

2023



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# TUM President's Foreword

## Shaping our future together

How can we effectively respond to the increasingly frequent shocks and attacks targeting our open society? How can we surmount the unique challenges confronting our generation, challenges so far unprecedented in our collective experience?

Our strength in research and teaching at TUM and the Institute for Advanced Study (TUM-IAS) is based on a climate of diversity, inclusion, fair competition, and mutual respect. Students and researchers from diverse cultures and backgrounds work together to expand the limits of knowledge, advance scientific progress, and shape a better future for humanity.

The future remains open, it does not follow predetermined paths. Our collective duty is to mold it, transcending disciplinary, institutional, national, and cultural boundaries with clarity, determination, and responsibility. We advocate for clearness in our values, exhibit an unwavering determination to uphold them, and acknowledge the responsibility we bear for the young minds shaping their futures under our guidance. As scientists, we recognize our role as exemplars of the values we cherish, fostering a sense of responsibility for the world we temporarily inhabit and will eventually pass on.

In line with this vision, TUM aspires to shape the future collaboratively and embraces an international ethos. Recognizing the pivotal role of open-minded pioneers as the catalysts for change, we acknowledge the transformative power of an international scientific community. This global perspective instills in us a deep respect for one another, fosters tolerance in thought and action, and instills trust in our collaborative partners.

Our commitment to this inclusive spirit is integral to being a truly international and diverse university. Over the past four years, TUM has welcomed two hundred new professors from a multitude of countries across the globe. Reflecting our global outreach, 44% of our 52,000 students hail from international backgrounds.

As a key component of our TUM Global South Initiative, we strategically deepen our collaborations with research institutions across South America, Asia, and Africa. This year, will be dedicated to the execution of additional projects and plans specifically tailored for the African continent. Notably, one of our crucial partner universities is KNUST in Ghana, with whom we are already engaged in twenty-five joint projects. In the realm of medicine, a clinical partnership has been initiated as well. TUM is actively involved in over 150 projects throughout Africa, demonstrating our commitment to impactful collaboration. The TUM-IAS Regional Fellowship stands as a further reinforcement, adding strength to these projects and fostering lasting partnerships.

The forthcoming Munich Medicine Alliance marks the amalgamation of TUM, LMU Munich, and their hospitals, as well as the Helmholtz Environmental Health Center and the German Heart Center Munich. While Munich is already recognized as a leading medical hub in Germany, this union is poised to elevate it to global prominence. Personally, I find it imperative that our pursuits in medical research and the education of thousands of young minds are conducted exclusively within the framework of diversity, inclusion, and utmost respect.

This principle extends to the field of data sciences as well. The Munich Data Science Institute plays a crucial role in integrating various data-driven research





activities across TUM as well as collaborative centers with LMU Munich, the German Aerospace Center, and the Helmholtz Centers. Recognizing the substantial responsibility inherent in working with and researching data, it is incumbent upon us all to approach these endeavors with care. In this context, as scientists, we must carry out research and education with a sense of responsibility, serving as exemplars and role models in our actions.

In response to the rightful demands of our students, our TUM Sustainable Futures Strategy gained considerable traction in 2023. We are actively shaping a Sustainability Transformation Roadmap, engaging our students profoundly by incorporating their ideas and suggestions. Significant initiatives aimed at large-scale reduction of CO<sub>2</sub> emissions are already in progress. The inaugural Sustainability Awards, organized in collaboration with the TUM-IAS and the Nobel Sustainability Trust, illustrate our commitment to sustainable practices.

Whether it is championing sustainability, fostering interdisciplinary research, or expanding connections to the Global South, the TUM-IAS occupies a pioneering and central position in all TUM endeavors.

The ongoing enthusiasm and fruitful collaborations among our students, researchers, and international guests consistently inspire me. These experiences convince me that collectively, we are actively contributing to a future worth living. ■

Prof. Thomas F. Hofmann  
President

# TUM-IAS Director's Message



Sustainability is the major challenge confronting society and science today. A look at the UN's 17 Sustainable Development Goals (SDG) reveals that research faces immense tasks. There are numerous opportunities to utilize the great potential of interdisciplinary, networked thinking and working collaboratively. The preventive approaches of the WHO "One Health" concept aim to defuse the most significant health problems of all, such as infectious diseases and many chronic diseases. Engineers are needed on many fronts to develop technologies geared toward creating humane and nature-friendly living conditions for everyone on our planet. The spectrum of work in the technology sector is extremely diverse and highly complex, and this also applies to basic scientific research. The latter creates the basis for translating or testing new, sustainable processes.

That is why research and other activities on sustainability are taking an increasingly prominent role at the TUM-IAS. In 2023, 49 of our 80 TUM-IAS Focus Groups worked on topics that were related to the UN's Sustainable Development Goals. Last year, we were able to award the Sustainability Awards supported by the Nobel Sustainability Trust for the first time. The winners were **Prof. Elena Bou** and **Lord Nicholas Stern**. The selection process was in the hands of the TUM-IAS, as was the content design for the Nobel Trust Summit held in November 2023 in Munich, where the prizes were awarded (see chapter "Actions, Awards, Events").

The new Dieter Schwarz Courageous Research Grant marks a new milestone for TUM and for the TUM-IAS. With annual funding of one million Euros, it represents the most extensive internal TUM research program and is entirely dedicated to Digitization and Sustainability. We, at the TUM-IAS are honored to lead and implement this new, groundbreaking program.

In addition, another Dieter Schwarz Fellowship supports research in subject areas offered by TUM on its campus in Heilbronn. The new programs expanded our activities significantly, and we were able to announce both of them for the first time last year. The first Fellows will be appointed in 2024 (see chapter "Actions, Awards, Events").

The new Seminar Series of European Universities on Sustainability, launched in autumn 2023, not only brings together scientists from research and academic institutions in Eastern, South-Eastern, and Central Europe, but also addresses "sustainability" as a core element of all seminars at the TUM-IAS. At present, the online event enables participants from more than eight universities to gain an overview of interdisciplinary sustainability research and to establish new contacts (see chapter "Actions, Awards, Events").

A funding line close to my heart is the Philosopher in Residence. Innovative research in the natural and health sciences, as well as in technical disciplines, raises numerous questions – both of an internal nature and of social significance. This necessitates deeper reflection and classification in the context of future-oriented social developments related to sustainability and resilience. Thanks to the support of the TÜV SÜD Foundation and the TUM Excellence Strategy, we were able to start this year with two philosophers: **Prof. Roberto Giuntini** from the University of Cagliari and **PD Rico Gutschmidt** from the University of Konstanz and ETH Zurich (see chapter "Welcoming Our New Fellows").

Lastly, on our website, you can now enjoy short video clips with some of our active and alumni Fellows from Argentina, Denmark, Ireland, Italy, Sweden, and the USA describing their TUM-IAS research projects – concisely and comprehensibly for non-experts!

I would like to express my gratitude to our friends and supporters: Siemens AG, the TÜV SÜD Foundation, the Dieter Schwarz Foundation, the Nemetschek Innovationsstiftung, and the Nobel Sustainability Trust. Your support is instrumental in bringing our ideas to life, getting new things off the ground, and possibly launching new initiatives. ■



Prof. Michael Molls  
Director



# Actions, Awards, Events

2023 has been a year of change, and of progress. It gave us ample opportunity for actions and new ventures.





# Actions

Sustainability is one of the biggest challenges facing science today. A glance at the UN's 17 Sustainable Development Goals (SDG) underscores the substantial tasks that research confronts in tackling global issues. Within this challenge lie many opportunities to utilize the great potential of networked thinking and national as well as international cooperation in interdisciplinary settings. Consequently, research and other activities on sustainability are taking an increasingly prominent place in the TUM-IAS.

TUM strategically focuses on six of the SDGs as thematic priorities. While remaining attentive to activities in other thematic areas, it applies its interdisciplinary strengths in research, teaching, and innovation to build on these SDGs:

- SDG 3 Good Health and Well-Being
- SDG 7 Affordable and Clean Energy
- SDG 11 Sustainable Cities and Communities
- SDG 12 Responsible Consumption and Production
- SDG 13 Climate Action
- SDG 15 Life on Land

At the TUM-IAS, 49 out of the 80 active Focus Groups (FG) directed their efforts to topics that were related to the UN's Sustainable Development Goals. Notably, a majority of these focused on Good Health and Well-Being (20 FG), Affordable and Clean Energy (9 FG), Responsible Consumption and Production (9), and Sustainable Cities and Communities (8). Additional efforts were directed toward Climate Action (2 FG) and Life on Earth (1 FG). This collaborative and multidisciplinary approach reflects our unwavering commitment to contribute meaningfully to global sustainability efforts.

## **Sustainability Awards supported by the Nobel Sustainability Trust**

For the first time, the Sustainability Awards supported by the Nobel Sustainability Trust Foundation (NST) were awarded in November 2023. The winners were selected by a panel of international experts as well as TUM professors organized by the TUM-IAS. The award ceremony was integrated into the Nobel Sustainability Trust Summit in Munich on 9 November 2023. The recipients of the awards were Professor Elena Bou, Innovation Director at EIT InnoEnergy (category "Outstanding Research and Development in the field of Energy") for achievements in supporting start-ups and scale-ups in the energy transition, and Lord Nicholas Stern, Professor at the London School of Economics and Politics (category "Leadership in Implementation"), honored for his work on the economics of climate change and sustainability.

The Nobel Sustainability Trust Summit featured keynote speakers from academia and enterprises, presenting their expertise on water, energy, and sustainability challenges to an audience of around 200 people, including academics, students and industry representatives, who engaged in insightful discussions.

## **New Funding: Dieter Schwarz Fellowships and Dieter Schwarz Courageous Research Grants**

With the support of the Dieter Schwarz Foundation (DSS), the TUM-IAS was able to add two new funding opportunities to its portfolio. The Dieter Schwarz Fellowship is based on the Hans Fischer (Senior) Fellowships but focuses on the thematic spectrum of the TUM campus in Heilbronn (information,

engineering, economics, and political or social sciences). The Dieter Schwarz Courageous Research Grant offers one million Euros to scientists proposing a radical solution to a major challenge in the research area of “digitization and sustainability” using pioneering technologies.

Demonstrating its sustained commitment, the DSS has expanded its support by endowing an additional ten professorships at the TUM School of Management and TUM School of Computation, Information, and Technology. This brings the total number of TUM professorships endowed by DSS since 2018 to 41, with 32 of the professorships in Heilbronn. The TUM Heilbronn campus has a unique, interdisciplinary profile at the intersection of management and informatics. The professorships will be fully financed by the foundation for an initial period of 30 years, covering equipment and infrastructure costs. The endowment funds are not subject to any conditions whatsoever, and the contract is based on the TUM Fundraising Code of Conduct, ensuring that contributors refrain from influencing research or teaching. Another objective of the expansion measures is to further enhance the internationalization of the TUM Heilbronn campus. The newly introduced Dieter Schwarz Fellowship aims to attract outstanding international professors to Heilbronn and, by also naming them Fellows of TUM-IAS, to build bridges to the TUM Garching campus.

### Seminar Series of European Universities on Sustainability

As part of the TUM-IAS's ongoing commitment to promoting scientific exchange and professional networks, we launched the Seminar Series of European Universities on Sustainability in 2023. This initiative aims to

bring together scientists from Eastern, South-eastern, and Central European research institutions to facilitate discussions on topics related to the United Nations' 17 Sustainable Development Goals. This series of seminars is a first step in overcoming geographical and academic barriers, fostering a scientific network, promoting joint research initiatives, and building lasting collaborations for a more sustainable future.

The seminars within this series are integrated into the Scientists Meet Scientists – Wednesday Coffee Talk series (Wednesdays, from 13:00, online). Every last talk of the month is dedicated to the sustainability seminar series. Currently, the network comprises the following universities and research institutions:

- **Dimitrie Cantemir Christian University**, Romania
- **National Technical University of Ukraine**, Ukraine
- **Poznań University of Life Sciences**, Poland
- **Riga Technical University**, Latvia
- **Wigner Research Centre for Physics**, Hungary
- **Technische Universität Wien**, Austria
- **University of Freiburg**, Germany
- **Institute for Advanced Study of Technical University of Munich**, Germany.

However, our vision for the future involves expanding the platform and seminar series on sustainability by inviting more research institutions from Eastern and Southeastern Europe, Austria, and Germany to participate and contribute.

We look forward to the growth and enrichment of this collaborative platform. ►

### Philosophers in Residence

The Philosopher in Residence Fellowship is a new program line at TUM-IAS. It is aimed at internationally leading and emerging representatives of the field of philosophy who wish to conduct joint projects with TUM professors from the fields of natural sciences, engineering, and life sciences, including medicine and health sciences, economics, and social sciences. The TUM-IAS recognizes that innovative developments in modern scientific and technical disciplines are often accompanied by implications that require philosophical consideration and embedding. The one-year Fellowship is to be located within the framework of the TUM Agenda 2030, which pursues a more robust integration of the humanities. Our new program is supported by the TÜV SÜD Foundation, for which we are very thankful.

We are pleased that the first two philosophers have started their Fellowships in 2023:

- **Roberto Giuntini** (Professor at University of Cagliari) works with his hosts, **Hans Joachim Bungartz** (Professor of Scientific Computing in Computer Science), **Stefania Centrone** (Professor of Philosophy and Philosophy of Science), and **Klaus Mainzer** (TUM Emeritus of Excellence) on the topic of “quantum logic and the second quantum revolution.”
- The project undertaken by **Rico Gutschmidt** (PD at University of Konstanz/ETH Zurich) and his host, **Eckhard Frick SJ** (Professor of Spiritual Care and Psychosomatic Health), explores “boundary situations and spiritual care.”

### New Siemens Fellows at the TUM-IAS

Thanks to the generous support of the Siemens AG, the TUM-IAS is expanding its

research initiatives. In 2023, two additional Hans Fischer Senior Fellowships have been awarded. A hearty welcome to our two new Fellows, **Elena Simperl**, Professor of Computer Science at King's College London, and **Rainald Loehner**, Professor of Computational Fluid Dynamics at George Mason University. We are grateful to Siemens for their continued support, which has made these new research projects in *Trustworthy AI* and *Digital Twin* possible. We look forward to closer cooperation at the Siemens Technology Center at the TUM Campus Garching.

### New TUM-IAS Program Manager for the Alexander von Humboldt Foundation's sponsorship programs at TUM

In an effort to intensify the long-standing contacts with the Alexander von Humboldt Foundation (AvH), TUM-IAS has now become the central administrative contact point at TUM for Humboldt Awardees and other AvH sponsorship programs. Since September 2023, Daniela Hägele has been responsible for all Humboldt-related inquiries beyond the postdoctoral level. Daniela will advise potential TUM host professors and international visitors coming to TUM within an Alexander von Humboldt program. You can reach her via [daniela.haegle@tum.de](mailto:daniela.haegle@tum.de).

### TUM Ambassadors

Over many years, numerous international researchers have repeatedly come to TUM as guest scientists or TUM-IAS Fellows and have made significant contributions to TUM through their research. Recognizing their exceptional impact, a cohort of distinguished international researchers was awarded the honorary title of TUM Ambassador. As new TUM-IAS Members, Ambassadors



are integrated into the academic life of the TUM-IAS, gaining access to offices and conference rooms; also, like TUM-IAS Alumni Fellows, they receive a certain amount of financial support for new projects.

### **Workshop of TUM-IAS Anna Boyksen Fellows**

The Anna Boysken Fellowships are designed to explore gender- and/or diversity-relevant topics in the context of the TUM subject portfolio. After 11 years of the Anna Boysken Fellowship Program at TUM-IAS, a workshop was held on 5 May 2023 to present and document the Fellows' findings, measures, and experiences within their research projects and at TUM. In addition, the Fellows proposed several recommendations for TUM in advancing toward enhanced diversity, inclusion, and equality. These suggestions included issues such as

- advertising multiple open academic positions beyond individual hires;
- revising the composition of the hiring committees and training on implicit bias and stereotypes;
- offering courses on inclusive leadership;
- adapting teaching materials for gender, diversity, and inclusion;
- introducing male mentor programs;
- actively seeking and supporting more professors and Fellows from Global South countries to diversify on an international scale.

### **Network of German Institutes for Advanced Study**

In Germany, more than 20 institutes for advanced study exist, each distinguished by varying structures, tasks, and governance. While the majority are university-based and

relatively recent establishments, others, such as the Wissenschaftskolleg Berlin or the Hanse Wissenschaftskolleg Delmenhorst, are much older and operate on the basis of their own foundation.

Annually, the German institutes for advanced study support more than 450 Fellows, more than 60% of whom come from abroad. In doing so, they make an important contribution to the internationality and diversity of the German research landscape. With their typically manageable size and flexibility to quickly embrace new research fields, they are successful with agile and innovative scientific operations. Collaboratively, these institutions aim to showcase their strengths and achievements through targeted public relations activities and to promote the initiation of new joint projects.

### **TUM-IAS Fellowship Call**

Anticipating the arrival of our new Fellows in 2024, we reflect on the 14 Fellowships granted in 2023, distributed among various Fellowship categories: Hans Fischer (Senior) Fellowship, Anna Boysken Fellowship, Albrecht Struppler Clinician Scientist Fellowship, and Philosopher in Residence Fellowship.

We are delighted to welcome these newly appointed Fellows from Denmark, Germany, Italy, United Kingdom, and USA!

To learn more about our newest Fellows, please consult the chapter "Welcoming Our New Fellows". For the current call, we are pleased to announce the opportunity to award up to 15 Fellowships (including the Dieter Schwarz Fellowship and Dieter Schwarz Courageous Research Grant). ►



**Rudolf Mößbauer Tenure Track Assistant Professorships**

For more than a decade, TUM has been selecting promising young talents as Tenure Track Assistant Professors (W2), after a thorough selection process organized by the TUM-IAS. The TUM Faculty Tenure Track represents a performance-oriented career model for young scientists with international experience, providing from the very beginning the realistic prospect toward advancing to a tenured W3 professorship.

This TUM-IAS Fellowship is named in honor of TUM professor Rudolf Mößbauer (1929–2011), a Nobel Prize laureate in Physics (1961)

for his groundbreaking research concerning the resonance absorption of gamma radiation and his associated discovery of the effect that bears his name. As the emphasis of the professorship lies on the creative development of a new field of science and/or technology, and as we intend to offer those young researchers the best possible career start, they are equally affiliated with the TUM-IAS as Fellows.

In 2023, three new Rudolf Mößbauer Tenure Track Assistant Professors were appointed. For detailed information on our new Fellows, please see chapters “Events” and “Welcoming Our New Fellows.” ■

# Awards



European Research Council  
Established by the European Commission

We are delighted and proud that our Fellows and partners have again received top-class awards in 2023:

## ERC Grants

**Jia Chen** and **Matthias Feige**, Alumni Rudolf Mößbauer Tenure Track Assistant Professors of TUM-IAS, received prestigious ERC Consolidator Grants. Jia Chen, Professor for Environmental Sensing and Modeling, works today in the search for greenhouse gas sources in cities. She is developing new types of sensors, methods, and models to precisely localize and quantify the emission sources of greenhouse gases and air pollutants in cities at high resolution. This can be used to efficiently reduce emissions, mitigate climate change, and reduce urban air pollution. Matthias Feige, Professor for Cellular Protein Biochemistry, is investigating how cells make and control important proteins. The objective is, among others, to find out how faulty membrane proteins are detected, which repair mechanisms exist, and how defective proteins, which cannot be repaired, are degraded. The results of the project should fundamentally advance our understanding of how our cells function and could provide new strategies for treating various severe diseases.

TUM-IAS Alumnus Rudolf Mößbauer Tenure Track Assistant Professor **Job Boekhoven**, Professor for Supramolecular Chemistry, is among the three TUM scientists who won ERC Consolidator Grants in 2023. This is already Job Boekhoven's second ERC Grant after securing an ERC Starting Grant for his proposal ActiDrops in 2019. In his project SynLife, he aims to create synthetic life by researching so-called active droplets. These tiny droplets of insoluble molecules exhibit life-like behavior: they only form when external energy is supplied and multiply by dividing

with sufficient energy. NASA defines life as a self-sustaining system capable of Darwinian evolution. In order to fulfill these criteria, Job Boekhoven wants to develop molecules that form a kind of genetic material. They are intended to influence properties such as the lifespan of the droplets, are passed on when a droplet divides, and can, in new ways, mutate and lead to new properties. Such artificial evolution could not only help provide insights into the origins of life but also make Darwinian evolution usable as a tool for designing new materials.

**Julien Gagneur**, TUM Professor for Computational Molecular Medicine, received an ERC Synergy Grant in 2023 and was made an TUM-IAS Honorary Fellow.

**Eitan Yaakobi**, TUM-IAS Alumnus Hans Fischer Fellow and Associate Professor at the Computer Science Department at the Technion – Israel Institute of Technology, was awarded an ERC Consolidator Grant in 2022 for his research in the field of DNA Storage. DNA storage is an innovative approach that is expected to revolutionize information storage while dramatically reducing storage volume, storing information for the very long term and significantly reducing energy and economic costs.

## Highly Cited Researchers

The frequency of citations of a study serves as a reliable indicator of research quality. Annually, Clarivate, a U.S.-based company, assesses the 'Web of Science' database it manages, compiling scientific publications across various disciplines. Through this evaluation, Clarivate identifies Highly Cited Researchers, each of whom has authored multiple Highly Cited Papers™ ranked in the top 1% by citations for their field(s) and publication year in the Web of Science™

over the past decade. However, citation activity is not the sole selection indicator. A preliminary list based on citation activity is refined through qualitative analysis and expert judgment.

The evaluation's latest edition shows the scientists cited most frequently in their respective fields. Researchers who are cited particularly often across different fields are listed in the "Cross-Field" category. In total, the list comprises around 7,125 scientists in no particular order, including the following TUM-IAS Fellows:

**Ib Chorkendorff** (Chemistry), Professor at DTU Copenhagen

**Naomi Halas** (Material Science), Professor at Rice University

**Laura Herz** (Cross-Field), Professor at University of Oxford

**Peter Nordlander** (Material Science), Professor at Rice University

**Melanie Schirmer** (Cross-Field), Professor at Technical University of Munich

**Yang Shao-Horn** (Chemistry), Professor at Massachusetts Institute of Technology

**Yang Shao-Horn** (Environment and Ecology), Professor at Massachusetts Institute of Technology

**Thaddeus S. Stappenbeck** (Cross-Field), Professor at Washington University.

#### Awards for further Outstanding Contributions

**Johannes Betz**, TUM-IAS Rudolf Mößbauer Tenure Track Assistant Professor, received the Golden Teaching Award 2023 by the Students' Association of Mechanical Engineering for his lecture titled "Fundamentals of Autonomous Vehicles".

**Ioannis Brilakis**, Laing O'Rourke Professor of Construction Engineering at Cambridge

University, and TUM-IAS Alumnus Hans Fischer Senior Fellow, was honored the Scherer Award at the European Council on Computing in Construction for 2023, as well as the Thorpe Medal at the European Council on Computing in Construction for 2022.

**Andrzej J. Buras** was awarded the J. J. Sakurai Prize for Theoretical Particle Physics by the American Physical Society (APS), which recognizes outstanding achievement in particle theory. He earned the prize "for exceptional contributions to quark-flavor physics, in particular, developing and carrying out calculations of higher-order QCD effects to electroweak transitions, as well as for drawing phenomenological connections between kaons, D mesons, and B mesons." Andrzej Buras is a Professor Emeritus of Theoretical Elementary Particle Physics at TUM and was Carl von Linde Senior Fellow at the TUM-IAS from 2008-2011.

**Roberto Giuntini**, TUM-IAS Philosopher in Residence and Professor at University of Cagliari, was elected Corresponding Member at the General Assembly of the Académie Internationale de Philosophie des Sciences (AIPS), held in Münster on 28 September 2023. The object of the Académie Internationale de Philosophie des Sciences is to reach a synthesis of the fundamental questions of the philosophy of the sciences in an interdisciplinary manner.

**Gustavo Goldman**, TUM-IAS Alumnus Hans Fischer Senior Fellow and Professor at University of São Paulo, was honored with the Mosello Schaechter Award 2021 of the American Society of Microbiology.

**Kim Kraus**, Physician at TUM University Hospital and TUM-IAS Albrecht Struppler Clinician Scientist Fellow, won the Innovation Prize of the German Society for ►



Radiation Oncology (DEGRO – Deutsche Gesellschaft für Radioonkologie). This prize is awarded to physicians, physicists and technicians who have developed and implemented advanced and innovative ideas in the field of medical technology and quality assurance in radiation oncology. Kim Kraus was awarded the prize for her work on “Microbeam therapy in Germany - on the way to the clinic.”

TUM-IAS Alumnus Hans Fischer Fellow **Luca Magri** won the “Artificial Intelligence research to enable UK’s net zero target” grant by UK Research and Innovation (UKRI). Endowed with more than 3 million GBP, the grant, for which Luca Magri applied together with Co-PIs, aims at using current AI technologies or developing and applying new AI capabilities to address net-zero challenges across the fields of energy, transportation, environment, and agricultural, and food systems.

**Andreea Molnar**, TUM-IAS Anna Boyksen Fellow and Associate Professor at Swinburne University of Technology, has been selected as one of the International Science Council Fellows.

TUM-IAS Hans Fischer Senior Fellow **Wil Schilders**, Professor at Eindhoven University of Technology, was one of three researchers awarded the prestigious NWO Stairway to Impact Award in 2022. This award is presented annually by the Dutch Research Council (NWO), one of the most important science funding bodies in the Netherlands, and aims to realize quality and innovation in science. The specific NWO Domain Science wishes to promote knowledge utilization. With the Stairway to Impact Award, NWO rewards scientists who take effective steps to utilize their scientific findings to tackle a societal problem and/or to make an economic contribution. In addition, Wil Schilders was awarded the high royal Dutch award Officier in de Orde van Oranje-Nassau from the Kingdom of the Netherlands. The award was given for his

extraordinary achievements for the Dutch and international mathematics community. Also, he was elected a Fellow of the European Academy of Sciences.

**Mathias Senge**, Hans Fischer Senior Fellow and Professor of Organic Chemistry at Trinity College Dublin, received the Trinity Research Excellence Award 2023 in the category “Foster and grow research talent” from Trinity College Dublin (2023).

TUM-IAS Hans Fischer Fellow **Natalia Shustova**, Professor at University of South Carolina, was honored with the Friedrich Wilhelm Bessel Research Award of the Alexander von Humboldt Foundation. The prize is awarded to researchers whose outstanding academic qualification is internationally recognized and demonstrated through corresponding successes in research. Moreover, they must present a well-founded expectation of future outstanding academic achievements that will have a lasting impact on their discipline beyond their immediate research area.

Every two years, the Applied Vision Association (AVA) honors the achievements of an outstanding scientist in vision research with the AVA David Marr Medal. This year, Rudolf Mößbauer Tenure Track Assistant Professor **Manuel Spitschan**, Professor of Chronobiology & Health at TUM, received the committee’s award for his research on how light affects human physiology. The award is named in memory of David Marr (1945-1980), one of the United Kingdom’s foremost neuroscientists in the field of the visual system. Spitschan’s research focuses on the effects of light in relation to human physiology and behavior, particularly the interplay of the biological clock, circadian rhythm, and sleep. The health scientist is providing new insights into the fundamental properties of melanopsin, a light-sensitive photoreceptor recently found in the human retina.

**Luisa Verdoliva**, TUM-IAS Hans Fischer Senior Fellow, became a Full Professor in April 2023 at the University Federico II of Naples, Italy.

**Antonia Wachter-Zeh**, Alumna Rudolf Mößbauer Tenure Track Assistant Professor of TUM-IAS, was awarded the bi-annual Johann-Philipp-Reis-Prize for significant innovations in telecommunications. In the field of post-quantum cryptography, she is working on procedures that are secure even when quantum computers are used. A second key area of her research is long-term data storage. As the volume of data continues to grow exponentially, the need for compact, secure, and long-term archiving solutions becomes increasingly critical. One promising approach involves storing data within a molecular biological system, mimicking the storage of genetic material in DNA.

#### Awards of the Alexander von Humboldt Foundation 2023

The Alexander von Humboldt Foundation Awardees are members of the TUM-IAS. We congratulate the recent awardees and welcome them as our new members.

#### Carl Friedrich von Siemens Research Award

**Meisong Tong**, Professor at Tongji University, Shanghai, at TUM Chair of High-Frequency Engineering (Prof. Eibert), Department of Electrical Engineering

**Polina Bayvel**, Professor at University College London, UK, at TUM Chair of Communications Engineering (Prof. Kramer), Department of Computer Engineering.

#### Friedrich Wilhelm Bessel Award

**Natalia Shustova**, Professor at University of South Carolina, USA, at TUM Chair of Inorganic and Organometallic Chemistry (Prof. Fischer), Department of Chemistry. ■

Hans Fischer  
Senior Fellow  
Alessandro Reali,  
TUM President  
Thomas Hofmann,  
and former  
TUM-IAS Director  
Ernst Rank (from  
left to right).



# Events

Seminars, workshops, and conferences are at the heart of TUM-IAS's activities. Throughout 2023, many of our Fellows hosted multi-day conferences on their research topics. In addition, over 150 other events were held at the TUM-IAS. Our Scientists Meet Scientists seminar series, with over 20 lectures annually, is now offered exclusively online. This makes it easier for the many TUM-IAS Fellows and Alumni Fellows from all over the world as well as all TUM members at six locations to participate in our current research topics seminars. Moreover, we continued to host our Fellow Lunches, and following the Covid-19 pandemic, reintroduced our public outreach program in the neighboring city of Garching with four public presentations.

## Nobel Sustainability Summit

For the first time, the Nobel Sustainability Trust (NST) and the Technical University of Munich (TUM) presented the Sustainability Awards supported by the NST. The first two honorees are Professor **Elena Bou**, Innovation Director of EIT InnoEnergy, for her contributions to promoting energy start-ups, and **Lord Nicholas Stern**, Professor at the London School of Economics and Political Science, for his achievements relating to the economic aspects of climate change.

The winners were selected by a panel of international experts and TUM professors organized by the TUM-IAS.

The prizes were presented on 9 November 2023 at the Nobel Sustainability Trust

Summit at the Bavarian Academy of Sciences and Humanities in Munich. Peter Nobel, Chairman of the Nobel Sustainability Trust, and TUM President Thomas Hofmann handed over the awards.

The Sustainability Awards supported by the NST are given annually to individuals or institutions who have made significant developments of great potential or contributions to implement sustainable solutions for the benefit of humanity.

In 2024, they will be given in the categories "Outstanding Research and Development in the field of Water", "Outstanding Research and Development in the field of Agriculture", and "Leadership in Implementation".





Elena Bou at the Award Ceremony and Nobel Sustainability Trust Summit 2023 in Munich.

**Elena Bou** said: “I am honored to receive this inaugural Nobel Sustainability Trust Award. This prize recognizes the determinant roles start-ups, innovation, and entrepreneurship play in the energy transition. Reaching net zero demands new ideas and approaches – it will truly shift the needle on the progress of sustainable energy solutions. Working at EIT InnoEnergy allows me to put this into action every day. Through my research and teaching at ESADE Business School, I hope to encourage and influence the next generation of changemakers.”

**Lord Nicholas Stern** said in his acceptance speech: “Overall, I am very optimistic about what we can do. We can see a path to a world with much stronger mitigation and adaptation and to a new, much more attractive model of growth and development: sustainable, resilient, and inclusive. However, I am deeply worried about what we will do. The scale and pace of structural, technological and social change must be large and rapid. That will require changes in behavior and institutions. It will require purposive and sustained political leadership and strong political pressure from society as a whole on decision-makers to deliver change.” ►

**More information can be found here:**

- ➔ <https://www.ias.tum.de/ias/news-events-insights/news/news/single-view/article/sustainability-awards-for-prof-elena-bou-and-lord-stern/>
- ➔ <https://nst-sustainabilityaward.events/>

## TUM-IAS General Assembly

Our General Assembly represents the highlight of our academic year, featuring talks from our Fellows and Focus Groups, poster presentations of doctoral candidates, and a keynote lecture. TUM-IAS Fellows attended our meeting enriching the discussions and exchanges.

**Julijana Gjorgjieva**, Professor for Computational Neuroscience at TUM School of Life Sciences and TUM-IAS Honorary Fellow, gave the 2023 Linde Lecture titled “Teaching the Brain to See: Models of Neural Circuit Development and Learning.” She presented her research on how diverse mechanisms work together to set up neural circuits shortly after an animal is born, enabling it to gradually acquire cognitive and behavioral capabilities. In her outlook, she mentioned recent work on understanding a higher cognitive function in human circuits, namely the ability to generate and understand language.

### Full Program

**Fast and Cost-Efficient Evaluation of Air Pollution Exposure in Urban and Rural Areas Using Machine Learning**, Frank Keutsch, Professor of Engineering and Atmospheric Science at Harvard University, Hans Fischer Senior Fellow

**Optimal Control for Highly Flexible Robots**, Karin Nachbagauer, Professor for Applied Mathematics at University of Applied Sciences Upper Austria, Hans Fischer Fellow funded by Siemens AG

**Quantum Computing and Quantum Simulation**, Christian Mendl, Rudolf Mößbauer Tenure Track Assistant Professor at TUM School of Computation, Information and Technology

**Detecting DeepFakes**, Luisa Verdoliva, Professor at the Department for Industrial En-

gineering at University Federico II of Naples, Hans Fischer Senior Fellow

**Factors Influencing Young Women to Enroll in IT at TUM**, Andreea Molnar, Professor at Swinburne University of Technology, Anna Boyksen Fellow

**Electrifying Chemical Production: Electrochemical Ammonia Synthesis**, Ib Chorkendorff, Professor in Heterogeneous Catalysis at Technical University of Denmark, Hans Fischer Senior Fellow

**Extreme Events on Structures. The Key Role of Multiphysics Simulation**, Antonia Larese, University of Padua, Hans Fischer Fellow

### Markets and Governance in the Digital Economy

Hans Fischer Senior Fellow, **Kathleen Thelen**, Professor at Massachusetts Institute of Technology, and her host, Eugénia da Conceição-Heldt, Professor at the TUM School of Social Sciences and Technology, organized a workshop on the topic “Markets and Governance in the Digital Economy” at the Hochschule für Politik München on 19 May 2023. It focused on the origins and evolution of political-economic institutions in rich democracies and their impact on contemporary political outcomes.

### Curriculum Comedy

Anna Boyksen Fellow, **Meike Schalk**, Professor at KTH Royal Institute of Technology, Stockholm organized together with SOFT – School of Transformation (TUM) the three-day symposium Curriculum Comedy at the Department of Architecture, TUM School of Engineering and Design, in November 2022.

This symposium took the form of a play and set the stage for conversations about the

architecture curriculum. Questions such as “How do we learn and work together?”, “What are the sources of our Canon, and who does it takes into account?”, and “What knowledge and experiences are we missing” were addressed. Three acts with lectures, workshops, and round tables dealt with the learning/unlearning of gender norms and unreflected biases in architecture, work cultures and well-being, and equitable pedagogies in humorous and serious ways.

