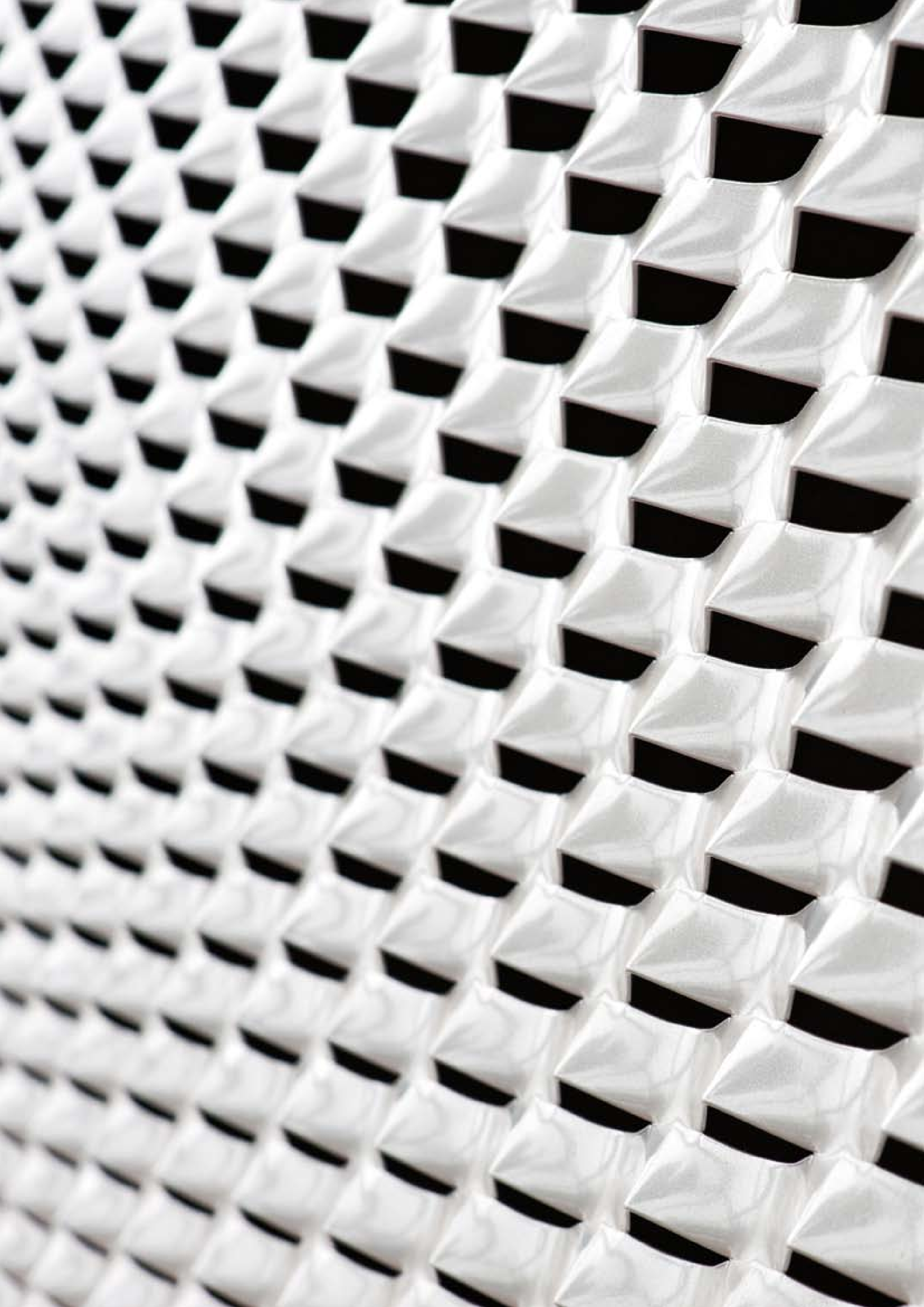
Annual Report

Technische Universität München

Institute for Advanced Study

2010



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Technische Universität München
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A dynamic new intellectual community has sprung up in our midst, given focus and vibrant life by the TUM Institute for Advanced Study. Beyond fostering scientific and technical excellence by freeing top researchers to pursue innovative and risky ideas, the TUM-IAS serves as a role model for interdisciplinary, international, intergenerational, and academic-industrial collaboration.

And while I could add, "just as we planned from the beginning," I also must say that the TUM-IAS continually delivers surprises, further proof that it has developed a life of its own. To give just one recent example: Where could one expect to find researchers in medicine, evolutionary biology, control theory and robotics, risk analysis and business economics, climate-change studies, and forest management devoting a day to understanding and helping to solve each other's scientific problems? A better question is: Where else?

And now, since October 2010, the TUM-IAS has an address, a fine address at the heart of the Garching Research Campus. The ten-million-euro headquarters building was paid for, built, and donated to our university – with no strings attached – by the BMW Group. We are grateful to BMW and our other benefactors for expressing, in such a tangible way, their faith in our entrepreneurial university and its most innovative ventures.

As this Annual Report documents, the TUM-IAS has a lot to show for such a young institution. Its development is largely the story of three ideas, beginning two centuries ago.

The first is Wilhelm von Humboldt's idea of the modern university, with its insistence on research-driven education and the freedom of research and teaching. Two hundred years ago, it was truly revolutionary to assert that leading scientific institutions must treat science as a problem never completely solved, and that they must therefore constantly engage in research, training the next generation of scientists in the process. Today it seems this idea is more alive in elite U.S. universities than in the country where it was invented, but I feel the very spirit of Humboldt lives here in the TUM-IAS.

The second key idea is embodied in the original Institute for Advanced Study, defined by the American educational innovator Abraham Flexner and founded in 1930 by philanthropists who believed in his vision. They offered a new "homeland for thought" to Albert Einstein, John von Neumann, Kurt Gödel and others. That ur-IAS set a new standard for both scholarly and institutional independence – as it stands apart even from nearby Princeton University – and has inspired many other Institutes, including our own.

What makes the TUM-IAS different and, we believe, unique is the idea of integrating an Institute for Advanced Study so completely within a technical university, specifically the technical university with the broadest research portfolio in Germany. Also, leveraging the fact that the Munich region is a heartland for science-based industries, ours is the only IAS worldwide that welcomes industrial researchers. Here it is only natural that unfettered research can and does – in addition to probing fundamental questions about our universe, our planet, and life itself – connect with the most pressing concerns of society, from human health and global change to renewable energy and sustainable economic growth.

From the very start, our TUM-IAS Fellows have made themselves at home in laboratories throughout the university and have welcomed TUM professors, postdocs, and students into their own workshops and events. An already lively circulation of people and ideas has been greatly enhanced by the opening of the headquarters building in Garching. I fully expect this trend to continue, and I also expect further, excellent surprises.

The idea brought to life in the TUM-IAS was the centerpiece of our winning proposal in the Excellence Initiative, a massive investment in the quality and competitiveness of German universities by the federal and state governments. The achievements and promise of the TUM-IAS will figure just as prominently in the next round of competition, now under way. Through its close connections to other major efforts launched by the first round – particularly the TUM Graduate School and the collaborative research centers known as Clusters of Excellence – the Institute has played a central role in their success. I am optimistic that it will have a similar role to play as we execute a second-phase program beginning in 2012.

Wolfgang A. Herrmann
President

2010 has been a most dynamic year for the TUM Institute for Advanced Study. Its physical setup has drastically changed, and its scientific operations have increased dramatically as well. There has been a rush forward toward what we could call a new mode of existence. For the first, as already stated by our President, the BMW Group is responsible; it created and donated our new headquarters, which we have been filling up with life since September. For the second, our Fellowship Program and our Fellows themselves have been the driving force.

Our opening ceremony and the inaugural workshop the next day showed the coming together of the two sides. The Institute had the pleasure of welcoming Dr. Wolfgang Heubisch, Bavarian State Minister for Science, Research and the Arts, and Dr.-Ing. Norbert Reithofer, CEO of the BMW Group, who opened the building officially and handed over the symbolic keys. The opening ceremony was immediately followed by our Inaugural International Symposium on the theme "Energy and Electromobility – Exploring the Fundamental Research Challenges," which brought together top scientists and developers from industry, from research institutes and from TUM itself, where the topic has received topmost attention by more than 30 research groups. In the enterprising style of the Institute, we chose as our keynote speaker one of our young scientists, doctoral candidate Christina Steinkohl, who has been developing statistical modeling for wind farms, using advanced statistical models combined with accurate physical modeling of the complex flow. Such predictions are key for optimizing sustainable energy production in the future.

The Institute has grown considerably in 2010, thanks to a large number of excellent proposals for new Fellows. The growth has been impressive in all Fellow categories, as is well accounted for in the following pages of this annual report. The Institute has put in place a keenly conceived evaluation system as a basis for selection. It is called a "Delphi process," because it tries to avoid both topic and committee bias as much as possible. Indeed, we award Fellowships across fields and have to compare, e.g., a proposal from the Faculty of Architecture with one from Electrical Engineering, and this on the basis of the excellence of the proposed candidate (demonstrated, for Senior Fellows, or potential for Junior). The Delphi process was originally developed by the RAND Corporation after World War II, and has proven to be as fair and effective as is humanly possible. A description of how it works can be found in our "Guidelines for Proposers" (also on our web site). In 2010 we used the Delphi method to select our five new Junior Fellows out of nine proposals. This was the third time we used it, and our Program Managers have proven increasingly adept and professional at executing it. The process is topped off by a final review by our Advisory Council, which carefully oversees the procedures and makes a final judgment, thereby combining the results of the blind ranking process, the goals of the Institute, and the financial possibilities.

Our Fellows have been prodigiously active in 2010. Besides developing their science and realizing their dreams in an uncommonly energetic manner, they and other members of our community have gone out of their way and out of their disciplines to organize a large number of events of various types: exploratory workshops, in which a modest number of top scientists are invited to chart new research avenues; public information workshops around major new themes; inaugural lectures, where Fellows present their ideas and views on the future; as well as lectures and lecture series in which new topics that are not normally covered in curricula are didactically presented. The Institute had the pleasure to welcome a large number of short-term visitors, Visiting Fellows, who each contributed substantially to our event program. Many of them are outstanding scientists with close connections to TUM. Some of our members really went out of their way to promote multi-disciplinarity and mutual understanding between fields; I want to mention Prof. Claudia Klüppelberg and Prof. Peter Wilderer as the most active performers in this respect.

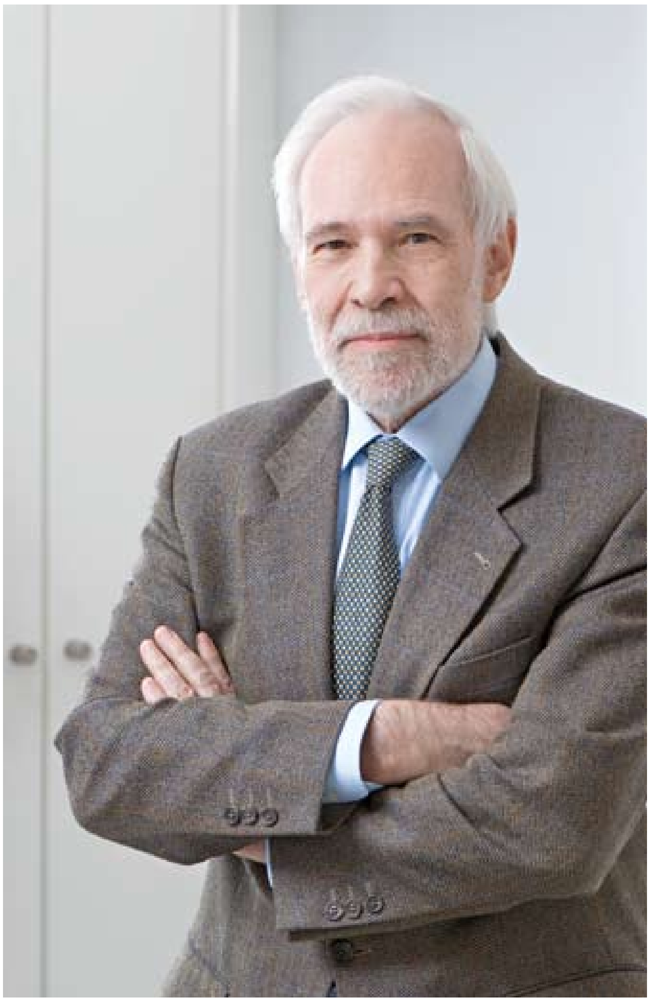
Our staff situation has been very dynamic as well, as detailed in the People section of this annual report – not only because of their enormous dedication and the changes in our operating environment, but also because of some inevitable personnel movements.

