of this transition at high baryon density.



Density distribution at highest compression, in the transverse plane of central Au+Au collisions at a beam energy of 3 AGeV, as expected with the CBM experiment at FAIR. We employed the new CMF.UrQMD model for the microscopic description of the QCD phase transition.

Dr.
Jan Steinheimer-Froschauer

Dr. Jan Steinheimer-Froschauer 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.

Collaboration with China

Jan Steinheimer is one of the initiators of the Xidian FIAS International Joint Research Center established 2019.

Projects @ FIAS: 3

Collaborations

HADES collaboration

Ralf Rapp, Texas A&M Universit

Abhijit Bhattacharyya, Calcutta University

Christoph Herold, Suranaree University

Volker Koch, LBNL Berkeley, USA

Yasushi Nara, Akita International University

Prof. Dr.
Jürgen Struckmeier

After finishing his diploma in physics 1978, Jürgen Struckmeier 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 the Goethe University Frankfurt. Having worked as a lecturer, he was appointed there as "Extracurricular Professor", in 2010. In 2016, he joined FIAS as Fellow.

New Book

We are currently working on a book project, titled "Canonical Covariant Gauge Theory of Gravitation and Cosmology", which will be published in 2022 by Springer.

Projects @ FIAS: 1

Collaborations

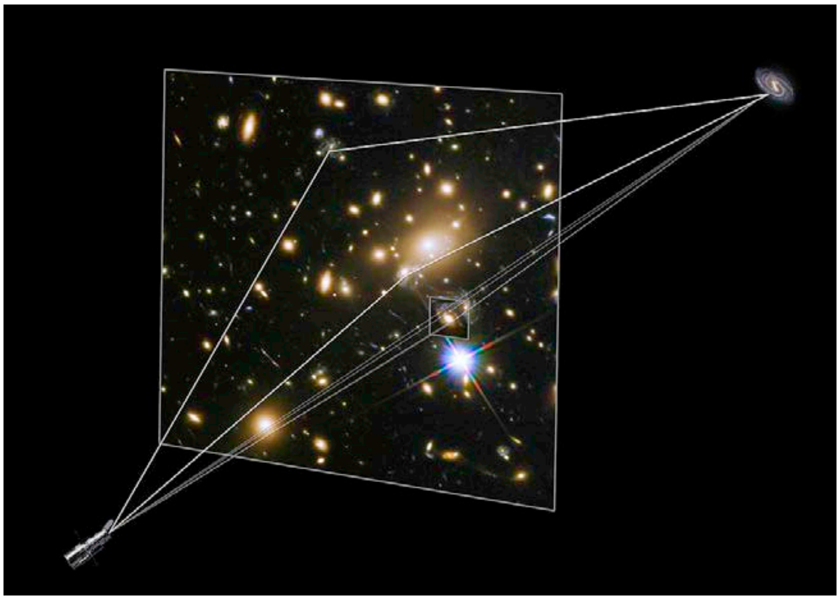
Eduardo Guendelman, Ben-Gurion University of the Negev;
Peter Hess, Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico;
Johannes Muench, University of Regensburg;
Friedrich Wilhelm Hehl, University Cologne;
Frank Antonsen, Copenhagen

Covariant Canonical Gauge Theory of Gravitation

We successfully derived Palatini-type gauge theories of gravitation based on canonical transformations in the covariant de Donder-Weyl Hamiltonian formalism of field theories. The canonical transformation theory ensures, by construction, that the form of the action functional to be maintained and thus complies with the requirement of diffeomorphism invariance -- historically referred to as the "Principle of General Relativity". The resulting Hamiltonian system describes self-consistently the coupled dynamics of matter fields and spacetime. This way, it is unambiguously determined how spin-0, spin-1, and spin-1/2 particle fields couple to spacetime.