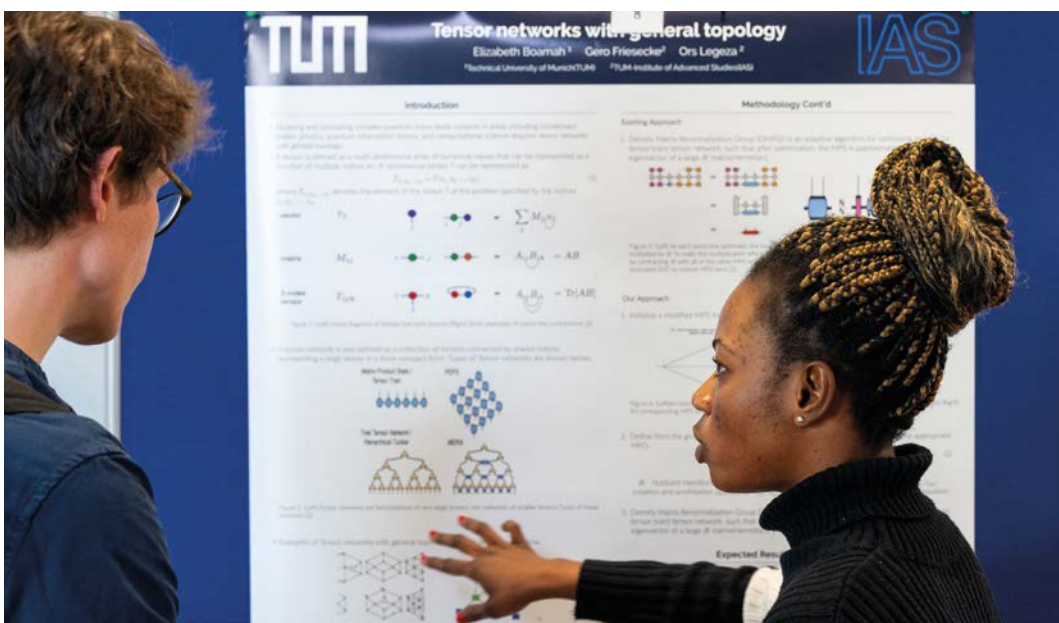
### Selection Symposium for Rudolf Mößbauer Tenure Track Assistant Professorships

For the last ten years, TUM-IAS has been responsible for selecting up to five Rudolf Mößbauer Tenure Track Assistant Professorships per year. From 22 to 24 March 2023, shortlisted candidates presented their research vision at the selection symposium “Selected Topics in Science and Technology”. The presentations were open to the public, and covered the following research areas:

- Cyber Security and Cryptography
- Green Hydrogen Production and Hydrogen Storage Technology
- Neutron-based Methods for Energy or Quantum Materials
- Participation and Diversity in Digital Societies
- Preventive Medicine
- Statistical Modelling and Uncertainty Quantification for Spatio-Temporal Data

Out of 138 applications received, 21 candidates were shortlisted and invited, and of those, 19 candidates presented for interviews. Individual and comparative peer reviews were collected for these candidates. Five candidates were proposed to the TUM Management Board for a Rudolf Mößbauer Assistant Tenure Track Assistant Professorship.

**Mathias Senge**, TUM-IAS Hans Fischer Senior Fellow and Professor at Trinity College Dublin, served as a member of the commission as an external expert. We owe him a debt of gratitude for his valuable advice and professional evaluations. ►



### Workshop on Optimal Transport, Mean-Field Models, and Machine Learning

TUM-IAS Hans Fischer Senior Fellow **Giuseppe Savaré**, Professor at Bocconi University, organized a workshop on Optimal Transport, Mean-Field Models, and Machine Learning (OTMFML) in April 2023. It aimed to highlight the interactions between optimal transport, mean-field control, and machine learning. It focused on innovative ideas to address crucial problems of high-dimensionality, nonlinearity, and nonconvexity, seeking the best examples and practice of successful deployment of mathematics to provide guarantees for practicable machine learning. The workshop was organized in cooperation with **Martin Burger**, Professor at Friedrich-Alexander-Universität Erlangen-Nürnberg, **Massimo Fornasier**, Professor of Applied Numerical Analysis at TUM, **Gabriel Peyré**, Professor in the Mathematics and Applications Department of the Ecole Normale Supérieure in Paris and TUM-IAS.

### Women In Science@TUM - WISTUM

The project is an initiative of Anna Boyksen Fellow **Shobhana Narasimhan**, Professor at Jawaharlal Nehru Centre for Advanced Scientific Research, India. In our society, there are significant elements of unequal treatment of different people, especially about their origin and gender or gender identity. Unfortunately, this also applies to the academic environment, including the STEM domain. In her project, Shobhana Narasimhan and her group have been developing a computer-based “cooperative discussion game” on diversity, equity, and inclusion in the scientific field. The game allows players to experience the stories and learnings of inspiring individuals who have overcome significant challenges due to inequality. Shobhana Narasimhan wants to increase the visibility and recognition of potentially successful but underrepresented groups of people. Unlike other passive media, a game allows players to actively engage with the issue and broaden their experience.



Shobhana Narashimhan (left), together with participants of the Women In Science@TUM - WISTUM workshop and speakers of the conference “Women in STEM - Voices from the Developing World”.



In her workshop on 8 and 9 May 2023, she also wanted to introduce the TUM community to a variety of perspectives and experiences of women in science from across the globe. It aimed to provide a platform for these women to share their stories, establish connections, and foster a supportive network. Additionally, the workshop sought to gather valuable insights that could contribute to the ongoing game project.

### Women in STEM – Voices from the Developing World

Another part of the WISTUM workshop was a one-day conference on “Women in STEM – Voices from the Developing World.” In the presentations, guests from around the world introduced themselves and shared their journey and experiences as female researchers in science in developing countries.

The international guests:

- **Shazrene Mohamed**, Professor of Computational Stellar Astrophysics, University of Miami, USA and University of Capetown, South Africa
- **Rabia Salihu Sa'id**, Professor of Atmospheric and Space-Weather Physics, Bayero University, Nigeria
- **Marta Antonelli**, TUM Ambassador and Head of the Laboratory of Perinatal Programming of Neurodevelopment, University of Buenos Aires, Argentina
- **Jinky Bornaes**, Vice Chancellor for Research and Extension and Project Leader of the Center of Innovation and Technopreneurship, Mindanao State University-Iligan Institute of Technology, Philippines

All speakers shared their experiences on how they were able to successfully pursue their scientific careers in hostile environments, which behavioral and communication methods were particularly helpful to them and offered recommendations based on their experiences.

**WOMEN IN STEM**

**VOICES FROM THE DEVELOPING WORLD**

8TH MAY 2023 | 17:00 PM | IAS AUDITORIUM  
LICHTENBERGSTRASSE 2 A  
85748 GARCHING

WE WARMLY INVITE EVERYBODY  
INTERESTED IN STEM TO JOIN.

FREE REGISTRATION.

**SPEAKER**

- **SHAZRENE MOHAMED** UNIVERSITY OF MIAMI, USA AND UNIVERSITY OF CAPETOWN, SOUTH AFRICA
- **RABIA SALIHU SA'ID** BAYERO UNIVERSITY, NIGERIA
- **MARTA ANTONELLI** UNIVERSITY OF BUENOS AIRES, ARGENTINA
- **JINKY BORNAES** MINDANAO STATE UNIVERSITY-ILIGAN INSTITUTE OF TECHNOLOGY, PHILIPPINES

WISTUM PROJECT

### CardioMRI Symposium - From MR Physics and Novel Hardware to Artificial Intelligence: making CMR a more Accessible and Affordable Imaging Modality

This workshop of Hans Fischer Senior Fellow **René M. Botnar**, Professor at King's College London, in July 2023 addressed cardiac MR (CMR) as a highly complex and rather expensive imaging exam that requires highly trained MR technicians and clinicians and is mainly performed in very specialized settings in tertiary academic hospitals. The workshop discussed how the latest developments in Artificial Intelligence (AI), MR acquisition/reconstruction, and low-field MRI, in combination ►

with knowledge gained from large CMR clinical trials/biobanks, could turn CMR into an easy-to-use and affordable mainstream imaging modality like computed tomography. More specifically, it was discussed how the latest developments in MR physics, motion correction, and image reconstruction can be harnessed to enable a self-driving CMR examination (no planning, no breath holds) that provides comprehensive disease characterization in a short, less than 10-minute scan. We asked how AI can enable automated image acquisition, reconstruction, processing, and analysis and create automated diagnosis and treatment planning. To better understand where CMR could play an increasing role in the patient pathway, lessons learned from large clinical trials/biobanks were taken. Finally, participants discussed the potential of AI to replace the use of gadolinium.

Learning outcomes:

- Understand how novel, more intelligent MR sequences, including quantitative multi-parametric MRI, can provide a comprehensive diagnosis with minimal user input.
- Understand how the latest developments in AI can facilitate automated processing and analysis of complex and multi-contrast MR datasets.



- Understand the value of clinical trials/biobanks in identifying new biomarkers and the economic value of CMR in comparison with other imaging modalities.

### Advocates and Allies - Male Allies for Gender Equality

On 19 June 2023, TUM-IAS Anna Boyksen Fellow **Andrea Erhardt** and Hans Fischer Senior Fellow **Gregory Erhardt**, Professors at University of Kentucky, organized a workshop on "Advocates and Allies - Male Allies for Gender Equality". The workshop aimed to address the underrepresentation of women in the sciences by engaging men as advocates and allies. Led by the instructors Gregory Erhardt, along with **Rolf Moeckl** and **Martin Elsner**, both Professors at TUM the workshop provided a platform for open dialogue on topics including implicit bias, workplace culture, effective communication, and handling resistance. Attendees explored best practices, shared relevant examples, and received guidance for future actions to promote gender equity in science.

### Gentoberfest - Crossing Bridges Between Bioinformatics and Clinical Research

This conference organized in October 2023 by Hans Fischer Senior Fellow **Lothar Hennighausen**, National Institute of Health, USA aimed at crossing the bridges between theory and clinical practice, hence, finding common ground between bioinformaticians and clinicians.

The sessions:

- **Discovery of Gene-Regulatory (Network) Mechanisms**  
Gene regulatory networks encompass a multitude of regulatory layers ranging from transcription factors to long non-coding RNAs, circRNAs or microRNAs. Furthermore, epigenetic mechanisms, such as DNA methylation or histone modifications,

are key determinants of gene activity. This session focused on current challenges and advances in discovering and understanding gene regulatory mechanisms and networks.

- **Using AI in Genetic Diagnostics**

Artificial intelligence (AI) has shown impressive results across fields and is starting to gain traction in the medical domain, especially in image processing. However, the expected breakthrough in genetics has not yet materialized despite countless genome-wide association studies. Considering the potential of AI in genetic diagnostics, this session focused on current challenges and future developments.

- **Implementing OMICS Technology in Clinical Practice**

OMICS technologies (e.g., genomics, transcriptomics, proteomics, and metabolomics) allow an understanding of the molecular landscapes in an unprecedented resolution. Even though OMICS technologies have shown potential for prognosis, diagnostics, and treatment monitoring, their use in clinical routine is still an exception. This session highlighted the successes of OMICS data in clinical practice and discussed how integrating different technologies can lead to more widespread and robust applications.

- **Data Storage and Sharing - Between FAIR Open Science and the GDPR and Ethics**

The unprecedented wealth of biological and genomic data that has already been generated, dwarfed by the OMICS data that will soon be routinely collected in clinical medicine. In spite of the huge potential of such data for research, the experience shows that the General Data Protection Regulation and other legislative barriers prevent researchers from leveraging such data towards improving the understanding

of diseases and the development of new diagnostic tools. This session provided an opportunity for discussing FAIR data sharing and usage of valuable datasets for scientific purposes in a GDPR-compliant fashion, to pave the way to open science.

- **Drug Target Prediction and Drug Repurposing**

Eroom's law shows that the costs for drug discovery have become prohibitively large such that alternative strategies are needed for widening the existing treatment options. Research highlights two avenues here. A better understanding of drug-target interactions will help develop more targeted therapies following the precision medicine paradigm. At the same time, a better understanding of disease mechanisms and drug-target interactions enables informed drug repurposing strategies, where existing drugs can be leveraged effectively and after shortened clinical trials for the benefit of the patients. For both strategies, the availability of high-quality datasets and the successful use of AI methods are imperative. This session was dedicated to assessing current advances in the fields of drug target predictions and drug repurposing.

- **Latest Developments in OMICS Technologies**

Since the introduction of microarrays in 1995, an ever-increasing variety of new technologies has provided new opportunities - among them, single-cell analyses, long-read, and spatial sequencing readouts. With new technologies, new challenges in data analysis arise and more advanced computational methods are needed to unearth the wealth of information from existing datasets. This session addressed the latest (sequencing) technological and methodological developments and their impact on clinical diagnostics. ►

### Workshop on Neuromorphic Computing and Rehabilitation

Neuromorphic computing is at the forefront of technological innovation, seeking to emulate the remarkable capabilities of the human brain in silicon. As students pursuing excellence in neural engineering, this workshop presented a unique opportunity to delve into the world of neuromorphic computation, interact with leading experts, and gain insights into the latest advancements in this fascinating field. The workshop was organized by Hans Fischer Senior Fellow **Nitish Thakor**, Professor of Biomedical Engineering at Johns Hopkins University, and his host Gordon Cheng, Professor at the TUM School of Computation, Information and Technology, in October 2023. The Hans Fischer Senior Fellowship of Nitish Thakor is funded by the Siemens AG.

### Quantumness: from Logic to Engineering and back

**Roberto Giuntini** is TUM-IAS Philosopher in Residence and Professor at the University of Cagliari. The leitmotiv of his research is based on the idea that quantum formalism finds applications beyond the realm of microphysics, encompassing the domains of cognitive and social sciences as well. The burgeoning research into quantum information and computation marks a significant milestone that can be dubbed “the second quantum revolution.” The first quantum revolution of the 20<sup>th</sup> century deeply changed

the fundamental concepts of physics and our understanding of the physical world. The second quantum revolution of the 21<sup>st</sup> century is leading to dramatic technological changes in our society and shaping new conceptual and logical paradigms. The new workshop series is dedicated to this topic. The first session on 6 December 2023, included **Guisepppe Sergiolo**, Professor at University of Cagliari, Roberto Giuntini and Rudolf Mößbauer Tenure Track Professor **Christian Mendl**, TUM School of Computation, Information and Technology.

### Exploring Global Governance Dynamics: Workshop on “The Evolution of International Regime Complexes”

In December 2023, **Eugénia da Conceição-Heldt**, TUM-IAS Carl von Linde Senior Fellow and Professor at the TUM School of Social Sciences and Technology, gathered scholars for a two-day workshop to delve into the intricate dynamics of international regime complexes. The workshop was hosted in collaboration with the American University and Temple University. It engaged in rigorous debates around the evolving nature of international regimes, focusing on both exogenous shocks and endogenous transformations that shape the global governance landscape. The insights gained from the discussions are expected to contribute to ongoing scholarly debates and inform future research on the evolution of international regime complexes. ■





TUM-IAS Fellows, their Focus Group members and other attendees during a poster session at the TUM-IAS General Assembly in 2023.

# Welcoming Our New Fellows

Meet our new Fellows and get inspired  
by their research projects.



# Fellowship Programs



## **Albrecht Struppler Clinician Scientist Fellowship**

three years for excellent senior physicians working at the TUM School of Medicine and Health, the TUM University Hospital and the German Heart Centre Munich.



## **Anna Boyksen Fellowship**

two years for outstanding female professors who intend to explore gender- and/or diversity-relevant topics within the TUM subject portfolio.



## **Carl von Linde Fellowship**

two years for excellent TUM faculty members.

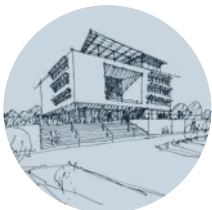


## **Hans Fischer Fellowship**

three years for outstanding early-career international scientists from outside TUM.

## **Hans Fischer Senior Fellowship**

three years for renowned international scientists from outside TUM.



## **Philosopher in Residence Fellowship**

one year for internationally leading and emerging representatives of the field of philosophy from outside TUM.



## **Rudolf Diesel Industry Fellowship**

three years for highly qualified researchers from industry.



## **Rudolf Mößbauer Tenure Track Assistant Professorship**

six years for outstanding, high-potential early-career scientists.

## Prof. Olga Boudker

Weill Cornell Medicine



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Claus Schwechheimer (TUM School of Life Sciences) | **Focus Group:** Toward Improved Nitrogen Efficiency – Amino Acid Transporters Take the Stage | **Research Area:** Fundamental Natural and Life Sciences

Plants require nitrogen for growth. However, producing inorganic nitrogen fertilizers is an energy-expensive process, and their application poses significant environmental problems. Amino acids are organic nitrogen-containing compounds in soil, which are the preferred nitrogen source for several plants. Breeding plants to increase the efficiency of amino acid intake and utilization is strategic alternative to the reliance on inorganic fertilizers. Amino acid transporters are proteins residing on the surfaces of plant cells, which take up amino acids from the environment and facilitate their distribution through plant tissues. While they are critical to the efficiency of nitrogen metabolism in plants, their molecular structure and mechanism are not understood. The Focus Group will use state-of-the-art electron microscopy to determine the near-atomic resolution structures of amino acid transporters and biophysical methods to investigate their function. Combined, these studies will reveal the mechanistic basis of transporter efficiency and pave the way to developing plants with improved amino acid utilization.

## Prof. Nathalie Bredella

Leibniz University Hannover



**Fellowship:** Anna Boyksen Fellowship | **Host:** Prof. Dietrich Erben (TUM School of Engineering and Design) | **Focus Group:** Feminism and Digital Cultures in Architecture | **Research Area:** Gender and Diversity in Science and Engineering

To encourage a critical engagement with the history of the digital in architecture, the Focus Group wants to explore methods of feminist practices in research and teaching. This Focus Group will bring together the chairs of Theory and History of Architecture, Art and Design, Architectural Informatics, Urban Design, Building Technology and Climate Responsive Design, Digital Fabrication, and History of Architecture and Curatorial Practice, in order to explore methods of writing history in the context of digital cultures. Who have been the protagonists in the development of digital practices, and how are they situated within local knowledge structures and their social, economic, and political contexts? What roles do activism, oral history, and reenactment play in understanding digital cultures? These are among the questions that the Focus Group will address as it explores methodologies and events that have not previously been included in architectural history. By focusing on the history of technology in collaboration with an international network of scholars, we will engage with situated precedents of digital practices and how they relate to contemporary discourse.

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## Prof. Priscilla A. Furth

Georgetown University



**Fellowship:** Anna Boyksen Fellowship | **Hosts:** Prof. Bernhard Küster, Prof. Markus List (TUM School of Life Sciences) | **Focus Group:** Gene-Regulatory Mechanisms | **Research Area:** Gender and Diversity in Science and Engineering

This Focus Group investigates gene-regulatory mechanisms through collaborative efforts in bioinformatics and targeted genetic research, utilizing preclinical models, gene editing, and human datasets. We aim to predict relevant regulatory elements governing normal development and physiology, alongside understanding pathophysiological changes leading to abnormal development or disease. Focusing on gene regulation as a multifactorial process, we leverage bioinformatics to gain insights into the genetic complexity of both normal physiology and disease. Our analyses investigate gene expression regulation across various levels, from chromatin and protein-DNA structures to regulatory RNA expression and subsequent protein-RNA interactions. Our goal is to contribute to the community through the development of new tools for bioinformatic analyses and to utilize these tools to elucidate specific regulatory mechanisms that lie behind normal and abnormal cytokine and hormonal responses. Currently, we are emphasizing genetic alterations impacting responses to viral diseases, vaccinations, and the development of hormonally mediated cancers such as breast cancer.

## Prof. Roberto Giuntini

University of Cagliari



**Fellowship:** Philosopher in Residence Fellowship (supported by the TÜV SÜD Foundation) | **Hosts:** Prof. Hans-Joachim Bungartz (TUM School of Computation, Information and Technology), Prof. Stefania Centrone (TUM School of Social Sciences and Technology), Prof. Klaus Mainzer (TUM Senior Excellence Faculty) | **Focus Group:** Quantum Logic and the Second Quantum Revolution | **Research Area:** Advanced Computation and Modeling

Our Focus Group seeks a unified model that harnesses the potential applications of key aspects of quantum formalism. We aim to construct a general model applicable to a range of phenomena beyond the realm of microphysics, with a special focus on practical and societal implications, particularly within the domain of machine learning and its potential ramifications for social, cognitive, and biomedical sciences. We will dedicate special attention to a comparative analysis of the behavior of artificial and human intelligences in processes involving concept recognition and object classification. Identifying an inherent “quantumness” in these natural and human processes promises a profound impact on knowledge advancement, fostering cross-disciplinary collaboration. The development of a new class of potentially faster and more accurate quantum-inspired classification algorithms, for instance, could strongly influence big data science, introduce novel predictive tools for cognitive and social sciences, and provide diagnostic support for biomedical research.



## PD Dr. Rico Gutschmidt

University of Konstanz / ETH Zurich



**Fellowship:** Philosopher in Residence Fellowship (supported by the TÜV SÜD Foundation) | **Host:** Prof. Eckhard Frick (TUM School of Medicine and Health/TUM University Hospital rechts der Isar) | **Focus Group:** Boundary Situations and Spiritual Care | **Research Area:** Health, Prevention, Care

Spiritual care addresses the spiritual needs of both religious and non-religious people. This project aims to address, in particular, to what extent this form of accompaniment can be made accessible to non-religious people. This study takes Karl Jaspers's notions of "boundary situation" and "philosophical faith" as its starting point. With regard to spiritual care, we will examine how these notions can be used to interrelate secular-existential and religious-spiritual forms of psychological support. The intention is to open up new possibilities for supportive forms of existential communication that would be independent of any religious or ideological background.

In a first, conceptual working step, spiritual care is examined and interpreted against the background of Karl Jaspers's philosophy. In a second, empirical working step, interviews with religious and non-religious patients facing boundary situations due to severe forms of physical or mental illness will be conducted within the framework of a qualitative study.

## Prof. Jiang Hu

Texas A&M University



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Ulf Schlichtmann (TUM School of Computation, Information and Technology) | **Focus Group:** A New and Scalable Methodology for Fast Machine Learning Accelerator Design | **Research Area:** Advanced Computation and Modeling

Machine learning (ML) has been generating phenomenal impact on human lives and society. The success of ML comes with immense cost of computation. It is well known that customized hardware computing is significantly more efficient than software computing on general purpose microprocessors. Therefore, hardware accelerators become a necessity for many ML applications. On the one hand, the growth of ML model complexity far outpaces the productivity of existing hardware chip design flows. On the other hand, increasing applications of ML demand fast design turn-around time for market competitiveness. Thus, there is a compelling need for a new ML accelerator design methodology that is fast and scalable to the growth in complexity. The goal of this research is to develop a new methodology that can reduce ML accelerator design turn-around time by an order of magnitude, and that will be scalable to ML models with trillions of parameters. This research goal will be achieved by developing a new design abstraction and algorithmic techniques that exploit design regularity in ML computations.

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## Prof. Heather J. Kulik

Massachusetts Institute of Technology



**Fellowship:** Hans Fischer Senior Fellowship | **Hosts:** Prof. Christopher J. Stein, Prof. Jennifer L.M. Rupp (TUM School of Natural Sciences) | **Focus Group:** Systematically Improvable Modeling of Electrochemical Processes | **Research Area:** Advanced Computation and Modeling

This Focus Group seeks to model electrochemical processes in batteries that are important for energy storage and electrocatalysts, which are key for energy utilization. To overcome present limitations, we aim to develop systematic approaches to bring high accuracy to low-cost methods and develop techniques to detect when lower-cost methods are insufficient. We are working to develop a machine learning (ML) framework for fitting low-cost methods to higher accuracy methodology, devise schemes for systematic multiscale modeling, and build ML model techniques to detect when low-level theories will fail. In doing so, we will address length and time scales in electrochemical modeling that have not been possible before, providing new insight into batteries and electrocatalysts to optimize next-generation aqueous, solid-state, and hybrid batteries by limiting the catalytic activity of electrode materials or, alternatively, to optimize electrocatalysts for oxygen evolution for fuel cells. This work is expected to provide both fundamental insights into electrochemical phenomena and provide opportunities for technological advances via novel design principles for battery technology.

## Prof. Chenchen Liu

University of Maryland



**Fellowship:** Hans Fischer Fellowship | **Host:** Prof. Ulf Schlichtmann (School of Computation, Information and Technology) | **Focus Group:** Enabling Neuromorphic Computing for Multi-tenant Artificial Intelligence | **Research Area:** Advanced Computation and Modeling

A distinctive trend in recent artificial intelligence (AI) applications is that they are evolving from singular tasks based on a single deep learning model – e.g., a deep neural network (DNN) – to complex “multi-tenant” scenarios with multiple DNN models being executed concurrently. The deployment of multi-tenant DNNs still presents significant difficulties. The goal of this research is to develop an innovative neuromorphic computing engine that can efficiently support multi-tenant AI. The neuromorphic engine not only can support complex multi-tenant DNNs computing with flexible resource and function configurations, but also can host model interactions across individual tenants’ computing instances with redefined multi-tenant data flow logistics and immediate computations. This research will benefit the computer system community at large by inspiring an interactive design philosophy between emerging complex AI applications, deep learning algorithms and their computing principles, and novel computing paradigms.



## Prof. Rainald Loehner

George Mason University



**Fellowship:** Hans Fischer Senior Fellowship (funded by the Siemens AG) | **Host:** Prof. Kai-Uwe Bletzinger (TUM School of Engineering and Design) | **Focus Group:** Adjoint-Based System Identification of Large-Scale Structures | **Research Area:** Advanced Computation and Modeling

Taking into account the increased loads due to climate change, the aging of structures, the advances in sensor technology, and the development of digital twins, a very fundamental question needs to be answered: Given measurements, can we pinpoint the location of weaknesses in structures? The potential benefits of being able to accomplish this are many: One could immediately and continuously assess the health of civil engineering structures during normal loads and extreme loads; the decision process of treating aging structures (demolish, upgrade, keep as-is) would be much more objective; being able to keep some aging structures operating longer would be less of a burden on the environment and reduce the carbon footprint; and overall safety would be improved.

## Prof. Lorenz Panny

TUM School of Computation,  
Information and Technology



**Fellowship:** Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Cryptography | **Research Area:** Communication and Information

Cryptography is a crucial part of modern life as the foundation of computer security. It is often unnoticed by the general public, yet we constantly rely on it for a wide variety of purposes, from messaging our friends to protecting critical infrastructure. Failures of these systems pose a great threat to individuals as well as society as a whole; thus, it is imperative that the risk of possibly catastrophic security breaches be minimized. One particular cause of concern is the possible emergence of large-scale quantum computers, which would be able to break most security systems deployed on the Internet today.

There are several major subtasks in designing cryptography and putting it into practice, ranging from the cryptanalysis of purported hard problems to developing efficient and reliable implementations. In the end, security is upper-bounded by the weakest link in this chain, and high- and low-level aspects must often be considered jointly to achieve the best outcome. This Focus Group works toward this goal: ultimately eliminating the possibility of cryptographic failures, with particular attention to the rapidly developing field of post-quantum cryptography.

## Prof. Bjørn Panyella Pedersen

Aarhus University



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Claus Schwechheimer (TUM School of Life Sciences) | **Focus Group:** Auxin Exporters as Targets for Herbicide Resistance | **Research Area:** Fundamental Natural and Life Sciences

In plants, auxins are essential hormones that regulate virtually all aspects of growth and development. Within the plant, auxins are transported in a polar fashion through auxin transporters. The central role of auxins in plant growth regulation has led to the design of synthetic auxins that cause uncoordinated overgrowth. These compounds are very important as agrochemicals, as they find wide use as herbicides; but it remains to be discerned how these compounds function at the molecular level and how they interfere with auxin transport.

The Focus Group will use state-of-the-art structural and biophysical methods to characterize the distribution and mode of transport of auxin herbicides in plant tissues. This will give fundamental insights into plant hormone transport pathways and will be a first step toward novel, efficient and environmentally safer herbicides for use in modern agriculture.

## Prof. Elizabeth Qian

Georgia Institute of Technology



**Fellowship:** Hans Fischer Fellowship (funded by the TUM Georg Nemetschek Institute) | **Hosts:** Prof. Daniel Straub, Dr. Iason Papaioannou (TUM School of Engineering and Design), Prof. Elisabeth Ullmann (TUM School of Computation, Information and Technology) | **Focus Group:** Model Reduction for Structural Reliability Analysis | **Research Area:** Advanced Computation and Modeling

Structural reliability analysis aims to quantify the probability of structural failure, an essential task in reliability and risk assessment for engineering structures and systems. Because failure events have low probability, standard sampling-based Monte Carlo methods for quantifying uncertainties require a large number of samples, making reliability analysis prohibitively expensive for many applications where the system model is high-dimensional and expensive to evaluate. This Focus Group will develop new efficient approaches to structural reliability analysis using projection-based reduced models, which are cheap, low-dimensional approximations to high-dimensional models that reflect the structure of the governing equations of the physical system. These approaches will be based on both existing reduced modeling methods and new reduced modeling methods tailored to the reliability analysis setting. The research will span the development of new methods, mathematical analysis of the methods, and practical demonstration of the computational benefits of the proposed approaches for real-world applications.

## Prof. Melanie Schirmer

TUM School of Life Sciences



**Fellowship:** Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Translational Microbiome Data Integration | **Research Area:** Medical Natural Sciences

The lab of Melanie Schirmer studies host-microbial interactions to uncover mechanisms behind microbiome-related diseases. The microbes that live in and on the human body are crucial for our well-being. Changes in these microbial communities are implicated in many inflammatory and autoimmune diseases. To identify and understand these changes, her lab analyzes and integrates large-scale multi-omics data from clinical cohorts, incorporating host and microbiome information to generate hypotheses on the functionality of the microbiome in disease. This research group combines these computational approaches with experimental validation of the immunogenicity and inflammatory activity of the identified bacterial strains and metabolites. The main goal is to understand (1) what role the microbiome plays in human health, (2) what the underlying mechanisms are that lead to aberrant host-microbial interactions in disease, and (3) how microbiome-based diagnostic and therapeutic approaches can be used to treat these diseases.

## Prof. Elena Simperl

King's College London



**Fellowship:** Hans Fischer Senior Fellowship (funded by the Siemens AG) | **Host:** Prof. Klaus Diepold (TUM School of Computation, Information and Technology) | **Focus Group:** Trustworthy Knowledge Graphs | **Research Area:** Advanced Computation and Modeling

Combined with machine learning, knowledge graphs (KGs) reduce the need for labeled data, facilitate transfer learning, and generate explanations. They are used in industrial AI applications, e.g., digital twins, enterprise data management, supply chain management, procurement, and regulatory compliance. The vision of the project is to advance trustworthy KG engineering for human-centric AI applications. We will define process blueprints for KG development, maintenance, and assessment that account for emerging human-in-the-loop practices where human, social, and machine capabilities are seamlessly mixed. We will then design and evaluate socio-technical methods that increase the transparency and accountability of the KG lifecycle and will assess biases and wider socio-environmental implications of KGs. We will apply the research in a legal compliance demonstrator, designed with the help of industry partners. It will include a legal knowledge graph and will guide compliance professionals when auditing industrial AI applications. We will document the results in a reusable, structured way and facilitate the discovery of best practices to streamline compliance efforts in organizations that deploy AI.

# 40

## Prof. Agnieszka Wykowska

Italian Institute of Technology



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Gordon Cheng (TUM School of Computation, Information and Technology) | **Focus Group:** Human Cognition in Neuroengineering | **Research Area:** Neuroengineering

The aim of this Focus Group is to address human cognitive mechanisms in the context of neuroengineering. When developing neurotechnological solutions for health care, one should not marginalize human cognitive mechanisms involved in interaction with such technology, and with the world (through such technology.) For example, the use and acceptance of exoskeletons or prostheses are highly dependent on how much sense of control the user experiences when acting upon the environment through such devices. When engaged in neurorehabilitation, the user should not experience excessive cognitive load or attentional demands that can interfere with the progress of the rehabilitation. With cognitive neuroscience methods (performance measures, EEG, eye tracking), this Focus Group will examine human cognition (sense of agency, attention, cognitive control) involved in the use of neuroengineering solutions.

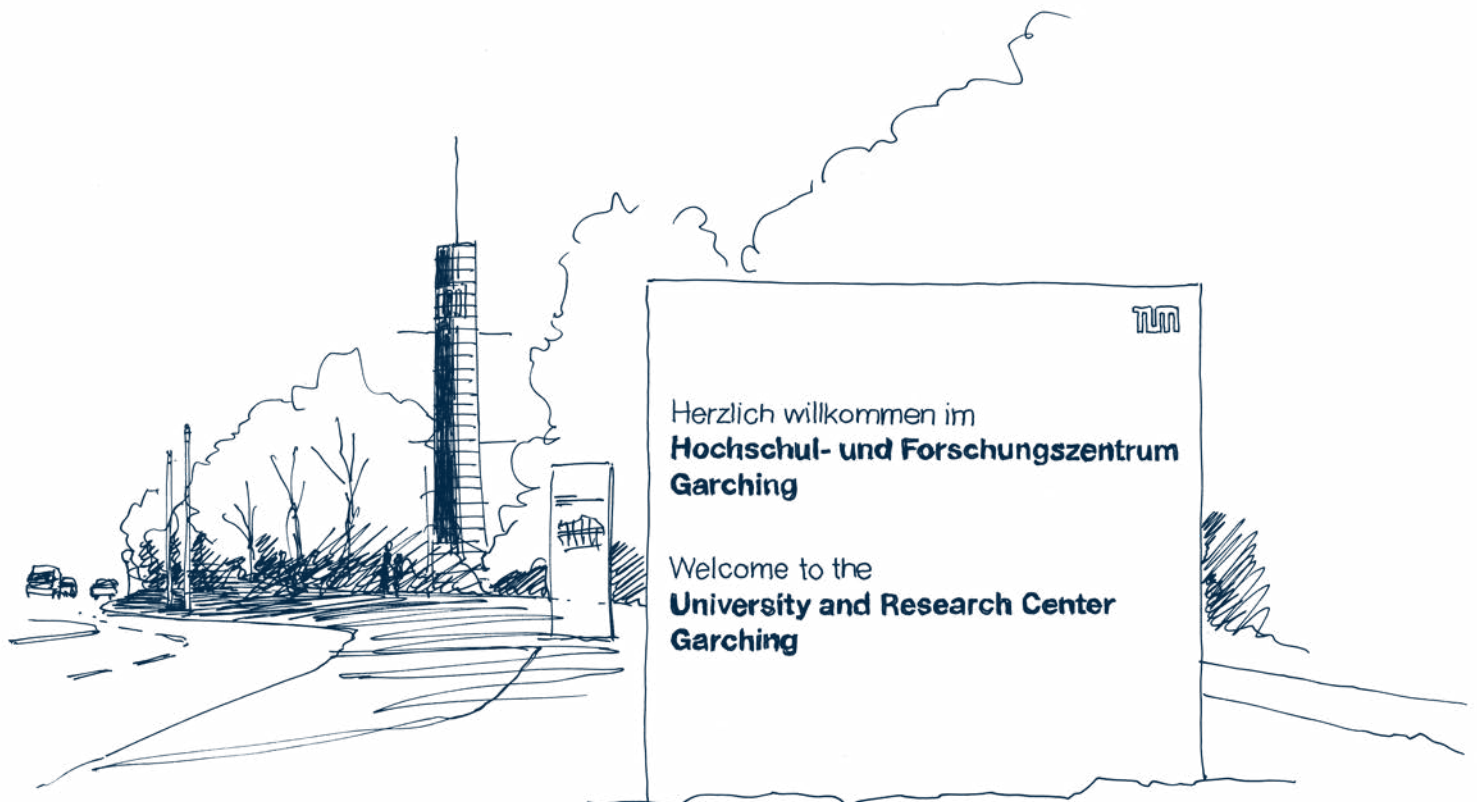
## PD Dr. Michael Zech

TUM University Hospital rechts der Isar |  
TUM School of Medicine and Health



**Fellowship:** Albrecht Struppler Clinician Scientist Fellowship | **Focus Group:** Linking Genomics with Computational Science | **Research Area:** Medical Natural Sciences

This research group, including Albrecht Struppler Clinician Scientist Fellow Priv.-Doz. Dr. med. Michael Zech (Institute of Human Genetics, TUM University Hospital Rechts der Isar), doctoral candidates, and TUM collaboration partner Prof. Dr. Julien Gagneur (TUM Computational Molecular Medicine), will bridge the disciplines of genomics and bioinformatics by establishing close trans-departmental relationships between the TUM School of Medicine and the TUM School of Computation, Information, and Technology, paving the way for big data-driven research in life sciences, optimized diagnostics, and personalized medicine. The collaborative team will harness high-throughput molecular methods, multiomics data, deep-learning informatics tools, shareable computational workflows, and cross-disciplinary thinking to ensure rapid translation of DNA base-pair technologies to bedside applications and to accelerate developments in bioinformatics. The Fellowship will demonstrate to the public the importance of the fields of genomics and computational molecular medicine with the goal of providing improved molecular diagnoses for patients and the identification of the underlying pathophysiology.