To make the Excellence Initiative a success, the coordinated efforts of all its constituents are needed, as well as their integration within our "Unternehmerische Universität," the "Entrepreneurial University." The TUM-IAS has profited greatly from the many cooperations in this context: the Clusters of Excellence; the TUM Graduate School, and particularly the IGSSE (International Graduate School of Science and Engineering) as the home base of many of our doctoral candidates; the Deans of our Faculties, who have contributed many nominations; UnternehmerTUM, TUM ForTe and its patent office; the Corporate Communications Center; the Offices of our President and our Chancellor, Dr. Albert Berger; and many Faculty offices.

The TUM-IAS is now in a position to develop as the intellectual center of the Garching Research Campus. It will put its full young energy to that task, in collaboration with all parties, inside and outside the Technische Universität München, who have a stake in making Munich shine as one of the main centers of scientific excellence in the world.

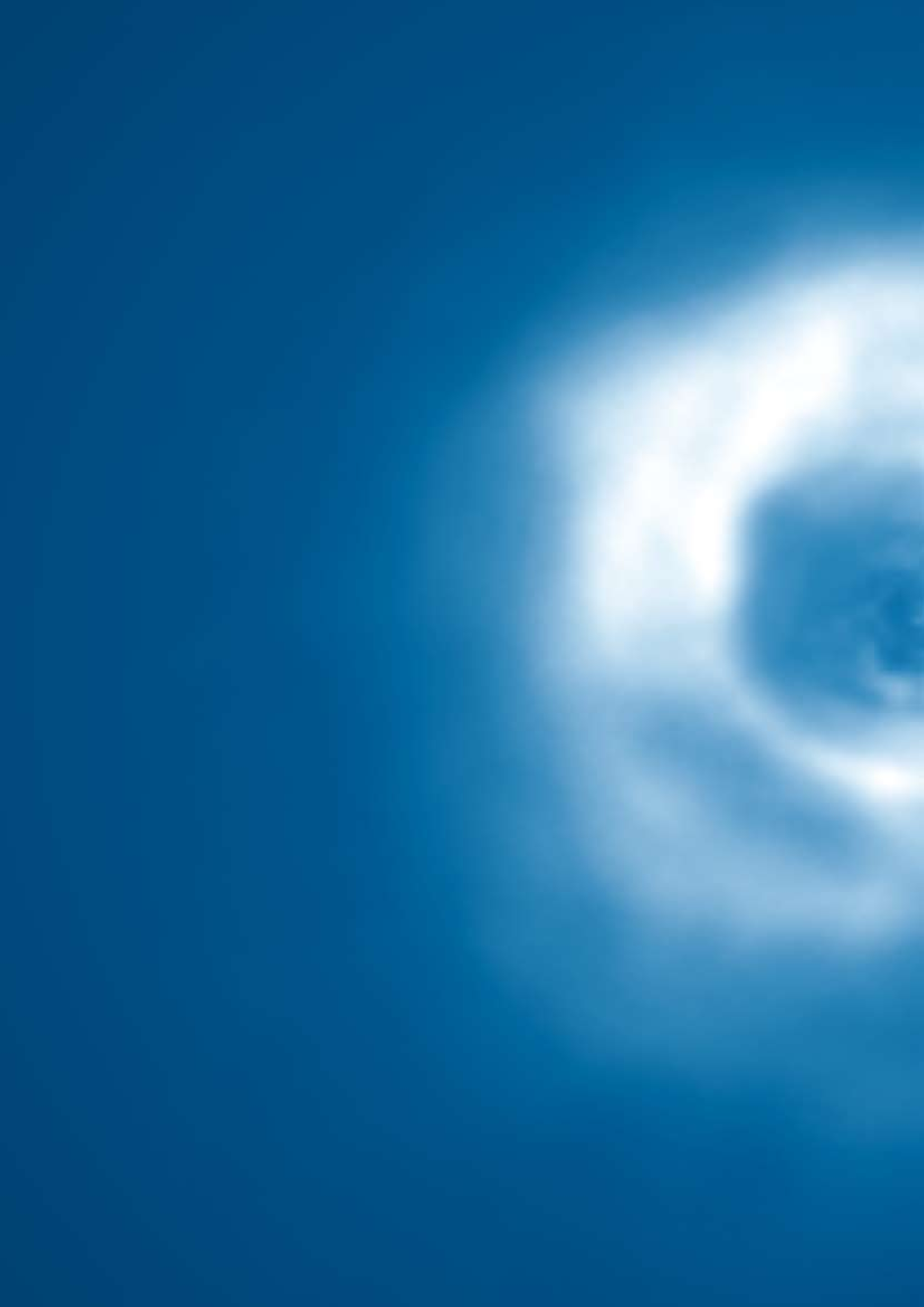
We shall put more efforts into action in the coming year. One will be the consolidation of our major "Research Areas." Through the strict Fellow selection process that we have been employing in the now more than five years of our existence, a few major areas of outstanding research have emerged, which we wish to nurture without compromising competition or our bias toward new and risky ideas.

In parallel and reinforcing that process, we want to increase our attractiveness to very promising young scientists and help TUM create a "tenure track" pool for their future junior professors, by giving them the chance to develop their creative ideas unimpeded by bureaucracy and duties that are irrelevant to their scientific progress. In particular, we want to be competitive with respect to the tenure track systems elsewhere, which have been drawing talent out of Europe by offering a more attractive environment for the most creative and capable young scientists.



Finally, we also want to provide our own contribution to easing "technology transfer," building bridges from science to society in such a way that both sides profit from the efforts. Engineering is inherently multidisciplinary and profits very much from being confronted with societal problems – as many of our projects show. Technology, the science of engineering, will only be worthy if it duly confronts its endeavors with the effects that they have.

Patrick Dewilde
Director



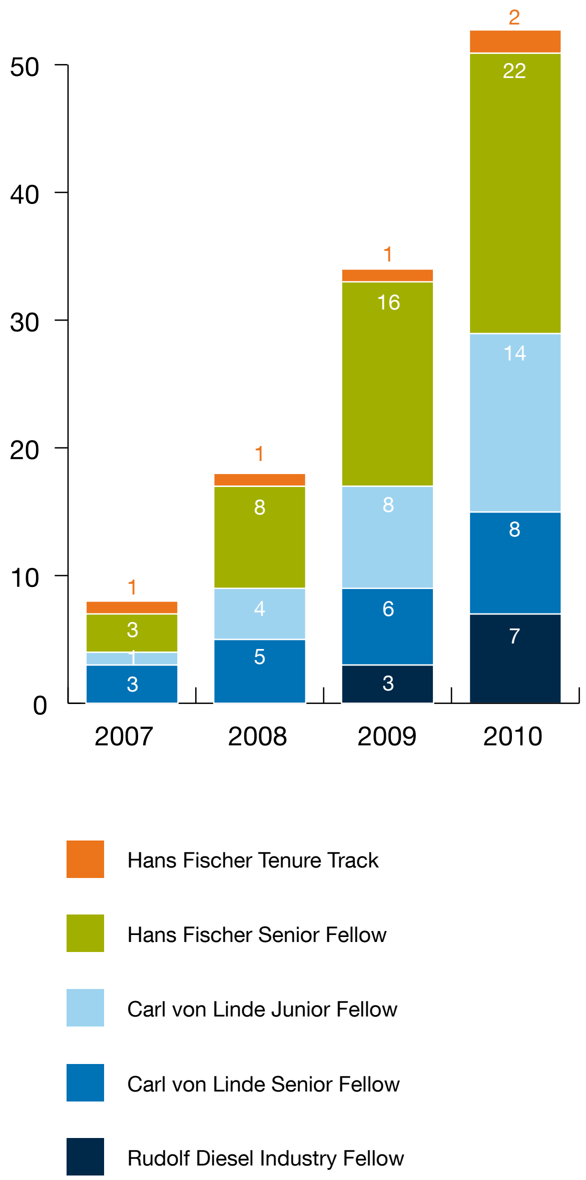
2010 Overview

2010 Overview

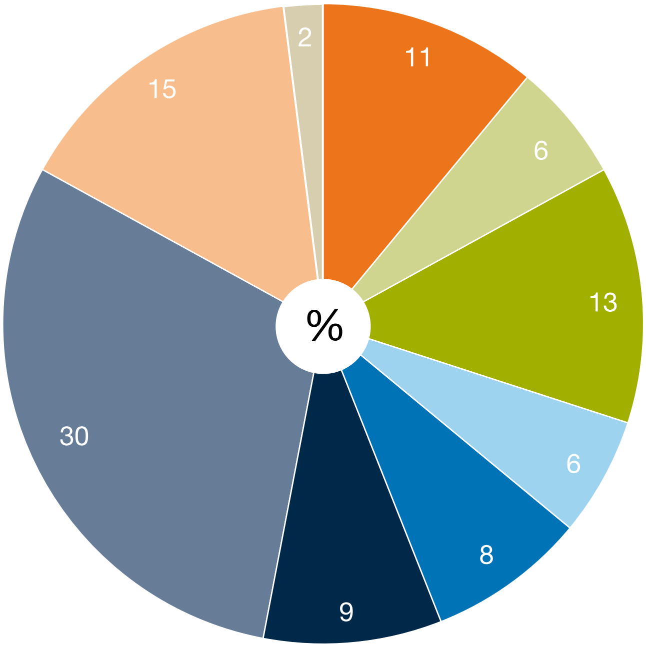
The TUM-IAS has awarded 19 new Fellowships in 2010, among them two Carl von Linde Senior Fellows, six Carl von Linde Junior Fellows, six Hans Fischer Senior Fellows, one Hans Fischer Tenure Track Fellow, and four Rudolf Diesel Industry Fellows.

The TUM-IAS Fellows come from diverse disciplines and from 12 different countries. Support for the TUM-IAS Fellows includes funding doctoral candidates (59) and postdocs (10), who collaborate closely with them.

Total Number of TUM-IAS Fellows

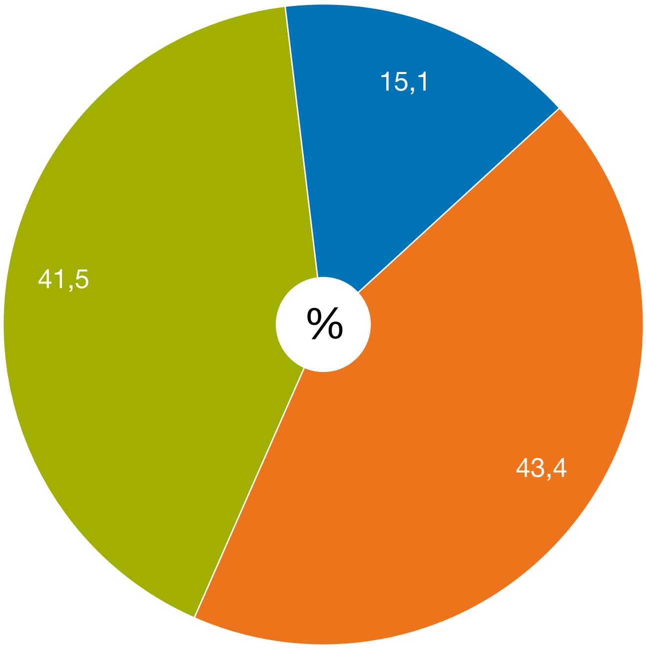


Distribution According to Faculties



- Informatics
- Chemistry
- Medicine
- Mathematics
- Mechanical Engineering
- Civil Engineering
- Physics
- Electrical Engineering
- Center of Life and Food Sciences Weihenstephan

Distribution According to Main Scientific Fields



- Life and Medical Sciences
- Engineering
- Natural Sciences

Focus Groups

TUM-IAS Focus Groups are the basic units of organization of the Institute. They are fully integrated in TUM and provide the social environment where Fellows, Hosts, their students, and collaborators meet to share the development of their topic, organize activities, and give mutual support. Ideally, these teams are also diverse in terms of disciplines and gender.