In Einstein's general theory of relativity, the description of the dynamics of the "free" (uncoupled to matter) gravitational field is postulated to be given by a linear term in the Lagrangian: the Ricci scalar. Therefore, spacetime lacks in this description a conjugate momentum field, which is required to enable a dynamical response to deformations of the metric. This is different in the "Covariant Canonical Gauge theory of Gravity" (CCGG) theory: the dynamical spacetime itself is attributed a conjugate momentum in analogy to all other classical field theories. This changes the description of compact astrophysical objects and of relativistic collapse dynamics, with significant impact on the description of binary neutron star structure, mergers and pulsar dynamics. The CCGG modifications of the Friedman equation suggests, for example, a non-standard running cosmological constant and a new interpretation of Dark Energy, and hence change the standard evolution scenario of the universe. Moreover, the spin-coupling of fermions entails a curvature-dependent effective mass term in the ensuing Dirac equation. Its implication on neutron star physics was studied in the master thesis of Julia Lienert, which was submitted in 2021.

Continuing the development of the Covariant Canonical Theory of Gravity now focuses on the self-consistent description of the coupling of spinors to gravity, whose first part was published in Astronomische Nachrichten (J. Struckmeier, D. Vasak). The actual research continues to work out the spin-torsion interaction and its cosmological implications.



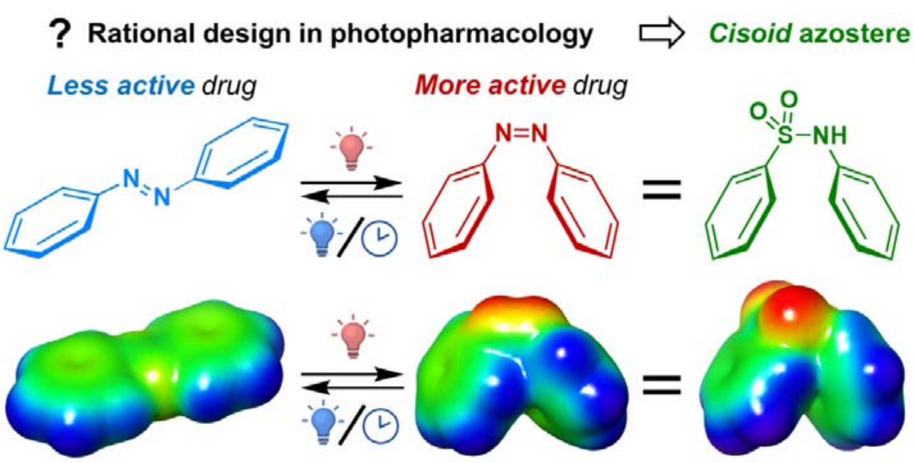
This sketch by NASA shows paths of light from a distant galaxy that is being gravitationally lensed.

Light-switchable pharmaceuticals derived from established drugs

In photopharmacology, light energy is used to switch pharmaceuticals between two forms. One of the forms is more active as a drug, the other one is less active. In order to be able to perform the switching, molecular fragments which change their properties upon light absorption, so-called molecular switches, have to be incorporated into a bioactive molecule. One strategy to do so is to start from an established drug and to look for opportunities to place the molecular switch. The challenge is to find a suitable part of the molecule which can be replaced by the molecular switch without altering important pharmaceutical properties.

In collaboration with researchers from the University of Groningen, we evaluated the potential of one class of drug molecules, biaryl sulfonamides. The idea was to replace the biaryl sulfonamide moiety by the common molecular switch azobenzene. To this end, we compared the properties of both molecules such as shape and dipole moment and concluded that biaryl sulfonamides are well-suited candidates for the development of light-switchable pharmaceuticals.

We tested our approach for two bioactive compounds, an inhibitor of a phospholipase and an FDA-approved histone deacetylase inhibitor for chemotherapy. First, we performed computational analysis to evaluate if the incorporated molecular switch is able to switch the inhibitor between more active and less active. Then, we performed experiments to validate the computational predictions. In both cases, it turned out that the two forms of the light-switchable inhibitors show different strengths of inhibition. Our results demonstrate how light-switchable pharmaceuticals can be designed based on known drugs containing biaryl sulfonamide moieties. In the future, we will use our computational toolbox to further improve light-switchable pharmaceuticals.