**In Focus**

# From Urban Air to Global Climate

Atmospheric chemists at Harvard, led by Frank Keutsch, probe basic processes taking place in the air. Jia Chen's group at TUM charts emissions of greenhouse gases and other pollutants with high resolution. Together they are generating new knowledge relevant to both human health and climate change.





## The air we breathe, the climate we bequeath

**Except in smoggy cities, the air we breathe is normally invisible. Yet it's plain to see that we depend on it, we interact with it, and we have changed it in ways that can harm human health, upset ecological balance, and even threaten civilization. For decades, the saying "out of sight, out of mind" has gone a long way toward explaining why many environmental problems of the Anthropocene – not just air pollution and global warming, but also phenomena such as the "sixth mass extinction" that appears to be under way – remain poorly understood and ineffectively addressed. Here science and engineering have a role to play, a challenge taken up by the TUM-IAS Focus Group on Air Pollution and Climate.**

Based at Harvard University, Hans Fischer Senior Fellow Frank Keutsch is a professor of Engineering and Atmospheric Science as well as Chemistry and Chemical Biology. His Host, Jia Chen, is a professor of Environmental Sensing and Modeling in the Department of Electrical Engineering at TUM. They are uniting largely complementary expertise in this Focus Group, with the ultimate goal of enabling policy makers to assess potential approaches to improving air quality and combating climate change.

For a closer look at how this collaboration works, what the researchers have learned, and what they envision for the future, science journalist Patrick Regan spoke with Frank Keutsch and Jia Chen by videoconference. Their conversation has been edited for clarity and length.

**Q: Your collaborative research ranges from basic chemistry to engineering and on to implications for public policy. What are you trying to find out? Why? And how?**

**Keutsch:** There are two reasons that come together why I and, I believe, Professor Chen, are conducting the research that we are doing. One is just trying to understand the world around us, in reality a small aspect of the world around us, and get an in-depth mechanistic understanding of how different aspects and processes couple together, and how they form the world around us. In our case that has to do with the atmosphere and air quality, and then both Professor Chen

and I do work in the direction of climate more broadly. It's really a question of how well we understand the air that we breathe, its composition, and what changes it. Part of that, at least for me, is a purely intellectual curiosity. I want to understand things. I find it frustrating when there's something I find fascinating that I don't understand.

Then again, of course, this is in many ways applied research, so there's also the motivation for the application. And that, fundamentally, is that if we better understand the air that we breathe and that interacts with plants and other things, perhaps we can also find ways to improve that air quality so that



Patrick Regan, Jia Chen and Frank Keutsch.

it has less harmful side-effects. In a sense, it is an applied science, so it is driven by the applied program of studying and improving air quality.

**Chen:** In my team, we are really good at developing sensors, and sensor networks, as well as automation and communications. And Frank's group is very strong in atmospheric chemistry. We are developing sensor networks and gathering the data, and together with Frank we can understand better how the metabolism of air pollution in the cities works, what are the drivers for the air pollution, where the air pollution is coming from, and so on.

**Q:** You're dealing with quite a range of time scales, aren't you?

**Keutsch:** The reason things are greenhouse gases is typically that they live a long time in the atmosphere, whereas the reactive species, usually from air pollution, are pretty short-lived. And so one of the big distinctions, for example between the greenhouse gases CO<sub>2</sub> and methane, is that CO<sub>2</sub> really does not get chemically processed in the atmosphere. It's in there, and it gets taken up by the earth's surface in some form or another. Methane actually can be chemically processed in the atmosphere, and then it's turned into CO<sub>2</sub>, a less effective greenhouse gas, but nonetheless, a greenhouse gas. And this turn-over rate of methane into CO<sub>2</sub> is determined primarily by one of the highly reactive species, the OH radical. It's a species that is very transient but is really the key to determining the atmospheric lifetime of methane.

You have to know the emission sources and the chemistry, and then you also need to know the different things that can happen, for example, when it gets deposited in the ground or taken up by plants. Uncertainty in any of those will drive uncertainty in what you predict a certain concentration will be. ►

**Chen:** Also, in the context of urban air monitoring, we have been able to detect and analyze changes over a period of days or weeks. What we learn could make it easier to predict how conditions might change on a comparable time scale.

**Keutsch:** There is also the question of how much humans have actually changed the world around us, in this case the air that interacts with living things, and to what degree we can control that. What's really interesting is the question: What is this interaction between things that we generally think of as natural and the human part? In some cases those can in essence build on each other and result in much worse air pollution, and in other cases they don't. What role do humans play, at a mechanistic level? One of the things we often want to know is how we've shaped and formed this planet. How well do we actually know what the planet was like before human interaction? People always talk about pre-industrial conditions. For many things, we can go back to pre-industrial conditions. You can take an ice core and see how much CO<sub>2</sub> is in it. We can go back and look at all kinds of historical records.

But when it comes to the chemical drivers of air pollution, there's an interesting conundrum: The actual compounds that drive chemical transformations in the atmosphere will be, by definition, very reactive. A chemical process will follow the easiest path, the fastest path, and that's the one that matters. That means these compounds do not survive in ice cores. To represent these correctly in models that can say, this is the condition pre-industrially, we have to rely on a fundamental understanding of chemical processes involving these most reactive species, commonly called radicals.

***“The ability to look back can give us confidence, not just for climate models, but also for reactive compounds that make air pollution.”***

FRANK KEUTSCH

**Q: Does that involve volatile organic compounds?**

**Keutsch:** Those are the things that get transformed by radicals. Volatile organic compounds are also reactive and mostly wouldn't survive in an ice core. There's a whole range of reactivity. The only way we can travel back in time and have an accurate understanding of the processes that would occur, and how they would occur, is if we understand the actual chemical processes.

**Q: So you can use proxies and models to work out what's happening?**

**Keutsch:** Exactly. So then we can say, we know these reactions, we know how these behave, and then you can integrate them into a model. For those things, the only way to travel back in time is then in “model world.”

**Q: What are some examples of these highly reactive substances?**

**Keutsch:** Nitrogen dioxide or NO<sub>2</sub> is a radical. This is a part of NO<sub>x</sub> that we're concerned about when it comes to cars and combustion. There's the OH radical. Even ozone, which is not a radical but is highly reactive, can't survive well in long historical samples. In a way, we use models not only to travel back in time, but also when we want to predict the future.



The ability to look back can give us confidence, not just for climate models, but also for reactive compounds that make air pollution. That also gives us some confidence that we understand the processes that would shape a future atmosphere where we've changed emissions into the atmosphere.

In my group, we have primarily specialized on measurements of an intermediate reactivity range. As hydrocarbons get emitted, those typically get processed via oxidative processes. We look at the precursors, the hydrocarbons, as well as the reaction products that are formed, and how fast this processing happens, from emissions into pollutants – in part to see where we need to have additional understanding.

We use tools from spectroscopy, an interaction of light with molecules and particles. We also use mass spectrometry, where we try to use the mass of individual molecules to identify them. Professor Chen's group uses primarily spectroscopy, but also electrochemical sensors, to measure some of these compounds we're interested in.

My group does this across a wide range of conditions. We try to find places on the planet that have very different conditions, that perhaps in some respect can get us closer to pre-industrial. We've done measurements in the middle of the Amazon, where there's very little of certain types of human interactions. That should be, in some coordinates, still fairly close to pre-industrial. We also do measurements in urban areas that are clearly anthropogenically influenced.

#### Q: Do you have data from polar regions?

**Keutsch:** Yes, we've done measurements on the ground and on ships. We were on an icebreaker going to Antarctica. Recently we've been doing a lot of measurements on stratospheric aircraft that go high into the atmosphere. We just did some measurements from Alaska. We've done that over the United States in the past few years with the idea of trying to understand these chemical processes under as many different conditions, in as many different places, as possible. Because after all, if we understand the processes correctly, we should be able to understand them regardless of where we are looking.

Now and again you find surprises. You may see a process you hadn't thought of before that you suddenly realize exists. And then you do laboratory studies. The problem is that the atmosphere is a messy place, especially the troposphere where we live. When we find something surprising, we typically go back to the lab to study that process in isolation, without all the uncertainties that the real system introduces. In my group, we do field measurements, and then lab measurements that tell you the detailed processes including reaction rates, how fast they occur. And then we go to models and see whether integrating that into the models actually improves agreement between the virtual model world and observations in the real world.

It's like a three-legged stool. You need a combination of measurements in the real world, models that try to represent the real world, and detailed specific studies of reactions to try to improve their representation in the models. ►



One of the sensors on a TUM rooftop for measuring urban greenhouse gas emissions.

**Q:** Looking at the present state of the atmosphere with an eye toward gaining a better understanding of both air pollution and climate change, you also have relatively high-resolution data from what could be called a “mission to Munich.” Could you give an overview of that work?

**Chen:** MUCCnet, the Munich Urban Carbon Column network, is a worldwide unique city sensor network measuring the total air column concentrations of greenhouse gases using the sun as a light source. We have sensor stations located both within and outside of Munich. You can look at the difference between the concentration in the column measured before and after the city, and the difference is a measure of the emission of the city.

Because of this uniqueness and also my expertise in developing sensors and models, Munich has been selected as a pilot city in the ICOS Cities PAUL project within the European Green Deal. ICOS stands for Integrated Carbon Observation System, and PAUL stands for Pilot Application in Urban Landscapes. The aim is to develop novel methods for monitoring city emissions, and they chose three pilot cities: Munich, Paris, and Zurich. I am the scientific lead for Munich. Within this project, we are adding more monitoring capacity on top of MUCCnet. We have 20 roof-level sensors, 100 street-level sensors, and then air quality sensors. So we have more than 170 sensors right now in Munich, to observe both greenhouse gases and air quality.

**Q: Particulate matter as well as gases?**

**Chen:** Yes, though only some of the sensors detect particulates. It's an integrated sensor network that is measuring all kinds of species that are relevant for climate and health.

**Q: How does that compare to the other cities involved in this EU project?**

**Chen:** Each city has its own strength. MUCNet is the strength of Munich. Some aspects are the same for all three cities. For example, Munich has roof-level sensors, same as Zurich and Paris. But only Munich and Zurich have street-level sensors, and only Munich and Paris conduct total column measurements.

**Q: Given that some of the sensors rely on sunlight, what do you measure at night?**

**Chen:** Well, it is difficult to measure anything at night if you use sunlight. Many people are saying that satellite observation is the future. If so, we can also use MUCNet to validate satellite measurements, to make the satellite data more accurate and then benefit from the global coverage. That's its advantage. But we also have sensors operating all the time, using an infrared light source inside the sensor. The disadvantage is that these are surface sensors measuring concentrations just at one point. The column sensor provides more information because it uses the sun as the light source and then integrates the concentration along the air column and correspondingly provides two-dimensional information instead of just one point.

**Q: What do you do to get the most information and knowledge out of the data?**

**Chen:** We are developing a modeling method, based on mathematical principles and employing machine learning, to localize, quantify, and characterize the emissions. This is also part of my successful proposal for the ERC Consolidator Grant, which is funded by the European Research Council.

**Q: Let's talk about how the models work and how they're used. Do you come to the models with hypotheses and test them in the model, and then test the model against the data?**

**Chen:** It can be thought of as two steps. You want to do some scientific experiment. You say you know the truth, and you test your model and see how well your model can recover the truth. And if you know that, and we have quantified the model's capability, we can deploy the model to the real-world data to get the emissions. In addition, you can imagine that we are measuring concentrations at different locations, in Munich for example, and we want to know where the emissions are coming from, how much a power plant or a car emits. Some sort of translation needs to be done between the emissions and the concentration that is measured. So this is what the model is supposed to be doing. That requires some knowledge of atmospheric transport. It requires mathematical knowledge as well. So together we can build the linkage, or what we refer to as the transfer function. Machine learning can help with this. ►

**Q: What are the benefits and limitations of machine learning in terms of extracting knowledge from data and applying that knowledge to real-world conditions?**

**Chen:** The model is partly to build this transfer function between the concentrations and the emissions. But machine learning can also help in making the sensor values more accurate. That's one application. And then secondly, if we measure concentrations, it's not the whole picture. Machine learning can also help us to interpolate the whole concentration field from the measured, sampled points to the whole map, for tracking air pollution in cities for example.

Machine learning can also help us to gain finer resolution for satellite pixels. Let's say you want to understand the urban biosphere, how much carbon is taken up by Westpark or the English Garden. You have some satellite observations. Still, that is very difficult to determine the urban biospheric fluxes. While the vegetation is doing photosynthesis, a certain amount of light is emitted back to space, usually in the red or infrared range. The satellite detects that part, and this is an indication of the photosynthetic activity of the vegetation. However, the satellite measurement pixel is very very coarse, say, five kilometers. You can have only a few pixels in Munich, and certainly you cannot determine the photosynthetic capacity of Westpark or the English Garden. Therefore, you need to develop some super-resolution technique, and that is what we have done using machine learning.

**Keutsch:** Machine learning can be very efficient computationally. And as an exploratory

tool, I think it's unbeatable, because it's much cheaper and faster.

We are both working to integrate machine learning and AI into our toolkits. Professor Chen's group has more expertise than my group in tools that have to do with detailed fluid dynamics modeling, for example air flow in the complex environment of a city. Where my group has more expertise is in the details of the chemical mechanisms and transformations. We do modeling as well, but using what's called chemical box models or chemical transport models.

Now, the way you have to imagine a chemical transport model is that it is trying to account for all the processes it can that exist in the real atmosphere, for every individual location. Each location has a certain size, and if you want to go to a more regional scale, you need a higher resolution. This increases the computational effort. Also, you're trying to include emissions into that, and a myriad of chemical reactions, transport processes, turbulence, and more. That is computationally quite expensive. In a way, you could say they're so computationally expensive that we can't possibly include all the processes that each research group thinks it's important to do. If you find a new chemical reaction, you really need to convince the chemical modelers that it's worthwhile for them to add another reaction into their model.

Machine learning models, on the other hand, are quite ignorant of all this. They have a lot of data available, which you can use to train them, and in a sense they'll find their own way to represent that internally. Which intellectually – I'll say as an atmospheric chemist – is

incredibly frustrating. Because it says: Who cares about this great detailed chemical reaction? About two years ago we found an absolutely fascinating phenomenon where formaldehyde can be a catalyst for the formation of sulphate particles, really weird.

Modeling with machine learning might make it easier to have decentralized, short-term forecasting of air quality. It's now being used for predicting weather, and if you stay in the short-term range, machine learning models are currently competitive with the big complicated models. If you try to predict farther out, they start going weird. This is not a replacement. My chemical transport models, like climate models, can run quite a bit into the future. But machine learning might potentially enable short-term air quality forecasting, perhaps even tailored to a specific region where you don't have measurement stations but want to make predictions.

We used it to predict changes in ozone, for example. It did a really good job of predicting this if you fed it with the right information. The idea is that you don't let it run free, but you set some of the boundary conditions, and this gets updated. It did quite well. The reason that matters is that we have air quality measurement stations only in very few locations. It's expensive, it takes effort, and they are predominantly in urban areas.

**Q: So when a machine learning approach yields results that are helpful in understanding real-world conditions, can it be transferable to different situations?**

**Keutsch:** Possibly, within limits. Transferability will likely be limited to locations that

span the same parameter range as where you trained your machine learning model.

**Q: Could it be useful in assessing the effectiveness of mitigation efforts?**

**Keutsch:** Yes, to the degree your mitigation efforts don't start moving you outside of the training data or boundary conditions that were available.

**Q: One striking result from the Focus Group is your study of the air in and around Munich before, during, and after Germany's Covid lockdown period. Was this to some extent a proof of concept for your measurement, modeling, machine learning, and analytical methods? And what did you learn?**

**Chen:** That was a very nice collaboration, which shows that together we can have really nice results. This work was done by my PhD candidate Vignesh Balamurugan, together with Frank and myself. Covid was very unfortunate, of course, but at the same time you see the emission reduction and a chance to study what kind of impact such a reduction in emissions has in terms of air pollution levels in cities.

**Keutsch:** If we went to the mayor's office in Munich and said, could you please stop all traffic for some number of days to reduce NOx, because we want to see whether our models and our understanding are right, we would get laughed out of the place. But Covid did it for us. Especially during the harder lockdown, traffic was reduced dramatically.

**Chen:** This enabled us to study what happened to several kinds of pollution. ►



For most people, if you talk about air pollution, especially in German cities, they think about NO<sub>x</sub>. That's what people are talking about in the media, often in relation to diesel bans or the diesel scandal. NO<sub>x</sub> is very relevant to health. People don't think too much about ozone and particulate matter, but these too are very harmful air pollutants, very harmful for health.

**Keutsch:** Ozone is a gas, fairly reactive and fairly short-lived, and particulate matter is much longer-lived. Both are of large significance, as is NO<sub>2</sub> itself, or NO<sub>x</sub>, which is a mixture of NO<sub>2</sub> and NO. Put simply, the more hydrocarbon emissions you have, the more pollution you're going to get. More ozone, more particulate matter. But how much you actually get depends on NO<sub>x</sub>, and it has a complicated dependence. The only source of ozone in the troposphere is actually photolysis of NO<sub>2</sub>. The first thought, of course, is the more NO<sub>2</sub> I have, the more ozone I'm going to make. However, through some very complicated coupled chemical reactions, what happens is at some point you have so much NO<sub>x</sub> that it actually suppresses the chemistry of ozone formation in the end, and with a further increase in NO<sub>x</sub> you actually have less ozone pollution.

**Chen:** What happened in the Covid lockdown is that we saw the NO<sub>x</sub> emissions reduced a lot, which was expected because we had less travel, less car transportation. But then ozone actually increased, and the particulate matter concentration stayed constant. So it's not a very simple story. OK, we reduced NO<sub>x</sub>, but that doesn't solve all our pollution problems. In this case ozone increases, because in German cities, the air is actually

in a NO<sub>x</sub>-saturated regime. That requires atmospheric chemistry to understand what's happening. In a NO<sub>x</sub>-saturated regime, if you reduce NO<sub>x</sub>, then ozone increases. So you need to reduce NO<sub>x</sub> much more, and then we can go to the other regime, which is a NO<sub>x</sub>-limited regime, so that ozone can also decrease.

**Keutsch:** Indeed, in all the larger urban areas in Germany, as Covid reduced NO<sub>x</sub> emissions, ozone went up compared to the previous year. We had to do a lot of checking, but finally, I would argue, it proved that we understand the general chemistry of it, and that we also understand the current status of German cities.

**Chen:** It is very important to understand which regime we are currently at in the German cities, and it turns out that we are in the NO<sub>x</sub>-saturated regime. Therefore, in terms of environmental policy, we need to consider this as well as other factors.

**Keutsch:** As we transition, let's say more and more to electric cars, and NO<sub>x</sub> goes down, that means ozone will initially increase until we get over that bump. I want to be very careful that things don't get misrepresented. No one should be able to say NO<sub>x</sub> emissions are good because they reduce ozone. The reason they do that is because we have such high NO<sub>x</sub> levels at present.

**Chen:** Either we reduce the NO<sub>x</sub> enough to reach the goal of ozone reduction also, or we need to really understand the atmospheric chemistry and think about the tradeoff.

**Q: Did you gain any new insights into particulates?**

**Keutsch:** Particulate matter is a much more complicated process. Lots of things contribute. Particulate matter you see in location A, as it lives longer, is influenced much more by being produced in some upwind location. And what we found is that while the reduction in NO<sub>x</sub> had a clear impact on the ozone, the particulate matter concentrations remained unchanged. We can't model particulate matter to the same degree of trust, I would say, as we can model ozone.

What we saw in our study is that reductions in NO<sub>x</sub> left particulate matter virtually unchanged. We were discussing what this might mean, and I had my own very convinced hypothesis, and Vignesh countered that it was more complicated and might have to do with the combination of nighttime and daytime chemistry. He did some further research and showed me he was right. There are many contributors to aerosols, and daytime production is associated with different chemical processes than nighttime. The idea is that it was buffered in that respect, by shifting away from one type of aerosol and more to another type, so the net amount stayed roughly the same. There's still a lot of work that needs to be done to really understand particulates better.

**Q: What other recent or upcoming research efforts would you like to highlight?**

**Keutsch:** We are joining together to do some actual atmospheric measurement campaigns in Munich. The first of these took place in August 2023. My instruments come from

the US in a container. The instruments of the Chen group are already there, of course. We also have instruments coming from KIT in Karlsruhe, and perhaps we'll also get one from China. The aim is to make very detailed measurements of the chemistry of the formation of ozone and particulate matter. We're doing very intensive campaigns to measure as much as we possibly can to try to understand the formation of aerosols. We were delayed significantly by Covid and trickle-down effects, but there will be quite a lot more output from this TUM-IAS effort over the next few years, where we look at measurements and modeling.

**Q: Do you see your collaboration continuing further, and deepening or broadening to involve other groups with different expertise and interests?**

**Keutsch:** Once we have our findings and we understand the foundations of what's happening, with regard to air quality in particular, I would be very interested in broadening the collaboration. At that point we will have a stronger basis for cooperation with people who understand public health, with people who understand the policy aspects, like Miranda Schreurs, or with the city of Munich.

With regard to climate change, I would also be very curious about broadening into the issues surrounding climate intervention. The Chen group is very focused on greenhouse gases, which are the cause. My group, while working on a general understanding of stratospheric science, is also looking into the feasibility and potential side-effects of measures like stratospheric aerosol injection. These are quite complementary fields. ►

One is trying to tackle the cause, and the other one is thinking about a potential Plan B if we do not address climate change rapidly enough. Some argue that no one should be doing research on this at all, because it's not a long-term solution. My concern is that if there is serious discussion of intervening in natural processes on such a scale – and there is – someone other than vested interests should be studying the matter scientifically and thinking seriously about what approval processes would be appropriate.

**Q: Returning to your goal of equipping decision makers to deal with air pollution and climate change, what can you do as scientists? How can you make effective connections between research and policy?**

**Keutsch:** In my view, the foundation of policy really should be on the physical sciences. What we as physical scientists do is provide information that then can be used by economists, and social scientists, and political scientists, to think about decision making. Especially when it comes to climate issues, there's a tendency to ask physical scientists about what decisions ought to be made, and I'm always apprehensive about that. Because I don't have any training in that, I have no mandate, and the actual decisions have to involve not only economics but also public perception and what the public wants. One of the key things is to have effective interaction and intermediaries between the physical science world and the world of economics, social science, and political science. That is one of the challenges, where you need to have very specialized people who in a sense

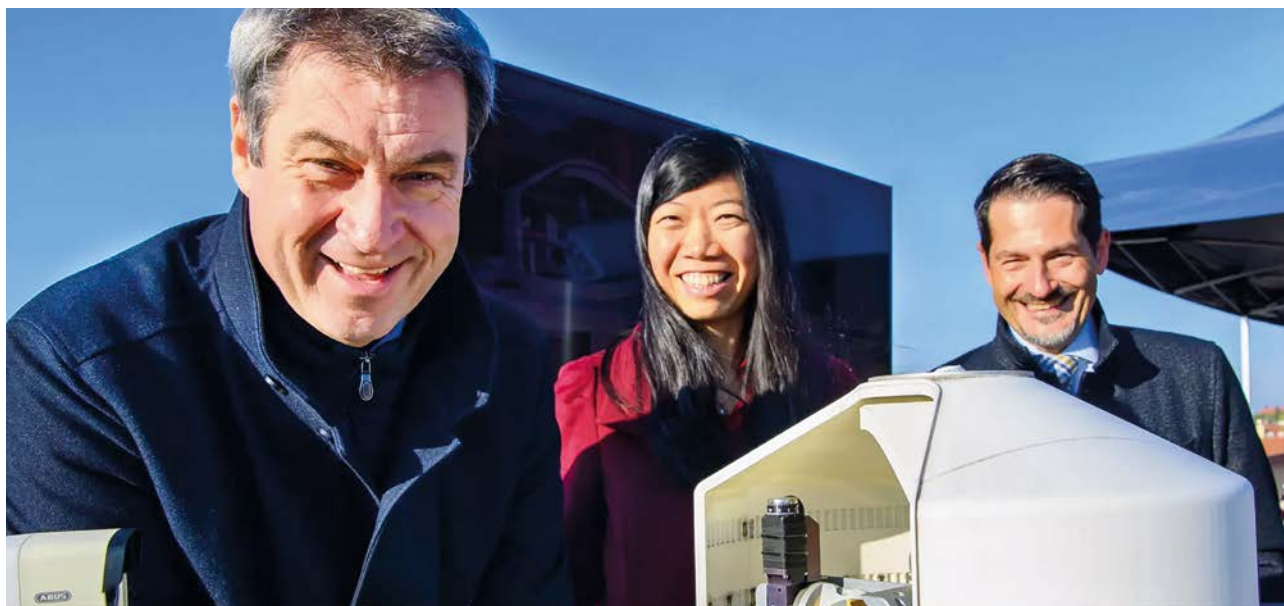
***“What we can do is provide scientific evidence and facts to the politicians, and we hope that they can make wise decisions based on our findings to improve climate and reduce air pollution.”***

JIA CHEN

understand both worlds, if you want to do it effectively.

**Chen:** What we can do is provide scientific evidence and facts to the politicians, and we hope that they can make wise decisions based on our findings to improve climate and reduce air pollution. I'm not developing policies or making decisions. But I hope that these kinds of scientific findings, such as the example of the Covid lockdown investigation, could bring more clarity to the politicians. We show measured emissions and concentrations to the politicians so they can, for example, have a better overview picture. This includes providing information on previously unknown emission sources. When decisions are to be made about where to make reductions, this may help them define a priority source to reduce first.

Over the last eight years, I've tried to make connections with people in the city of Munich. And now I have good connections at the city level in a number of different departments. I would say that's a success. I also got the city to support participation in the ICOS Cities project. This is very good, that they see the necessity of measuring greenhouse gases



Bavaria's Minister-President Dr. Markus Söder (left) learns about TUM's sensor network for measuring urban greenhouse gas emissions. Climate researcher Prof. Jia Chen and TUM President Prof. Thomas F. Hofmann explain the system to him.

and not just calculating them, and that they support this project in particular. Within the project they are also providing us with a lot of information that will help us accomplish the science.

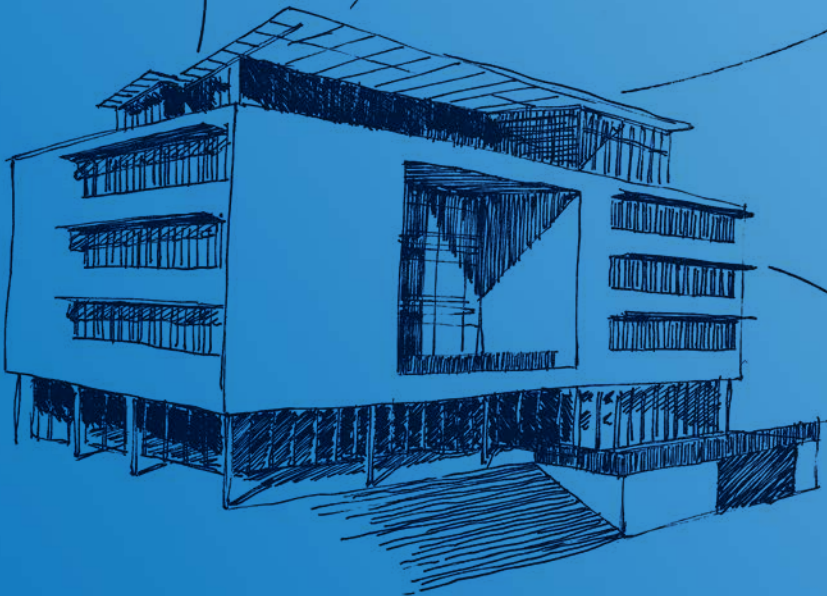
We organize workshops, inviting city officials and other stakeholders to attend. Here I'm working with TUM Professor Miranda Schreurs, the chair of Climate and Environmental Policy at the Bavarian School of Public Policy. [See "Pollutants and Sustainability Governance" in the TUM-IAS Annual Report for 2020.]

TUM President Thomas Hofmann and I hosted a rooftop visit to MUCCnet by Bavarian Minister President Söder, who was very interested in our work. He commented on our sensor systems as "Small box, big impact" (German: kleine Kiste, große Wirkung).

I'd say all of this shows we're making headway, and while our main focus is on the research itself, we will keep pushing to make sure the results are available to people who can make a difference in addressing air pollution and climate change. ■

Advanced Computation and Modeling

Gender and Diversity  
in Science and Engineering



Fundamental Natural  
and Life Sciences

Communication and Information



# Scientific Reports

When their research projects come to an end, we ask our Fellows to provide a final Scientific Report presenting their achievements. At the same time, true to our philosophy “once a Fellow, always a Fellow,” we are happy to welcome them as Alumni Fellows.

## Focus Group: Data-Driven Dynamical Systems Analysis in Fluid Mechanics

Prof. Mirko R. Bothien (Ansaldo Energia Switzerland, now Zurich University of Applied Sciences and NTNU Trondheim), Alumnus Rudolf Diesel Industry Fellow | Host: Prof. Thomas Sattelmayer (TUM)



Prof. Mirko  
R. Bothien

# Decarbonizing power generation with hydrogen gas turbines

**To fulfill the goals of the Paris Agreement, the share of power generation from renewable sources will increase rapidly, resulting in fluctuations in electric power output. A reliable way to compensate for this volatility is the use of gas turbines operated on CO<sub>2</sub>-free fuels. The work of the Focus Group tackles one of the major challenges in the development of clean combustion technologies: combustion stability.**

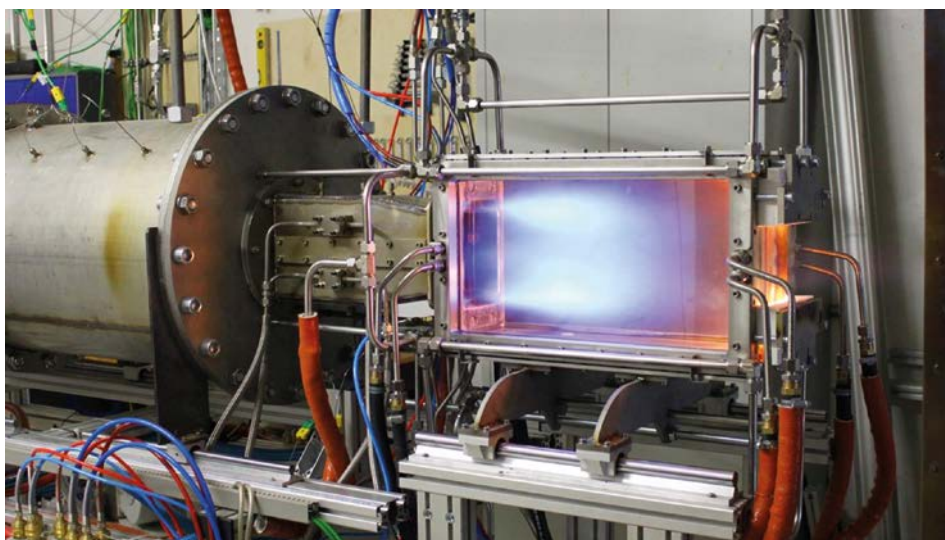
### Introduction

By 2050, net CO<sub>2</sub> emissions must be reduced to zero to fulfill the goals of the Paris Agreement. To achieve this, the share of power generation from non-dispatchable renewable energy sources (RES), i.e., wind and solar, will increase rapidly. As a result, fluctuations in electric power output from these RES will increase in amplitude and impact, requiring robust and rapid grid-stabilization measures. A reliable way to compensate for this (seasonal) volatility is the use of gas turbines operated on alternative, CO<sub>2</sub>-free fuels that can stabilize the grid and provide dispatchable power. Alternative fuels such as hydrogen and ammonia are optimally suited for seasonal, large-scale chemical storage in periods of overproduction from non-dispatchable RES and can be burned in gas turbines at times when RES do not satisfy the need.

Most gas turbine manufacturers are using axially staged or sequential combustion sys-

tems in their newest engines. Consisting of two combustion chambers arranged in series, this concept is the method of choice for alternative fuels because of its superior fuel flexibility obtained by different flame stabilization mechanisms. This is especially important for the transition phase from 2030 onward, in which the supply of alternative fuels will be unsteady, and the engines will need to handle and seamlessly switch between a broad variety of different fuel compositions.

Besides fulfilling stringent emission regulations, one of the major challenges in the development of any clean combustion technology is to ensure dynamic stability, also referred to as thermoacoustic stability. A system can get thermoacoustically unstable due to a constructive coupling of fluctuating heat release with the system's acoustics, severely limiting engine operation. Up to now, the thermoacoustics of the second stage



**Fig. 1,** Atmospheric reheat combustion rig for experimental investigations.

combustor have been studied much less than those of the first stage. Flame stabilization in the second stage is achieved by autoignition. Hence, the involved physics and methods substantially differ from the well-studied propagation-stabilized first stage flames. The work in the Focus Group targets better understanding and modeling of the thermoacoustics of autoignition flames, making it possible to identify and solve instability issues in an early design stage.

### Project results

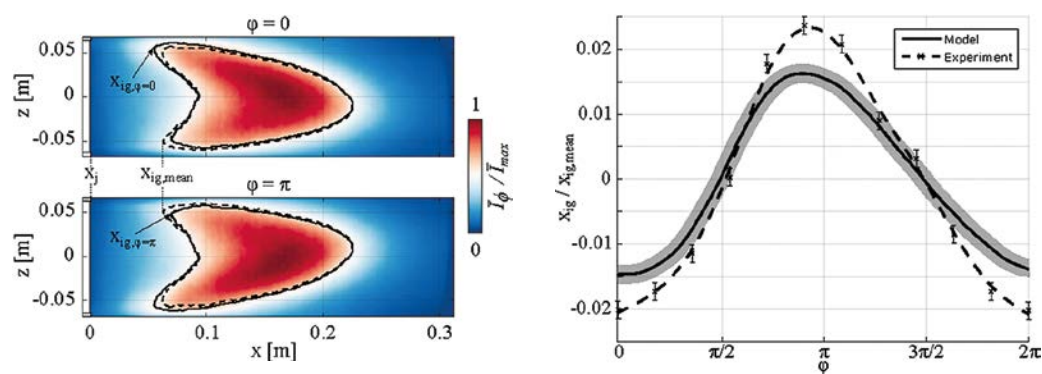
Funding for two doctoral candidates was successfully secured from the German Science Foundation (High-Frequency Flame-Acoustic Interaction Mechanisms in Reheat Flames, Jonathan McClure) and the Research Council of Norway (Dynamic Behaviour of Hydrogen Flames in Sequential Combustion Systems, Florian Franke), making it possible to perform the research. In the following, re-

sults of the former project from Jonathan McClure are presented.