Advanced Cardiac Mechanics Emulator
Prof. Michael Ortiz | California Institute of Technology
Host: Prof. Wolfgang A. Wall | Computational Mechanics, TUM

Advanced Computation
Prof. Matthew Campbell | University of Texas
Host: Prof. Kristina Shea | Product Development, TUM

Prof. Peter Schröder | California Institute of Technology
Host: Prof. Rüdiger Westermann | Computer Graphics and Visualization, TUM

Advanced Construction Chemicals and Materials
Dr. Tsuyoshi Hirata | Nippon Shokubai, Ltd., Japan
Host: Prof. Johann Plank | Construction Chemicals, TUM

Advanced Stability Analysis
Prof. Raman I. Sujith | Indian Institute of Technology Madras
Host: Prof. Wolfgang Polifke | Thermodynamics, TUM

Aircraft Stability and Control
Dr. Matthias Heller | CASSIDIAN Air Systems, EADS Deutschland GmbH
Host: Prof. Florian Holzapfel | Flight System Dynamics, TUM

Biochemistry
Prof. Horst Kessler | Organic Chemistry and Biochemistry, TUM

Biomedical Engineering
Prof. Axel Haase | TUM
Host: Prof. Markus Schwaiger | Clinic for Nuclear Medicine, TUM

Prof. Walter Kucharczyk | University of Toronto
Host: Prof. Tim Lüth | Micro Technology and Medical Device Technology, TUM

Biophysics
Prof. Robijn Bruinsma | University of California, UCLA
Prof. Hendrik Dietz | TUM
Prof. David A. Weitz | Harvard University
Host: Prof. Andreas Bausch | Molecular and Cellular Biophysics, TUM

Clinical Cell Processing and Purification
Prof. Stanley Riddell | University of Seattle
Dr. Christian Stemberger | TUM
Host: Prof. Dirk Busch | Medical Microbiology, Immunology and Hygiene, TUM

Cognitive Technology
Dr. Alexandra Kirsch | TUM
Dr. Kolja Kühnlenz | TUM
Prof. Mandayam A. Srinivasan | MIT
Dr. Georg von Wichert | Siemens, Munich
Dr. Dirk Wollherr | TUM
Host: Prof. Martin Buss | Automatic Control Engineering, TUM

Computational Biology
Dr. Marco Punta | TUM
Host: Prof. Burkhard Rost | Bioinformatics, TUM

Computational Biomechanics
Prof. Zohar Yosibash | Ben-Gurion University, Israel
Host: Prof. Ernst Rank | Computation in Engineering, TUM

Fundamental Physics
Dr. Martin Gorbahn | TUM
Prof. Gino Isidori | Frascati National Laboratories
Prof. Stefan Pokorski | University of Warsaw
Host: Prof. Andrzej Buras | Particle Physics, TUM

Global Change
Prof. Tim Sparks | Anglia Ruskin University, Cambridge
Host: Prof. Annette Menzel | Ecoclimatology, TUM

High-Performance Computing (HPC)
Prof. Markus Hegland | Australian National University
Dr. Miriam Mehl | TUM
Host: Prof. Hans-Joachim Bungartz | Scientific Computing, TUM

Networked Dynamical Systems
Prof. Anuradha M. Annaswamy | MIT
Dr. Dragan Obradovic | Siemens, Munich
Host: Prof. Sandra Hirche | Automatic Control Engineering, TUM

Neuroscience
Prof. Thomas Misgeld | TUM
Prof. Bert Sakmann | MPI for Neurobiology, Martinsried
Host: Prof. Arthur Konnerth | Neuroscience, TUM

Satellite Geodesy
Prof. Gerhard Beutler | University of Bern
Dr. Adrian Jäggi | University of Bern
Host: Prof. Reiner Rummel | Astronomical and Physical Geodesy, TUM

Risk Analysis

Engineering Risk Analysis
Dr. Chin Man Mok | AMEC Geomatrix, Inc., Oakland, California
Host: Prof. Daniel Straub | Engineering Risk Analysis, TUM

Risk Analysis and Stochastic Modeling
Prof. Richard Davis | Columbia University
Dr. Robert Stelzer | TUM
Host: Prof. Claudia Klüppelberg | Mathematical Statistics, TUM

Energy

Diesel Reloaded
Prof. Gernot Spiegelberg | Siemens, Munich
Host: Prof. Alois Knoll | Robotics and Embedded Systems, TUM

Molecular Aspects in Interface Science
Dr. Julia Kunze-Liebhäuser | TUM
Host: Prof. Ulrich Stimming | Interfaces and Energy Conversion, TUM

Nanoscience

Functional Nanosystems
Prof. Shuit-Tong Lee | City University of Hong Kong
Dr. Ian Sharp | TUM
Host: Prof. Martin Stutzmann | Experimental Semiconductor Physics, TUM

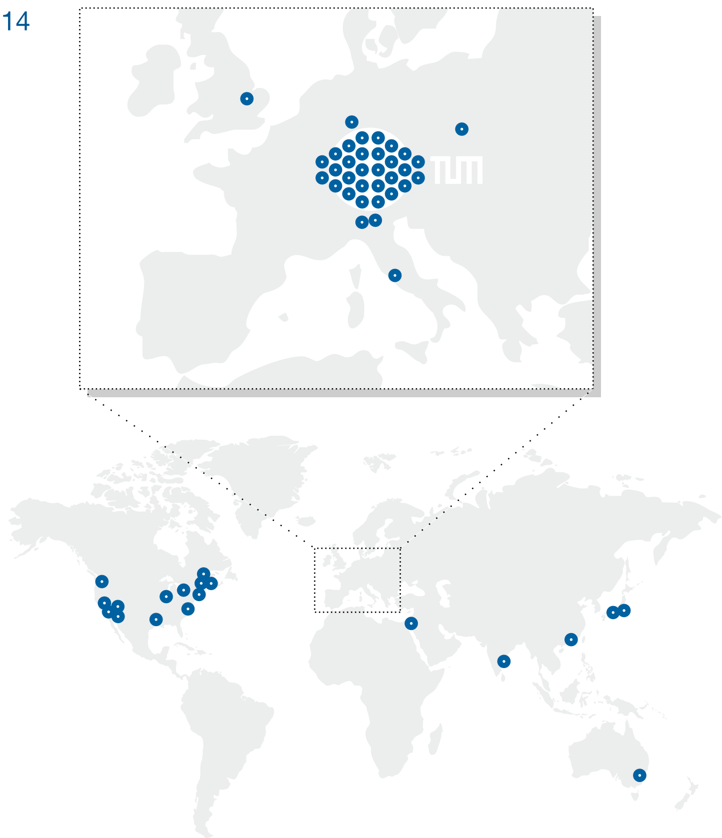
Nanoimprint and Nanotransfer
Prof. Khaled Karrai | Attocube Systems AG, Munich
Prof. Wolfgang Porod | University of Notre Dame
Host: Prof. Paolo Lugli | Nanoelectronics, TUM

Nanophotonics
Prof. Yasuhiko Arakawa | University of Tokyo
Dr. Ulrich Rant | TUM
Host: Prof. Gerhard Abstreiter | Experimental Semiconductor Physics, TUM

Nanoscale Control of Quantum Materials
Dr. Wilhelm Auwärter | TUM
Prof. Douglas Bonn | University of British Columbia
Host: Prof. Johannes Barth | Molecular Nanoscience and Chemical Physics of Interfaces, TUM

Nonequilibrium Statistical Mechanics at the Nanoscale
Dr. Vladimir García Morales | TUM
Host: Prof. Katharina Krischer | Interfaces and Nonlinear Dynamics, TUM

Where do the TUM-IAS Fellows come from?



Start-up Funding

Biaxial Tractor
Prof. Wolfgang A. Wall | TUM

Imaging System
Prof. Arthur Konnerth | TUM
Prof. Thomas Misgeld | TUM
Prof. Bert Sakmann | MPI for Neurobiology, Martinsried

Molecular Aspects in Interface Science
Dr. Julia Kunze-Liebhäuser | TUM

Molecular Tissue Analysis
Prof. Karl-Friedrich Becker | TUM
Prof. Heinz Höfler | TUM

Nanomagnetic Computing
Prof. Doris Schmitt-Landsiedel | TUM

Scanning Tunneling Spectroscopy
Prof. Johannes Barth | TUM
Prof. Douglas Bonn | University of British Columbia

STED microscope
Prof. Andreas Bausch | TUM
Prof. David A. Weitz | Harvard University

Technology Push
Prof. Klaus Diepold | TUM
Steven D. Edelson | Shadow Laboratories, USA

Telehaptics for Nanoassembly
Prof. Mandayam A. Srinivasan | MIT
Andreas Schmid | TUM
Dr. Stefan Thalhammer | Helmholtz Center
Ramesh Yechangunja | Yantric, Inc., USA

Understanding Complex Biological Systems
Prof. Chris-Carolin Schön | TUM

Vision in Quadrocopters
Prof. Florian Holzapfel | TUM
Prof. Alois Knoll | TUM

Watching a Single Protein Molecule Fold in a Cellular Environment
Prof. Matthias Rief | TUM

Prof. Andrzej Buras

- “FLAVOUR,” ERC Advanced Investigator Grant, European Research Council, 2011–2016
- Schrödinger Guest Professor of the University of Vienna (Oct. 17–Nov. 10)
- Election to Ordinary member of the Bavarian Academy of Sciences and Humanities.

Prof. Hendrik Dietz

- “DNA ORIGAMI DEVICES,” ERC Starting Independent Researcher Grant, European Research Council
- Arnold Sommerfeld Preis of the Bavarian Academy of Sciences and Humanities.

Prof. Walter Kucharczyk

- Distinguished Service Medal (Distinction), Fellow (FISMRM) (Distinction), and Outstanding Teacher Award, International Society of Magnetic Resonance in Medicine, Stockholm, Sweden.

Focus Group Neuroscience

- DFG-Graduiertenkolleg (GRK 1373) “Brain signaling: from neurons to networks” (Speaker: Prof. Arthur Konnerth), funding until 2015
- Prof. Thomas Misgeld, Prof. Arthur Konnerth and teams from Israel and Italy: “High-speed two-photon imaging for *in vivo* analysis of brain disease” (Speaker: Prof. Arthur Konnerth), EU grant within the ERA-Net NEURON framework
- Prof. Thomas Misgeld: “Sachmittelbeihilfe” from Alexander von Humboldt Foundation for a two-photon microscope
- PhD student Hongbo Jia, “Scopus Young Neuroscientist Award.”

Prof. Horst Kessler

- Honorary Membership “Fachgruppe Magnetische Resonanzspektroskopie,” German Chemical Society
- Klassensekretar, Mathematisch-Naturwissenschaftlichen Klasse of the Bavarian Academy of Sciences and Humanities.

Prof. Shuit-Tong Lee

- Research Grants Council of Hong Kong SAR “High-efficiency photocatalyst design based on up-converted carbon nanoparticles.”

Prof. Wolfgang Porod

- Prof. Wolfgang Porod, Prof. Paolo Lugli, Prof. Doris Schmitt-Landsiedel, and industry partners IBM and Grandis, Inc.: “NanoMagnet Logic,” DARPA-funded project for 4.5 years
- “NanoMagnet Logic,” Midwest Center for Nanoelectronics Discovery (MIND), second phase of funding.

Prof. Stanley Riddell

- Election to the Association of American Physicians
- E. Donnall Thomas Lecture, American Society of Blood and Marrow Transplantation.