Azobenzene is a common molecular switch used in light-switchable bioactive molecules. It can be used to switch a drug between a less active (blue Lewis structure) and a more active form (red Lewis structure). A good candidate to be replaced by azobenzene is a biaryl sulfonamide (green Lewis structure). Both molecules have similar structural (top row) and electronic properties (bottom row). Figure taken from P. Kobauri et al., Chem. Commun. 57, 4126 (2021).

Dr. Sebastian Thallmair

Sebastian Thallmair 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 was appointed as a Fellow in October 2020.

Active Students

In 2021, Cristina Gil Herrero, PhD student in the Thallmair group, became one of the student representatives of FIAS.

Projects @ FIAS: 1

Collaborations

Stefan Knapp (GU Frankfurt)
Clemens Glaubitz (GU Frankfurt)
Irene Burghardt (GU Frankfurt)
Balázs Fábián (MPI Biophysics)
Dominik Oliver (Philipps University Marburg)
Paulo C. T. Souza (CNRS Lyon)
Pablo Rivera-Fuentes (ETH Zürich)

**Prof. Dr.
Jochen Triesch**

Jochen Triesch 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.

Making AIs learn more autonomously

Most of today's AI systems are trained with large numbers of labeled training examples, an approach called supervised learning. For example, it is common to train systems that recognize cats or dogs with millions of training images that have been annotated by humans as containing a cat or a dog. In sharp contrast, human infants do not need such excessive labeling. They can learn much more autonomously as they explore their environments. Members of the Triesch lab asked whether it is possible to emulate such infant-like learning in AI systems and, if so, whether such systems could reach the performance of supervised approaches. To answer these questions they explored a new approach called „Contrastive Learning Through Time." This approach simulates how infants interact with and learn about objects, exploiting the temporal structure of the visual input and using it as a replacement for explicit labeling. In particular, the approach works by learning an internal code for the images such that images that are viewed in succession receive a similar encoding, a mechanism that can be summed up by „close in time, will align." The team showed that, indeed, this approach allows the system to learn without any labels while approaching the performance of a fully supervised method. Furthermore, they could establish how the quality of the learned representations depends on the temporal structure that the system experiences during learning. Finally, the team also related their approach to classic findings from Neuroscience, reproducing findings showing that objects that are systematically viewed in succession will be represented similarly by the brain.

Winter hike

In December 2021, the Triesch lab enjoyed a winter hike in the Taunus mountains.

Reference:

Contrastive Learning Through Time. F Schneider, X Xu, MR Ernst, Z Yu, J Triesch. 3rd Workshop on Shared Visual Representations in Human and Machine Intelligence (SVRHM 2021) of the Neural Information Processing Systems (NeurIPS) conference, Virtual.

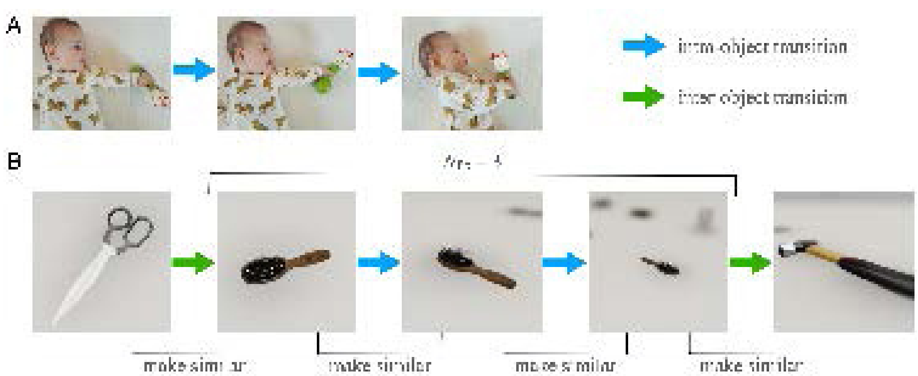
Link:

https://openreview.net/pdf?id=HTCRs8taN8

Projects @ FIAS: 7

Collaborations

Bert E. Shi (Hong Kong)
Maria Fronius (Frankfurt)
Felix Rosenow (Frankfurt),
Elke Hattingen (Frankfurt),
Frederic von Wegner (Sydney)