To investigate the flame-acoustic coupling mechanisms driving thermoacoustic instabilities in reheat flames, the following research topics were investigated to support predictive models:

- 1) Development of an autoignition modulation model
- 2) Comparison of model results with experimental observations
- 3) Influence of additional superposed driving mechanisms
- 4) Impact of real engine conditions.

A thermoacoustic driving mechanism based on the local modulation of the autoignition delay time by acoustic perturbations ►



**Fig. 2.** Left: Phase-locked ensemble-averaged chemiluminescence images of the reheat flame at opposing peaks of the acoustic oscillation. The dashed contour illustrates the mean flame boundary, while the solid contour shows the perturbed boundary for each image. Right: Comparison of ignition length variation over a full oscillation cycle between the flame response model and experimental measurements.

was proposed and modeled numerically. Model results indicate that this mechanism represents significant driving potential when regions of high acoustic pressure amplitudes overlap with the autoignition flame. Comparison with experimental measurements confirms this as a key driver of thermo-acoustic instabilities in reheat flames.

Experiments were carried out on the unique, industrial-size reheat test rig at the Technical University of Munich (Fig. 1) over a range of conditions, using synchronous acoustic and optical diagnostics to characterize the reheat flame response.

Investigation of the acoustic data from a range of experiments revealed two distinct unstable high-frequency modes. One mode experienced high-amplitude limit-cycle oscillations and was highly sensitive to fuel reactivity and power level. This

indicates that the driving of the limit-cycle oscillations is strongly linked with autoignition. Investigation of the flame dynamics associated with the limit-cycle oscillations showed an axial motion of the flame in the areas near the walls where the acoustic oscillations are strongest. This motion occurred in-phase with the acoustic oscillations and is illustrated in Fig. 2 (left).

By scaling a numerical estimation of the acoustic field with experimentally measured pressure amplitudes, it is possible to determine the pressure oscillations experienced by the fuel-air mixture as it is advected through the test rig. This is then used as an input for the reduced order model developed in the project to directly compare the predicted flame motion. The comparison can be seen in Fig. 2 (right) indicating that the in-phase motion predicted by the model is indeed present in experiments. Furthermore, the predicted

magnitude of the ignition delay variation is approximately 70% of that observed in experiments, suggesting that the autoignition modulation mechanism is the dominant mechanism behind the observed flame dynamics.

The project results provide important insight into the physics of autoignition flame dynamics relevant for industrial-size combustors. The findings will help in modeling and mitigating thermoacoustic instabilities in the early design stage of new combustors for alternative fuels and are a starting point to include the important effect of mean pressure level.

#### **Fostering the exchange between academia and industry**

The Focus Group organized the Symposium on Thermoacoustics in Combustion – Industry meets Academia (SoTiC) in 2021. A total of

170 participants attended the online symposium, with 64 papers presented, making SoTiC 2021 one of the largest – if not, the largest – event with respect to combustion dynamics so far. The symposium attracted interest from the technical and scientific community working in the field of combustion instabilities. Attendees enjoyed a week of interesting presentations on current research in the field of combustion instabilities in gas turbines and rocket engines. The format is now well established. In 2023, Mirko Bothien and Thomas Sattelmayer co-organized SoTiC at ETH Zurich in Switzerland. More than 120 thermoacousticians from 15 countries attended outstanding invited talks and 60 high-quality technical presentations followed by lively discussions. SoTiC 2025 will take place at NTNU Trondheim, Norway, where Mirko Bothien holds an Associate Professorship. ■

#### **Selected publications**

McClure, J., Bothien, M. R. & Sattelmayer, T. High-Frequency Mode Shape Dependent Flame-Acoustic Interactions in Reheat Flames. *Journal of Engineering for Gas Turbines and Power* 145(1), p. 011014 (2022).

McClure, J., Bothien, M. R. & Sattelmayer, T. Autoignition Delay Modulation by High-Frequency Thermoacoustic Oscillations in Reheat Flames. *Proceedings of the Combustion Institute* 39(4), pp. 4691–4700 (2022).

Gruber, A., Bothien, M. R., Ciani, A., Aditya, K., Chen, J. & Williams, F. Direct Numerical Simulation of hydrogen combustion at auto-ignitive conditions: ignition, stability and turbulent reaction-front velocity.

*Combustion and Flame* 229, p. 111385 (2021).

Gant, F., Bunkute, B. & Bothien, M. R. Reheat flames response to entropy waves. *Proceedings of the Combustion Institute* 38(4), pp. 6271–6278 (2021).

Bothien, M. R., Ciani, A., Wood, J. P. & Fruechtel, G. Toward Decarbonized Power Generation With Gas Turbines by Using Sequential Combustion for Burning Hydrogen. *Journal of Engineering for Gas Turbines and Power* 141(12), p. 121013 (2019).

**For a full list of publications, please visit**  
[www.ias.tum.de/ias/bothien-mirko-ruben-1/](http://www.ias.tum.de/ias/bothien-mirko-ruben-1/)



## Focus Group: Built Environment Digital Twinning

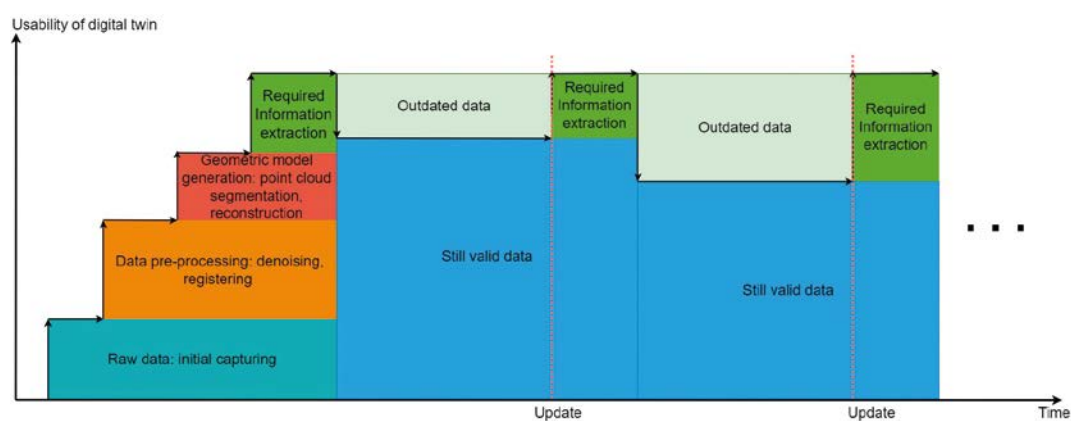
Prof. Ioannis Brilakis (University of Cambridge), Alumnus Hans Fischer Senior Fellow  
| Dr. Yuandong Pan (TUM, now University of Cambridge), Alumnus Doctoral Candidate | Host: Prof. André Borrmann (TUM)



Prof. Ioannis  
Brilakis

# Automatically creating digital twins of built environments

Digital twins have been starting to penetrate built environments because they can provide substantial benefits to all stakeholders. The process of creating such a digital twin is extremely time-consuming and requires very high human effort. This project aims to reduce the human effort in this process by proposing methods that apply advanced deep learning technologies to automate the process.



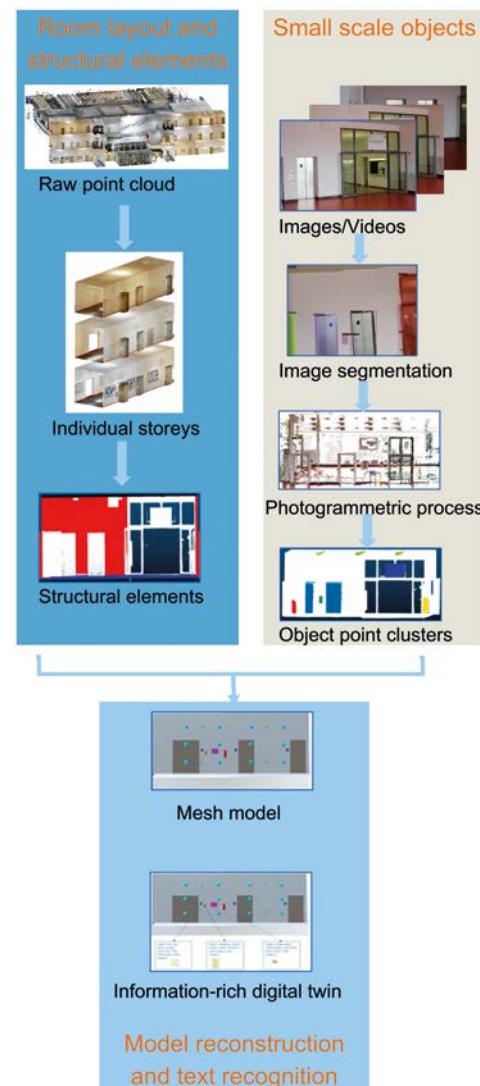
**Fig. 1,** Concept of usability changing for digital twin of facility management over time.

The adoption of digital twins (DTs) in the built environment sector is gradually increasing, as DTs can offer substantial value to all of the associated stakeholders. DTs can be used to construct, manage, maintain, and monitor physical facilities. There are mainly two reasons for this situation. The first reason is that many facilities have no pre-existing digital models from when they were constructed. Secondly, even if digital models exist, they are not updated throughout the assets' life cycle. Hence, digital models are missing all asset modifications. This substantially reduces the reliability and usability of the data.

Data are continuously accumulated throughout the life cycle of the asset in the update process. However, it needs to be noted that more data cannot always guarantee a better representation of the facility. If we use the term "usability" to describe how accurate and useful the data in a digital twin will be, it needs to be noticed that although the data are continuously added to the digital twin throughout the life cycle of a facility, the usability of the digital twin would start to drop while the data are starting to be outdated. Subsequently, usability starts to be restored when the digital twin receives newly updated data. This concept is illustrated in Fig. 1.

Existing capturing technologies such as laser scanning or photogrammetry allow the automation of data acquisition for geometric models. However, the generation of semantically rich DTs is a complex process that is extremely labor-intensive. This project aims to reduce the human effort in this process by proposing methods that apply state-of-the-art deep learning technologies to automate the process.

The overall proposed approach, as illustrated in Fig. 2, uses laser-scanned point clouds and images as input. First, it starts with segmenting a point cloud of a multi-story build-



**Fig. 2,** Proposed approach to create a digital twin from point clouds and images.

ing into individual stories. Subsequently, two different approaches are proposed for buildings depending on whether they do or do not fulfill the Manhattan-world assumption. Both approaches use the semantic information extracted by point cloud deep learning. The void-growing method, designed ▶

for Manhattan-world buildings, starts with extracting the void spaces inside rooms. Space-bounding elements are then extracted on the basis of the extracted void spaces. For buildings that do not fulfill the Manhattan-world assumption, planes in point clouds are extracted, intersected, and selected by a method based on energy optimization.

The next step is reconstructing small objects, where images are used to improve the results; this approach is based on the finding that recognition of small objects in images outperforms that in point clouds. The photos taken by the camera can be registered with laser-scanned point clouds by the photogrammetric process, which means the photogrammetric point cloud works as a bridge to fuse data from different sources. Subsequently, state-of-the-art artificial neural networks of image segmentation are implemented. Then, the recognized semantic information in the images is mapped to the laser-scanned point clouds by the camera matrices from the photogrammetric process. Predefined geometric primitives are then fitted to the point clusters with semantic information and added to the digital twin as simplified geometric information. In model enrichment, state-of-the-art deep learning models for text detection and recognition are applied to the images. Text information, such as serial numbers of objects and room numbers, is extracted from images and then mapped to the reconstructed objects in 3-D space.

The proposed approach in this project uses point cloud data and images as input to create an information-rich digital twin of indoor environments. The final output of the approach contains geometric and semantic

information for space-bounding elements and small elements. The created digital twin can be used with regard to different aspects throughout various assets' life cycles. For historical assets that have been completed for many years but do not yet have any digital records, the created digital twin can help to start and keep a recording of their current conditions for making better decisions, especially in facility maintenance and renovation. For those assets with available digital representations, the proposed approach provides the possibility to enrich the current digital model with more useful information as well. Keeping the digital twin dynamic and up-to-date can improve the asset's real-time progress monitoring, quality control, diagnostics, and prognostics for facilities. Furthermore, the created final output can also be used in capital investment projects before the design and construction of the facility. It is efficient and convenient to simulate the performance with its digital twin to assist decision- and strategy-making in various predictive scenarios.

In practice, the proposed approach can heavily reduce the human effort in the process of reconstructing indoor environments from point clouds and photos. The human modelers do not need to measure the locations and dimensions of elements in the environments. Instead, they could just check the automatically created models and fix the corresponding parts if errors or inconsistencies are found. The cost to create a digital twin for indoor environments could be heavily reduced, which also provides the possibility to digitize more facilities. These digital twins can be used in various use cases and bring benefits to all stakeholders of the facility.

For the whole society, when more and more digital twins of various facilities are available, the current geometric conditions of these assets can be visually monitored. Furthermore, by putting different kinds of sensors into the physical assets and updating the corresponding data in digital twins, the data between digital and physical twins can be linked effectively. This could be a starting point to make smart buildings or smart cities. Decision-makers can effectively collect information for buildings and cities in the digital twin.

In the future, research could be conducted to address aspects such as the following: First, more component categories could be considered, such as staircases, handrails, furniture, and so on. The digital twin can be further enriched by including more object classes. Second, components with more complicated structures can be considered. Finally, data from other sensors can also be included, such as thermal sensors, which can enrich the information in digital twins. The multimodal data in digital twins can provide more potential use cases. ■

#### Selected publications

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Pan, Y., Braun, A., Brilakis, I. & Borrmann, A. Enriching geometric digital twins of buildings with small objects by fusing laser scanning and AI-based image recognition. *Automation in Construction* 140, 104375 (2022).

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Pan, Y., Noichl, F., Braun, A., Borrmann, A. & Brilakis, I. Automatic creation and enrichment of 3-D models for pipe systems by co-registration of laser-scanned point clouds and photos. *Proceedings of the 2022 European Conference on Computing in Construction* (2022).

**For a full list of publications, please visit**  
[www.ias.tum.de/ias/brilakis-ioannis/](http://www.ias.tum.de/ias/brilakis-ioannis/)

## Focus Group: Data-Informed Decisions for Structures and Infrastructures

Prof. Eleni Chatzi (ETH Zurich), Alumna Hans Fischer Fellow (funded by the TÜV SÜD Foundation) | Antonios Kamariotis (TUM), Doctoral Candidate | Host: Prof. Daniel Straub (TUM)



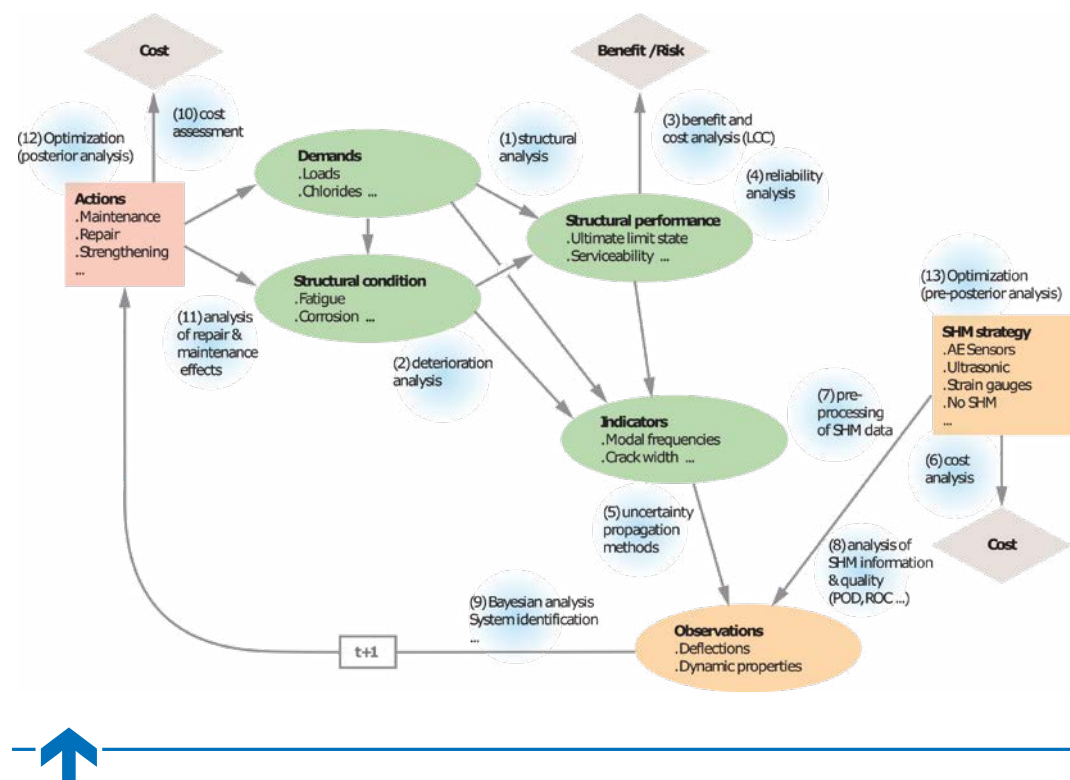
Prof. Eleni  
Chatzi

# The value of monitoring for infrastructure management



Prof. Daniel  
Straub

Structural health monitoring (SHM) systems are potent tools for decision support. Our Focus Group's research centered on quantifying the value generated through the systematic integration of SHM in the operation and maintenance decision-making process for engineering structures and infrastructure systems.



**Fig. 1.** Influence diagram of the SHM process for a Bayesian decision analysis to quantify the Vol. (Kamariotis, A., Chatzi, E. & Straub, D. Value of information from vibration-based structural health monitoring extracted via Bayesian model updating. *Mechanical Systems and Signal Processing* 166, 108465 (2022))



This report summarizes our Focus Group's investigations into the application of structural health monitoring (SHM) systems for enhancing decision-making for engineering structures and infrastructure systems. Our research centered on evaluating and quantifying the impact of SHM on the operation and maintenance decision-making processes, highlighting its pivotal role in improving the management of engineering structures and infrastructure systems through data-informed decision-making.

In our first publication [1], we explored the concept of value of information (VoI) in structural health monitoring (SHM). Our focus was on understanding how long-term vibration-based SHM systems can assist in decision-making, particularly in maintenance planning. We introduced – for the first time in literature – a comprehensive framework that captures the entire process of SHM, from data collection to decision-making (see Fig. 1). This framework was applied to a bridge system example, demonstrating how to assess the optimality of SHM in different decision contexts.

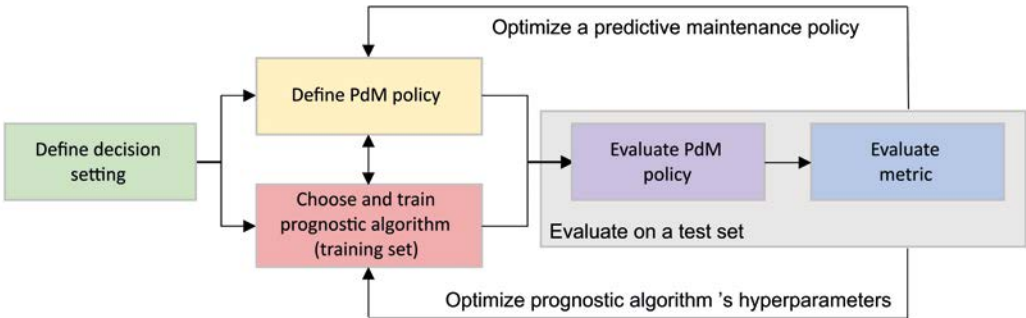
Our second publication [2] presented a framework for quantifying the expected gains that continuous SHM-aided maintenance planning can provide when compared against the currently dominant approach of intermittent inspection-based maintenance planning. A novel metric, the value of SHM (VoSHM) metric, was introduced for formally computing these expected gains. The presented framework can be used as an actionable decision support tool for guiding decisions on whether or not to install an SHM system on a structure, for a wide range of SHM use cases. Using a bridge model, we explored several actionable SHM use cases, demonstrating the substantial economic advantages of SHM in certain decision-making contexts.

Stochastic models describing time-evolving deterioration processes are instrumental for facilitating a predictive maintenance planning paradigm. In the modern data-centric landscape, Bayesian methods can exploit monitoring data to sequentially update knowledge on underlying model parameters. The precise probabilistic characterization of these parameters is indispensable for several real-world tasks, where decisions need to be taken in view of the evaluated margins of risk and uncertainty. Our third publication [3] investigated and compared on-line and off-line Bayesian filters and adapted the former for posterior uncertainty quantification of time-invariant parameters of deterioration models. We showed that tailored on-line particle filters are competitive alternatives to computationally prohibitive off-line Bayesian filters.

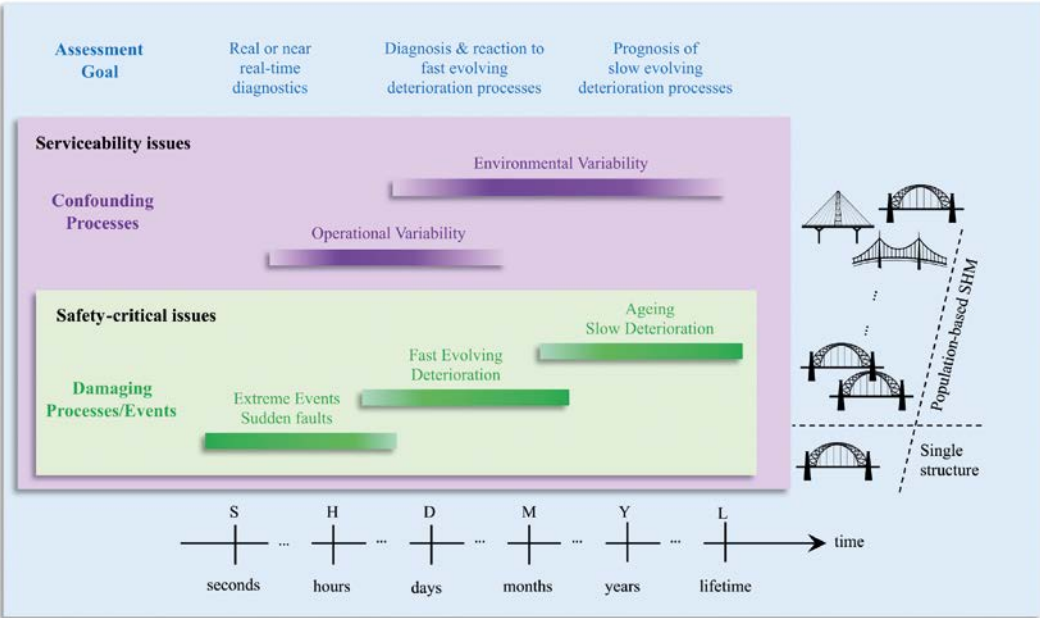
In our fourth publication [4], we focused on purely data-driven prognostic algorithms based on monitoring. Specifically, we proposed a novel metric for assessing and optimizing such algorithms in the context of predictive maintenance (PdM). This metric, distinct in its approach, uses the algorithms' output – predictions of the system's remaining useful life (RUL) – as inputs to PdM decision-making policies that eventually inform decisions. The application of the proposed framework for evaluating this metric, shown in Fig. 2, was demonstrated using theoretical and real-world case studies, including one involving degrading turbofan engines.

In addition to the above publication output, our Focus Group engaged with global leaders in related research areas, organizing a workshop and an online speaker series. The virtual workshop in October 2020, titled *Frontiers in Monitoring-Supported Decision Making for Structures and Infrastructures*, included presentations from ten research leaders. ►

- [1] Kamariotis, A., Chatzi, E. & Straub, D. (2022).
- [2] Kamariotis, A., Chatzi, E. & Straub, D. (2023).
- [3] Kamariotis, A., Sardi, L., Papaioannou, I., Chatzi, E. & Straub, D. (2023).
- [4] Kamariotis, A., Tatsis, K., Chatzi, E., Goebel, K. & Straub, D. (2024).



**Fig. 2,** Summary of the proposed framework for a decision-oriented, uncertainty-aware performance assessment and optimization of data-driven prognostic algorithms. (Kamariotis, A., Tatsis, K., Chatzi, E., Goebel, K. & Straub, D. A metric for assessing and optimizing data-driven prognostic algorithms for predictive maintenance. *Reliability Engineering & System Safety* 242, 109723 (2024))



**Fig. 3,** SHM use cases across dimensions that influence decision-making for monitored structures. (Kamariotis, A., Chatzi, E., Straub, D., Dervilis, N., Goebel, K., Hughes, A.J., Lombaert, G., Papadimitriou, C., Papakonstantinou, K.G., Pozzi, M., Todd, M. & Worden, K. Monitoring-Supported Value Generation for Managing Structures and Infrastructure Systems. Submitted to: *Data-Centric Engineering* (2024))

Its primary aim was to foster extensive discussions and idea exchange. Following this, in May and June 2021, we held a speaker series featuring 12 experts, which attracted a wide audience, including TUM's Master's students. This collaborative knowledge exchange led to drafting a position paper on Monitoring-Supported Value Generation for Managing Structures and Infrastructure Systems [5] (see Fig. 3), submitted in January 2024.

Overall, this project contributed to the deepening of our understanding on the means and ways by which SHM impacts the decision-making process. We believe that interdisciplinary, collaborative efforts, similar to the one conducted in our Focus Group, are key to reaching a reliable synergy between SHM and decision-making. ■

[5] Kamariotis, A. *et al.* (submitted 2024).

#### Selected publications

Kamariotis, A., Chatzi, E. & Straub, D. Value of information from vibration-based structural health monitoring extracted via Bayesian model updating. *Mechanical Systems and Signal Processing* 166, 108465 (2022). [www.doi.org/10.1016/j.ymssp.2021.108465](https://doi.org/10.1016/j.ymssp.2021.108465).

Kamariotis, A., Chatzi, E. & Straub, D. A framework for quantifying the value of vibration-based structural health monitoring. *Mechanical Systems and Signal Processing* 184, 109708 (2023). [www.doi.org/10.1016/j.ymssp.2022.109708](https://doi.org/10.1016/j.ymssp.2022.109708).

Kamariotis, A., Sardi, L., Papaioannou, I., Chatzi, E. & Straub, D. On off-line and on-line Bayesian filtering for uncertainty quantification of structural deterioration. *Data-Centric Engineering* 4, e17 (2023). [www.doi.org/10.1017/dce.2023.13](https://doi.org/10.1017/dce.2023.13).

Kamariotis, A., Tatsis, K., Chatzi, E., Goebel, K. & Straub, D. A metric for assessing and optimizing data-driven prognostic algorithms for predictive maintenance. *Reliability Engineering & System Safety* 242, 109723 (2024). [www.doi.org/10.1016/j.ress.2023.109723](https://doi.org/10.1016/j.ress.2023.109723).

Kamariotis, A., Chatzi, E., Straub, D., Dervilis, N., Goebel, K., Hughes, A.J., Lombaert, G., Papadimitriou, C., Papakonstantinou, K.G., Pozzi, M., Todd, M. & Worden, K. Monitoring-Supported Value Generation for Managing Structures and Infrastructure Systems. Submitted to: *Data-Centric Engineering* (2024).

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## Focus Group: Theory of Functional Energy Materials

**Prof. David Egger (TUM)**, Alumnus Rudolf Mößbauer Tenure Track Assistant Professor | **Dr. Sebastián Caicedo-Dávila (TUM)**, Postdoctoral Researcher | **Christian Gehrmann, Maximilian Schilcher, Xiangzhou Zhu (TUM)**, Doctoral Candidates



**Prof. David  
Egger**

# The jiggling and wiggling of atoms in energy materials

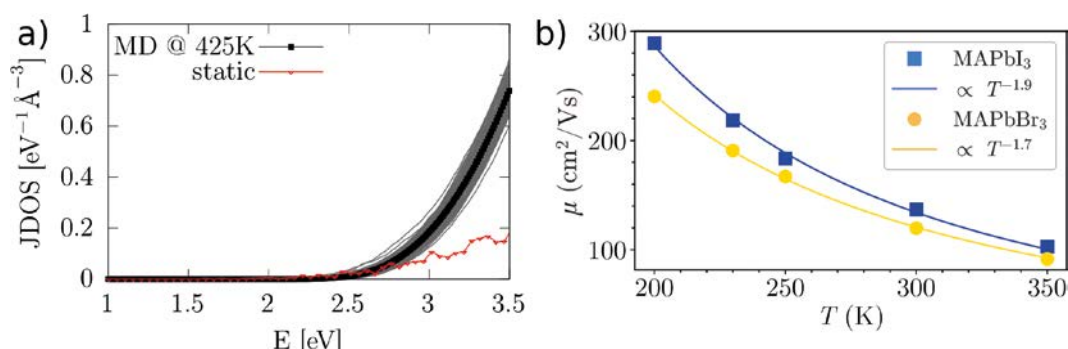
**Energy materials are the key ingredients to convert the sun's energy into electrical energy and store it in batteries. Yet predicting the properties of these materials under technologically relevant conditions has been a major challenge for researchers. The team led by David Egger develops new theoretical methods in order to discover energy materials and improve devices made from them.**

It is exciting to explore the “wiggling and jiggling of atoms,” as famously coined by Richard Feynman, in the molecules and materials all around us, because virtually every physical and chemical process depends on how atoms are moving about. In energy materials, which are important components in devices for energy conversion or storage such as solar cells or batteries, atomic motions at higher temperatures are important to understand when we want to make these technologies more efficient or less expensive. This is because novel types of energy materials, such as halide perovskites (HaPs), exhibit intriguing atomic motions that deviate from the canonical, wavelike oscillations found in materials such as diamond or silicon. Instead, the atomic behavior is more anharmonic and perturbs the crystal in ways that are not fully understood today. The goal of this Focus Group, which was established in 2019, is to develop and apply theoretical models in order to characterize these motions and their consequences for energy materials on the atomic scale.

### Research focus and progress

Since its establishment, the Focus Group has assembled a team of approximately 15 members from nine different countries. Their research work has been published in close to 30 articles. In the following, examples from two research areas, namely on HaPs and solid-state ionic conductors (SSICs), will be summarized to showcase how the atomic wiggling and jiggling impact important properties of energy materials.

HaPs are promising materials for photovoltaics: Solar cells made from them have already surpassed the 25% power-conversion efficiency threshold, which is the single most important quantity for technological exploitation of photovoltaics. What is more, combination of HaPs with silicon in so-called tandem devices is getting close to reaching 35% efficiency. In our group, we study the fundamental properties of these materials using quantum-mechanical calculations.



**Fig. 1,** (a) Joint density of states (JDOS) of the HaP CsPbBr<sub>3</sub>, calculated for a static cubic structure (red) and for a structure where atoms move according to molecular dynamics (MD) simulations at 425 K (black). Thin-black lines show the JDOS of individual MD snapshots and the thick-dotted line their average. (*Adv. Sci.* 9, 2200706, (2022))  
(b) Temperature-dependent charge transport in MAPbI<sub>3</sub> and MAPbBr<sub>3</sub>: carrier mobilities computed in a multi-scale tight-binding model and quantum dynamics. The lines represent fits to the power-law behavior of the temperature-dependent data. (*Phys. Rev. Materials* 7, L081601 (2023))

Fig. 1a shows how atomic motions influence key characteristics of HaPs: the joint density of states, which determines how efficiently the material can absorb sunlight, is found to rise significantly more steeply when the atoms move instead of standing still. In Fig. 1b, temperature-dependent carrier mobilities are reported. These are key quantities because they tell how easy it is to transport charge throughout the crystal. Developing a new multi-scale model, we found that anharmonic atomic motions are correlated with carrier transport in HaPs. Switching the composition from MAPbI<sub>3</sub> to MAPbBr<sub>3</sub> we were able to tune carrier-transport characteristics through these phenomena. This exemplifies how a better understanding of dynamic effects can lead to new ways of controlling important macroscopic properties of materials.

In regard to atomic motions, SSICs share several characteristics with HaPs and other related energy materials. A key difference, however, is that long-range ion migration oc-

curs as the defining feature of SSICs through, e.g., a diffusion mechanism. When SSICs are exploited technologically in new types of batteries, it is crucial to improve the conductivity of mobile ionic species while balancing other material parameters such as the energy density or cost. Our group is interested in revealing how the complex dynamic atomic properties in these materials impact their ionic conductivity.

We investigated the perhaps best known SSIC, namely AgI in its superionic  $\alpha$ -phase (see Fig. 2a). In this phase, the material shows a high ionic conductivity and the Ag<sup>+</sup> ion dynamically hops among various sites. When this occurs, the mobile ionic species ought to enter a potential-energy region of the material that is significantly anharmonic (see Fig. 2b). Together with our experimental partners (group of Dr. Yaffe at the Weizmann Institute of Science, Israel), we showed that the host lattice surrounding the mobile ions plays an important role in the conduction process. Specifically, the anharmonic vibrational

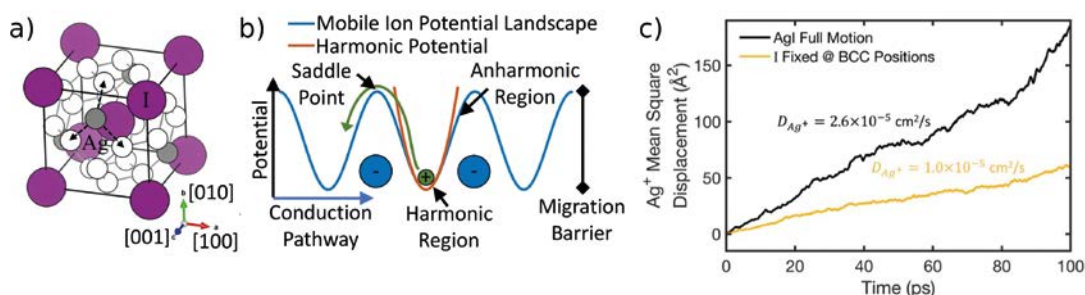


coupling among mobile ions and the ones of the host lattice was found to manifest in an interesting duality of crystalline and liquid behavior in AgI. In our molecular dynamics (MD) calculations, we could show that freezing out the atomic motions of the host lattice significantly reduces the ionic conductivity (see Fig. 2c). More recently, we discovered similar types of phenomena in Na-based SSICs, which are among the most promising materials to augment current battery technologies based on Li and other elements.

These findings highlight again how interplay of dynamic effects on the atomic scale determine macroscopic functionalities of important types of energy materials with relevance for technological applications.