Prof. Reiner Rummel

- Bayerischer Maximiliansorden für Wissenschaft und Kunst.

Prof. Ulrich Stimming

- Electrochimica Acta Gold Medal.

Prof. David A. Weitz

- Election to the National Academy of Sciences, USA
- Election to the American Academy of Arts and Sciences.

Prof. Zohar Yosibash

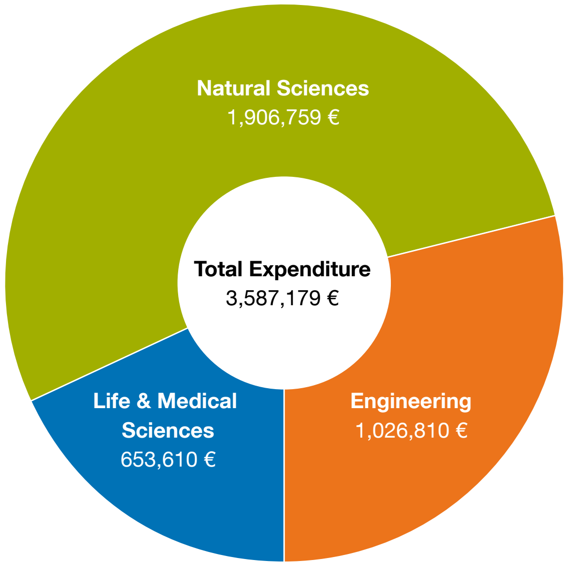
- German Research Foundation, “Electro-thermo-mechanical modeling of Field Assisted Sintering Technology using high-order finite elements validated by experiments” (Prof. Ernst Rank, Prof. Zohar Yosibash et al.), funding for two years
- Israel Ministry of Health grant “Novel computational methods for predicting bone fractures due to metastatic/benign tumors,” funding for two years.

Resources and Data

In this section a brief survey of the financial data is given. All expenditures of TUM-IAS are covered by the current “third funding line” of the Excellence Initiative. The Institute has reached now full financial capacity.

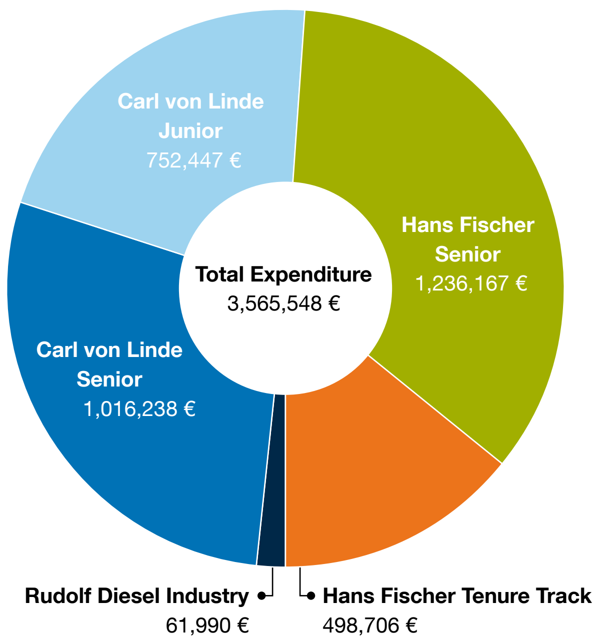
In 2010 with 53 Fellows we have exceeded the targeted size of 50. The expenditures reflect this fact, showing an increase of around one million euros in comparison with the previous year.

Expenditures per Main Scientific Fields in 2010



This chart shows the expenditures of the different Fellows grouped into the TUM scientific fields. The majority of TUM-IAS projects/programs are interdisciplinary, and therefore a distribution by the individual faculties is not meaningful. Of course, cooperation among these four different fields also occurs, but it is not shown in the chart. Information about these interactions can be found in the Fellow reports. The TUM-IAS Fellowships are awarded solely according to quality criteria, and no quotas have to be filled.

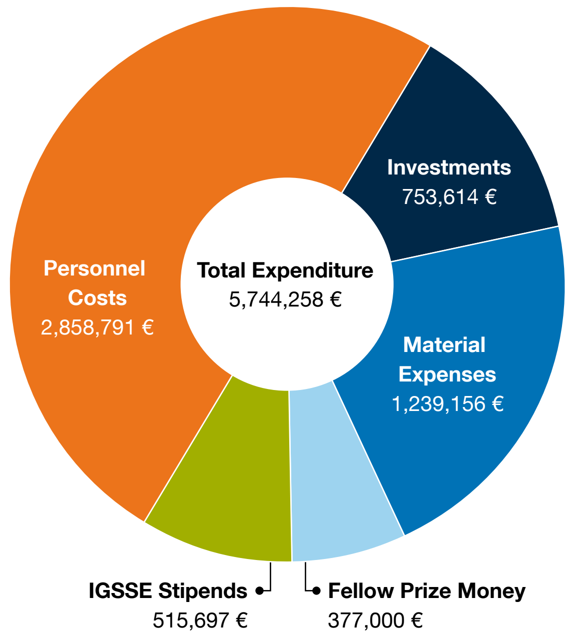
Expenditures per Fellowship Category in 2010



This chart shows that during 2010 the TUM-IAS Fellowship program has been fully established. In the Rudolf Diesel category we were able to nominate four Fellows in the past year, but most of the expenditures will be accounted for in 2011. The contribution for the internationalization of TUM is quite visible, as the TUM-IAS Fellowship that dominates the program in costs is the Hans Fischer Senior category. These Fellowships are an important and successful contribution to the TUM internationalization strategy and are immensely valuable regarding exchange of complementary expertise and grooming of emerging fields.

The Carl von Linde Senior Fellowship reached full capacity in 2010, and one further nomination per year is planned for the coming years. The Carl von Linde Junior category (less cost-intensive than the Senior category) has also developed extremely well and is a successful instrument in the development of new fields in science, giving good opportunities and a material base to promising young scientists. Not accounted for in the chart are the positions of the PhD students coached by the Junior Fellows, as they are financed by the Start-up Fund.

Total Expenditures in 2010



The total expenditures have increased from 2009 to 2010. Although the material costs and investments remained almost identical to the former year (investments even decreased), the personal costs and stipends increased significantly, reflecting the increase in the numbers of active Fellows and attached PhD and postdoc positions.

Highlights and Achievements

Fundamental Physics

Neuroscience

Satellite Geodesy

Nanoscience

- Nanophotonics
- Functional Nanosystems
- Nanoimprint and Nanotransfer

Biochemistry

Biomedical Engineering

Computational Biology

Computational Biomechanics

Advanced Computation

Risk Analysis and Stochastic Modeling

Networked Dynamical Systems

Cognitive Technology

Introduction

In this section, most of our currently active Focus Groups present the highlights of their research in 2010 and some of their most important publications. (We do not duplicate with the section in which our new Fellows are presented, so some of our Focus Groups are covered there.) With our diverse, very active and innovative community of researchers, it should be hard to discover and impose anything like an all-embracing order in which all, or at least most, results presented would fit; we can, however, describe a number of far-reaching commonalities. We will also address the question, certainly legitimate, of whether it is worthwhile to construct a community consisting of researchers from such different fields.

Indeed, in the diversity of highlights and research results presented, some strong "fields of force" appear. We would characterize them through poles of attraction from which they originate. One such pole is undoubtedly the need to have a much better mathematical grip on the physical situation. In our Institute this is very apparent in multiple ways. One is the reported great improvement obtained in advanced techniques for numerical modeling. Prof. Ernst Rank, Prof. Zohar Yosibash and their students have been able to push human bone modeling to an impressive level of accuracy, beating everything done so far. Prof. Burkhard Rost, Dr. Marco Punta, and their group have succeeded in characterizing function from genetic material in some very important types of proteins. Prof. Reiner Rummel, Prof. Gerhard Beutler, Dr. Adrian Jäggi, and the GOCE group have demonstrated their impressive computational talents by inverting the set of equations that determines gravity from mass distribution, to reveal new and unexpected structures on Earth. Prof. Claudia Klüppelberg, Dr. Robert Stelzer, and a large group of prize winners and doctoral candidates have been able to extend the boundaries of non-Gaussian, Lévy-driven statistical modeling to include effective modeling of such complicated dynamical systems as spot markets and wind farms. Our new Carl von Linde Junior Fellow Dr. Miriam Mehl has been developing "multi-physics" methods in which modeling and simulation packages from different fields collaborate at the time-step level to gauge how physical phenomena in different domains interact. In almost any field of endeavor, mathematical modeling and the use of advanced simulation techniques play a determining role. The need for more accurate and more powerful numerical modeling brings researchers from different fields together, facilitated by the language of mathematics, which evidently is the common language of all science.

It is clear that the biologists and the mathematicians have found each other in recent years, and that our Institute can greatly facilitate this process further. However, there is much more. Biology, biochemistry, supramolecular chemistry and nanoscience are very quickly finding each other as well, and creating an impressive array of new devices. Dr. Ulrich Rant, Dr. Ian Sharp, and their group have been exploring the integration of DNA-type molecules on a silicon substrate – defining heterostructures between biomolecules and semiconductors – and have been expanding into advanced graphene-based bioelectronic systems.

This has brought our top chemists much closer to our nanotechnology researchers, who are mostly physicists or electrical engineers. At one end of that spectrum, we have the very impressive results obtained by the Prof. Horst Kessler group, with applications ranging from drug discovery to biologically inspired materials (the group has been capable of reproducing artificially the reactions that take place when a spider spins her web). At the other end we have the work of Prof. Yasuhiko Arakawa, Prof. Gerhard Abstreiter, and doctoral candidates in producing new types of lasering quantum dots, with frequency characteristics that can be designed almost at will, and the work of Prof. Wolfgang Porod and Prof. Paolo Lugli on developing new techniques for nanoimprinting, thereby creating new process technology that is realistic and industrially feasible.

This Highlights section starts out rightly with our groups in what we could call fundamental science. While they are not in the majority (most of our research is technology-oriented), they do contribute an essential component and provide a very needed injection of basic science in our discussions. Prof. Andrzej Buras, Dr. Martin Gorbahn, Prof. Gino Isidori, and Prof. Stefan Pokorski have produced headlines and made headway in charting the future of the Standard Model, investigating its shortcomings and exploring testable avenues for the future theory of elementary particles. Prof. Arthur Konnerth, Prof. Bert Sakmann, and Prof. Thomas Misgeld have been building on their already formidable reputation as *in vivo* observers of the behavior of neurons by adding double-photon imaging to their imaging arsenal in addition to the probe-based techniques for which they are famous, leading not only to new understanding of neural mechanisms, but also to potential new therapies for axon degeneration and hope for important new medical applications.

This brings us to a further very common endeavor in our community of researchers, the building of new instrumentation to “see better.” Central here is the development or incorporation of new techniques in our experiments. We already mentioned two-photon imaging. We also have a very important effort going into the development of new NMR instrumentation (Prof. Axel Haase), often in conjunction with the analysis of new types of molecules. We have worked at further developing STED (Prof. Andreas Bausch and his group) and STM surface measurement techniques (Prof. Douglas Bonn, Prof. Johannes Barth, Dr. Willi Auwärter). Also haptics at the micro- and nano-scale have received attention (Prof. Mandayam A. Srinivasan, Prof. Martin Buss, and students), and these efforts have combined with the interests of Diesel Fellow Prof. Khaled Karrai of Attocube, toward creating new instrumentation for the field of nanoscience.

Building new devices and new instruments is certainly one of the central activities in the Institute, but we have also been very active at what I would call the “system side,” covered by extensive work in robotics (Dr. Dirk Wollherr, Dr. Kolja Kühnlenz, Dr. Alexandra Kirsch, Dr. Georg von Wichert, and students), networked dynamical systems (Prof. Martin Buss, Prof. Anuradha M. Annaswamy), and smart grids (Dr. Dragan Obradovic, Prof. Sandra Hirche). Clearly, distributed system control and system intelligence play a major role here.