Contrastive Learning Through Time (CLTT). A. Infants learn about objects during extended interactions, where they experience different views of an object before directing their attention elsewhere. B. Our CLTT approach mimics the essence of such interations. A certain number Nfix of object views are sampled before directing attention to another object. Latent representations of successive views (both intra-object and inter-object transitions) are made more similar.

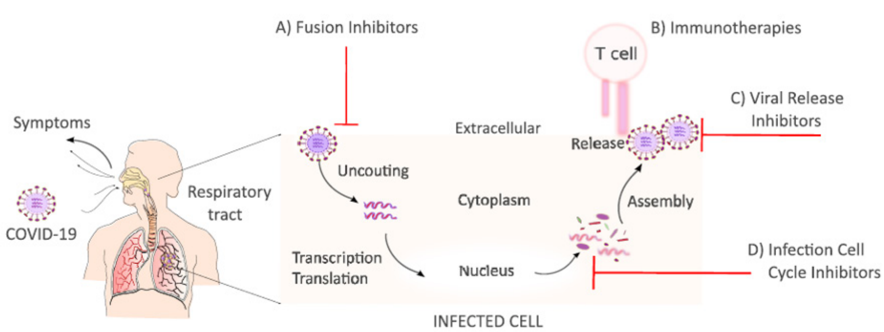
Systems Medicine of Infectious Diseases

Our research group has a special interest Throughout history, we have witnessed alarming high death tolls derived from infectious diseases around the globe. Last year 2020 has uncovered one of the biggest pandemics in history, the novel coronavirus SARS-CoV-2 that was first reported in Wuhan, Hubei Province, China in December 2019 (CDC, 2020). 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 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.

Current research focusses:

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.



After the binding to receptors of the host cell, the virus RNA is uncoated in the cytoplasm. Then, transcription/translation processes take place to generate new viral RNA material and proteins. Virus assembly occurs within vesicles followed by virus release. Once the virus is released can infect other cells.
Ref: In-host Mathematical Modelling of COVID-19 in Humans. EA Hernandez-Vargas, JX Velasco-Hernandez. Annual Reviews in Control, 2020

Dr. Esteban A. Hernandez-Vargas

FIAS Fellow Esteban Hernandez-Vargas obtained a PhD in Mathematics at the National University of Ireland. Esteban 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 holds a Research Fellow funded by the Alfons und Gertrud Kassel-Stiftung, at FIAS Frankfurt.

International Group

His lab members are living at three different continents working together by zoom.

Projects @ FIAS: 2

Collaborations

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

Prof Dr.
Christoph von der Malsburg

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

Visiting Professor

Invitation to serve as Visiting Professor at ETH in 2022 and as Senior Fellow of Collegium Helveticum.