### Outlook

Atomic-scale modeling has reached an exciting level of sophistication and has become an indispensable tool in the discovery and characterization of new materials. We



**Fig. 2.** (a) Schematic representation of AgI crystal. (b) Sketch showing the conventional ion transport mechanism: a mobile ion (grey circle) hops across barriers in the generally anharmonic potential energy surface that is due to the host lattice (blue circles) and surrounding mobile ions. The orange line indicates a harmonic potential. (c) Mean square displacement as a function of time for Ag<sup>+</sup> ions and their calculated diffusion coefficient,  $D_{Ag^+}$ , for different scenarios: all atomic motions allowed (black line) and I ions fixed at BCC lattice positions (yellow). (*Phys. Rev. Materials* 4, 115402 (2020))

witnessed an enormous acceleration in the field prompted by the advent of artificial intelligence, data science, and machine learning. In our most recent work, we exploited the great opportunities offered by these methods to develop a new theoretical methodology. It allows for atomistic material modeling under more realistic conditions, treating to the full extent the atomic motions as well as their consequences for important properties. We anticipate that further advances in these directions will eventually bring

the theoretical and computational research closer to the experimental and technological reality of materials, e.g., in regard to defects and other crystalline irregularities. Bridging computational modeling to the lab and fab will offer new perspectives for revealing fundamental phenomena in materials and exploiting them in technological applications. ■

#### Selected publications

Righetto, M., Caicedo-Davila, S., Sirtl, M. T., Lim, V. J.-Y., Patel, J. B., Egger, D. A., Bein, T. & Herz, L. M. Alloying Effects on Charge-Carrier Transport in Silver-Bismuth Double Perovskites. *J. Phys. Chem. Lett.* 14, 10340 (2023).

Schilcher, M. J., Abramovitch, D. J., Mayers, M. Z., Tan, L. Z., Reichman, D. R. & Egger, D. A. Correlated Anharmonicity and Dynamic Disorder Control Carrier Transport in Halide Perovskites. *Phys. Rev. Mater* 7, L081601 (2023).

Gehrmann, C., Caicedo-Dávila, S., Zhu, X. & Egger, D. A. Transversal Halide Motion Intensifies Band-To-Band Transitions in Halide Perovskites. *Adv. Sci.* 9, 2200706 (2022).

Schilcher, M. J., Robinson, P. J., Abramovitch, D. J., Tan, L. Z., Rappe, A. M., Reichman, D. R. & Egger, D. A. The Significance of Polarons and Dynamic Disorder in Halide Perovskites. *ACS Energy Lett.* 6, 2162 (2021).

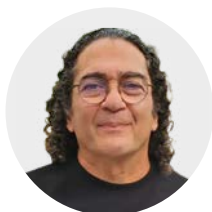
Brenner, T., Gehrmann, C., Korobko, R., Livneh, T., Egger, D. A. & Yaffe, O. Anharmonic host Lattice Dynamics Enable Fast Ion Conduction in Superionic. *Agil. Phys. Rev. Mater* 4, 115402 (2020).

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## Focus Group: Fungal Sensing and Signaling of the Environment

Prof. Gustavo H. Goldman (University of São Paulo), Alumnus Hans Fischer Senior Fellow | Lisa Meyer (TUM), Doctoral Candidate | Host: Prof. J. Philipp Benz (TUM)



Prof. Gustavo H. Goldman



Prof. J. Philipp Benz

# Carbon catabolite repression in filamentous fungi

Filamentous fungi are important for the production of lignocellulolytic enzymes. Carbon catabolite repression (CCR) plays an important role in this process. We studied CCR in two of the most important reference fungi, *Aspergillus nidulans* and *Neurospora crassa*. We investigated the regulation of the transcription factor CreA in CCR and the role played by F-box proteins during the CCR regulation.

**[1]** Brown, N. A., Ries, L. N. A., Goldman, G.H. How nutritional status signalling coordinates metabolism and lignocellulolytic enzyme secretion. *Fungal Genet. Biol.* 72, 48–63 (2014).

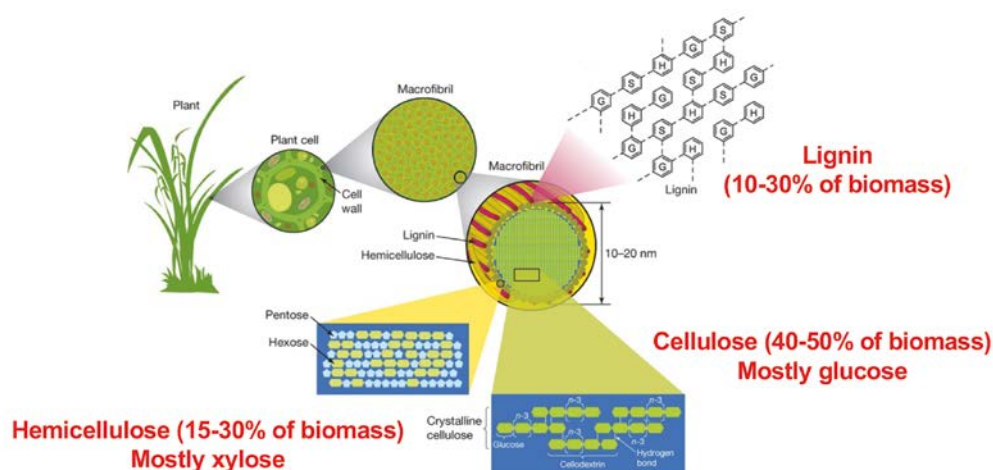
**[2]** de Assis, L. J. et al. (2021).

Filamentous fungi are of particular interest for biotechnological applications due to their natural capacity to secrete carbohydrate-active enzymes (CAZy) that target plant biomass (Fig. 1). The presence of easily metabolizable sugars, such as glucose, whose concentrations increase during plant biomass hydrolysis, results in the repression of CAZy-encoding genes in a process known as carbon catabolite repression (CCR), which is undesired for the purpose of large-scale enzyme production. Glucose is the preferential carbon source for most microorganisms, because it is rapidly metabolized, generating quick energy for growth. In the filamentous fungi *A. nidulans* and *N. crassa*, CCR is mediated by the transcription factor CreA/CRE-1, a C2H2 finger domain DNA-binding protein [1] (Fig. 2). The main aims of our project were: (i) to understand the regulation of the transcription factor CreA/CRE-1 during CCR and (ii) to investigate the role played by F-box proteins during the regulation of CCR. Our project is unique in the field, considering that, in investigating

the regulation of this process, we are looking at both transcriptional and post-translational regulation.

CreA has been described as the major carbon catabolite repressor in *Aspergillus* spp., although little is known about the role of post-translational modifications in this process. We have identified S262, S319, S268, and T308 as phosphorylation sites. Sites S262, S268, and T308 are important for CreA protein accumulation and cellular localization, DNA binding, and repression of enzyme activities [2]. Site S319 was not important for several here-tested phenotypes but is key for CreA degradation and induction of enzyme activities. All sites were shown to be important for glycogen and Wtrehalose metabolism [2].

The utilization of different carbon sources in filamentous fungi underlies a complex regulatory network governed by signaling events of different protein kinase pathways. An initial screening of a library of 103 *A. nidulans*



**Fig. 1,** The main structural components of plant biomass. (Modified from Rubin, E.M. Genomics of cellulosic biofuels. *Nature* 454, 841-845 (2008))

non-essential protein kinase (NPK) deletion strains identified several mitogen-activated protein kinases (MAPKs) to be important for CCR [3]. We selected the MAPKs Ste7, MpkB, and PbsA for further characterization and showed that they are pivotal for HOG pathway activation, protein kinase A activity, and CCR via regulation of CreA cellular localization and protein accumulation, as well as for hydrolytic enzyme secretion. Protein-protein interaction studies show that Ste7, MpkB, and PbsA are part of the same protein complex that regulates CreA cellular localization in the presence of xylan and that this complex dissociates upon the addition of glucose, thus allowing CCR to proceed [3]. Glycogen synthase kinase (GSK) A was also identified as part of this protein complex and shown to potentially phosphorylate two serine residues of the HOG MAPKK PbsA [3].

The attachment of one or more ubiquitin molecules by SCF (Skp-Cullin-F-box) complexes to protein substrates targets them for subsequent degradation by the 26S proteasome,

allowing the control of numerous cellular processes. Glucose-mediated signaling and subsequent CCR are processes relying on the functional regulation of target proteins, ultimately controlling the utilization of this carbon source. There are 74 genes encoding F-box proteins in *A. nidulans* [4]. The Fbx23 protein was identified as being involved in CCR and the  $\Delta fbx23$  mutant presented impaired xylanase production under repressing (glucose) and derepressing (xylan) conditions [5, 2]. Mass spectrometry showed that Fbx23 is part of an SCF ubiquitin ligase complex that is bridged via the GskA protein kinase to the CreA-SsnF-RcoA repressor complex, resulting in the degradation of the latter under derepressing conditions [5, 2]. Upon the addition of glucose, CreA dissociates from the ubiquitin ligase complex and is transported into the nucleus. Furthermore, casein kinase is important for CreA function during glucose signaling, although the exact role of phosphorylation in CCR remains to be determined [5, 2]. ►

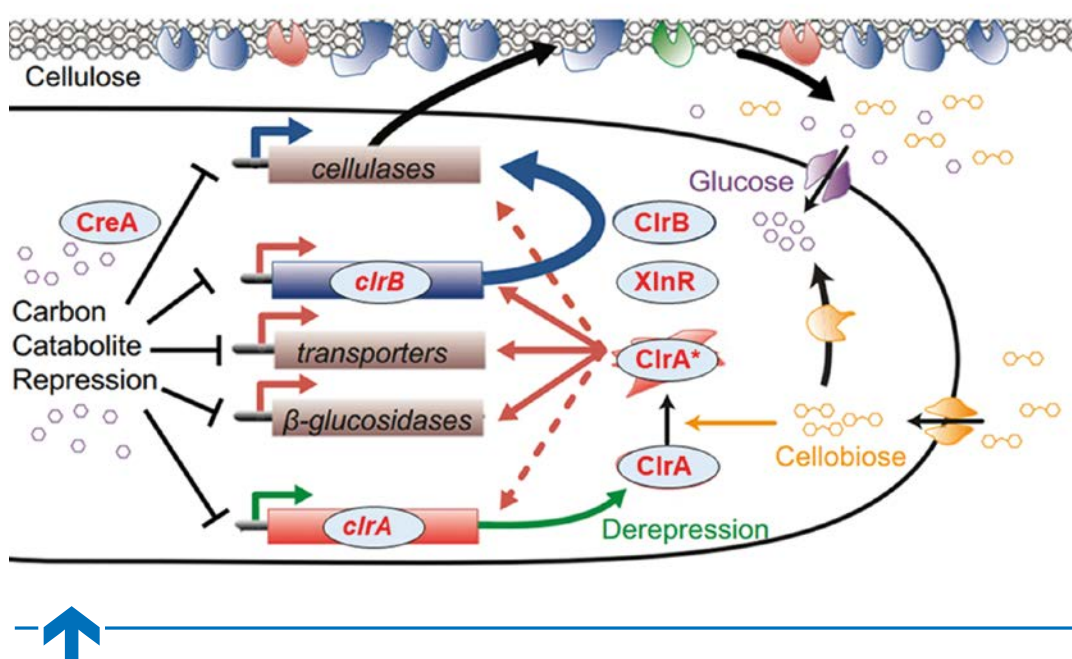
[3] de Assis, L. J. *et al.* (2020).

[4] Sarikaya Bayram, Ö. *et al.* (2022).

[5] de Assis, L. J. *et al.* Regulation of *Aspergillus nidulans* CreA-Mediated Catabolite Repression by the F-Box Proteins Fbx23 and Fbx47. *mBio.* 9, e00840-18 (2018).

The attachment of one or more ubiquitin molecules by SCF (Skp-Cullin-F-box) complexes to protein substrates targets them for subsequent degradation by the 26S proteasome, allowing the control of numerous cellular processes. Glucose-mediated signaling and subsequent CCR are processes relying on the functional regulation of target proteins, ultimately controlling the utilization of this carbon source. There are 74 genes encoding F-box proteins in *A. nidulans* [4]. The Fbx23 protein was identified as being involved in CCR and the  $\Delta fbx23$  mutant presented impaired xylanase production under repressing

(glucose) and derepressing (xylan) conditions [5, 2]. Mass spectrometry showed that Fbx23 is part of an SCF ubiquitin ligase complex that is bridged via the GskA protein kinase to the CreA-SsnF-RcoA repressor complex, resulting in the degradation of the latter under derepressing conditions [5, 2]. Upon the addition of glucose, CreA dissociates from the ubiquitin ligase complex and is transported into the nucleus. Furthermore, casein kinase is important for CreA function during glucose signaling, although the exact role of phosphorylation in CCR remains to be determined [5, 2].



**Fig. 2.** Regulation of the production of cellulases and hemicellulases in filamentous fungi, depicting the strong repressive function of CreA/CRE-1. (Modified from Coradetti, S.T. *et al.* Conserved and essential transcription factors for cellulase gene expression in ascomycete fungi. *PNAS* 109(19), 7397-7402 (2012))

**The main conclusions of our work are:**

(i) Several novel aspects of the post-translational regulation of *A. nidulans* and *N. crassa* CreA/CRE1 and CCR were identified, highlighting for example the importance of CreA phosphorylation for the regulation of CCR.

(ii) Our work provides a model where phosphorylation events and the correct integration of PKA, HOG, and GSK signaling are required for the utilization of different carbon sources.

(iii) Finally, our screen of F-box-encoding genes demonstrates how targeted protein

degradation is necessary for the fungal ability to switch between metabolic conditions.

These CreA/CRE-1 sites are interesting targets for biotechnological strain engineering without the need to delete essential genes, which could result in undesired side effects. These novel functions serve as a basis for additional research in fungal carbon metabolism with the aim of potentially improving fungal industrial applications. Future work will address the possibility of constructing genetically improved strains for increased enzymatic production. ■

**Selected publications**

Horta, M. A. C. *et al.* Broad Substrate-Specific Phosphorylation Events Are Associated With the Initial Stage of Plant Cell Wall Recognition in *Neurospora crassa*. *Front. Microbiol.* 10, 2317 (2019).

de Assis, L. J. *et al.* The High Osmolarity Glycerol Mitogen-Activated Protein Kinase regulates glucose catabolite repression in filamentous fungi. *PLoS Genet.* 16, e1008996 (2020).

Gabriel, R. *et al.* The F-box protein gene exo-1 is a target for reverse engineering enzyme hypersecretion in filamentous fungi. *Proc. Natl. Acad. Sci. USA* 118, e2025689118 (2021).

de Assis, L. J. *et al.* Carbon Catabolite Repression in Filamentous Fungi Is Regulated by Phosphorylation of the Transcription Factor CreA. *mBio.* 12, e03146-20 (2021).

Sarikaya Bayram, O. *et al.* F-box receptor mediated control of substrate stability and subcellular location organizes cellular development of *Aspergillus nidulans*. *PLoS Genet.* 18, e1010502 (2022).

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## Focus Group: Visual Computing

Prof. Leonidas J. Guibas (Stanford University), Alumnus Hans Fischer Senior Fellow |  
Manuel Dahnert (TUM), Doctoral Candidate | Host: Prof. Matthias Nießner (TUM)



Prof. Leonidas  
J. Guibas

# Inferring actionable information from visual data in 3-D environments

**This project aims to improve the perception and semantic understanding of 3-D environments, with the goal of aiding interactions with that environment. We have developed neural techniques that allow us to complete missing geometry, localize cameras, capture objects with high-quality textures, predict object affordances, and understand natural language references to objects in the scene.**

### Focus Group goal and effort rationale

For both humans and autonomous robotic agents, the action of perceiving an environment and its objects typically aims at planning and execution of future actions. Traditional computer vision, however, has focused either on object recognition, where the goal is to detect and assign semantic classes to objects, or on reconstruction, where the aim is to build full 3-D models of objects. Our goal in this project has been to develop the algorithms and datasets that support object-centric actionable information extraction from visual data – that is, low-dimensional information sufficient for planning and executing actions to bring the environment into a desired state.

Our efforts have aimed to generate scene understanding that informs robotic agents operating in indoor environments as well as helping humans who, due to age, disability,

or lack of skill, may need assistance in performing various tasks. This has motivated the study of natural language object references and understanding in a scene context, so as to facilitate communication between the human and an assistive agent.

The Fellowship period (2018–2022) coincided with the Covid-19 pandemic, which severely restricted international travel. Despite the reduced number of physical visits and stays, the Stanford and TUM groups maintained an active collaboration that resulted in significant progress in 3-D computer vision.

### Stanford and TUM-IAS collaborative research highlights

Inspired by the above goals, our Stanford/TUM-IAS collaborative activities have focused on the following areas:

### Embedding spaces for 3-D geometry

Models of 3-D shapes can come either from *ab initio* design or from scanning real objects. These two modalities often contain complementary information toward understanding environments. However, establishing a mapping is a challenging task due to strong, low-level differences. We learn a novel joint embedding space [1] using 3-D deep learning, where semantically similar objects from both domains lie close together, which can be exploited in retrieving designed models similar to scanned real-world objects, enabling scan denoising and completion.

### Texture acquisition and generation

The creation or capture of 3-D models requires good texture modeling. Our TextureNet work [2] establishes consistent local parametrizations on meshes, making it easier to learn high-resolution signals such as textures. We also address issues in learning textures coming from misaligned images by proposing a novel adversarial loss based on a patch-based conditional discriminator that guides the texture optimization to be tolerant to such misalignments.

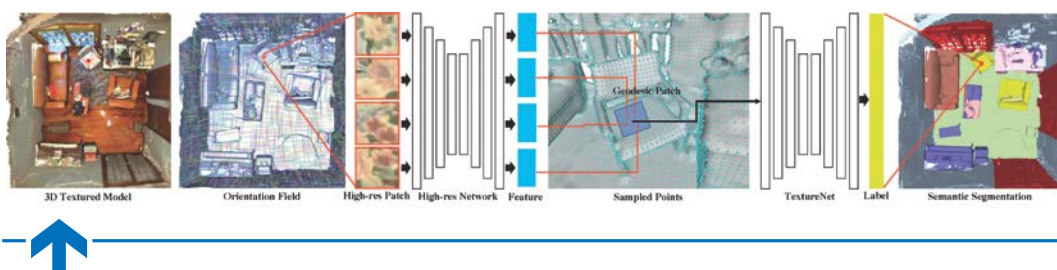
### Camera localization and pose estimation

Acting on the objects in an environment requires accurate estimation of both agent and object pose. We introduced a novel passive-active camera localization strategy where the agent actively moves to better localize the camera [4]. We also developed a unified framework (CAPTRA) that can handle 9DoF (nine degrees of freedom) pose tracking for novel rigid object instances as well as per-part pose tracking for articulated objects from known categories.

### Affordances and manipulation action prediction

We have explored the use of simulators in learning how robotic agents can interact with articulated objects. We addressed the design of networks that can extract highly localized actionable information related to elementary actions such as pushing or pulling [4]. For example, given a drawer, our network predicts that pushing anywhere on the surface of the drawer can help close it, while only applying a pulling force on the handle or drawer edge will help open it. We also extended these basic motions to longer trajectories that accomplish a specific goal and have shown how to learn articulated object affordances with a minimal number of interactions. ►

- [1] Dahnert, M., Dai, A., Guibas, L. J. & Nießner, M (2019).
- [2] Huang, J. *et al.* (2019).
- [3] Fang, Q. *et al.* (2022).
- [4] Mo, K., Guibas, L. J., Mukadam, M., Gupta, A. & Tulsiani, S. (2021).



**Fig. 1,** (from [2]). TextureNet uses a 4-way rotationally symmetric (4-RoSy) field to parametrize a mesh, extracting oriented patches for 3-D semantic segmentation through networks with 4-RoSy convolutional operators.

- [5] Achlioptas, P., Abdel-reheem, A., Xia, F., Elhoseiny, M. & Guibas, L. J. (2020).

### Language understanding and generation for objects in scenes

We studied the challenging problem of using referential language to identify common objects in real-world 3-D scenes, focusing on multi-instance and semantically fine-grained objects. To ameliorate to the scarcity of data for this problem, we developed two large-scale and complementary visio-linguistic datasets to demonstrate how to combine linguistic and geometric information and creating multi-modal (3-D) neural listeners that can perform fine-grained object localization and discrimination [5].

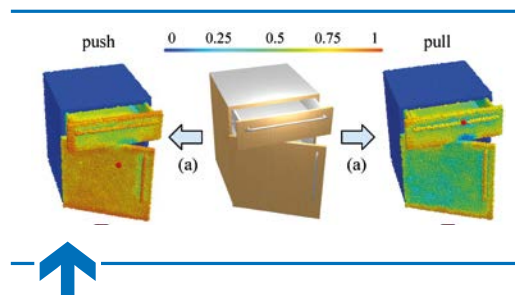
### Synergistic activities

#### International workshop: Machine learning for 3-D understanding (TUM-IAS 2018)

With 23 invited international speakers from both academia (TUM, Imperial College, Harvard, Stanford, and others) and industry (including Google, Facebook, and Intel), the workshop covered a wide range of topics between machine learning and geometry, and it fostered an engaging atmosphere to allow for interdisciplinary exchange of ideas.

#### TUM-IAS doctoral candidate research stay with Prof. Leonidas Guibas's group at Stanford (spring 2019)

In spring 2019, the TUM-IAS supported the research stay of TUM-IAS doctoral candidate Manuel Dahnert with Leonidas Guibas's research group at Stanford University, USA, to deepen international and in-person collaboration. The goal of the stay was to develop a novel generative approach for modeling 3-D shapes using graph neural networks. The three-month stay was concluded with the presentation of another TUM-IAS project: Avetisyan et. al., Scan2CAD, at CVPR 2019, which was accepted as an oral presentation.



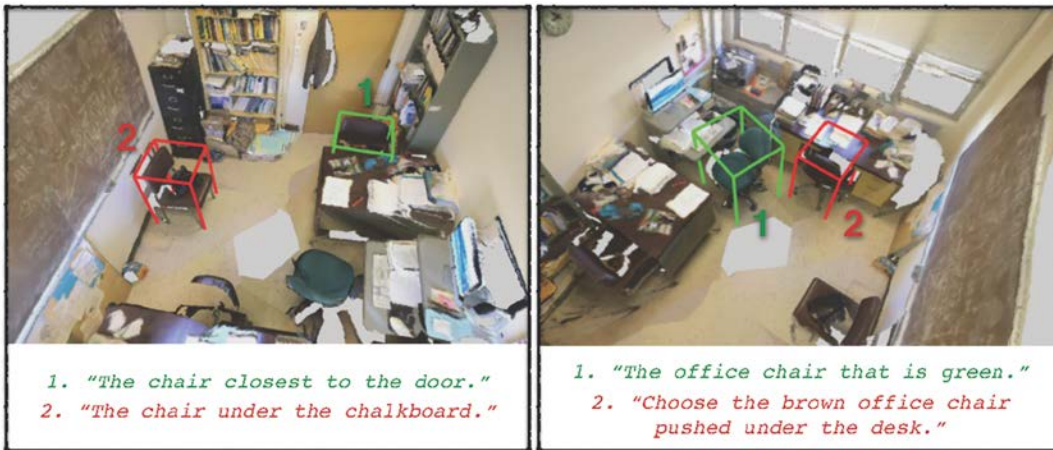
**Fig. 2.** (from [4]). Where2Act uses a simulation environment (SAPIEN) to explore different affordances for object parts, such as doors or drawers of cabinets. Note that the successful “active site” can be quite different, depending on the desired action (push/pull) or (open/close).

#### First workshop on language for 3-D scenes (CVPR 2021)

In 2021, our inaugural workshop on natural language and 3-D object understanding (<https://language3dscenes.github.io/>) at CVPR aimed to unite researchers in the field and benchmark the progress in connecting natural language with 3-D object representations of the physical world. Attended by 80 participants, it received 17 code submissions on two “language-assisted 3-D object localization” tasks. Furthermore, our underlying dataset papers (ScanRefer, ReferIt3-D) have been cited more than 70 times, since appearing at ECCV 2020, showing strong interest from the CV/CL communities.

#### Second workshop on language for 3-D scenes (ECCV 2022)

Following that success, we organized a second installment of the Workshop on Language for 3-D Scenes at ECCV, Tel Aviv, Israel. The program featured six international keynote speakers and the presentation of several accepted submissions of the three accompanying challenges. ■



**Fig. 3,** (from [5]). ReferIt3-D showcases the ability to understand and generate referential language that makes fine-grained differentiation among objects in the same class.

### Selected publications

Dahnert, M., Dai, A., Guibas, L. J. & Nießner, M. Joint Embedding of 3-D Scan and CAD Objects. *IEEE/CVF International Conference on Computer Vision (ICCV)*, 8748-8757 (2019).

Huang, J. *et al.* TextureNet: Consistent Local Parametrizations for Learning from High-Resolution Signals on Meshes. *IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, 4435-4444 (2019).

Fang, Q. *et al.* Towards Accurate Active Camera Localization. *European Conference on Computer Vision (ECCV)*, 122-139 (2022).

Mo, K., Guibas, L. J., Mukadam, M., Gupta, A. & Tulsiani, S. Where2Act: From Pixels to Actions for Articulated 3-D Objects. *IEEE/CVF International Conference on Computer Vision (ICCV)*, 6793-6803 (2021).

Achlioptas, P., Abdelreheem, A., Xia, F., Elhoseiny, M. & Guibas, L. J. ReferIt3-D: Neural Listeners for Fine-Grained 3-D Object Identification in Real-World Scenes. *European Conference on Computer Vision (ECCV)*, 422-440 (2020).

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## Focus Group: Population Epigenetics and Epigenomics

**Prof. Frank Johannes (TUM)**, Alumnus Rudolf Mößbauer Tenure Track Assistant Professor |  
**Prof. Robert J. Schmitz (University of Georgia)**, Alumnus Hans Fischer Fellow |  
**Yadollah Shahryary (TUM)**, Doctoral Candidate



**Prof. Frank  
Johannes**

# Exploring epimutational processes across time scales

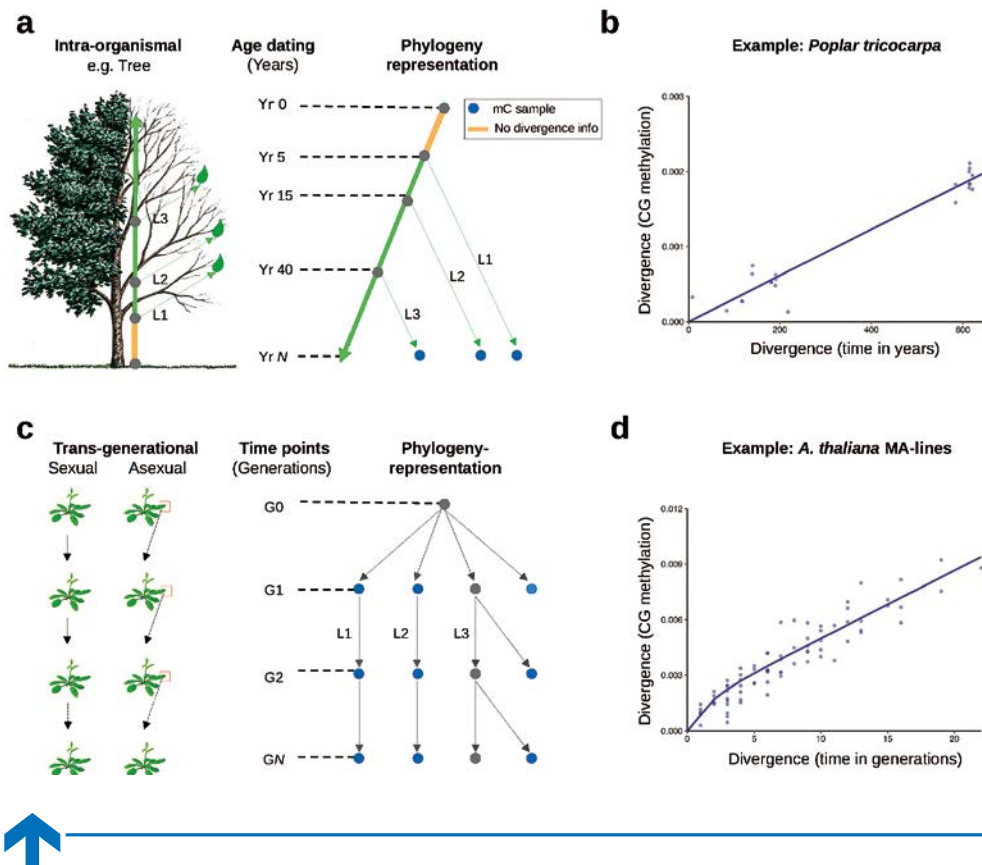
**The field of epigenetics studies heritable changes in genome function that cannot be explained by alterations in the underlying DNA sequence. Our group is interested in understanding how genetic, environmental, and stochastic factors induce epigenetic modifications in plants, how these modifications are propagated over time, and whether they have agricultural and evolutionary consequences.**

Heritable gains or losses of cytosine methylation can arise stochastically in plant genomes independently of DNA sequence changes. These so-called “spontaneous epimutations” appear to be a by-product of imperfect DNA methylation maintenance. There is continued interest in the plant epigenetics community in trying to understand the broader implications of these stochastic events, as some have been shown to induce heritable gene expression changes, to shape patterns of methylation diversity within and among plant populations and to be responsive to multi-generational environmental stressors. In collaboration with Hans Fischer Fellow Robert J. Schmitz, a central research aim of our Focus Group has been to study the rate and spectrum of spontaneous epimutations, their molecular origins, and their patterns of somatic and trans-

generational accumulation. To that end, we have combined mathematical modeling and high-throughput DNA methylation data with various experimental (epi)mutation accumulation systems (Fig. 1).

### Plant genomes harbor epimutation hotspots

Multigenerational studies in plants have shown that the rate of spontaneous epimutations varies substantially across the genome, with some regions harboring localized “epimutation hotspots.” Using the model plant species *A. thaliana*, we were able to show that epimutation hotspots are indexed by a specific set of epigenomic features that map to a subset of genes. Although these regions comprise only ~12% of all CGs (cytosine-guanine dinucleotides) in the ▶



**Fig. 1.** Studying spontaneous epimutations using (epi)mutation accumulation systems. (A) Left panel: Construction of multi-generational (G0 to GN) mutation accumulation (MA) lines through sexual (selfing or sibling mating) or asexual (clonal) propagation. The different lineages (L1 to L3) can be represented as a phylogeny. The branch point times and the branch lengths are typically known, *a priori*, from the experimental design. DNA methylation (mC) sampling can be performed at selected generations, either from plant material of direct progenitors or from siblings of those progenitors. Right panel: DNA methylation between individuals/lineages diverges approximately linearly with divergence time (in generations). Divergence increases according to a neutral epimutation process and depends only on the stochastic methylation gain and loss rates at individual sites as well as the Mendelian segregation and fixation of *de novo* epimutations. (B) Left panel: A tree can be interpreted as an intra-organismal phylogeny. The topology (i.e., branching structure) is typically known, and the branch points and branch lengths can be dated by coring. Only three branches are highlighted (L1, to L3) for simplicity. Leaf mC measurements can be obtained and used as the basis to calculate DNA methylation divergence. Similarly, divergence times (in years) for pairs of leaves can be calculated by tracing back the ages of the branches to their most recent common branch point. This can only be done down to the tree's earliest branch point (in this case, Yr = 5) but not to earlier time points (orange segment). Note: tree image was modified from [www.photos.com](http://www.photos.com). Right panel: DNA methylation of leaves sampled from different branches of the single tree diverge approximately linearly with divergence time (in years). Divergence increases according to a neutral epimutation process, and depends only on the stochastic methylation gain and loss rates at individual sites. (Schmitz, J. R., Johannes, F. Epimutations Define a Fast-Ticking Molecular Clock in Plants. Trends Genet. 37(8), (2021))



genome, they account for ~63% of all epimutation events per unit time. Molecular profiling revealed that these regions contain unique sequence properties, harbor steady-state intermediate methylation levels, and act as putative targets of antagonistic DNA methylation pathways. We further demonstrated that experimentally-induced shifts in steady-state methylation in these hotspot regions are sufficient to significantly alter local epimutation intensities.

#### Epimutations accumulate during somatic development

Although our work with experimental (epi)mutation accumulation lines (Fig. 1A) has allowed us to gain quantitative insights into the process by which DNA methylation maintenance mistakes arise and are propagated across generations, we actually had no clear understanding of where in the plant life cycle these mistakes originate. One hypothesis was that they occur continuously during somatic development. To test this, we used trees as a model system. Given their exceptional longevity and well-defined modular architectures, trees act as natural (epi)mutation accumulation systems and permit unprecedented insights into the dynamics, mitotic stability, and functional impact of spontaneous epimutations over time scales that have been inaccessible to previous prospective studies. We developed novel analytical methods that treat the tree branching topology as an intra-organism phylogeny and used this approach to show that somatic epimutations accumulate

gradually throughout development (Fig. 1B). Moreover, we found that this accumulation was clock-like and that information about somatic epimutations could be used to estimate the chronological age of trees.

#### Epimutations define a fast-ticking evolutionary clock

Since spontaneous epimutations are also heritable across generations, we sought to test if their clock-like properties could be used, more generally, as a molecular clock to date evolutionary events over longer time scales. In evolutionary biology, DNA-based molecular clocks are classically used for dating the divergence between lineages over macroevolutionary time scales ( $\sim 10^5$  to  $10^8$  years). However, these classical DNA-based clocks tick too slowly to inform us about the recent past. We were able to demonstrate that stochastic DNA methylation changes at a subset of cytosines in plant genomes define an epimutation-based evolutionary clock whose tick-rate is orders of magnitude faster than DNA-based clocks. This new clock enabled us to perform phylogenetic explorations on a scale of years to centuries. We showed experimentally that the use of epimutation clocks recapitulate known topologies and branching times of intraspecies phylogenetic trees in the self-fertilizing plant *A. thaliana* and the clonal seagrass *Z. marina*, which represent two major modes of plant reproduction. This discovery will open new possibilities for high-resolution temporal studies of plant biodiversity.

**Future research**

Our group continues to dissect the molecular and phenotypic properties of spontaneous epimutations in plants. We have begun to employ single-cell sequencing technologies to be able to detect the origin of somatic epimutations within a small population of stem cells from in which they most likely arise. Using cell lineage-based mathematical models, we further seek to understand how somatic epimutations originating in this stem

cell population are propagated in the plant morphological architecture throughout development, as well as how they are eventually transferred to the cell lineages that form the next generation. In parallel to these efforts, we aim to calibrate epimutation-based evolutionary clocks in various plant species to help resolve evolutionary questions about time scales that are difficult to resolve with DNA-based mutation data. ■

**Selected publications**

Yao N. *et al.* An evolutionary epigenetic clock in plants. *Science* 381, 1440-1445 (2023).

Hazarika, R.R. *et al.* Molecular properties of epimutation hotspots. *Nature Plants* 8, 146-156 (2022).

Zhang Y. *et al.* Heterochromatin is a quantitative trait associated with spontaneous epiallele formation. *Nature Communications* 12, 6958 (2021).

Shahryary D.Y. *et al.* AlphaBeta: Computational inference of epimutation rates and spectra from high-throughput DNA methylation data in plants. *Genome Biology* 21, 260 (2020).

Lauss K. *et al.* Parental DNA methylation states are associated with heterosis in Arabidopsis epigenetic hybrids. *Plant Physiology* 176, 1627-1645 (2018).

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[www.ias.tum.de/ias/johannes-frank/](http://www.ias.tum.de/ias/johannes-frank/)

## Focus Group: Inclusion and Diversity in Physics

Dr. Sara Lucatello (INAF Osservatorio Astronomico di Padova), Alumna Anna Boyksen Fellow | Host: Prof. Laura Fabbietti (TUM)



Dr. Sara Lucatello

# Tackling biases and unveiling disparities in astrophysics

**Through an anonymous survey, we have collected data on demographics, professional activities, career development, workplace environment, and work-life balance for a large sample of European astrophysicists. One of the most striking results is that the field has a systemic bullying problem, which disproportionately affects women and minorities.**

The under-representation of women and, more generally, the lack of diversity in hard sciences, is a long-standing issue: Women, racial minorities, and people from socio-economically underprivileged backgrounds have a harder time successfully pursuing an academic career (see, e.g., [1]). This suggests that the metrics adopted, in spite of being generally reduceable to numerical indexes that allow easy comparison, are not as unbiased as assumed (see, e.g., [2], [3]).