All the general areas mentioned (advanced computations, modeling, devices, biochemistry, instrumentation, systems) have of course important interactions with each other. They are not clearly delimited.
A modern scientist or technologist needs more than a working knowledge of each of them; she/he needs basic understanding of what the novel contributions in fields other than her/his own are. That is where our Institute can and does play a major role. Engineering is definitely the art of multidisciplinary fusion, bringing the best techniques together and making the whole much more powerful than the parts. Take the future scene of sustainable energy: We will need advanced stochastic modeling (to predict output), smart grids (to accommodate multiple sources), new catalysis (for better batteries and fuel cells), and new ideas in city planning, automotive design, and renewable sources of energy. In the case of TUM-IAS, almost each important direction has a “champion” interested in how he or she can influence developments elsewhere, and being influenced by them in turn. Much of our program is geared toward catalyzing these interactions, guided by opportunities for deepening understanding and communicating abilities wherever they appear.

Focus Group **Fundamental Physics**

Prof. Andrzej Buras | Carl von Linde Senior Fellow
Dr. Martin Gorbahn | Carl von Linde Junior Fellow
Prof. Gino Isidori | Hans Fischer Senior Fellow
Host: Prof. Andrzej Buras, Particle Physics, TUM

Andrzej Buras, Martin Gorbahn, Gino Isidori, and Stefan Pokorski

At the threshold of big discoveries

Fundamental physics – more specifically, elementary particle physics – stands on the threshold of new and exciting era of discovery. The next generation of experiments, including both the Large Hadron Collider (LHC) at CERN and high-precision measurements of very rare processes in Europe and Japan, will explore new energy domains and will improve the resolution of the shortest distance scales by a factor of 20 to 100. They will measure the properties of elementary constituents of matter and their interactions with unprecedented accuracy, and they will uncover new phenomena such as new particles and new elementary interactions. Efforts to solve long-standing puzzles such as the origin of mass, the huge hierarchies in the mass spectrum of elementary particles, and their flavor-violating interactions as well as the matter-antimatter asymmetry of the universe, which is essential for our existence, will soon benefit from these new discoveries. This resembles the early days of quantum physics; however, about hundred years later, the open questions are now profoundly different from those addressed by Planck, Bohr, Heisenberg, Schrödinger, Born, and Einstein.

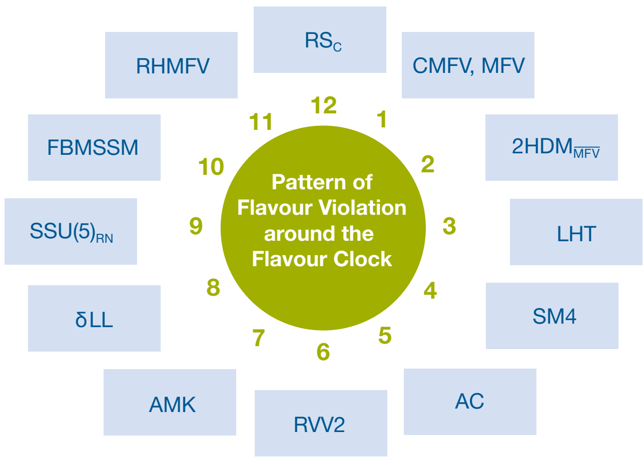
Within the Focus Group Fundamental Physics the preparations for this exciting era are concentrated on flavor physics, that is, the physics describing the different kinds (flavors) of leptons and quarks, their mixing via weak interactions, and their masses.

As of April 2011 we have a good knowledge of fundamental physics on scales down to 10^{-18} m, namely just above the scale where the mechanism giving rise to all masses of the observed particles (the so-called Higgs mechanism) is expected to occur. This scale is a key threshold in fundamental physics, and the investigation of physical phenomena below this threshold will be substantially improved in this decade: LHC will directly probe distance scales down to 10^{-19} m while, thanks to quantum fluctuations, the flavor-violating rare processes studied in our Focus Group and under experimental investigation in Europe and Japan will provide information about phenomena occurring at even smaller scales (possibly of the order of 10^{-20} m). In this context during 2010 our group performed several detailed analyses of various extensions of the Standard Model (SM) of fundamental interactions. We have identified patterns of flavor violation and correlations between various observables that, with the help of future precise experimental results, would allow us to uncover what kind of dynamics, new interactions, and new particles exist at the scales below 10^{-18} m. The highlights of our research in 2010 can be summarized as follows:

- The study of a model with new quarks and leptons has demonstrated that these new particles, while helping to explain certain deviations from the SM expectations in CP-symmetry-violating processes observed at Fermilab (USA), could simultaneously help to explain the observed size of matter-antimatter asymmetry in the universe [1].

- A different study, of a model with one additional Higgs field and a special flavor structure named Minimal Flavor Violation (a concept formulated in 2001-2002 by Prof. Andrzej Buras, Dr. Martin Gorbahn, and their collaborators in Munich and by Prof. Gino Isidori and his Italian collaborators), has shown that several deviations from the SM expectations can be explained through this new field in a correlated manner [2]. Moreover, it has been pointed out that the pattern of flavor violation in this model is rather different from the one with new quarks and leptons mentioned above. In a following analysis, within the same model, electric dipole moments of atoms and leptons have been calculated demonstrating very impressive correlations between these observables and the violation of CP symmetry in B-meson decays [3]. Our analysis has shown that the explanation of the deviations from SM prediction in B-meson decays would automatically imply enhancements by several orders of magnitude of the electric dipole moments in question over the corresponding SM predictions. These impressive correlations will be tested experimentally within the next five years.

- One of the main properties of the SM regarding flavor-violating processes is the left-handed structure of the charged weak current processes, in accordance with the maximal violation of parity observed in low-energy experiments. Yet the SM is expected to be only the low-energy limit of a more fundamental theory in which, in principle, parity could be a good symmetry – implying the existence of right-handed (RH) charged weak currents. The presence of such currents could help to explain certain anomalies (from the point of view of the SM) seen



Working day and night on patterns of flavor violation in different extensions of the Standard Model.

in experimental data on B-meson decays. Assuming that RH currents provide the solution to the problem at hand, there is an important question whether the strength of RH currents required for this purpose is consistent with other observables and whether it implies new effects somewhere else that could be used to test this idea more globally. This question has been addressed in [4]. Similarly to the other analyses mentioned above, various predictions and correlations for a multitude of observables have been worked out and compared with the predictions of other models studied in our group since 2008.

- The high precision of future experiments requires very precise calculations. Martin Gorbahn and his two younger collaborators improved significantly the precision of the theory for rare Kaon and CP-violating processes by calculating thousands of very complicated Feynman diagrams with difficulty at the forefront of the present state of the art [5,6,7].

Publications:

[1] A. J. Buras, B. Duling, T. Feldmann, T. Heidsieck, C. Promberger and S. Recksiegel, “Patterns of Flavour Violation in the Presence of a Fourth Generation of Quarks and Leptons,” *J High Energy Phys.* 1009: 106, 2010.

[2] A. J. Buras, M. V. Carlucci, S. Gori and G. Isidori, “Higgs-mediated FCNCs: Natural Flavour Conservation vs. Minimal Flavour Violation,” *J High Energy Phys.*, 1010: 009, 2010.

[3] A. J. Buras, G. Isidori and P. Paradisi, “EDMs vs. CPV in B-mixing in two Higgs doublet models with MFV,” *Phys. Lett. B*, 694: 402, 2011.

[4] A. J. Buras, K. Gemmler and G. Isidori, “Quark flavour mixing with right-handed currents: an effective theory approach,” *Nucl. Phys. B*, 843: 107, 2011.

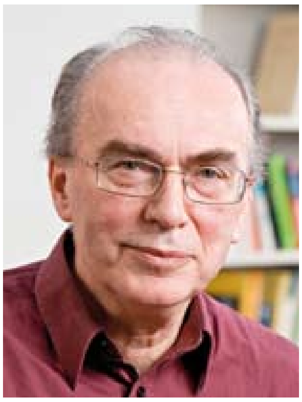
[5] J. Brod and M. Gorbahn, “Epsilon(K) at NNLO: The Charm-Top-Quark Contribution,” *Phys. Rev. D*, 82: 094026, 2010.

[6] J. Brod, M. Gorbahn and E. Stamou, Two-Loop Electroweak Corrections for the K->pi nu bar nu Decays, in arXiv:1009.0947 [hep-ph].

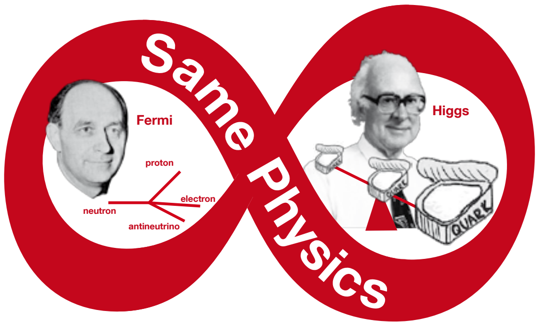
[7] J. Brod, M. Gorbahn, E. Stamou, Two-loop electroweak corrections for the $K \to \pi\nu\bar{\nu}$ decays; selected for a Viewpoint in Physics; *PHYSICAL REVIEW* D 83, 034030 (2011); DOI: 10.1103/PhysRevD.83.034030.

Focus Group **Fundamental Physics**

Prof. Stefan Pokorski | Hans Fischer Senior Fellow
Prof. Andrzej Buras, Particle Physics, TUM



Stefan Pokorski



The research conducted by Prof. Stefan Pokorski within the Fundamental Physics Focus Group has been, like that of other members, strongly linked to the Large Hadron Collider (LHC) era. It is now well appreciated that the very successful Standard Model (SM) has its limitations and can only be an approximate theory of elementary interactions. The SM cannot explain the observed hierarchies in quark and charged lepton masses, the origin of the neutrino masses, or cosmological facts such as the presence of dark matter in the universe, and baryon-antibaryon asymmetry. The SM is also not entirely satisfactory from a theoretical standpoint since it does not dynamically explain the origin of the Fermi scale, which determines, e.g., the "strength" of the neutron beta decay into proton, electron, and antineutrino. From the SM, one cannot even understand the reasons for quantum stability of the Fermi scale (gauge hierarchy problem).

The experiments at the LHC will shed important, new light on the latter issues and should discriminate between various theoretical concepts, such as supersymmetry or extra space dimensions, that have been proposed as dynamical theories of Fermi scale origin and solutions to the gauge hierarchy problem. In parallel, one has to understand the origin of the hierarchical fermion mass pattern. The two problems are not disconnected from one another. Peter Higgs has conjectured the existence of a new particle, the Higgs boson, as an explanation for both the Fermi scale and the non-zero fermion masses but not of their hierarchical structure. Theories of fermion mass hierarchies generate new sources of FCNC and CP violation; when combined with solutions to the gauge hierarchy problem, they are strongly constrained phenomenologically. In the papers cited below, theories of fermion mass hierarchies and their predictions for FCNC and CP violation are investigated in the framework of supersymmetric theories.

Explicit, family symmetry-based fermion mass theories usually predict stronger FCNC and CP violation effects than those predicted by the hypothesis of Minimal Flavor Violation, and such theories can be tested experimentally [2]. That is one highlight of these investigations. Furthermore, such theories are compared to another set of fermion mass theories based on the concept of wave function renormalization in supersymmetric models [1]. An important conclusion is that different theories, each correctly predicting the fermion mass pattern, can lead to very different and experimentally testable predictions for the FCNC and CP violation effects.