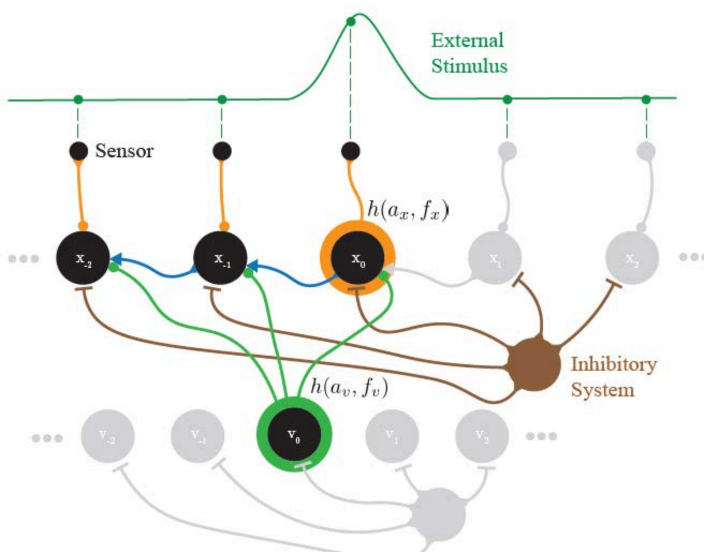
Collaborations

Rodney Douglas,
Benjamin Grewe, both INI, Zürich.
Irving Biederman, USC, Los Angeles.
Tomas Fernandes, Hongshi Technologies, Wuhan.

Handling of Uncertainty in the Brain

The brain has to establish and dynamically maintain estimates of large numbers of variables relating to the environment, such as positions and velocities of objects. This task is complicated by noise, ambiguity and partial absence of sensory signals. The brain presumably deals with this difficulty by representing variables by probability distributions and by constraining variable values by previously established relations between them. This general idea is captured in the literature by a broad range of probabilistic formulations. A generally unsolved problem, however, is how such formulations are implemented in the neural tissue of the brain, that is, exclusively in terms of neural signals.

On the example of a Kalman Filter, we generated such implementation. The variables object position and velocity are represented by two rows of neural units (each a set of neurons), each neural unit standing for a particular value and probability distributions being represented by activity distributions over units. So far this is a conventional approach. When it comes, however, to the step of updating probability distributions by merging several signals (in our case current sensory position input and velocity model prediction) we are, to our knowledge, the first to propose a concrete neural implementation. To dynamically handle neural activity distributions we introduce a simple evolution equation that dynamically normalizes the distributions (as required in probability theory) and lets them contract around the values that are favored by the combined input from several sources. The relative weight given to current position signals vs. velocity-model predictions and other features of the Kalman filter can be regulated by parameters, but we haven't found yet mechanisms to set these parameters automatically. Simulations of our Neural Kalman Filter compare well to the standard analytical formulation. More work is needed to arrive at a general formulation of the problem of handling large networks of variables in the brain referred to above.



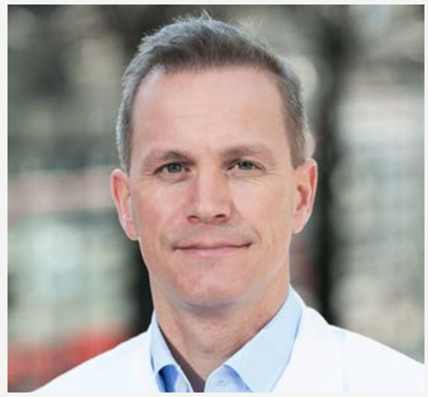
Neural Kalman Filter. Position and velocity of a moving object are estimated. Position sensors (small circles, second row) receive noisy signals (probability distribution, upper row). The sensor signals feed into a row of neural units (large circles, third row) acting as position value units. Position units fuse information they get from position sensors (second row) and motion estimation units (fourth row). Motion estimation is based on coincidences between delayed signals (blue arrows) and current activity in position units, picked up by green neurites (so-called Reichardt detector). Motion units generate position prediction as products of signals on converging blue and green fibers (the green fibers conducting in both directions). The inhibitory systems are responsible for normalization of activity distributions of position units and velocity units.

Systems Pathology

Building accurate models for cancer is a challenging task due to high levels of intra-tumor heterogeneity (ITH) displayed by human cancers. Tumor samples typically consist of a mixture of cells (tumor, stromal, immune and vascular cells), and cancer sub-clonal populations that coexist together and evolve through competition for resources and survival. Genomic heterogeneity generates large clinical variability in major clinically important phenotypes such as the ability to metastasize or resistance to therapy. Particularly, distinct diagnostic signatures can be found in different biopsies from the same tumor, and different clonal populations may exhibit different sensitivities to drugs.