The problem is particularly severe in Germany, with the under-representation of women in hard sciences being consistently more pronounced than in most EU countries across all academic levels. Building a fair and equitable system is a crucial step in improving diversity, which is linked to innovation (see, e.g., [4]). This is of fundamental importance at this time, as post-secondary education in Europe will see a large influx of second-generation immigrants as a result of recent waves of migration.

The goal of our efforts was to improve awareness of the conscious and unconscious biases affecting the selection and evaluation systems in natural sciences, and in particular in the European astrophysics community. In fact, while awareness of the problem of under-representation of women and lack of diversity is improving, there is still a widespread belief in the scientific community that it is only marginally affected by this matter.

During the funding period, the Focus Group has undertaken a number of activities.

On the one hand, we have been working on organizing events aimed at improving the awareness of conscious and unconscious bias in academia. With this goal, we have held unconscious bias training workshops in major research institutions: at the Collaborative Research Center “Neutrinos and Dark Matter in Astro- and Particle Physics” (SFB 1258) general meeting in Munich (more than

100 attendees), at the European Southern Observatory headquarters (more than 50 attendees), and at the Faculty of Physics at the Pontificia Universidad Católica de Chile in Santiago (more than 50 attendees). A larger number of events were originally planned; several of them were canceled because of the pandemic, while others were turned into virtual events, such as those at INAF (more than 100 attendees) and the DARK center of the University of Copenhagen (50+ attendees).

We also held three international meetings on the topic. The first, “Working toward an equitable, diverse, and inclusive astronomy” was organized as a special session within the European Astronomical Society (Lyon in June 2019), a meeting that attracted more than 1,200 attendees.

Following the success of that meeting, we worked with the European Astronomical Society to institute an EAS Advisory Committee on issues related to Equity, Diversity, and Inclusion, which started its activities in 2019.

We also coordinated the organization of two editions of the EAS yearly Inclusion and Diversity event for the European Astronomical Society. Both Inclusion Day 2020 and Diversity and Inclusion Day 2021 were virtual due to pandemic disruption.

On the other hand, we have worked on the administration of a survey aimed at examining

the demographics of astrophysics communities in Europe. Originally intended to take place in mid-2020, its schedule was affected by considerable delays associated with the pandemic.

The survey was designed to explore dimensions related to professional activities, career development, workplace environment, and work-life balance, as well as to probe the impact that COVID-19 had on such activities. It was developed with input from experts in the field and was run in collaboration with the European Astronomical Society. Data collection was completed in late 2022, resulting in more than 1,300 responses from 68 countries, the largest survey sample collected to date from professional astrophysicists.

Data analysis is currently being completed, and we have an agreement with Nature Astronomy for publication. One of the striking results emerging from the data is that the community is affected by a systemic bullying problem: One in five people report having been subjected to instances of bullying or harassment in the workplace, and women and minority groups are disproportionately affected. Women and non-binary people in the field are at least twice as likely as men to be bullied or harassed. Moreover, one in three members of the LGBTIQ+ community report having been subjected to instances of bullying and harassment. ►

- [1] Lucatello, S. & Diamond-Stanic, A. Diversity and inclusiveness in large scientific collaborations. *Nature Astronomy* 1 (6), 0161 (2017).
- [2] Larivière, V., Ni, C., Gingras, Y. *et al.* Bibliometrics: Global gender disparities in science. *Nature* 504, 211–213 (2013).
- [3] Boyle, P., Smith, L., Cooper, N. *et al.* Gender balance: Women are funded more fairly in social science. *Nature* 525, 181–183 (2015).
- [4] Jones, G., Chirino Chace, B. & Wright, J. Cultural diversity drives innovation: empowering teams for success. *International Journal of Innovation Science* 12, 323–343 (2020).

Another interesting and unexpected result involves remote participation in conferences. The annual meeting of the European Astronomical Society is the largest astronomical conference in Europe, regularly attracting well over a thousand professional astronomers from 50+ countries in Europe and beyond. Participants based in countries where research is not funded at the level of Western Europe (e.g., Eastern Europe, Africa, and Latin America) account for roughly one-sixth of the attendees.

Due to the pandemic, the 2020 and 2021 meetings were held virtually, with considerably reduced registration fees. The number of attendees for these two events was larger than usual, reaching 2,200 for the 2021 edition. The expectation was that the availability of affordable remote access would widen

the pool of participants, in particular to scientists based in countries where research is poorly funded, or to holders of non-powerful passports.

The fraction of attendees from these countries, however, did in fact have a moderate decrease with respect to those for in-person meetings (2022, 2019, 2018, and 2017), while there was a clear increase in participation of scientists based in affluent countries beyond Europe (e.g., USA, Canada, Japan, and Australia). While there is no doubt that allowing remote attendance increases the accessibility of meetings, our results suggest that this facilitates the participation from minorities based in western-world countries, but does not seem to have the same positive effect among other communities. ■



**Selected publications**

Schiappacasse-Ulloa, J. & Lucatello, S. Neutron-capture elements in NGC 6752 multiple populations. *Monthly Notices of the Royal Astronomical Society* 520(4), 5938–5949 (April 2023). [www.doi.org/10.1093/mnras/stad486](https://www.doi.org/10.1093/mnras/stad486).

Jin, S., Trager, S., Dalton, G., *et al.* The wide-field, multiplexed, spectroscopic facility WEAVE: Survey design, overview, and simulated implementation. *Monthly Notices of the Royal Astronomical Society*, stad557 (2023). [www.doi.org/10.1093/mnras/stad557](https://www.doi.org/10.1093/mnras/stad557).

Schiappacasse-Ulloa, J., Lucatello, S., Rain, M., *et al.* Lithium abundances as a tracer of asymptotic giant branch star pollution in the globular cluster NGC 6752. *Monthly Notices of the Royal Astronomical Society* 511 (1), 231–240 (March 2022). [www.doi.org/10.1093/mnras/stab3795](https://www.doi.org/10.1093/mnras/stab3795).

Gratton, R., Bragaglia, A., Carretta, E. *et al.* What is a globular cluster? An observational perspective. *Astron Astrophys Rev* 27, 8 (2019). [www.doi.org/10.1007/s00159-019-0119-3](https://www.doi.org/10.1007/s00159-019-0119-3).

**For a full list of publications, please visit**  
[www.ias.tum.de/ias/lucatello-sara-1/](https://www.ias.tum.de/ias/lucatello-sara-1/)

## Focus Group: Building Bridges To Promote Gender Diversity In Science

Prof. Shobhana Narasimhan (Jawaharlal Nehru Centre for Advanced Scientific Research), Alumna Anna Boyksen Fellow | Prof. Gudrun Klinker, Daniel Dyrda (TUM), Collaborators | Hosts: Prof. Johannes Barth, Dr. Eva Sandmann (TUM)



Prof. Shobhana Narasimhan

# Fixing gender inequity in science: From statistics to games

**We seek to understand why women are a minority in science, and we wish to spread awareness of the chilly climate they often encounter in academia. We find surprising patterns in statistics for female participation in science worldwide. Using narratives from across the world, we designed computer games that raise awareness about these issues and hope they will help improve the situation.**

[1] UNESCO Institute for Statistics, Women in Science, Fact Sheet No. 55 (June 2019). FS/2019/SCI/55.

[2] [www.hdr.undp.org/gender-development-index#/indicies/GDI](http://www.hdr.undp.org/gender-development-index#/indicies/GDI)

[3] Huyer, S. Is the gender gap narrowing in science and engineering? UNESCO Science Report: towards 2030. 85-103. Paris: UNESCO (2015).

[4] Database of the World Economic Outlook reports, International Monetary Fund <https://www.imf.org/en/Publications/WEO> retrieved on 11/12/2020.

### Motivation

It is recognized today that the low numbers of women in science constitute a problem that has to be confronted and addressed. It is interesting that many developing countries have a much higher percentage of women scientists than is found in Europe or the USA [1]. However, women scientists in the developing world frequently face additional challenges due to economic and cultural factors. We wished to increase the engagement of the TUM community with these women. We also wished to use the stories and experiences collected from this group to design games that bring out the problems, challenges, and joys of being a woman in science. We note that our primary focus was active intervention, rather than academic research.

### Reorientation of goals

As the initial years of the Fellowship period coincided with the pandemic, we had to reorient many of our initial goals. Travel re-

strictions made impossible our original plan to have a cohort of foreign women scientists visit TUM. While in lockdown, one of us (SN) instead worked on a project (described below) to compare and analyze statistics for women's participation in science around the world. Later, a short but highly productive international workshop was held at the TUM-IAS. A major part of our effort and budget was redirected toward the development of computer games.

### Statistics: Some surprising correlations

We used statistics available publicly [1]-[4] to explore whether there were hitherto undetected patterns in the worldwide participation of women in science.

### We made three important findings:

1. The percentage of women in the scientific workforce of a country shows an interesting and surprising correlation with its per capita

income (adjusted for purchasing power parity). The data fall on an inverted U, i.e., the poorest and richest countries have very few women in science. The largest number of women in science is found in countries where the per capita income is neither very low nor very high (see Fig. 1a).

If one looks at the countries in Europe alone, one finds an inverse correlation: The richer the country, the lower the percentage of women in science (see Fig. 1b). Some of this inverse correlation can be attributed to the poorer economies being countries that were formerly socialist or communist, and therefore having a more firmly embedded feminist ideology.

The inverted U pattern is extremely surprising, as it is well known in labor economics that the participation of women in the workforce as a whole follows the exactly opposite trend of a right-side-up U [5],[6].

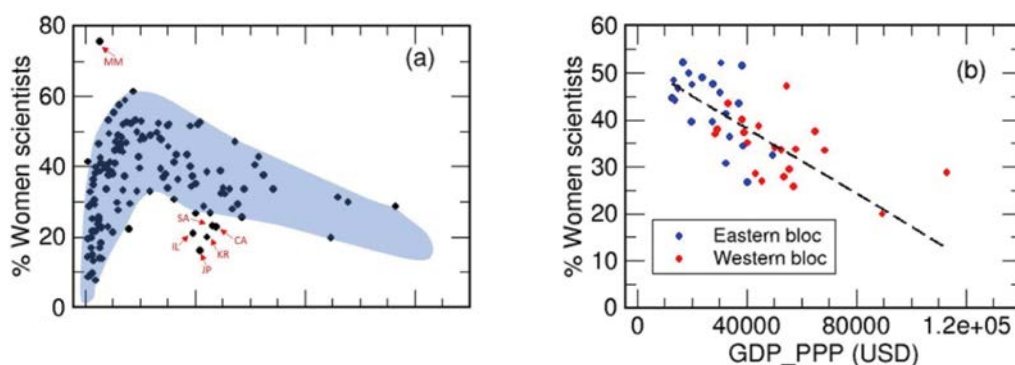
2. There have been claims in the literature that the percentage of women in science is anticorrelated with the degree of gender equity in the country. This has been used to argue that when gender biases do not operate, women exhibit their “natural” preference for non-science subjects. We do not find this; instead, we find that the percentage of women in science is positively correlated with the gender development index [2] of the country.

3. We find very different patterns of retention of women in science in countries in the Global South and Global North. In the former, the percentage of women in science is high at the school and college level, but drops significantly afterward. In the latter, however, the percentage is low at all stages, though there are exceptions.

This work was published in a special edition of the IUPAC flagship journal *Pure and Applied Chemistry* devoted to articles about women in science. ▶

[5] Lechman, E. & Kaur, H. Economic Growth and Female Labor Force Participation – Verifying the U-Feminization Hypothesis. New Evidence for 162 Countries Over the Period 1990–2012. SSRN (2015).

[6] Gaddis, I. & Klasen, K. Economic Development, Structural Change and Women’s Labor Force Participation A Reexamination of the Feminization U Hypothesis. *Courant Research Centre: Poverty, Equity and Growth, Discussion papers* 71 (2011).



**Fig. 1,** Scatter plots showing the percentage of women working in science in a country (PW) vs. the per capita GDP of the country in US Dollars, adjusted for purchasing power parity. (a) Data for 138 countries throughout the world for which data were available; the light blue shaded inverted-U-shaped boomerang is a guide to the eye, which contains most of the points. Outlier countries, which fall outside the blue-shaded boomerang, are labeled: MM (Myanmar), JP (Japan), KR (South Korea), IL (Israel), CA (Canada), and SA (Saudi Arabia). (b) Data for countries in Europe. The blue points correspond to countries that were in the former “Eastern bloc” and the red points correspond to the remaining “Western bloc” countries. The dashed line is a linear regression to the data. The data for PW were obtained from Ref. [1], and those for the per capita GDP-PPP from Ref. [4]. (Reproduced from Narasimhan, S. Participation of women in science in the developed and developing worlds: inverted U of feminization of the scientific workforce, gender equity and retention. *Pure and Applied Chemistry* 93, 913-925, 2021))

### Workshops at the TUM-IAS

A workshop was conducted at the TUM-IAS on 8 and 9 May 2023. This WISTUM workshop aimed to introduce the TUM community to diverse perspectives and experiences of women in science from around the world, to create a space where these women could share their stories and form a network, and to collect insights that could contribute to the game project.

The workshop had 29 participants, of whom 16 were from outside TUM. The 11 international participants were from Argentina, Croatia, India, Italy, Zimbabwe, Nigeria, the Philippines, the USA, Ukraine, Romania, and New Zealand; the participants with German affiliations also had diverse backgrounds and nationalities. The participants included two historians of science and a drama therapist.

At the workshop, drama and dialogue were used to collect stories and experiences of women in science. In a session called Voices from the Developing World, open to the entire TUM community, Shazrene Mohamed from Zimbabwe, Marta Antonelli from Argentina, Rabia Salihu Sa'id from Nigeria, and

Jinky Bornaes from the Philippines shared the stories of their personal trajectories and described their research work. This session showed that while the pleasures and intellectual challenges of scientific research are universal, women scientists from the Global South have to deal with not only a paucity of resources, but often a toxic combination of sexism and racism.

### Computer games

We have been working on developing computer games on women in science, in collaboration with Gudrun Klinker the Games Engineering Department of TUM: Daniel Dyrda (project lead, designer and programmer); Chrysa Bika, Mary Hardisty, and Lorena Kneipp Vitale (content and game designers); and Alina Fetoski, Paul Hemming, Felix Stieglbauer, and Damian Schneider (programmers).

These games can be played online using mobile phones or desktop computers, in either single-player or multi-player mode. Playing these games is intended to make one aware of what it feels like to be a woman in science, and to spark discussion when played in a group.



**Fig. 2.** At the WISTUM workshop in May 2023: Rabia Salihu Sai'd from Nigeria, Marta Antonelli from Argentina, and Shobhana Narasimhan from India. © Jinky Bornaes



**Fig. 3,** Former TUM student Chrysa Bika (now at LMU) leads a playtesting session of the computer games with students from TUM. © Felix Stieglbauer

The game has six modules: Unconscious Bias, Journey in Science, Being a Mentor, Juggling, Discrimination and Coping, and Fuel the Fire. Each of these deals with a different aspect of the challenges faced by women in science. The first four modules are complete and have already undergone two rounds of play tests. The remaining two

modules are partially complete. We are in the process of further tweaking the structure and content of the games in response to the feedback received.

We hope to launch these games and make them publicly available during 2024.

### Open questions and the future

The correlations found in statistics of the worldwide participation of women in science are unexpected and fascinating. They raise obvious questions about whether there is a causal relationship, and if so, why. Further research is needed to study this; social scientists have expressed interest in exploring these issues together.

The game modules need to be refined in response to player feedback, and also be expanded to capture more diverse experiences. We are also looking for a catchy name for the game, and suggestions are welcome! ■

### Selected publications

Narasimhan, S. Participation of women in science in the developed and developing worlds: inverted U of feminization of the scientific workforce, gender equity and retention. *Pure and Applied Chemistry* 93, 913-925 (2021).

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[www.ias.tum.de/ias/narasimhan-shobhana/](http://www.ias.tum.de/ias/narasimhan-shobhana/)



## Focus Group: China in Global Economic Governance

Prof. Susan Park (University of Sydney), Alumna Hans Fischer Senior | Julia Esser-Grimm (TUM), Doctoral Candidate | Host: Prof. Eugénia da Conceição-Heldt (TUM)



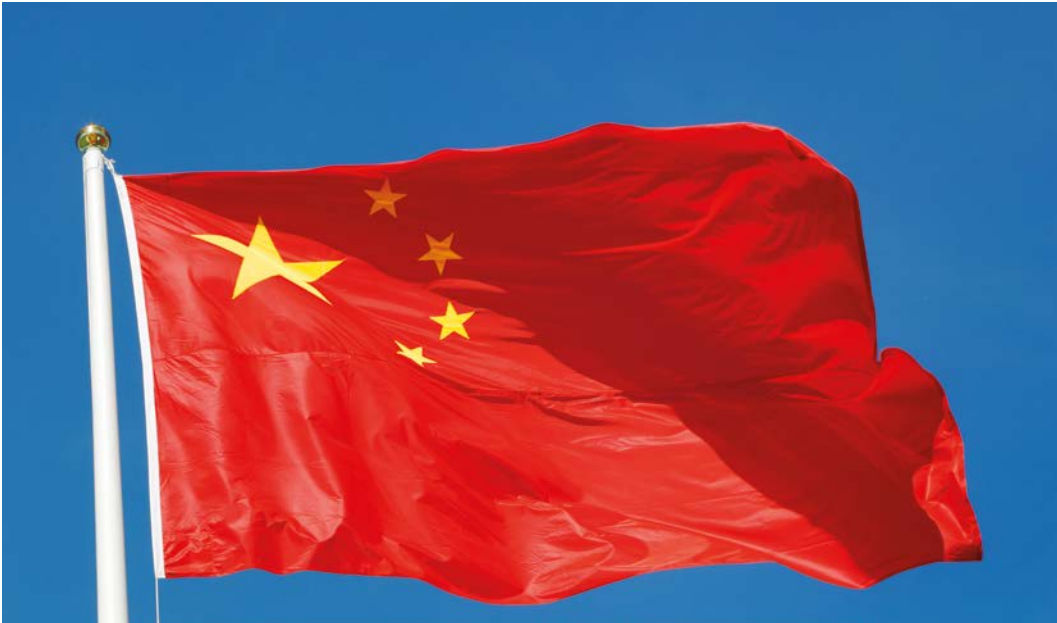
Prof. Susan  
Park

# Analysis of China's role in global economic governance

**The China's rapid economic ascent has raised questions as to how it is reshaping the international order. This is already affecting international trade agreements and monetary cooperation. In global development, aid lending is increasingly contested between the US and China. This Focus Group maps China's role in global economic governance and the multilateral development banks in particular.**

The rapid rise of China's economic and political influence is changing the configuration of global economic governance. In some cases, Chinese initiatives have improved and complemented global governance structures, rather than fundamentally altering and undermining them. In other cases, the political status quo endures. This project examines China's role in global economic governance, specifically pertaining to its impact and influence on international institutions. Until recently, the rising economic power of China, ahead of other rising powers such as India and Brazil, has not been matched by a reconfiguration of the global economic order to better accommodate their new financial and political weight through institutional reforms. This misalignment between representation and economic weight has led to China's contestation and dissatisfaction with the liberal international order

(LIO) comprised of formal inter-governmental organizations and informal institutions. This discontent culminated in the creation of new international organizations (IOs) – including the Asian Infrastructure Investment Bank (AIIB) and the New Development Bank (NDB) – by rising powers, under Chinese, Indian, and Brazilian leadership, respectively. Until now, scholars have focused on theorizing the impact of China on the international order without specific knowledge and understanding of how international institutions operate. The Focus Group is interested in providing a detailed analysis of how China is operating within international institutions, such as the multilateral development banks, to better understand how well China's actions are explained by dominant theories regarding its preference for maintaining or changing the international system.



The research conducted sought to identify the main activities of China within global economic governance. Currently, scholars tend to identify China's activities as either supporting or undermining the Western liberal international order. Our Focus Group recognizes that China's activities, and those in response to China, are reconfiguring the international order. This is not an either/or proposition; it is both/and. In other words, even when China is engaging in cooperation, this can still reshape international institutions such as the World Trade Organization and the Paris Club. The research highlights instead a continuum of activity, from limited support and limited contestation to robust cooperation and existential challenge. Limited support refers to a mode of engagement that is supportive but that requires fewer resources and less investment than the robust cooperation mode. China

accepts the rules, norms, and principles of an existing global economic institution. However, it is not willing to contribute substantially to providing resources, enforcing rules, deepening cooperation, or improving institutional performance [1]. Limited contestation is where China accepts the broad thrust of cooperation but contests specific rules for how it is being enacted or the realm in which the rules are being applied. Robust cooperation means that China engages in global economic institutions in a supportive way by accepting underlying rules, norms, and principles. We see this mode of engagement in multilateral development lending, where China took the lead in creating the Asian Infrastructure Investment Bank and making extensive resources available to support this new multilateral organization [2]. Existential challenge defines a mode of engagement that questions and rejects ►

**[1]** Heldt, E., Schmidtke, H. & Serrano, O. Multilateralism à la Carte: China's Engagement in Global Economic Institutions. *Review of International Political Economy* (under review, 2023).

**[2]** Heldt, E. & Schmidtke, H. Explaining Coherence in International Regime Complexes: How the World Bank Shapes the Field of Multilateral Development Finance. *Review of International Political Economy* 26(6), 1160–1186 (2019).

**[3]** Park, S. (2023).

the purposes, rules, norms, and principles of a global economic institution. This mode is evident when China's actions challenge, undermine, and eventually replace existing multilateral governance structures. In this way, China acts as a disruptor by explicitly refusing to join or comply with the rules of an existing IO [1]. This continuum clarifies what drives China's interactions in multilateral fora and how this contributes to the debate over the liberal international order. Such analytical categories provide greater utility for understanding China's behavior beyond the increasingly simple binary of for or against the liberal international order, which itself has become highly politicized.

The Focus Group undertook two workshops at the Technical University of Munich (one virtual in 2021 and one in-person in 2023) and a panel at the 2023 annual International Studies Association conference in Montreal, Canada. More dissemination activities would have been possible except for the border closures during the global pandemic.

The results of the workshops have culminated in a submission of a special issue [1] submitted to the international peer-reviewed

journal the *Review of International Political Economy*. The special issue is still under review at this time.

The major result of this research is an attempt to shape the debate in international relations to go beyond simply binaries of how China's economic governance activities are viewed, and to better identify how its activities are shaping global economic institutions including the World Trade Organization, the International Monetary Fund, and the World Bank. The significance of the research is to highlight that political posturing portraying China as either good or bad overlooks the much more complicated picture of how China both supports and undermines global institutions for its own benefit. The final outcomes of the project will be used to inform the scholarly community and policy makers of the importance of working with Chinese counterparts in meaningful ways to establish the means for cooperation and to build toward supporting an inclusive international economic order. Future research will be needed to advance better understanding of China's intentions in international monetary relations, development finance, and environmental governance [3]. ■

**Selected publications**

Park, S. Meeting in the Middle? Multilateral Development Finance, China, and Norm Harmonization. *Asia Policy* 18(4), 61-70 (2023). [www.doi.org/10.1353/asp.2023.a911619](https://www.doi.org/10.1353/asp.2023.a911619).

Gunaydin, E. & Park, S. Accountability Enablers? The Role of Transnational Activism in the Use of the Multilateral Development Bank Grievance Mechanisms. *Policy and Society* (2023). [www.doi.org/10.1093/polsoc/puad014](https://www.doi.org/10.1093/polsoc/puad014).

Park, S. The African Development Bank and the Accountability Policy Norm: Endogenous Change, Norm Conformance, and Regime Complex Coherence. *Global Governance* 26(1), 61-84 (2023). [www.doi.org/10.1163/19426720-02901003](https://www.doi.org/10.1163/19426720-02901003).

Park, S. *The Good Hegemon: United States Power, Accountability as Justice, and the Multilateral Development Banks*. Oxford: Oxford University Press (2022).

Park, S. Policy Norms, the Development Finance Regime Complex, and Holding the EBRD to Account, *Global Policy* 12(4), 90-100 (2021). [www.doi.org/10.1111/1758-5899.12881](https://www.doi.org/10.1111/1758-5899.12881).

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## Focus Group: Optimal Transport in Science, Technology and Society

**Prof. Giuseppe Savaré (Bocconi University)**, Alumnus Hans Fischer Senior Fellow | **Dr. Giacomo Enrico Sodini (TUM, now University of Vienna)**, Doctoral Candidate | Hosts: **Prof. Massimo Fornasier, Prof. Daniel Matthes (TUM)**



**Prof. Giuseppe Savaré**

# New paradigms for optimal transport

**Optimal transport is a rich and deep mathematical theory, primarily concerned with studying the best way to move available resources to a target configuration of destinations. In our Focus Group, we developed new frameworks for theoretical and computational investigations that greatly extend the scope of the theory, with promising applications to other relevant branches of mathematics.**

**[1]** Kantorovitch, L. On the translocation of masses. *C. R. (Doklady) Acad. Sci. URSS (N.S.)* 37, pp. 227–229 (1942).

**[2]** Ambrosio, L., Gigli, N. & Savaré, G. Gradient flows in metric spaces and in the space of probability measures. *Lectures in Mathematics ETH Zurich* (2), pp. x+334. Basel: Birkhäuser Verlag (2008).

**[3]** Villani, C. Optimal transport: Old and new. *Grundlehren der Mathematischen Wissenschaften* (338), pp. xxii+973. Berlin: Springer Verlag (2009).

**[4]** Peyré, G. & Cuturi, M. Computational Optimal Transport. *Foundations and Trends in Machine Learning* 11(5–6), pp. 355–602 (2019).

The modern formulation of optimal transport problems is mainly due to the Nobel laureate Leonid Kantorovich [1]. Roughly speaking, they concern the best way to move a given distribution of resources to a prescribed new configuration (Fig. 1). Depending on the meaning assigned to the terms “resource,” “best,” “move,” and “configuration,” one can obtain an amazing variety of different situations: for example optimal allocation of economic resources (the original motivation of Kantorovich’s work that earned him the Nobel Prize), the comparison of probability distributions of random events or statistical data sets, the physical motion of masses or charges, the evolution of particle systems, the modeling of congested crowded motion, the interpolation or generation of images, and so on.

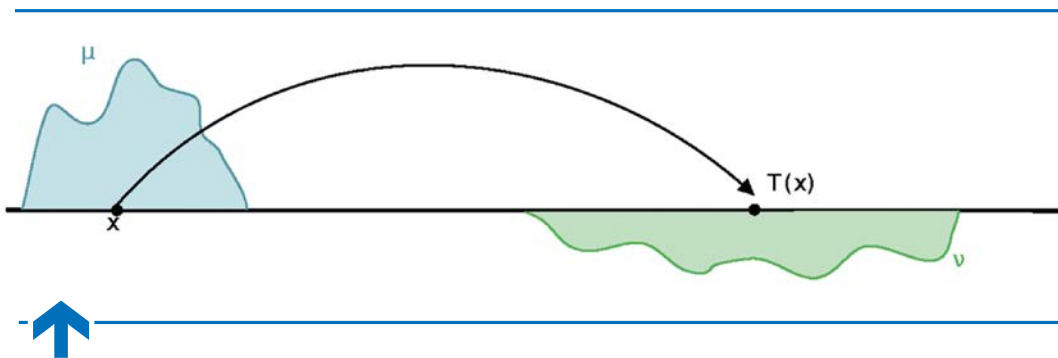
The versatility of the theory [2,3,4] depends on the one hand on its formulation based on general variational principles and on the other on the very powerful combination of measure/probability theory, differential models expressed by partial differential equations, and a geometric perspective. Such a gener-

al approach then requires the development of sophisticated numerical methods to be applied to real problems.

The goal of this Focus Group was to bring together the theoretical knowledge of the Fellow and the more application-oriented expertise of the hosts to create a fruitful collaboration while supervising a talented doctoral candidate. This was done along four main directions dealing with optimal transport for unbalanced mass distributions, evolution models for probability measures, new discrete and geometric structures for nonlinear quantum drift diffusion models, and functional analytic and computational tools in probability metric spaces for deep learning.

### Unbalanced optimal transport

The classical theory of optimal transport typically concerns moving a given distribution (which mathematically is represented by a finite positive measure) to a target location able to receive precisely the aforementioned quantity of resources (still represented by a positive measure with the same total mass).



**Fig. 1,** An illustration of the Monge-Kantorovich problem: the blue mass is moved to the green target location. © Giacomo Sodini

A very natural and important question is how to describe the same kind of phenomenon in case the problem becomes unbalanced and there may be a gain or a loss of mass during the transport. This is particularly relevant in the case of unnormalized distributions, such as images or more general data. Such a problem has been considered in some specific cases, inspired by a dynamic viewpoint [5,6,7]. We discovered a general approach based on convex relaxation on the metric cone generated by the ambient spaces [8], which is the natural setting for unbalanced optimal transport problems in full generality.

### Evolutions of probability measures

Many relevant models for describing the interaction of agents/particles, also in the context of optimization and machine learning, can be represented by the evolution in time of probability measures. A very important class of such evolutions is provided by gradient flows [2], which are driven by suitable functionals and typically converge to their minimum. However, the gradient structure is quite rigid, and even simple perturbations easily destroy such a property. We developed a general notion of evolution that reproduces at the infinite dimensional measure setting some features of more familiar dynamical

systems. They are characterized by the notion of measure probability vector fields: Heuristically, each point in the support of a probability measure evolves according to a probability distribution on the space of admissible velocities, whose law is dictated by the nonlocal interaction of the evolving state. This can be thought of as an evolving system in which uncertainty affects both the position and velocity of the particles, depending on some probability distribution. We elaborated on a rather flexible theory that allows for discrete-to-continuous limits and provides a deep connection to the general theory of dissipative evolutions in Hilbert spaces [9,10].

### Discrete and geometric structures for non-linear quantum drift-diffusion models

We addressed the challenging fourth-order Derrida-Lebowitz-Speer-Spohn nonlinear partial differential equation arising in quantum drift-diffusion. Inspired by the geometric and dynamical insights of optimal transport, we introduced [11] a suitable discretization that is able to capture the amazing structures of this remarkable equation, and we also showed a novel gradient flow formulation in terms of a metric that generalizes Martingale transport. The discrete ►

[5] Chizat, L., Peyré, G., Schmitzer, B. & Villard, F.-X. Unbalanced optimal transport: dynamic and Kantorovich formulations. *J. Funct. Anal.* 274(11), pp. 3090–3123 (2018).

[6] Kondratyev, S., Monsaingeon, L. & Vorotnikov, D. A new optimal transport distance on the space of finite Radon measures. *Adv. Differential Equations* 21(11-12), pp. 1117–1164 (2016).

[7] Liero, M., Mielke, A. & Savaré, G. Optimal entropy-transport problems and a new Hellinger-Kantorovich distance between positive measures. *Invent. Math.* 211(3), pp. 969–1117 (2018).

[8] Savaré, G. & Sodini, G.E. (2023).



[9] Cavagnari, G., Savaré, G. & Sodini, G.E. (2022).

[10] Cavagnari, G., Savaré, G. & Sodini, G.E. A Lagrangian approach to dissipative evolutions in Wasserstein spaces. *arXiv* :2305.05211 (2023).

[11] Matthes, D., Rott, E.-V., Savaré, G. & Schichtling, A. A structure-preserving discretization for the Derrida-Lebowitz-Speer-Spohn equation based on diffusive transport. *arXiv*:2312.13284 (2023).

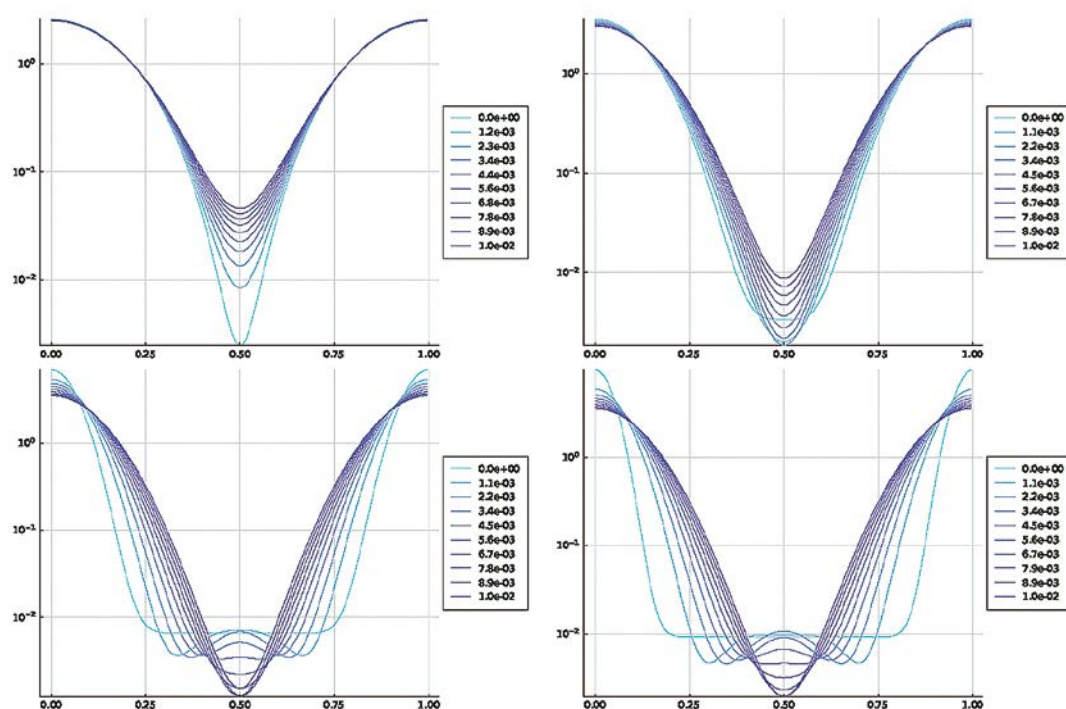
[12] Fornasier, M., Savaré, G. & Sodini, G.E. (2023).

[13] Sodini, G.E. The general class of Wasserstein Sobolev spaces: density of cylinder functions, reflexivity, uniform convexity and Clarkson's inequalities. *Calculus of Variations and Partial Differential Equations* 62, p. 212 (2023).