Publications:

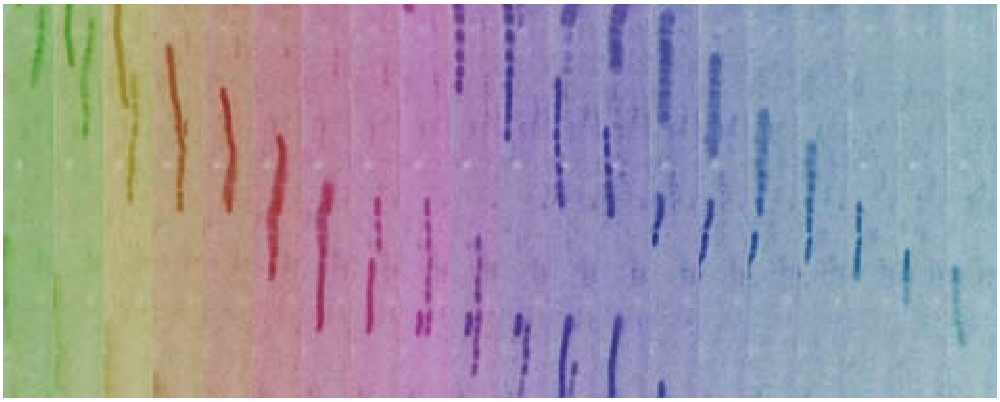
[1] E. Dudas, G. von Gersdorff, J. Parmentier, and S. Pokorski, "Flavour in supersymmetry: Horizontal symmetries or wave function renormalisation," *J High Energy Phys.*, no. 12, pp. 1-20, 2010. doi: 10.1007/JHEP12(2010)015.

[2] Z. Lalak, S. Pokorski, and G. G. Ross, "Beyond MFV in family symmetry theories of fermion masses," *J High Energy Phys.*, no. 8, pp. 1-34, 2010. doi: 10.1007/JHEP08(2010)129.

Focus Group **Neuroscience**

Prof. Arthur Konnerth | Carl von Linde Senior Fellow
Prof. Thomas Misgeld | Hans Fischer Tenure Track Fellow
Prof. Bert Sakmann | Hans Fischer Senior Fellow
Prof. Arthur Konnerth, Neuroscience, TUM

Of mice and microscopes



The TUM-IAS Neuroscience Focus Group, comprising the labs of Prof. Bert Sakmann, Prof. Arthur Konnerth and Prof. Thomas Misgeld, focuses on electrophysiology- and microscopy-based explorations of nervous system function and malfunction. Over the past decades, new technologies that permit recording of cellular signaling by light ("optophysiology") and others that allow optical modulation of cellular biology ("optogenetics") have ushered in a dramatic change in how the nervous system can be probed in living animals. However, such exploration faces a number of challenges: First, as more and more probes (genetically encoded and otherwise) become available from studies in cell culture, we need to devise ways to evaluate such probes for *in vivo* use and deliver them to the intact nervous system of mammals. Second, given the enormous complexity of neuronal circuits, with numerous cell types intermingling, it is necessary to restrict such probes to well-defined cell populations. Third, microscopy needs to be pushed to its limits, as signals that can be reported and modulated by such probes originate in minute tissue volumes and very short periods of time – typically in the submicron and millisecond domains.

Our research focuses on developing integrated approaches to address such challenges and apply the resulting methodology to questions of circuit function and plasticity in the healthy and diseased nervous system. The efforts we undertake are generally two-tiered. On the one hand, microelectrode-based, transgenic or viral expression technology is devised to transfer new probes to specified populations of neural cells. On the other hand, we further develop microscopy techniques, especially two-photon *in vivo* imaging, to probe progressively smaller volumes and shorter time intervals. Together, such technology development has allowed us in 2010 to obtain fundamental new insights into how signals are processed by healthy cells in the adult brain, and how the structural changes in neurological disease emerge.

Sakmann Group

Bert Sakmann

Mice and other rodents use whiskers to explore their immediate environment. The sensory signals collected with the whiskers are processed by the somatosensory thalamus before reaching the cortex. We use this system as a model of bidirectional cortico-thalamic information flow – in particular, to explore how feedback from specific cortical output cells influences traditionally "lower level" processing in the somatosensory thalamus. Feedback from the mammalian cortex is provided by two major cell types, each having a distinct anatomy and function in the cortico-thalamic circuit. In order to study the influence of the two connections on thalamic sensory processing separately, we further developed optogenetic techniques to control neuronal activity in a cell type-specific manner. This allowed us to expand the current understanding of cortical feedback to include a scheme in which few but strong cortical connections integrate with equally strong brainstem inputs to control firing of thalamic integrator neurons (in collaboration with Laszlo Acsady, Budapest). The second cortical output consists of numerous connections that control the firing mode in the thalamus rather than directly driving activity. We are currently studying how switches in firing mode influence information processing, and preliminary data show that particular sensory features may be selectively transmitted according to cortical feedback-induced switches in firing mode.

While this work focuses on the role of connections from cortex to thalamus, our anatomical studies have shown that the cortical neurons providing the strong output to thalamus are likely to receive thalamic signals from the neurons they innervate. These cell type-specific bidirectional connections between thalamus and cortex suggest the possibility of closed loops in which sensory signals might be amplified or maintained over time. To test this hypothesis, we established a method that allows us to selectively activate thalamic inputs while recording from individual cortical neurons. These experiments confirm the presence of a closed loop – e.g., the output of the thalamic cell population that is driven by cortical feedback serves in turn to boost cortical sensitivity to sensory signals. A central resource in this effort was the establishment in 2010 of a viral production facility (maintained together with the other Neuroscience Focus Group labs), which allows for the production of adeno-associated virus particles, which can be used to deliver optophysiological modulators to select cell populations of the mouse cortex.

Together, these data about cortical and thalamic communication help us to understand network processing of sensory signals. As a next step, we would like to relate this functional circuit analysis to sensory-guided behavior – more specifically, sensory sampling via exploratory whisker movements. To this end, we have established a behavioral protocol (in collaboration with Tansu Celikel, University of Southern California) that allows us to quantify learning and sensory exploration by freely moving mice in a sensory-motor task. In combination with our approach of cell type- and/or region-specific manipulation of neural activity, this protocol will allow us to systematically probe the role of particular cortico-thalamic loops in both behavior and the whisker movements that guide behavior. With this combined approach, we hope to clarify functional links between single-neuron physiology, networks, and behavior.

Key Publication:

[1] A. Groh*, H. Bokor*, R. A. Mease, V. M. Plattner, B. Hangya, E. Scharifullina, A. Stroh, M. Deschenes, B. Sakmann, and L. Acsady. "Convergence and Integration of Top Down Cortical and Bottom Up Sensory Signals in Thalamus", unpublished. *equal first authorship

Konnerth Group

Arthur Konnerth

In sensory cortex regions, neurons are tuned to specific stimulus features. For example, in the visual cortex, many neurons fire predominantly in response to moving objects of a preferred orientation. However, the characteristics of the synaptic input that cortical neurons receive at the level of their dendrites to generate their output firing pattern remained unclear. One of the most effective ways to analyze dendritic signals relies on the imaging of the dynamics of intracellular Ca^{2+} concentration. Previously, synaptic input-related dendritic Ca^{2+} transients were identified and studied in detail in *in vitro* brain slice preparations, while *in vivo* work had mostly explored action potential-related dendritic Ca^{2+} signals. However, virtually nothing was known about the nature of subthreshold sensory-evoked input signals in the dendrites of mammalian cortical neurons. A detailed knowledge of sensory input signals would represent an important step forward for a better understanding of dendritic computation. An intriguing open question is whether sensory inputs with similar features are clustered on the same dendrite of a neuron or dispersed throughout the dendritic tree. Clustered inputs are capable of generating dendritic spikes and may form neuronal computational subunits *in vivo*, as they do under certain experimental conditions *in vitro*. Alternatively, sensory inputs that are not clustered, but widely distributed, may underlie different rules of integration and formation of neuronal output signals – such as, for example, the linear summation of excitatory inputs.

In an article by Jia et al., 2010, representing the highlight of our work during this year, we reported a novel approach for the visualization and functional mapping of sensory inputs to the dendrites of cortical neurons *in vivo*. By combining two-photon imaging with electrophysiological recordings, we were able to identify for the first time local subthreshold calcium signals that corresponded to orientation-specific synaptic inputs. These hot spots represented novel dendritic calcium signals *in vivo* and were found in all layer 2/3 neurons of the visual cortex, irrespective of their output firing pattern. Afferent sensory inputs with the same orientation preference were widely dispersed throughout the dendritic tree. Interestingly, even neurons with a highly tuned output signal were found to receive input signals that were heterogeneous and coded for multiple orientations and/or directions.

Taken together, the new results indicated that orientation-tuned neurons can compute their characteristic firing pattern by integrating spatially distributed synaptic inputs coding for multiple stimulus orientations (see Nature*: News & Views* by Priebe and Ferster, 2010). The results support a neuronal integration model involving summation of distributed inputs, rather than models that stress the role of convergent inputs to single dendrites. We are confident that the approach introduced in this study will open the way to a detailed analysis of various types of neurons followed by the construction of functional wiring diagrams of sensory pathways *in vivo*.

Key Publication:

[1] H. Jia, N. L. Rochefort, X. Chen, A. Konnerth, "Dendritic organization of sensory input to cortical neurons *in vivo*," *Nature*, 464 (7293):1307-12, 2010.

Misgeld Group

Thomas Misgeld

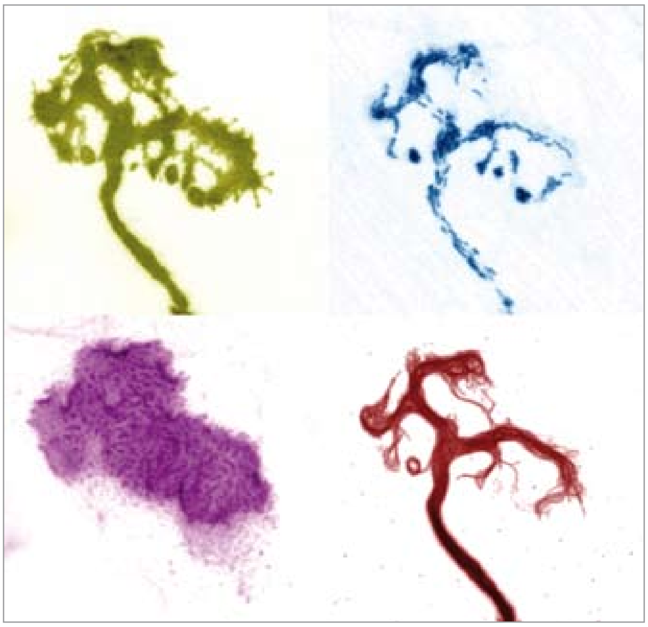
Nerve cells use long, thin cellular processes (axons) to convey signals over long distances – in the longest axons of the human body, over distances of up to one meter. Not surprisingly, given their geometry, axons are highly vulnerable to injury during disease processes, such as neurodegeneration, trauma, or neuroinflammation. Together with our collaborators (Martin Kerschensteiner, LMU, and Derron Bishop, Indiana), we have started to explore the changes within axons that precede their injury using live imaging.

For us, the most fascinating insight from these efforts was that axons can show signs of injury transiently and then recover. One example of such reversible damage can be found in models of multiple sclerosis, a common neurological disease that accounts for a significant part of neurological disability in younger people. Here axons are exposed to immune cells that invade the nervous system and cause damage to axons and their sheaths (myelin), which results in axon degeneration. We found that preceding these overt signs of axonal demise, there is an intermediate state, in which axons already show changes in shape, and also contain damaged organelles such as mitochondria (Nikić et al, *Nature Medicine*, in press). Mitochondria are essential cellular organelles that generate energy substrates, but they also possess the capacity, when damaged, to produce toxic intermediates themselves. Remarkably, axons can remain in this "sub-lethal" injury state for several days and then recover, most likely as inflammation abates and a less stressful local environment is again established. Central mediators of such axon damage appear to be "reactive oxygen species," aggressive derivatives of oxygen that are produced by immune cells and also result from mitochondrial disruption. Our current aim is to understand the subcellular mechanisms that underlie such stable and reversible states of axon injury.

Together with the other Neuroscience Focus Group labs, we have started developing the necessary infrastructural requirements for this quest. To visualize intra-axonal structures that might be altered prior to overt axon loss, we have turned to developing transgenic and viral expression systems to deliver reporters of subcellular damage to nerve cells. With support of the TUM-IAS, we inaugurated in 2010 a new mouse breeding facility and established a viral production facility. Using these resources, we have generated a number of transgenic mice that allow visualizing mitochondria and reactive oxygen species production, to measure transport of organelles in axons and the dynamics of the cellular "tracks" (cytoskeleton) that such transport depends upon. (See figure.)