The clonal evolution of e.g. malignant pleural mesothelioma (MPM) is poorly understood. The Systems Pathology Lab lead by Peter Wild investigated the sub-clonal genomic alterations and characterized the intra-tumor heterogeneity in MPM samples through whole exome sequencing and targeted ultra-deep sequencing. MPM is a rare but fatal lung cancer and is associated with asbestos exposure. Due to the lack of many alternative treatment options, standard clinical therapy regimens include a platinum-based therapy in combination with an antifolate. However, chemotherapy only shows effectiveness in about a third of all MPM patients, exposing two thirds of them to unnecessary and mostly severe side effects. In our project, we screened a cohort of 67 MPM patients undergoing similar cisplatin-based treatment for a genetic marker predictive of response to chemotherapy and found that alterations in BAP1 were a negative predictor of MPM outcome. Using different MPM cell lines, we demonstrated that the absence of BAP1 in vitro is causative for cisplatin resistance. We, therefore, suggested that BAP1 mutational status could be used for patient stratification before chemotherapeutic treatment.

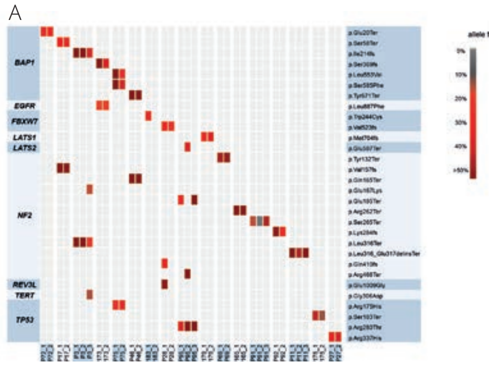
For some of the MPM patients, the genetic composition of the tumor varied between the different phases, reflecting the spatial and temporal heterogeneity in MPM. For a better visualization of the data (Fig. A), we modeled the tumor evolution of two patients from the amplicon sequencing data (Fig. B). The models are based on the assumption that mutations of a high allele frequency are present in a higher fraction of tumor cells and are, therefore, of early clonal origin. Thus, in patient 1, the BAP1 mutation arose before the NF2 mutation and both mutations did not change during chemotherapy (Fig B, left panel). In the relapsing phase, two other mutations in TERT and NF2 occurred. In patient 2, by contrast, TP53 was mutated rather early during MPM development, followed by an NF2 mutation (Fig B, right panel).



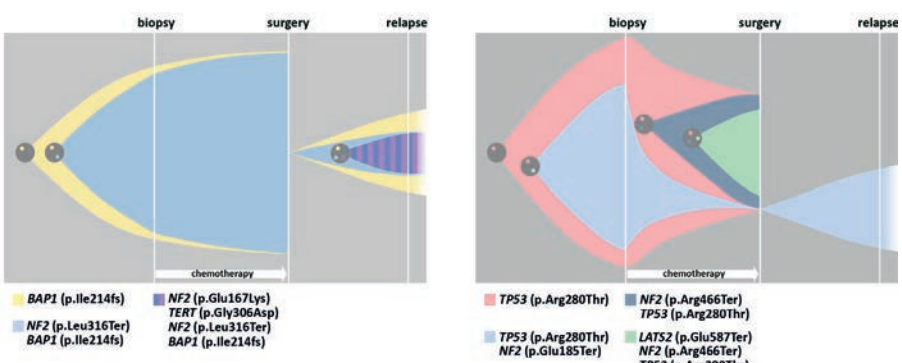
**Prof. Dr.
Peter Wild**

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. In April 2018 he was appointed director of the Dr. Senckenberg Institute of Pathology (SIP), at the University Medical Center Frankfurt and joined FIAS in September 2020.