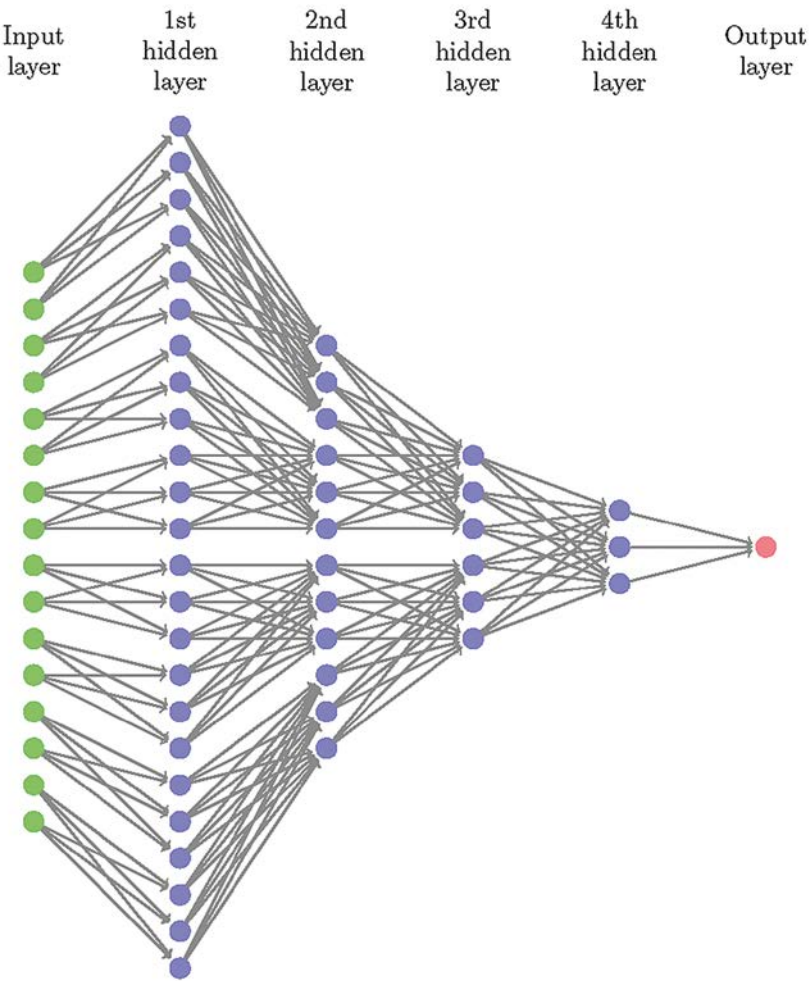
dynamics inherit this gradient flow structure as well as further properties, such as contractivity in the Hellinger distance and monotonicity of several Lyapunov functionals. Using all these features, we are able to perform a precise approximation of the solutions, showing also anti-diffusive behavior and delicate effects when the positive solution approaches 0 at some point (Fig. 2).

### Approximation theory, computing, and deep learning on the Wasserstein space

The challenge of approximating functions in infinite-dimensional spaces from finite samples is widely regarded as formidable. We devoted part of our investigation to the problem of the numerical approximation of Sobolev-smooth functions defined on probability spaces. Since measures can be used to represent data in an efficient way and can be used in problems of image comparison or character classification, it is thus relevant to provide a general functional analytic framework. First of all, we studied a notion of Sobolev space on the Wasserstein spaces of probability measures, [12,13] ►



**Fig. 2.** (from [11]). Logarithmic plot of numerical solutions exhibiting anti-diffusive behavior.



**Fig. 3,** (from [15]). The architecture of the neural network representing the maxima function in the Euclidean space of dimension 16.

**[14]**Heinonen, J., Koskela, P., Shanmugalingam, N. & Tyson, J.T. Sobolev spaces on metric measure spaces: an approach based on upper gradients. *New Mathematical Monographs* (27), pp. xii+434. Cambridge: Cambridge University Press (2015).

**[15]**Fornasier, M., Heid, P. & Sodini, G.E. Approximation Theory, Computing, and Deep Learning on the Wasserstein Space, *arXiv:2310.19548* (2023).

and connected it with the theory of Sobolev spaces in metric measure spaces [14]. We then leveraged the theory of metric Sobolev spaces and combined it with techniques from optimal transport, variational calculus, and large deviation bounds [15]. In our numerical implementation, we used appropriately designed neural networks to serve as basis functions (Fig. 3). This approach allows us to approximate functions that can be rapidly evaluated after training. As a result, our constructive solutions significantly increased the evaluation speed while maintaining the same accuracy, improving state-of-the-art methods by several orders of magnitude.

These themes were at the heart of the workshop Optimal Transport, Mean-Field Models, and Machine Learning (OTMFML), which we organized at the end of the Focus Group activity in collaboration with Martin Burger and Gabriel Peyré. The aim of the workshop was to highlight the interactions between optimal transport, mean-field control, and machine learning, to address the crucial problems of high dimensionality, nonlinearity, and nonconvexity, and to look for best examples and practices of successful use of mathematics to provide guarantees for practicable machine learning. ■

**Selected publications**

Ambrosio, L., Fornasier, M., Morandotti, M. & Savaré, G. Spatially Inhomogeneous Evolutionary Games. *Communications on Pure and Applied Mathematics* 74(7), pp. 1353-1402 (2021). [www.doi.org/10.1002/cpa.21995](http://www.doi.org/10.1002/cpa.21995).

Cavagnari, G., Savaré, G. & Sodini, G.E. Dissipative probability vector fields and generation of evolution semigroups in Wasserstein spaces. *Probability Theory and Related Fields* (2022). [www.doi.org/10.1007/s00440-022-01148-7](http://www.doi.org/10.1007/s00440-022-01148-7).

Fornasier, M., Savaré, G. & Sodini, G.E. Density of subalgebras of Lipschitz functions in metric Sobolev spaces and applications to Wasserstein Sobolev spaces. *Journal of Functional Analysis* 285(11), (2023). [www.doi.org/10.1016/j.jfa.2023.110153](http://www.doi.org/10.1016/j.jfa.2023.110153).

Liero, M., Mielke, A. & Savaré, G. Fine Properties of Geodesics and Geodesic  $\lambda$ -Convexity for the Hellinger-Kantorovich Distance. *Arch. Ration. Mech. Anal.* 247(6), p. 112 (2023). [www.doi.org/10.48550/arXiv.2208.14299](http://www.doi.org/10.48550/arXiv.2208.14299).

Savaré, G. & Sodini, G.E. A relaxation viewpoint to Unbalanced Optimal Transport: duality, optimality and Monge formulation. *arXiv:2401.00542* (2023). [www.doi.org/10.48550/arXiv.2401.00542](http://www.doi.org/10.48550/arXiv.2401.00542).

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## Focus Group: Rethinking Patterns of (In)equity and Diversity in Architectural Education and Professional Practice

Prof. Meike Schalk (KTH Royal Institute of Technology, Stockholm), Alumna Anna Boyksen Fellow | Prof. Dietrich Erben (TUM), Prof. Uta Graff (TUM), The Parity Board (TUM), Prof. Paula-Irene Villa Braslavsky (LMU), Collaborators | Host: Prof. Benedikt Boucsein (TUM)



Prof. Meike  
Schalk

# Equity and diversity in architecture

**This Focus Group was concerned with cultures and institutionalized patterns of equity and diversity within the field of the built environment, both in professional practice and in higher education. We aimed to show how (in)equalities are embedded, produced, and reproduced in architectural representations, discourses, norms, policies, curricula, and working regimes.**

[1] Schalk, M. *et al.* (2022).

[2] Schalk, M. *et al.* (2023).

We defined five areas of action: 1) diversifying research education through online courses; 2) strengthening the work of the TUM School of Engineering and Design's Parity Board; 3) curriculum workshops; 4) gender research on professional practice; and 5) future European research collaboration on EDI (equality, diversity, and inclusion) and learning.

### Diversifying research education in architecture

We developed an online, one-year-long program for doctoral training, [Approaching Research Practice in Architecture](#), with the BauHow5 Alliance – TUM, Delft University of Technology, ETH Zurich, Chalmers University of Technology in Gothenburg, University College London (UCL) – and the Swedish research school ResArc (KTH Royal Institute of Technology, Lund University). The program ran twice, 2020-2021 and 2021-2022, starting with an [international workshop](#) for doctoral candidates in October 2020 and 2021. Due to its accessibility, the online program could include doctoral candidates

from universities in Africa, Asia, Europe, and the Middle East. Broadening the participation made us review the standard Eurocentric references and rework literature lists, agendas, and research questions, making each module critical and meaningful for a more diverse group of 25-30 doctoral candidates. The program concluded with the publications “Species of Theses and Other Pieces” (2022) [1], and “Material Practices” (2023) [2]; the latter was also conceived as an exhibition and shown at AJA 2023, the annual exhibition of the TUM Department of Architecture (Fig.1).

### Parity Board and Parity Jour Fixes

The Focus Group is part of the [Parity Board](#) (PB) at the TUM School of Engineering and Design, an exemplary self-organized and student-led entity, which includes students as well as teaching and administrative staff on all levels. It works to strengthen gender equality, diversity, and equal opportunities by formulating aims, developing strategies, and critically monitoring the progress of the implementation of EDI policies. The PB orga-



**Fig. 1.** Approaching Research Practice in Architecture, a two-year-long research education program, concludes with its second publication and an exhibition at AJA 2023, Jahresausstellung, TUM Dept. of Architecture, 9-14 October 2023. © Isabel Mühlhaus

nizes public [Parity Jour Fixes](#) that foreground structural discriminations within institutions and respond to and discuss actual issues at TUM. Public events include joint activities with similar groups at related architecture departments, i.e., in Switzerland, Austria, Sweden, and the USA. The PB also conducted a study visit to KTH in 2022 (Fig. 2).

#### Curriculum workshops

Two workshops on curriculum changes and learning were held in December 2021 with

students, junior staff, and the invited guests, Ann Fontayne of ETH Zurich, Khensani de Klerk of Matri-Archi(tecture) and ETH Zurich, and Rosario Talevi (Floating University Berlin). The workshops led to the emergence of new networks among the students and the co-organization of the symposium [Curriculum Comedy](#) in October 2022. Twenty interviews were conducted with the symposium speakers on curricula and pedagogies in the face of climate and social justice crises to be published in the forthcoming Curriculum Report (2024) [3]. ►

[3] Schalk, M. *et al.* in press (2024).



- [4] Schuster, S. *et al.* Women in Architecture. Munich: Technical University Munich, Chair of Architectural Design and Timber Construction (2018).
- [5] Stjernberg, M. S. "Gender balance on architectural companies' boards". *Arkitekten* (2019). [www.arkitekten.se/nyheter/sa-ar-konsfordelningen-i-arkitektforetagens-styrelser/](http://www.arkitekten.se/nyheter/sa-ar-konsfordelningen-i-arkitektforetagens-styrelser/)

### Gender equity in architectural practice research

The ongoing pilot research project Invisible Labor: Women Steering Large Architectural Firms (IL) is inspired by the TUM pilot research project Women in Architecture [4], which presented statistical data on gender gaps and experiences through interviews with women working within architecture in Germany. IL has gathered comparative Swedish data and conducted interviews with leading women architects in two of the largest Swedish architectural companies, which are predominantly led by women (59%) [5]. The study asks how these equitable gender

relations regarding status and income were made possible and where the Swedish model also fails. Based on the findings of the two studies, the Focus Group aims to develop a larger research application that goes beyond the category of gender equality to include intersectional perspectives on architectural labor and alternative professional practices.

### Future research collaboration

The Focus Group collaborates with the BauHow5 EDI group in the research proposal Mapping and Intervening in Obstacles to Inclusive Built Environment Design and Ed-



**Fig. 2**, Parity Jour Fixe No. 29: Code of Conduct, at TUM Pavillon 333, on 21 July 2023. Workshop with staff and students of TUM Dept. of Architecture on equitable and sustainable working culture, with presentations by Torsten Lange, Uta Leconte and Meike Schalk, curated by the student initiative SOFT – School of Transformation. © Matthias Faul

education, which was submitted to Horizon Europe. It states that future learning needs to innovatively tackle intersecting obstructions to inclusive learning in the built environment sector to support students marginalized by inequalities, such as poverty, racism, LGBTQ+, mental health, or disability. The proposal extends from an understanding that built environment learning methods still predominantly privilege competitive behaviors and higher-income/educated familial backgrounds. This issue undermines the sector's ability to create cohesive societies and respond effectively to critical challenges. The application proposes intervening through

co-development, with students and staff, of inclusive learning resources to mitigate against discrimination. The aim is to prioritize EDI in the education of future generations of built environment designers to meet the complex societal and environmental challenges that shape our cities and communities.

The main aims of this Focus Group were to raise awareness of existing inequities in studies and practices of architecture and to address possible cultural and structural changes within the TUM Department of Architecture. ■

#### Selected publications

Schalk, M., Lange, T., Putz, A., Stevanovic, T. & Markus, E. Species of Theses and Other Pieces. Dimensions. *Journal of Architectural Knowledge* 2(3), 13-22, (2022). [www.doi.org/10.14361/dak-2022-0302](https://doi.org/10.14361/dak-2022-0302).

Schalk, M., Reisinger, K., Markus, E. & Leconte, U. Material Practices: Positionalities, Methodologies, Ethics. Munich: TUM School of Engineering and Design (2023). Publication and exhibition posters. Retrieved from <https://mediatum.ub.tum.de/1725721>.

Schalk, M., Schmidt, J., & SOFT – School of Transformation (TUM). Curriculum Report. Munich: TUM School of Engineering and Design, in press (2024).

Schalk, M. Bredella, N., Hallama, D. & Lange, T. Frauen in großen Architekturbüros. Figuren von Gender. Berlin: TU Berlin University Press, in press (2024).

**For a full list of publications, please visit** [www.ias.tum.de/ias/schalk-meike/](http://www.ias.tum.de/ias/schalk-meike/)

## Focus Group: Simulation and Digital Twin

**Prof. Barbara Solenthaler (ETH Zurich)**, Alumna Hans Fischer Fellow (funded by the Siemens AG) | **Erik Franz (TUM)**, Doctoral Candidate | Host: **Prof. Nils Thürey (TUM)**



**Prof. Barbara Solenthaler**

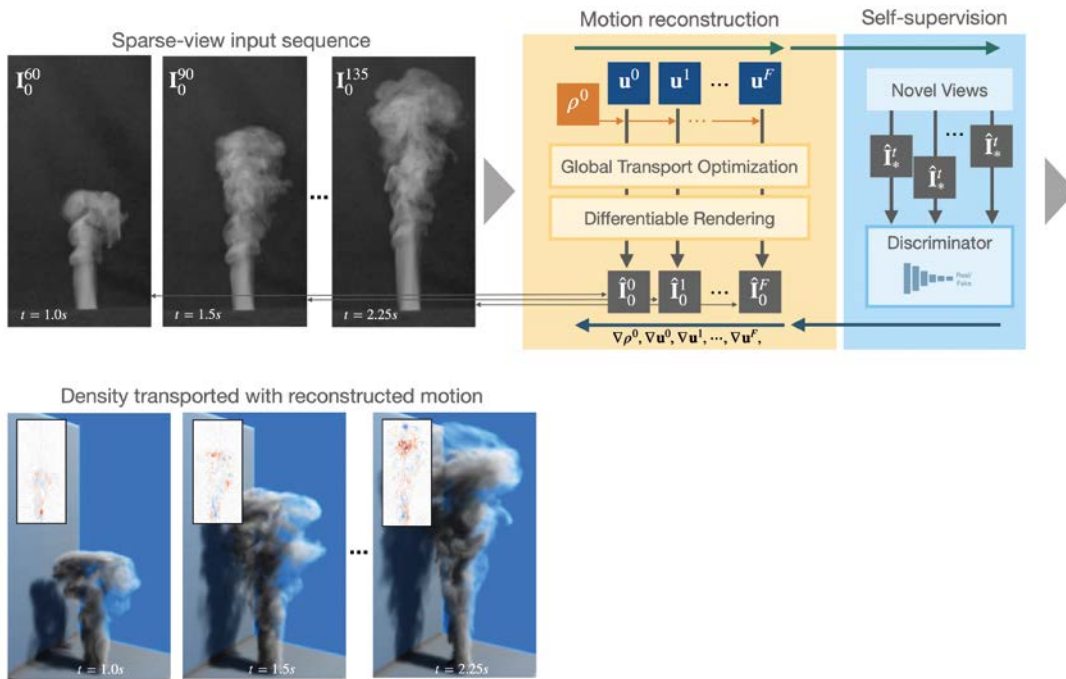
# Data-driven flow capture and reconstruction

**The Focus Group devised data-driven techniques for reconstructing 3-D motion in flows using sparse and single-view video inputs. Our approach introduces a global transport formulation, establishing a connection between real-world capture data and a differentiable physics solver. We conducted training for neural networks to infer 3-D motion from monocular videos in the absence of 3-D reference data.**

The Simulation and Digital Twin Focus Group conducted research on fluid capture and the comprehensive description of flow dynamics. Traditional fluid capture methods often entail intricate hardware configurations and calibration procedures, creating a demand for simpler systems. An example is the video-based flow capture stage developed within Thürey's research group at TUM. Estimating motion from input videos presents a formidable challenge due to motion being a secondary quantity, indirectly derived from changes observed in transported markers

such as density. Unlike the single-step estimation in optical flow, motion estimation typically involves multiple interconnected steps to achieve stable global transport. Additionally, in this context, the volume distribution of markers is usually unknown and requires concurrent reconstruction during motion estimation.

In our TUM-IAS project, we utilized a high-resolution dataset acquired through Thürey's multi-view capture setup for precise tomography reconstructions. In the



**Fig. 1,** We present a novel algorithm that reconstructs the motion of a single initial state over the full course of an input sequence, i.e., its global transport. On the basis of a learned self-supervision, our algorithm yields a realistic motion for highly under-constrained scenarios such as a single input view.

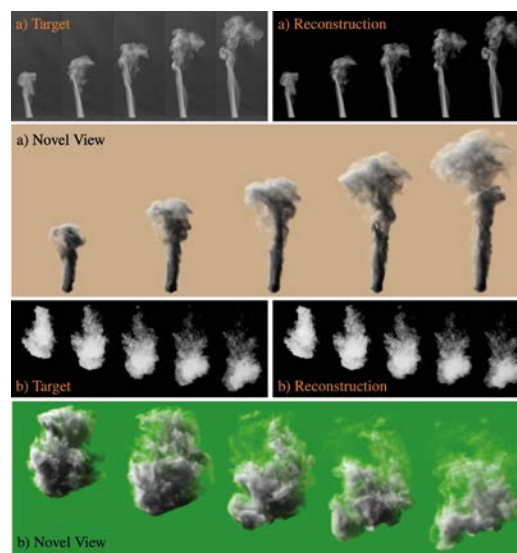
initial phase of the project, we integrated real-world captured data into a differentiable physics solver and employed optimization techniques to reconstruct volumetric flows from sparse views, employing a global transport formulation. Rather than deriving the space-time function of observations, our approach reconstructs motion on the basis of a single initial state. Additionally, we introduced a learned self-supervision mechanism, which imposes constraints on observations from unseen angles. These visual constraints are interconnected through

transport constraints and a differentiable rendering step, resulting in a robust end-to-end reconstruction algorithm (Fig. 1). This enables the reconstruction of highly realistic flow motions, even from a single input view. Through a range of synthetic and real flow scenarios, we demonstrated that our proposed global reconstruction of the transport process significantly enhances the reconstruction of fluid motion. ►

We observed a notable interest in single-view motion estimation, achieved by incorporating physical priors in the form of governing equations. However, despite robust priors, dealing with the fully unconstrained depth dimension in a single viewpoint remains a challenge. In the latter part of the project, we introduced a deep learning-based approach where a neural network learns to represent underlying motion structures. This allows almost instantaneous, single-pass motion inference without relying on ground truth motion data – a crucial aspect, especially for complex volumetric motions where direct acquisition of reference motions is impractical. Addressing the challenge of training neural networks to infer 3-D motions from monocular videos without available 3-D reference data, we employed an unsupervised training approach using observations from real-world capture setups. This involved generating an initial prototype volume, which is then moved and transported over time without volumetric supervision. Our method relies solely on image-based losses, an adversarial discriminator network, and regularization. It demonstrates the ability to estimate stable long-term sequences, closely matching targets for inputs such as rising smoke plumes (Fig. 2).

A current limitation in our methods is their exclusive support for white smoke, necessitating an extension of the rendering model for scenarios involving anisotropic scattering, self-illumination, or alternative materials. Additionally, our transport model relies on advection without obstructions, suggesting the potential for extensions to accommodate obstacles or multi-phase flows. To enhance long-term stability further, the method could be expanded to convey information about future time steps, offering improved guidance.

In summary, our TUM-IAS project successfully achieved its initial objective of bridging real-world flow-captured data with physics simulations through deep learning methods, facilitating a high-quality mapping between diverse data sources. Notably, we demonstrated that our networks can be effectively trained with single-view data and short time horizons, maintaining stability for extended sequences during inference. The resulting global trajectories from the neural global transport are both qualitatively and quantitatively competitive with single-scene optimization methods that demand significantly longer runtimes. This establishes our approach as a crucial factor for practical translation. ■



**Fig. 2.** Single-view reconstructions. Top left: input views; top right: reconstruction from input view; bottom: different viewpoint with modified lighting. Our algorithm successfully reconstructs realistic motions for wispy smoke (a), as well as thicker volumes (b).

**Selected publications**

Franz, E., Solenthaler, B. & Thürey, N. Learning to Estimate Single-View Volumetric Flow Motions without 3-D Supervision. *International Conference on Learning Representations (ICLR)* (2023).

Franz, E., Solenthaler, B. & Thürey, N. Global Transport for Fluid Reconstruction with Learned Self-Supervision. Conference on *Computer Vision and Pattern Recognition (CVPR)* (2021).

Wiewel, S., Kim, B., Azevedo, V.C., Solenthaler, B. & Thürey, N. Latent Space Subdivision: Stable and Controllable Time Predictions for Fluid Flow. *Computer Graphics Forum* 39(8), 15-25 (2020).

Kim, B., Azevedo, V.C., Thürey, N., Kim, T., Gross, M. & Solenthaler, B. Deep Fluids: A Generative Network for Parameterized Fluid Simulations. *Computer Graphics Forum* 38(2), 59-70 (2019).

Tang, J., Kim, B., Azevedo, V.C. & Solenthaler, B. Physics-Informed Neural Corrector for Deformation-based Fluid Control. *Computer Graphics Forum* 42(2), 161-173 (2023).

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## Focus Group: Comparative-Historical Perspectives on Platform Capitalism

Prof. Kathleen Thelen (Massachusetts Institute of Technology), Alumna Hans Fischer Senior Fellow | Patrick Baldes (TUM), Doctoral Candidate | Host: Prof. Eugénia da Conceição-Heldt (TUM)



Prof. Kathleen Thelen

# Comparative-Historical Perspectives on Platform Capitalism

**The projects undertaken during my Fellowship year explored the regulation of new digital platform firms in a broad comparative-historical perspective.**

[1] Thelen, K. (forthcoming).

[2] Foster, C. *et al.* (2023a).

[3] Foster, C. *et al.* (2023b).

In a wide range of industries, the advent of the new platform business model poses a host of new regulatory challenges. Among other things, new global giants such as Amazon and Google have put competition and antitrust policy at the top of the public policy agenda. The activities I undertook – both individually and in collaboration with colleagues at TUM – during my research year focused on analyzing these changes in a broad comparative-historical perspective. The results of the projects I undertook over the course of my Fellowship are summarized below.

I completed a book entitled *Attention, Shoppers! American Retail Capitalism and the Rise of the Amazon Economy* [1]. This book situates the development of retail capitalism in the United States in a comparative-historical perspective. It traces the origins of the Amazon economy to the late 19<sup>th</sup> century as large-scale retailers capitalized on the uniquely permissive regulatory landscape of the American political economy to outgrow the capacity of the government to regulate them. While their counterparts in Europe faced strong countervailing forces and a far less congenial regulatory landscape, large-

scale retailers in the United States enjoyed judicial forbearance and often active government support as they expanded to national scale. Where they encountered resistance, the fragmented regulatory landscape invited venue arbitrage and outright rule-breaking. And as they grew, America's large discount retailers were able to assemble an ever-growing political support coalition that could be weaponized to head off subsequent regulatory efforts.

I presented this work twice while I was at TUM, once at the Garching campus and once within the Political Science Department at the TUM School of Social Sciences and Technology.

The book is now forthcoming with Princeton University Press.

In addition, I collaborated with TUM post-doctoral researcher Chase Foster on two additional articles.

The first of these, entitled "Brandeis in Brussels? Bureaucratic Discretion, Social Learning, and the Development of Regulated

Competition in the European Union,” [2] explores parallels between proposals for a revision in American antitrust advanced by so-called “neo-Brandeisians” and features of the contemporary EU competition regime.

Within the United States, neo-Brandeisian legal scholars have recently revived the ideas of Supreme Court Justice Louis Brandeis, who championed state regulation that preserved market competition and economic liberty in the face of concentrated private power. Yet ultimately and perhaps paradoxically, it has been Europe and not the United States that has proved more hospitable to accommodating key features of the Brandeisian approach. We explain this outcome by tracing the evolution of EU competition law to gain insight into the social learning processes through which such regimes change over time. We argue that the EU’s administrative system, which provides the European Commission with significant bureaucratic discretion, has facilitated processes of ongoing deliberative adjustment to policy and practice, which over time has resulted in a system of ‘regulated competition’ with striking similarities to the Brandeisian vision. The analysis highlights how administrative law institutions condition how regulatory regimes evolve in response to acquired experience and knowledge.

This article has been published in the meantime, appearing online first in December 2023 in *Regulation and Governance*.

Chase Foster and I also published a short, more policy-oriented blogpost based on this article, and that appeared in the blog *Law and Political Economy*.

Chase Foster and I are currently working on a second article that we also initiated during my Fellowship year. This article is entitled “Coordination Rights, Competition Law and Varieties of Capitalism,” [3] and it provides a new framework for analyzing changes in competition regimes and their impact on the organization of markets.

Competition law – the rules governing where interfirm coordination is allowed and where competition is required – is a key constitutive institution in capitalist markets. Yet comparativists have spent decades debating the varieties of capitalism framework – which places the issue of coordination at the center of the distinction between coordinated and liberal market economies – while paying virtually no attention to cross-national variation in competition regimes. This article develops an original theoretical framework to conceptualize the relationship between competition law and the organization of capitalism. Building on seminal work on US antitrust law by the legal scholar Sanjukta Paul (2020), we identify the distinct ways in which competition regimes in Europe and the United States have enabled and protected different forms of coordination, with important implications for capitalist market structures. We go ►

beyond the usual binaries – “coordinated” versus “liberal market economy,” “restrictive” versus “permissive” antitrust regimes – to disentangle two dimensions of the law that fundamentally shape patterns of coordination and competition both across regulatory jurisdictions and over time. Applying our framework to analyze the evolution of European and American competition law, we show how a comparative coordination rights framework can be used to conceptualize key institutional changes within contemporary capitalist systems.

This article is currently a “Revise and Resubmit” in Comparative Political Studies.

In addition, my host Eugénia da Conceição-Heldt and I convened a workshop on 19 May

2023, on “Governing the Digital Economy” that we hope will result in a special journal issue.

Finally, together with Eugénia da Conceição-Heldt, I co-advised the work of the doctoral candidate Padrick Baldes on the theme “Regulating New Platform Firms,” which will advance our understanding of the regulation of new technologies within the European Union.

In addition, my host Eugenia da Conceicao-Heldt and I convened a workshop on May 19, 2023, on “Governing the Digital Economy” that we hope will result in a special journal issue (Fig. 1). ■



**Fig. 1.** Workshop on “Governing the Digital Economy” on 19 May 2023. © Astrid Eckert

**Selected publications**

Thelen, K. *Attention, Shoppers! American Retail Capitalism and the Origins of the Amazon Economy*. Princeton: University Press (forthcoming).

Foster, C. & Thelen, K. Brandeis in Brussels? Bureaucratic Discretion, Social Learning, and the Development of Regulated Competition in the European Union. *Regulation and Governance* (2023a). [www.doi.org/10.1111/rego.12570](http://www.doi.org/10.1111/rego.12570).

Foster, C. & Thelen, K. Brandeis in Brussels: What American Reformers Can Learn from the European Union. In blog *Law and Political Economy* (LPE project) (2023b). Retrieved from [www.lpeproject.org/blog/brandeis-in-brussels-american-anti-trust-reform-european-union/](http://www.lpeproject.org/blog/brandeis-in-brussels-american-anti-trust-reform-european-union/).

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## Focus Group: Network Dynamics

**Prof. Krasimira Tsaneva-Atanasova (University of Exeter)**, Alumna Hans Fischer Senior Fellow | **Prof. Christian Bick (Vrije Universiteit Amsterdam)**, Alumnus Hans Fischer Fellow | **Tobias Böhle, Elena Gonzalez Herrero (TUM)**, Doctoral Candidates | Host: **Prof. Christian Kuehn (TUM)**



**Prof. Krasimira  
Tsaneva-Atanasova**

# Interconnections that govern crucial aspects of our lives



**Prof. Christian  
Bick**

**Many systems that govern our lives – from transportation networks to the human brain – can be seen as networks of interconnected dynamical units. The coordinated dynamics of all units, such as synchronization, are intricately linked to the system function. This Focus Group develops fundamental insights into factors that determine network dynamics to elucidate the function of real-world networks and to design effective interventions in case of malfunction.**

**[1]** Bick, C., Böhle, T. & Kuehn, C. (2023).

The function of systems of interconnected dynamical units – for example, the human brain, which contains billions of individual neural cells – depends on their emergent dynamical properties. Collective dynamics in networks, such as synchronization, where individual units behave in unison, is intricately linked with the function of these networks. Indeed, coordinated beating of heart cells makes the heart function, while excessive synchrony in the human brain is associated with malfunction and disease. The Focus Group Network Dynamics gains fundamental insights into the factors that govern the collective dynamics of coupled dynamical units, over both short and long time scales. Our results cover both fundamental mathematical theory (such as bifurcations in dynamical systems) and applications to models relevant for real-world networks such as the human heart and brain to build the basis for new intervention techniques to restore healthy function.

Having many interconnected dynamical units is a common feature of systems with complex dynamics. For example, the human brain consists of billions of interconnected neuronal cells. The sheer number of units, however, is an obstacle to obtain mathematical insights. Hence, methods to reduce the complexity and dimensionality of the problem become crucial to understand how, for example, synchrony emerges in these network dynamical systems. In Ref. [1], we develop new approaches for phase reduction, a complexity reduction technique that is applicable to networks where each unit is oscillatory. Our theoretical approach elucidates two important aspects. First, we clarify how the geometry of the oscillation affects the synchronization behavior of the network dynamical system. Second, our technique is applicable beyond commonly applied first-order approximations that are only valid for very weak coupling. In particular, it highlights how (and what)



**Fig. 1,** Many complex systems can be seen as networks: Individual units interact with each other along network connections. For example, the human brain consists of billions of nerve cells that exchange and integrate information using electrical pulses.

nonpairwise nonlinear phase interactions, that is, interactions between three or more units, arise in the reduced network that may be relevant for synchronization behavior if the coupling is stronger.

If network function is linked to synchronization behavior, it is critical to understand whether synchronization persists as the system parameters are varied. For example, only sufficiently strong coupling may lead to synchronization of oscillators with distinct frequencies. Transitions in synchronization behavior can be continuous (a small change in a parameter leads to a small change in the synchrony properties) or discontinuous (small changes can lead to jumps in synchronization behavior – in the latter case, such synchronization transitions are also known as “explosive” transitions due to the rapid change in system dynamics. In phase oscillator networks, for example, explosive transitions can be observed when nonpairwise,

higher-order interactions (which become relevant for stronger coupling) are present. Using an approach from bifurcation theory in Ref. [2], we uncover a universal route to explosive transitions in dynamical systems by showing that variations of generic system parameters can turn a continuous transition into a discontinuous transition. This not only explains how nonpairwise interactions lead to explosive synchronization transitions, but also shows that it is not specific to these nonpairwise interactions but rather a universally expected effect.

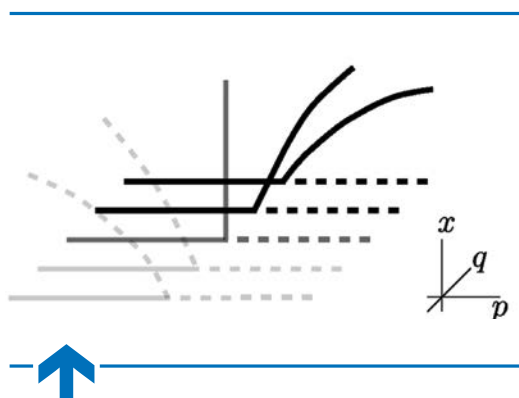
Apart from these universal results, we obtained further insights for specific examples of oscillator networks with a given coupling structure. In Ref. [3], we consider ring-like networks of phase oscillators that give rise to rotating wave solutions – think of synchrony in the form of a merry-go-round or a wave in a stadium. We showed that nonpairwise higher-order interactions can stabilize ►

**[2]** Kuehn, C. & Bick, C. (2021).

**[3]** Bick, C., Böhle, T. & Kuehn, C. (2023).

**[4]** Gonzalez Herrero, M.E., Kuehn C. & Tsaneva-Atanasova K. (2021).

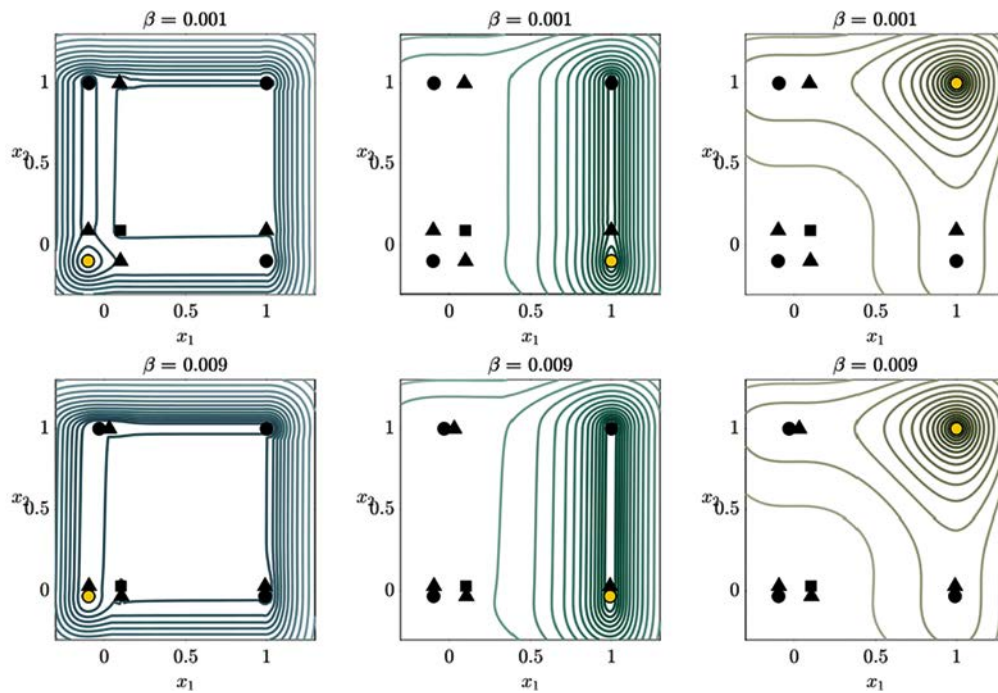




**Fig. 2.** Sketch of changes of criticality in a synchronization transition. Where the solid horizontal line becomes dashed indicates a synchronization transition point as a parameter  $p$  is varied; at this point a second line emerges in the  $x$  direction. Whether the second line is solid or dashed determines whether the synchronization transition is continuous (emerging line is solid) or discontinuous (emerging line is dashed). We show that varying an additional parameter  $q$  (changing shading) generically changes the criticality of the transition from continuous to discontinuous and vice versa. (Kuehn, C., & Bick, C. A universal route to explosive phenomena. *Science Advances* 7(16), (2021))

such solutions, an insight that is beneficial if one wanted to control synchrony in these systems. Moreover, we show that nonpairwise interactions can also turn a continuous transition away from a uniform rotating wave solution to an explosive transition – in line with the universal results expected from our previous research in Ref. [2].