In parallel, we are broadening the scope of disease processes that we are studying to include conditions where the initial insult does not involve immune cells, but either disruptions of endogenous detoxification of reactive oxygen species (e.g., some forms of motor neuron disease) or non-transecting axonal injuries during trauma, where endogenous rather than exogenous sources of noxious mediators might induce transient axonal injury.

Finally, we are investing in improving technologies to correlate *in vivo* light microscopy with electron microscopy, to characterize changes in axonal ultrastructure that precede overt axonal injury. Here we developed a new technique ("near infrared branding," NIRB), that allows delivering fiduciary marks into fixed tissue surrounding fluorescent axons that were identified previously using *in vivo* imaging. Such correlated imaging is highly challenging, but it overcomes a fundamental limitation of light microscopy, namely its limited resolution in the subcellular domain.



Confocal microscopy images of a neuromuscular synapse as studied by the Misgeld lab. Yellow - axonal cytoplasm; Cyan - mitochondria; Magenta - synaptic neurotransmitter receptors; Red- cytoskeletal tracts.

Key Publication:

[1] I. Nikić, D. Merkler, C. Sorbara, M. Brinkoetter, M. Kreutzfeldt, F. M. Bareyre, W. Brück, D. Bishop, T. Misgeld*, and M. Kerschensteiner*, "A reversible form of axon damage in multiple sclerosis and its animal model," *Nature Medicine*. In press.*equal contributing senior authorship.

Prof. Reiner Rummel | Carl von Linde Senior Fellow
Astronomical and Physical Geodesy, TUM

Reiner Rummel

Seeing planet Earth in the "light" of gravity

The European Space Agency satellite GOCE (Gravity and steady-state Ocean Circulation Explorer) has been operational since November 2009. General summaries of its objectives, principles, and current state have been published recently, e.g., by B. Röthlein in "Wie man ins Innere der Erde schaut" (*TUM Faszination Forschung* 7, 2010: 36) and by Quirin Schiermeier in "Weighing the world" (*Nature* 467, 2010: 647).

Analysis of the first two months of data proved that global gravity gradient maps of excellent quality could be produced. Through comparison with the best available models of the Earth's gravitational field, it was demonstrated that GOCE is significantly improving the field's fine scale features, in particular for areas where terrestrial gravity measurements are poor or sparse. In the context of TUM-IAS activities, an emphasis is currently placed on analyzing the characteristics of individual gravity gradient components. Figure 1 shows a first map of vertical gravity gradients in the Antarctic region.

A further goal of the GOCE mission is the determination of global ocean circulation patterns. The actual mean ocean surface, as derived from more than ten years of continuous satellite radar altimetry, is combined with the "geoid" (global gravity field level surface) computed from GOCE data. As an example, Figure 2 shows the geostrophic velocities in the Antarctic Circumpolar Current. Because this area is one of the "tipping points" of our climate system, better knowledge of ocean mass and heat transport there is of great importance.

Publications:

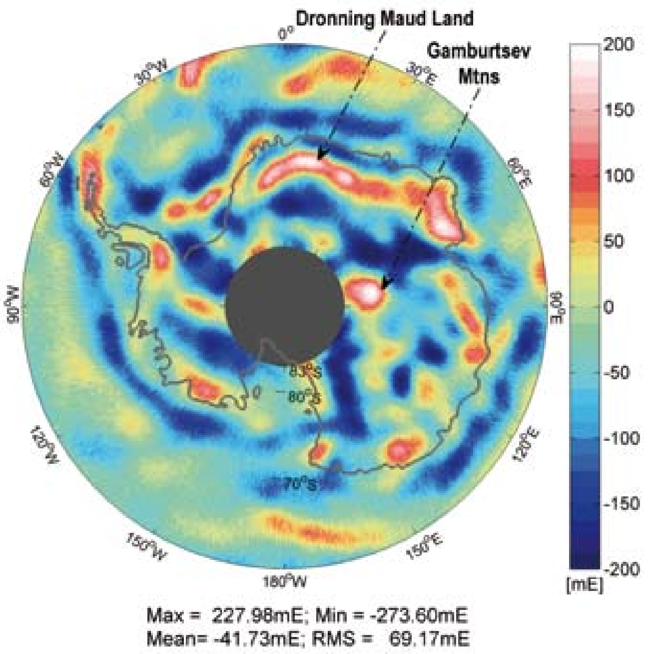
[1] R. Rummel and A. Schlicht, "Großer Aufwand für klein g," *Physik Journal*, vol. 9, no. 3, pp. 35-40, 2010.

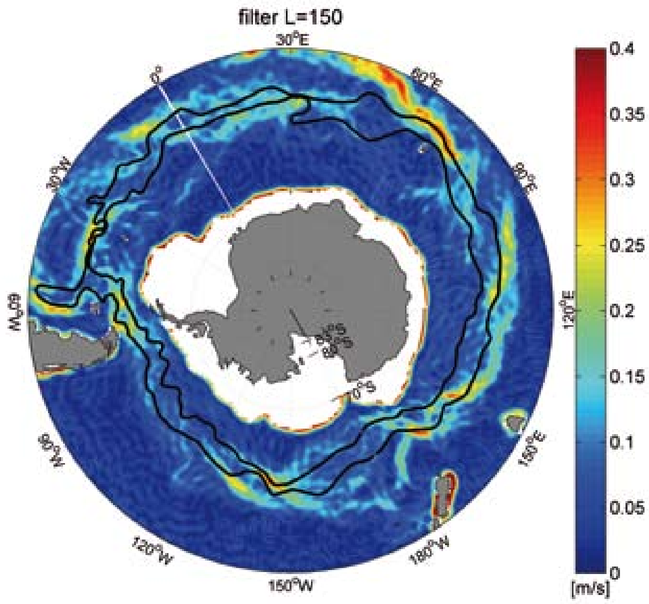
[2] R. Rummel and T. Gruber, "Gravity and steady-state ocean circulation explorer GOCE." In *System earth via geodetic-geophysical space techniques, (Advanced technologies in earth sciences)*, edited by F. Flechtner et al., 203-212. Berlin Heidelberg: Springer, 2010.

[3] R. Rummel, "GOCE: Gravitational gradiometry in a satellite." In *Handbook of Geomathematics*, edited by W. Freeden, M.Z. Nashed and T. Sonar, ch. 22. Berlin Heidelberg: Springer, 2010.

[4] R. Rummel, "Die Satellitenmission GOCE – Geodäsie aus dem Weltraum," *Mitteilungen des DVW-Bayern*, vol. 62, no. 4, pp. 471-476, 2010.

[5] R. Rummel, M. Horwath, W. Yi, A. Albertella, W. Bosch, and R. Haagmans, "GOCE, satellite gravimetry and Antarctic mass transports", *Surveys in Geophysics*. Accepted for publication (2011).





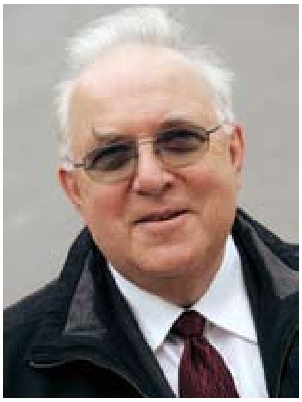
1 | Showing band-pass filtered vertical (i.e., radial) gravity gradients for the Antarctic region as derived from GOCE's first measurements cycle (November and December 2009) for all ascending arcs. The gradients reveal some prominent tectonic features of Antarctica that are covered under the ice shield, such as Dronning Maud Land and the Gamburtsev Mountains. The data gap at the pole is marked in black.

2 | Geostrophic velocities are computed from the mean dynamic topography of the Antarctic Circumpolar Current (ACC), as derived from the difference of a multi-year and multi-mission altimetric mean ocean surface and the GOCE geoid (based on model GOCO-01s). Fronts are shown as black lines and are deduced from in-situ ocean data.

Focus Group **Satellite Geodesy**

Prof. Gerhard Beutler | Hans Fischer Senior Fellow
Dr. Adrian Jäggi | Carl von Linde Junior Fellow
Prof. Reiner Rummel, Astronomical and Physical Geodesy, TUM

Satellite Geodesy, the Swiss contribution



Gerhard Beutler

Adrian Jäggi

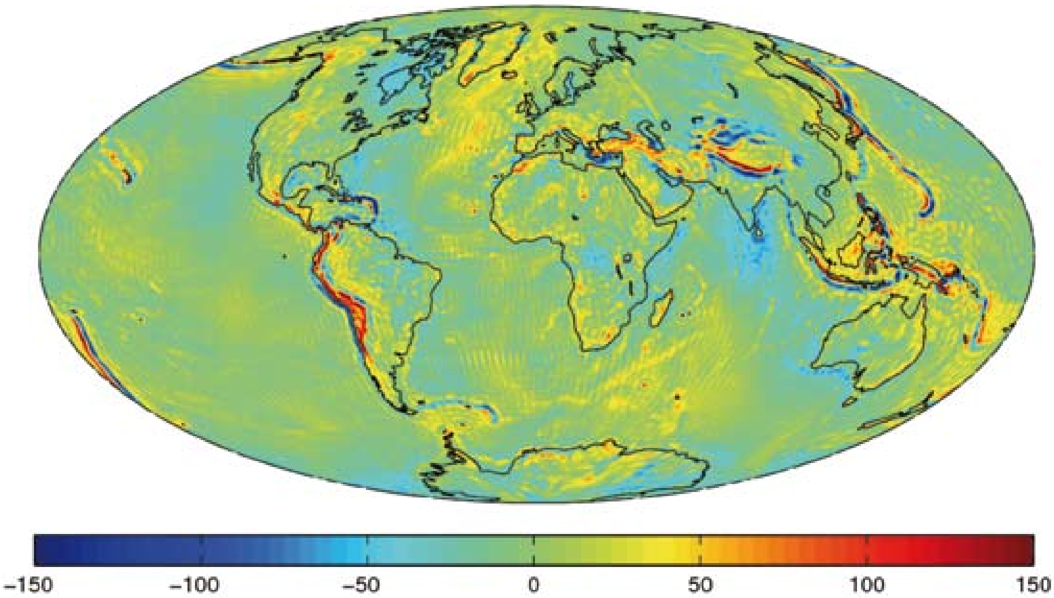
Contributions to the Satellite Geodesy project by the Astronomical Institute of the University of Bern and the Technical University of Prague officially end in 2011. The project started in 2007 with the six-month sabbatical of Prof. Gerhard Beutler (Hans Fischer Senior Fellow) and Dr. Adrian Jäggi (Carl von Linde Junior Fellow). All in all, the two Fellows spent about one calendar year each between 2007 and 2011 at the Institute for Astronomical and Physical Geodesy (IAPG) in Munich. Leos Mervart, the informatics expert of the group, supported the team during visits to Munich and in Bern. The Swiss National Science Foundation co-sponsored the project between 2007 and 2010.

The results of the project greatly exceed the 2007 expectations. Directly attributed to the project are five international journal articles and two articles reviewed in the International Association of Geodesy (IAG) Symposia book series. Two additional articles containing key results are in preparation. The project stimulated work in related areas, particularly in the field of precise orbit determination (POD), at the University of Bern, the Technische Universität München, and other research institutions. So far, we count a total of 15 articles in journals and reviewed proceedings (not included in the reference list) that were heavily influenced by TUM-IAS activities.

The development and refinement of the Celestial Mechanics Approach (CMA) stood at the center of our TUM-IAS-related activities. The theoretical foundations and interesting related studies performed with the CMA are documented in Ref. [1]–[2]. First, very promising results were published by Dr. Jäggi (Ref. [3]–[5]). Important technical issues were resolved and discussed by Meyer et al. (Ref. [6]) and Jäggi et al. (Ref. [7]). Figure 1 shows the gravity anomalies analyzed within this TUM-IAS project and derived from the yet unpublished gravity field model AIUB-GRACE03S, which includes more than six years of data from GRACE (Gravity Recovery and Climate Experiment), a joint mission of NASA and the German Aerospace Center (DLR).