A

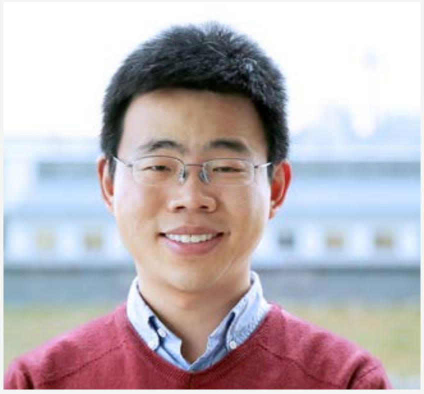


B



A and B: Results of deep sequencing (A) and graphical illustration of the clonal evolution of two MPM patients (B). The allele frequency of the mutations was taken as a measure for emergence of the respective clone and is depicted in the width of the diagram (Permission by Clinical Cancer Research 2021).

Physics-informed deep learning for inverse problem solving



Dr.
Kai Zhou

Dr. Kai Zhou recieved 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.

COVID-19 Research

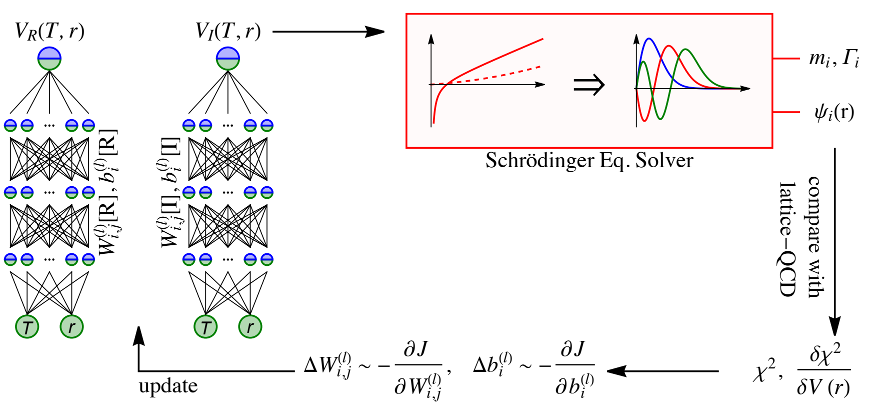
We transferred our physics and AI experience into COVID-19 risk spatio-temperal evolution studies .

Projects @ FIAS: 3

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

One research focus of my group is AI for inverse problems (IP). IPs occur in many research areas, especially in the context of ErUM related fundamental physics, also in other scientific and engineering areas. I recently devised a methodology within automatic differentiation (AD) which integrates our physics-priors into the specific IPs and deep learning representation together to perform Bayesian inference on the IPs. We demonstrated the developed methodology in several IPs raised in high energy nuclear physics (can also be easily generalized to other physics areas as well). (1) We first deploy the above AD-based approach to reconstruct spectral functions from Euclidean correlation functions which has been proven ill-posed especially with limited and noisy measurements. In our method the spectral is represented by DNNs while the reconstruction turns out to be optimization within AD under natural regularization to fit the measured correlators. We demonstrated and proved that the network with weight regularization can provide non-local regulator for this IP. Compared to conventional maximum-entropy-method (MEM), our method achieved better performance in realistic large-noise situation. It's for the first time to introduce non-local regulator using DNNs for the problem and is an inherent advantage for the method, which can promisingly lead to substantial improvements in related problems and IPs. (2) We applied the method to reconstruct the fundamental QCD force – heavy-quark potential – from lQCD calculated bottomonium in-medium spectrum. Both the radius and temperature dependence of the interaction are well reconstructed via inverse the Schroedinger equation given limited and discretized bottomonium low-lying states mass and width. (3) We also demonstrated the method's ability to infer neutron star EoS from astrophysical observables, with exciting results on closure tests for reasonable EoS reconstruction based on finite noisy M-R observables. Compared to conventional approaches our method holds unbiased representation for the EoS and bare interpretable Bayesian picture for the reconstruction.



Flow chart of heavy quark potential reconstruction scheme – using generalized back-propagation to optimize the network represented potential coupled to a Schroedinger equation solver.

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. In 2020, 3 junior research groups were funded by private donors. We thank all supporters and look forward to continued cooperation!

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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:

2020: Quandt Research Group on Mathematical Immuno-Epidemiology Dr. Maria Barbarossa
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

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