Interactions between individual units are crucial for the functioning of systems that we depend on in our daily lives: Electric signals between excitable heart cells called cardiomyocytes are vital for making the heart contract properly, which is essential for its healthy functioning. By contrast, signaling going wrong can lead to heart problems such as irregular heartbeats (arrhythmia). It is hence crucial to explore different methods to better understand how these heart cells transmit signals, with the goal of finding ways to improve medical treatments. Heart cell behavior is complex and difficult to study using rigorous mathematical analysis. In Ref. [4], we compare two simpler models that capture the important aspects



**Fig. 3,** Illustration of quasipotentials for a three-node network system. Potentials are computed from the yellow-colored dots marked in each panel for different strengths of coupling. The number of metastable states changes with increase in coupling. (Ashwin P, Creaser J, Tsaneva-Atanasova K. Quasipotentials for coupled escape problems and the gate-height bifurcation, *Phys. Rev. E* 107(1), (2023))

of how heart cells work: One mimics how heart cells get excited (the FitzHugh-Nagumo model), and the other is made specifically to mimic heart cells' excitable behavior (the polynomial Karma model). We employ geometric singular perturbation theory to study the dynamical properties of the models. We also look at how these models act in

a one-dimensional space, studying excitable wave propagation. Finally, we run computer simulations to see how changing certain aspects of the models affects how the waves propagate. Our study helps us understand what these models have in common and what makes them different. ►

[5] Ashwin P., Creaser J. & Tsaneva-Atanasova K. (2023).

Brain networks can transition between synchronized and desynchronized states, reflecting various cognitive and physiological conditions in health and disease. Elucidating these transitions is essential to understand healthy brain function. Our focus is on understanding transitions from a “quiescent” to an “active” attractor in networks of multi-stable systems in the presence of random noise. Coupling such systems leads to qualitatively different transient behaviors depending on the coupling strength. With weak coupling, transitions are stochastic, while strong coupling promotes synchronous transitions, which we called a “fast domino” regime. An intermediate regime, called a “slow domino,” shows transitions that can be arbitrarily long. Our previous work has described transition

timings and sequences using potential landscape bifurcations in the low noise limit. In Ref. [5] we now examine noise-induced transitions employing a quasipotential (QP) in scenarios where the coupled system lacks potential, as is often the case in models of real-world systems. Gates, represented by points on the boundary of the basin of attraction with minimal QP concerning the attractor, help characterize the escape rates from the basin. However, alterations in the coupling strength can cause these gates to undergo a global shift. This global gate-height bifurcation marks a general qualitative change in the escape characteristics of parameterized non-gradient dynamical systems subject to small noise. ■

**Selected publications**

Bick, C., Böhle, T. & Kuehn, C. Higher-Order Network Interactions through Phase Reduction for Oscillators with Phase-Dependent Amplitude. *ArXiv* (2023). [www.arxiv.org/abs/2305.04277](http://www.arxiv.org/abs/2305.04277).

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Ashwin P., Creaser J. & Tsaneva-Atanasova K. Quasipotentials for coupled escape problems and the gate-height bifurcation, *Phys. Rev. E* 107(1), (2023). [www.doi.org/10.1103/PhysRevE.107.014213](http://www.doi.org/10.1103/PhysRevE.107.014213).

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## Focus Group: Coding for DNA Storage

**Prof. Eitan Yaakobi (Technion – Israel Institute of Technology)**, Alumnus Hans Fischer Fellow | **Dr. Rawad Bitar (TUM)**, Postdoctoral Researcher | **Andreas Lenz, Lorenz Welter, Anisha Banerjee (TUM)**, Doctoral Candidates | Host: **Prof. Antonia Wachter-Zeh (TUM)**



**Prof. Eitan Yaakobi**

# Coding for Insertions/Deletions and DNA Storage

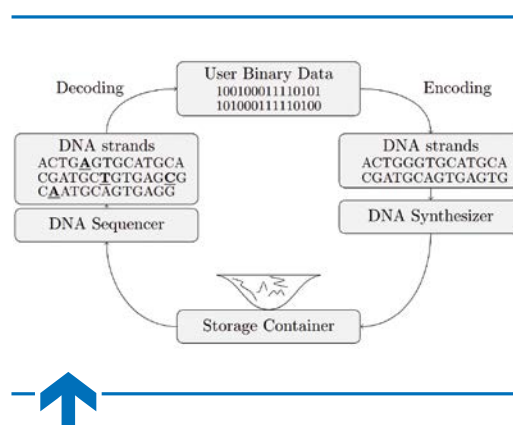


**Prof. Antonia Wachter-Zeh**

**Codes for correcting insertions and deletions, first proposed for communication applications, have particular importance in DNA storage, which is recently attracting attention as a dense and robust storage solution. The data is written on DNA strands by synthesis and read by sequencing. DNA storage has to cope with sequence losses, loss of ordering, and errors such as insertions and deletions.**

In the past decade, drawing on advances in biotechnology, several experiments have demonstrated the viability of DNA as a storage medium that can offer unprecedented information density, archival durability, and device independence. One major impediment to the adoption of this technology is that data coding requirements are fundamentally different from those of existing storage media. To overcome this and realize the full potential of DNA-based storage, it is necessary to establish the technology's information-theoretic limits and to develop coding methods to achieve these limits. To attain this goal, our collaboration focused on several fundamental problems in coding and information theory to improve the reliability and performance of DNA-based storage solutions.

A typical DNA storage system consists of three components (see Fig. 1): (1) DNA synthesis that produces the molecules encoding the data. In state-of-the-art technology acceptable error rates are achieved for synthetic oli-



**Fig. 1.** Illustration of a DNA-based storage system.

gos of length no more than 250-300nt; (2) a storage container to store the synthetic DNA; (3) a DNA sequencing device that serves for reading and for retrieving the data. The encoding and decoding are external processes that convert the binary data into molecules of DNA in a way that enables reconstruction even under errors. From a coding perspective

DNA as a storage system has several attributes that distinguish it from other storage systems. The most prominent one is that the oligos are not ordered in the memory and thus it is not possible to know the order in which they were stored. One solution uses indices, or barcodes, that are stored as part of the oligos. Furthermore, errors in DNA are typically substitutions, insertions, and deletions, while the error rates depend upon the specific technology used for synthesis and sequencing.

In [1], we studied error-correcting codes for the storage of data in synthetic DNA. We investigated a storage model where a data set is represented by an unordered set of  $M$  sequences, each of length  $L$  (see Fig. 4). Errors within that model are a loss of whole sequences and point errors inside the sequences, such as insertions, deletions, and substitutions. We derived Gilbert-Varshamov lower bounds and sphere packing upper bounds on achievable cardinalities of error-correcting codes within this storage model. We further proposed explicit code constructions that can be encoded and decoded efficiently.

Comparing the sizes of these codes to the upper bounds, we showed that many of the constructions are close to optimal.

To explore the information theoretical limits of DNA-based data storage, we studied in [2] a communication system where information is conveyed over many sequences in parallel. The receiver cannot control the access to these sequences and can only draw from these sequences, unaware which sequence has been drawn (see Fig. 2). Further, the drawn sequences are susceptible to errors. We considered a suitable channel model that models this input-output relationship and computed its information capacity for a wide range of parameters. We believe that this analysis can guide future DNA-based data storage experiments by establishing theoretical limits on achievable information rates and by proposing decoding techniques. In [3], we studied coding for the synthesizing DNA, which is the most costly part of existing systems. As a step toward more efficient synthesis, we designed codes that minimize the time and number of cycles to produce the DNA strands. We considered a popular synthesis ►

[1] Lenz, A. *et al.* (2020).

[2] Lenz, A. *et al.* (2023).

[3] Lenz, A. *et al.* (June 2020).

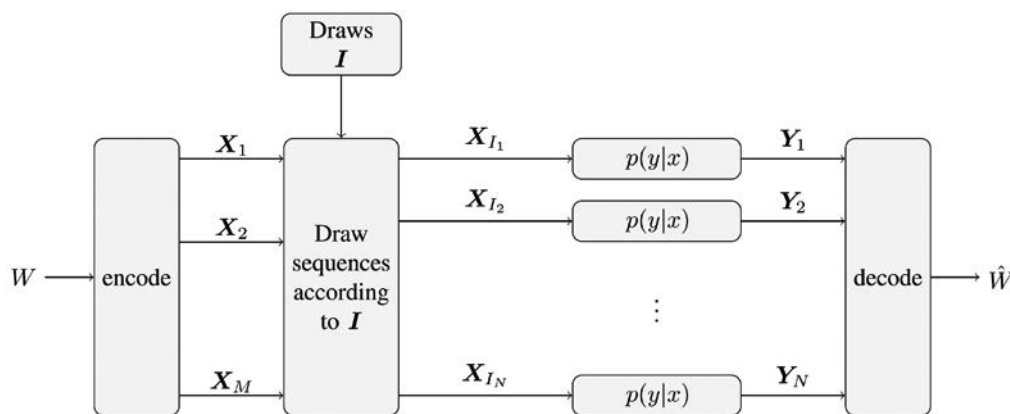
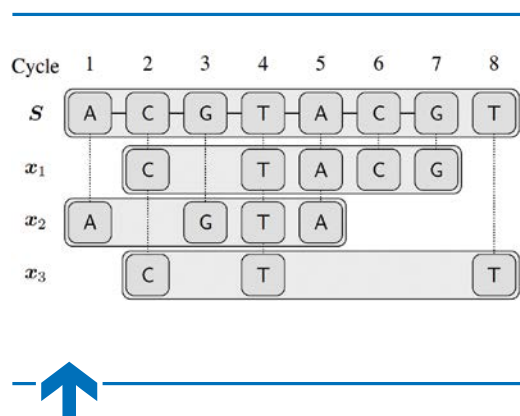


Fig. 2, Visualization of the noisy drawing channel of DNA storage.





**Fig. 3.** The cycle order of synthesizing DNA strands.

[4] Banerjee, A. *et al.* (2023).

[5] Bitar, I. *et al.* (2021).

process that builds many strands in parallel in a step-by-step fashion using a fixed supersequence  $S$ . The machine iterates through  $S$  one nucleotide at a time, and in each cycle, it adds the next nucleotide to a subset of the strands (see Fig. 3). The synthesis time is determined by the length of  $S$ . We showed that by introducing redundancy to the synthesized strands, we can significantly decrease the number of synthesis cycles. We derived the maximum amount of information per synthesis cycle assuming  $S$  is an arbitrary periodic sequence. To prove our results, we exhibited new connections to cost-constrained codes.

In [4], we analyzed synthetic polymer-based data storage, which involves designing molecules of distinct masses to represent the respective bits, followed by the synthesis of a polymer of molecular units that reflects the order of bits. Reading out the stored data requires the use of a tandem mass spectrometer that fragments the polymer into shorter

substrings and provides their corresponding masses, from which the composition, i.e., the number of 1s and 0s in the concerned substring, can be inferred. Prior works have dealt with the problem of unique string reconstruction from the set of all possible compositions, called composition multiset. Additionally, error-correcting schemes to deal with substitution errors caused by imprecise fragmentation during the readout process have also been suggested. Our work built on this research by extending previously considered error models, mainly confined to substitution of compositions. To this end, we defined new error models that consider insertions of spurious compositions and deletions of existing ones, thereby corrupting the composition multiset. We analyzed if the reconstruction codebook proposed in a previous work is indeed robust to such errors and, if not, proposed new coding constraints to remedy this. In [5], we extended the study of codes correcting deletions and insertions to the problem of constructing codes correcting deletions in arrays. Under this model, it is assumed that an array can experience deletions (insertions) of rows and columns. These deletion errors are referred to as crisscross deletions (insertions). We first showed that the problems of correcting crisscross deletions and crisscross insertions are equivalent. Our focus was on code correcting one row and one column deletion. A non-asymptotic bound assures that the redundancy is at least  $2n - 3 + 2\log n$  bits, and a code construction with an existential encoding and an explicit decoding algorithm was presented. The redundancy of the construction is at most  $2n + 4\log n + 7 + 2\log e$ . ■

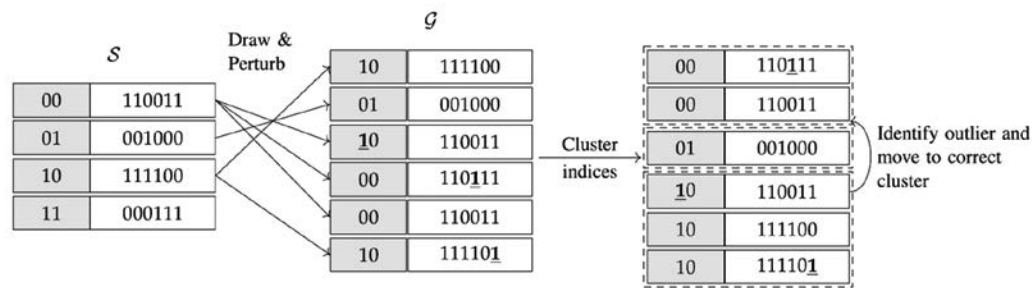


Fig. 4, Exemplary realization of the DNA channel model.

**Selected publications**

Lenz, A., Siegel, P.H., Wachter-Zeh, A. & Yaakobi, E. Coding over Sets for DNA Storage. *IEEE Trans. Inform. Theory* 66, 2331–2351 (2020).

Lenz, A., Siegel, P.H., Wachter-Zeh, A. & Yaakobi, E. The Noisy Drawing Channel: Reliable Data Storage in DNA Sequences. *IEEE Trans. Inform. Theory* 69, 2757–2778 (2023).

Lenz, A., Liu, Y., Rashtchian, C., Siegel, P.H., Wachter-Zeh, A. & Yaakobi, E. Coding for Efficient DNA Synthesis. *IEEE Int’l Symp. on Information Theory*, Los Angeles, California, 2903–2908 (June 2020).

Banerjee, A., Wachter-Zeh, A. & Yaakobi, E. Insertion and Deletion Correction in Polymer-based Data Storage. *IEEE Trans. Inform. Theory* 69, 4384–4406 (2023).

Bitar, R., Smagloy, I., Welter, L., Wachter-Zeh, A. & Yaakobi, E. Criss-Cross Insertion and Deletion Correcting Codes. *IEEE Trans. Inform. Theory* 67, 7999–8015 (2021).

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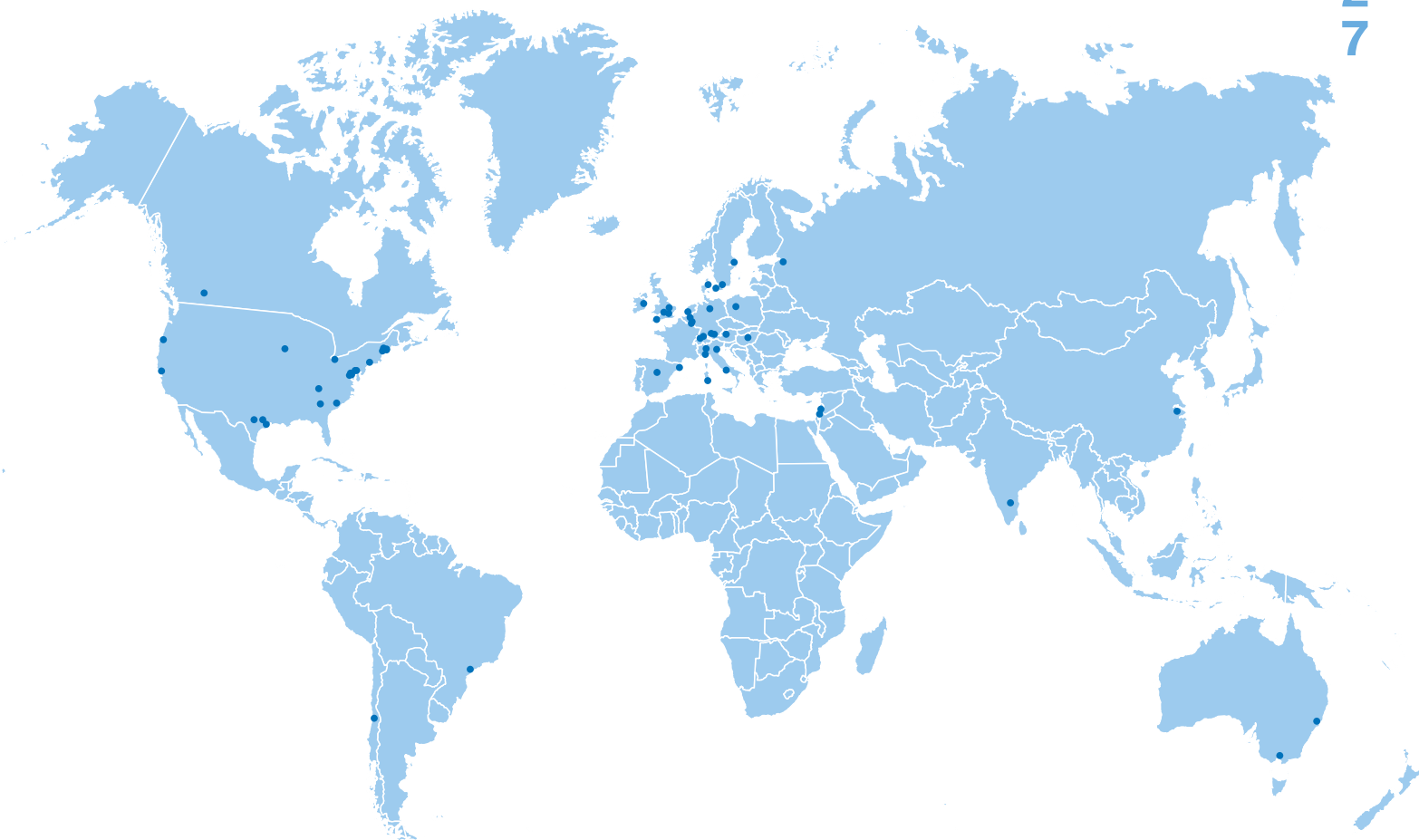
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## Excellence Strategy, Clusters of Excellence, and TUM Budget

After having played a central part in the first two rounds of the Excellence Initiative (2006–2012 and 2012–2019), the TUM-IAS became a permanent institution of TUM, financed out of the general TUM budget.

In addition, the TUM-IAS receives funding from the current Excellence Strategy, thanks to its Anna Boyksen and Albrecht Struppler Clinician Scientist Fellowships, and the Philosopher in Residence program. In addition, the TUM-IAS is collaborating with the Cluster of Excellence e-conversion, which finances several TUM-IAS@e-conversion Hans Fischer Senior Fellowships. A total of three Fellowships are currently funded within this program.

## Third-party funding

### TÜV SÜD Foundation

In 2023, two Philosophers in Residence were appointed for the first time. This new one-year Fellowship is funded by the TÜV SÜD Foundation and the Excellence Strategy. Two more Philosophers in Residence can be appointed in 2024 and 2025.

The TUM-IAS has a long collaboration history with the TÜV SÜD Foundation: after having

funded short-term Visiting Professorships for several years, the foundation funded two Hans Fischer (Senior) Fellows in 2016 and 2019 respectively. With its support for these Fellowships, the foundation aimed to promote research in the fields of energy efficiency and climate protection, test procedures, product and plant safety, and compliance management.

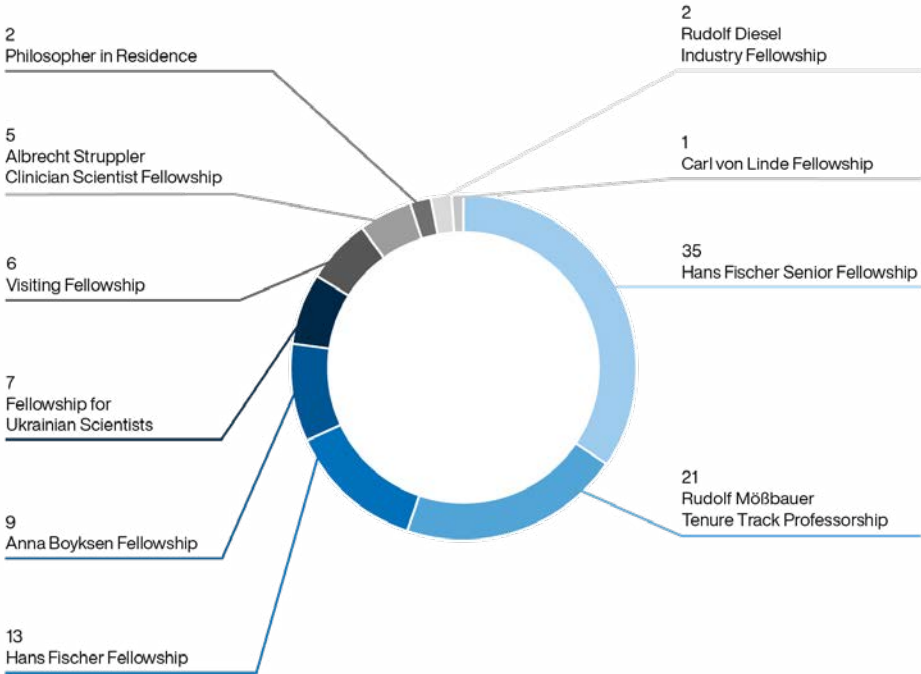
### Siemens AG

Since 2018, the Siemens AG has provided TUM-IAS with a total of EUR 4.6 million over two funding periods, enabling the appointment of two additional Hans Fischer (Senior) Fellowships per year. After the first six Siemens-funded Fellowship concentrated on the areas of Simulation and Digital Twin as well as Future of Autonomous Systems/Robotics, the focus is now on the Industrial Metaverse. So far, eight Fellowships funded by the Siemens AG have been appointed at TUM-IAS.

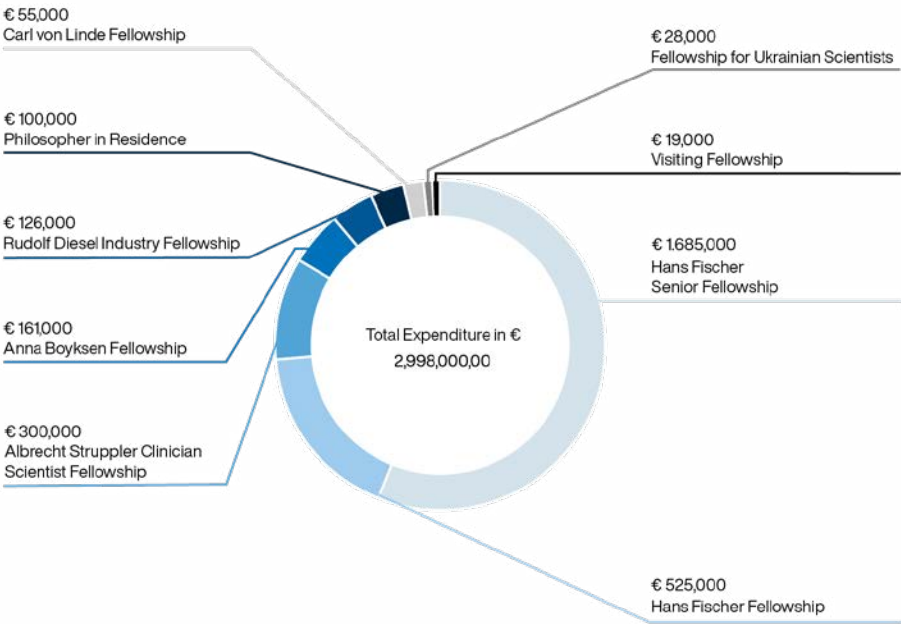
### Georg Nemetschek Institute Artificial Intelligence for the Built World

Since 2022, the Georg Nemetschek Institute has provided funding for one Hans Fischer (Senior) Fellowship per year, focusing on the field of Artificial Intelligence for the Built World. A second Fellowship was awarded in 2023 (please see chapter “Welcome Our New Fellows”).

**Fellow Distribution  
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Category in 2023**

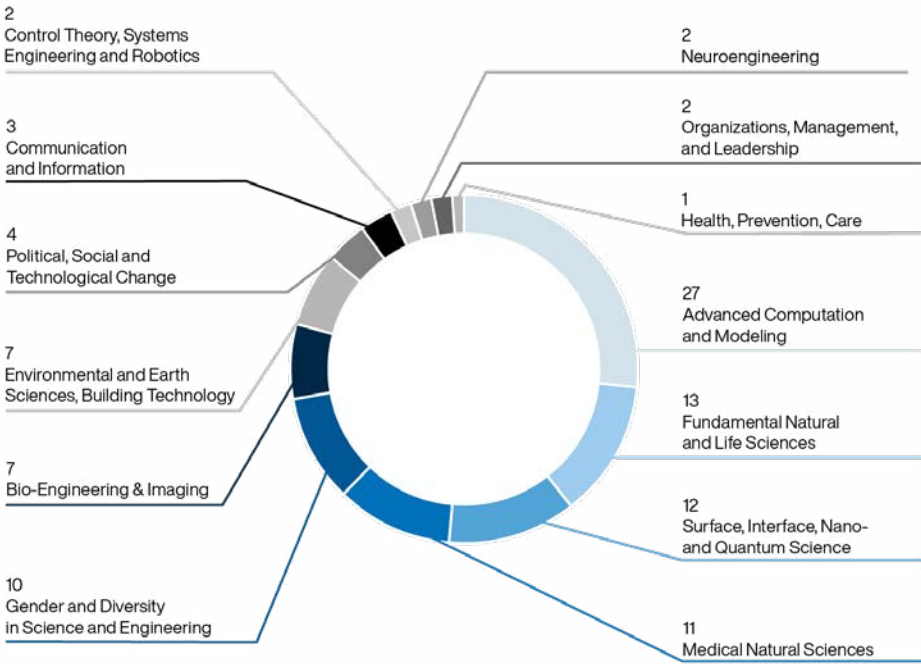


**Expenditure per  
Fellowship Category  
in 2023**

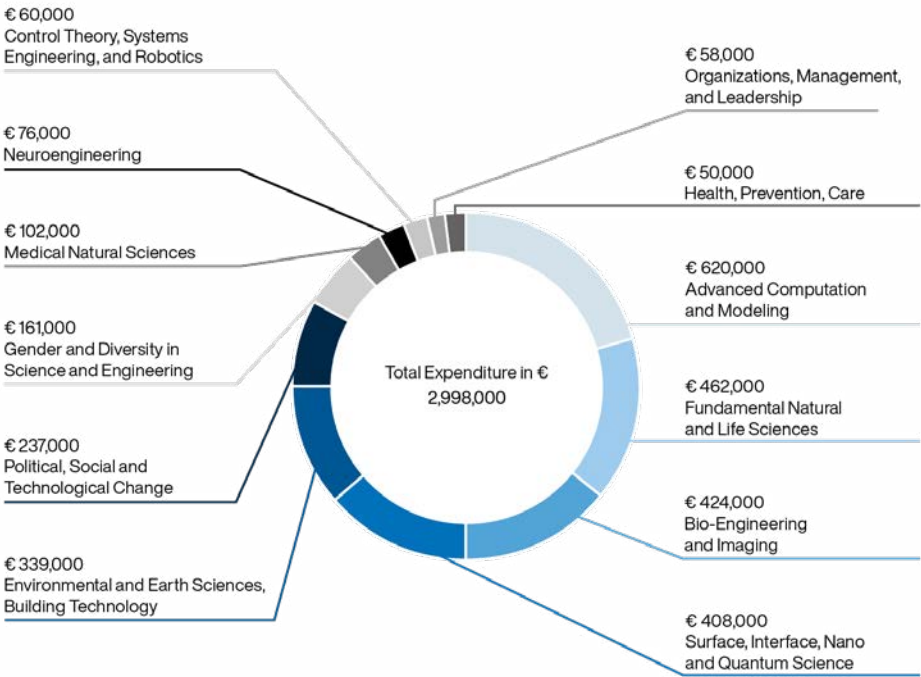




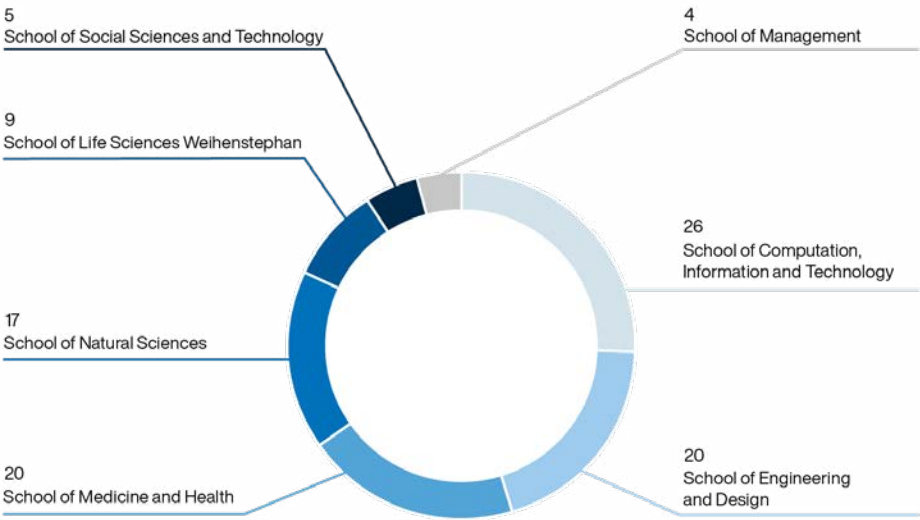
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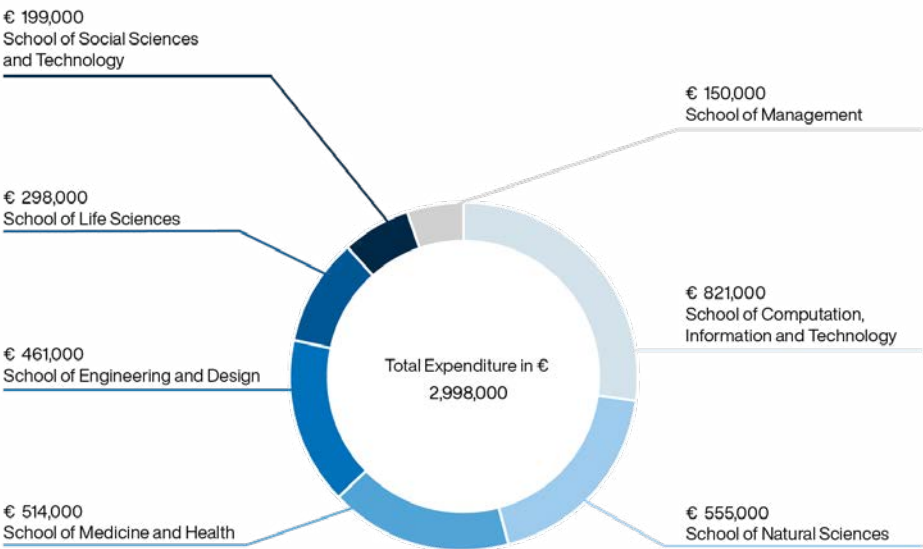
Expenditure  
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**Fellow Distribution  
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**Expenditure  
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in 2023**



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The Board of Trustees is formed by a group of international advisors from academia, research support organizations, and industry. It advises the TUM-IAS director on general scientific, organizational, and technical issues. The Board also defines the general strategy and standards of the TUM-IAS.

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(status: January 2024)

The TUM-IAS Advisory Council is composed mainly of TUM faculty, representing the different research areas of the university and the TUM-IAS. One of its prime functions is advising on the suitability and ranking of Fellow nominations the TUM-IAS receives for its various Fellowship programs. In addition, the Council advises on the scientific and technological course of the TUM-IAS, on the basis of an assessment of the potential and needs of the university. The Advisory Council usually meets three times a year.

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(status: January 2024)

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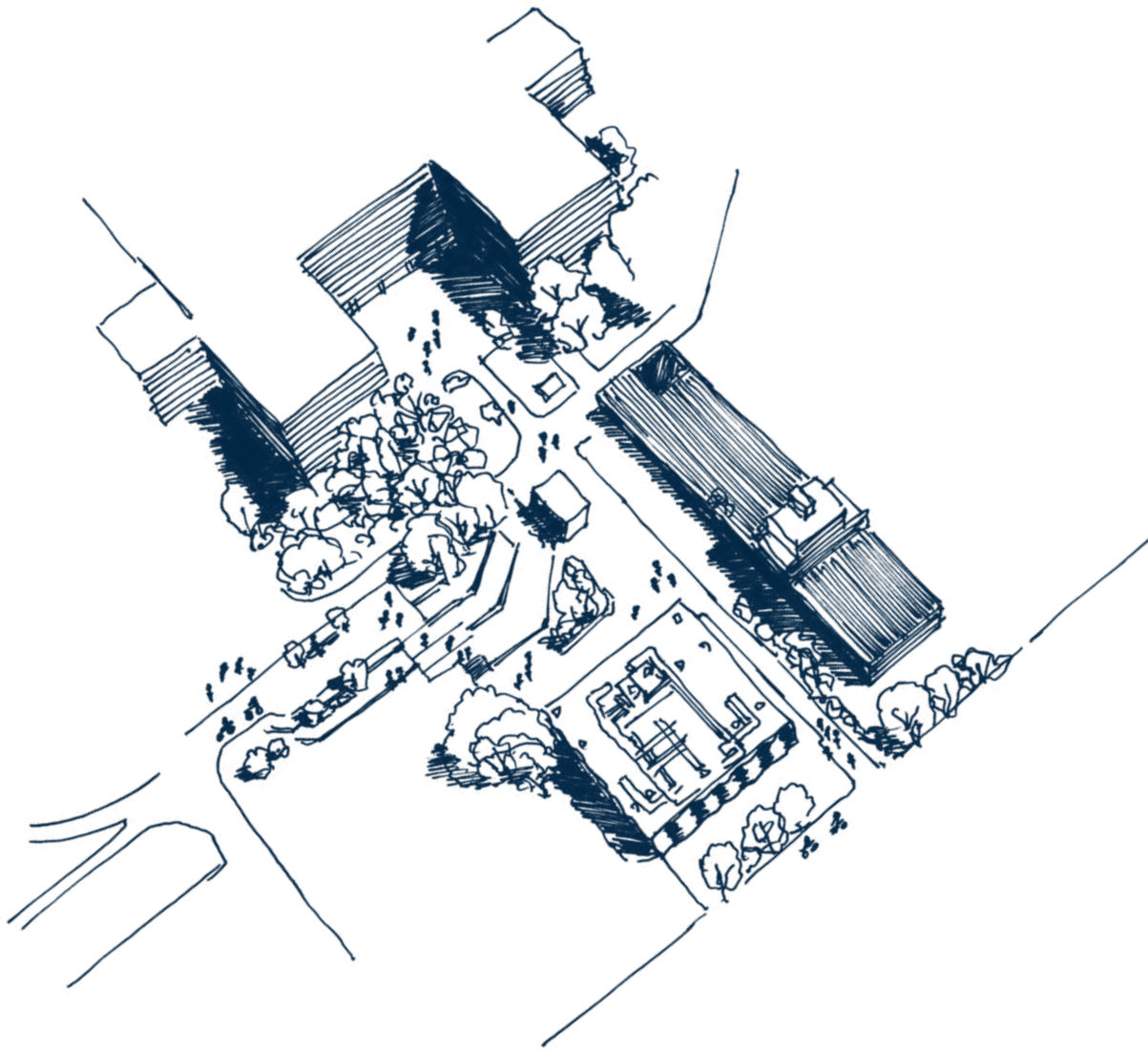
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