The TUM-IAS Satellite Geodesy project initiated what we hope will be a long-lasting collaboration between IAPG and AIUB. Common research projects and proposals to the German and Swiss science sponsoring agencies are under way.

The authors of this short report wish to express their gratitude to TUM-IAS for its generous support of this challenging and fascinating research project.



Gravity anomalies (in mgal) as derived from AIUB-GRACE03S.

Publications:

[1] G. Beutler, A. Jäggi, L. Mervart, and U. Meyer, "The celestial mechanics approach: theoretical foundations," *Journal of Geodesy*, vol. 84, no. 10, pp. 605–624, October 2010. accessed March 2011, doi 10.1007/s00190-010-0401-7.

[2] G. Beutler, A. Jäggi, L. Mervart, and U. Meyer, "The celestial mechanics approach: application to data of the GRACE mission," *Journal of Geodesy*, vol. 84, no. 11, pp. 661–681, November 2010. accessed March 2011, doi: 10.1007/s00190-010-0402-6.

[3] A. Jäggi, G. Beutler, and L. Mervart, "GRACE Gravity Field Determination Using the Celestial Mechanics Approach - First Results," in *Gravity, Geoid and Earth Observation*, ed. S.P. Mertikas, IAG Symposia, 2010, vol. 135, 177–184, accessed March 2011, doi: 10.1007/978-3-642-10634-7_24.

[4] A. Jäggi, G. Beutler, U. Meyer, L. Prange, R. Dach, and L. Mervart, "AIUB-GRACE02S - Status of GRACE Gravity Field Recovery using the Celestial Mechanics Approach," IAG Symposia, Springer, in press 2010.

[5] A. Jäggi, H. Bock, L. Prange, U. Meyer, and G. Beutler, "GPS-only gravity field recovery with GOCE, CHAMP, and GRACE," *Advances in Space Research*, vol. 47, no. 6., pp. 1020–1028, March 2011. accessed March 2011, doi:10.1016/j.asr.2010.11.008.

[6] U. Meyer, A. Jäggi, and G. Beutler, "The Impact of Attitude Control on GRACE Accelerometry and Orbits," IAG Symposia, Springer, in press 2011.

[7] A. Jäggi, L. Prange, and U. Hugentobler, "Impact of covariance information of kinematic positions on orbit reconstruction and gravity field recovery," *Advances in Space Research*, in press 2011. accessed March 2011, doi: 10.1016/j.asr.2010.12.009.

Yasuhiko Arakawa and Gerhard Abstreiter at the International Symposium on Advances in Nanoscience organized jointly by TUM-IAS and the Excellence Cluster Nanosystems Initiative Munich for October 25-26, 2010 in the new TUM- IAS building in Garching.

Focus Group **Nanophotonics**

Prof. Yasuhiko Arakawa | Hans Fischer Senior Fellow
Prof. Gerhard Abstreiter, Experimental Semiconductor Physics, TUM

Clearing basic hurdles on the way to practical silicon light emitters

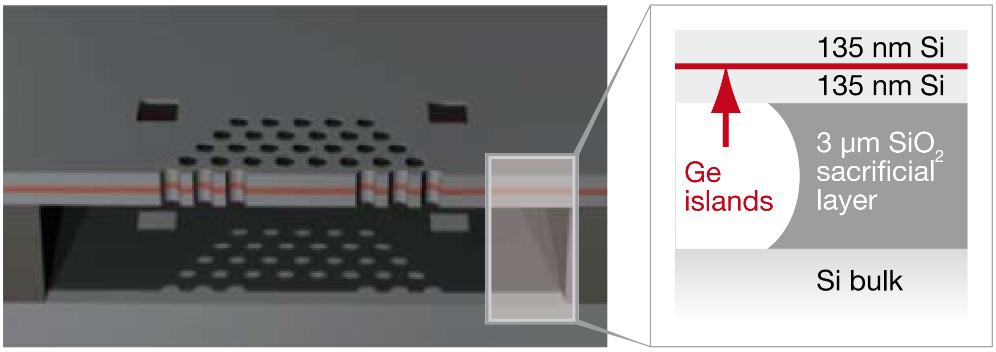
Due to its indirect electronic band gap, crystalline silicon is rarely used as the active emitter in semiconductor optics. Interband light emission is predominantly a phonon-assisted process, and in that respect silicon has very poor quantum efficiency. The development of efficient silicon-based light emitters would, however, pave the way toward CMOS-compatible, monolithic optical interconnects and thus signal processing speeds much higher than those currently provided by silicon microelectronics. Enhanced light emission from crystalline silicon can be achieved by using two-dimensional photonic crystals with point-defect photonic nanocavities. Such defect photonic crystal nanocavities modify the spatial emission profile of light, and a much larger fraction of light is emitted perpendicular to the slab due to the in-plane photonic band gap.

During the past year, we studied in detail the optical spectrum and the temperature stability of the photoluminescence emission from crystalline silicon photonic crystal nanocavities. Indeed, we found efficient light emission up to room temperature. Details of the achieved results can be found in Ref. 1. In further work, we imbedded germanium islands as active emitters into silicon photonic crystal nanocavities and studied the correlation between emission intensity and the nanocavity quality factor [Ref. 2]. Surprisingly, we found a clear increase in mode emission intensity as the quality factor decreased. The experimental results can be understood qualitatively by simulations that describe a cavity weakly coupled to an ensemble of emitters. Based on this model, we propose strategies for enhancing the radiative efficiency of entirely group IV photonic crystal nanostructures.

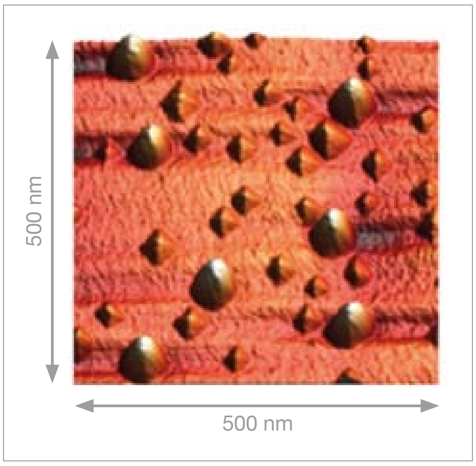
Publications:

[1] N. Hauke, T. Zabel, K. Müller, M. Kaniber, A. Laucht, D. Bougeard, G. Abstreiter, J. J. Finley, and Y. Arakawa, “Enhanced photoluminescence emission from two-dimensional silicon photonic crystal nanocavities,” *New J. Phys*. 12, May 2010: 053005.

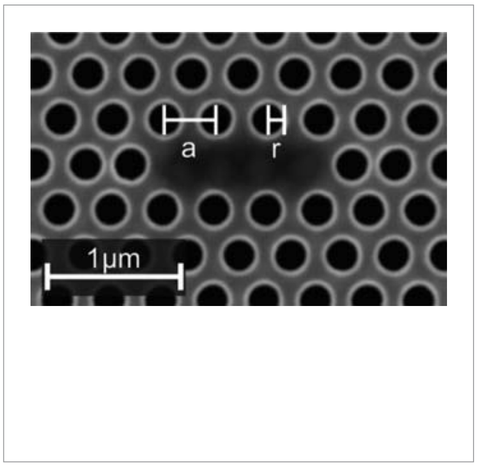
[2] N. Hauke, S. Lichtmannecker, T. Zabel, F. P. Laussy, E. del Valle, A. Laucht, M. Kanniber, D. Bougeard, G. Abstreiter, J. J. Finley, and Y. Arakawa, “A Correlation between the Emission Intensity of Self-assembled Germanium Islands and the Quality Factor of Silicon Photonic Crystal Nanocavities,” preprint, submitted for publication.



1 | Left panel: schematic cross-sectional representation of the photonic crystal nanocavity structure
Right panel: layer sequence in the active region



2 | AFM image of germanium islands



3 | SEM image showing a photonic crystal cavity from the top

Dr. Ulrich Rant | Carl von Linde Junior Fellow
Prof. Gerhard Abstreiter, Experimental Semiconductor Physics, TUM

Ulrich Rant

Analysis of molecular interactions with electrically switchable biosurfaces

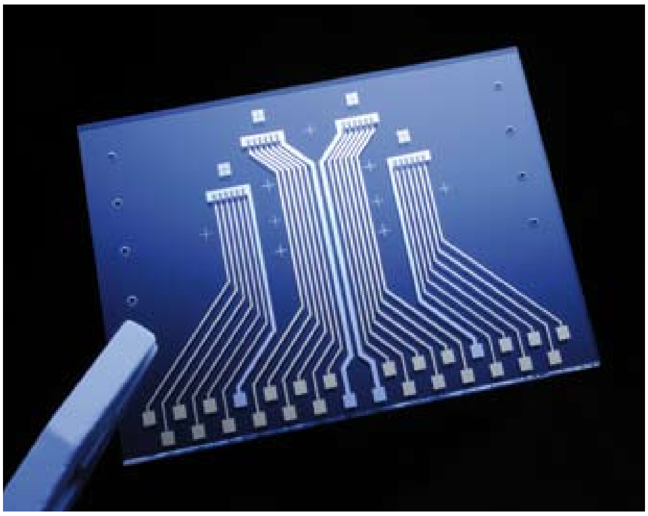
Interactions between molecules are in many ways like romantic encounters. The following questions may arise in a gossip magazine just as well as during the development of new drugs or in an attempt to understand signaling pathways in cells: How and when do partners meet? How long will they stay together? How does a partner's appearance (shape/size) influence its "attractiveness"? Is one of the partners polygamous and maybe already engaged in interactions with others? In which way does the new relationship affect other possible binding partners? Biosensors typically provide information like binding rates or affinities, but this is often not enough to understand the behavior of complex biomolecules, where form defines function.

On the basis of our research of electrically switchable DNA layers on metal surfaces, we devised a novel concept for a label-free biosensor platform termed *switch*SENSE. Short (~20 nm) DNA molecules are tethered at one end to microelectrodes on a chip. By applying alternating electric voltages to the electrodes, the charged DNA molecules are dynamically switched between a standing and lying conformation. "Target" molecules (e.g., antibodies), which bind to designated receptors (antigens) that are attached to upper DNA ends, change the molecular switching behavior; in particular, they affect the dynamics of the electrically driven motion. This opens up new possibilities beyond the performance of state-of-the-art biosensors. Because the target molecules slow the switching motion in a characteristic way, their size or shape can be inferred from a time-resolved measurement. Thus, the principle can be employed to analyze biomolecules following their detection directly on-chip. Applications include investigations of the changes of the folding state of proteins, protein-protein interactions, agglomerations, and modifications of proteins, etc., with important implications for the engineering of antibodies for therapeutic purposes. In addition to demonstrating the extraordinary sensitivity of the method, we devised a time-resolved measurement mode and implemented it in a prototype device. In conjunction with the developed biochip, the system forms a platform that can be easily adapted to a variety of different targets. Our future efforts will concentrate on making the *switch*SENSE technology available to a broad range of researchers working in biotechnology and drug development.

European patent application EP 10 180 282.5 (2010)

Publication:

[1] W. Kaiser and U. Rant, "Conformations of End-Tethered DNA Molecules on Gold Surfaces: Influences of Applied Electric Potential, Electrolyte Screening, and Temperature," *J. Am. Chem. Soc.*, vol. 132, no. 23, pp. 7935–7945, 2010.



1 | *switch*SENSE platform for molecular interaction analysis: biochip with 24 micro-electrodes and 4 flow-channels.

2 | *switch*SENSE platform for molecular interaction analysis: device prototype.

Focus Group **Functional Nanosystems**

Prof. Shuit-Tong Lee | Hans Fischer Senior Fellow
Prof. Martin Stutzmann, Experimental Semiconductor Physics, TUM

Shuit-Tong Lee

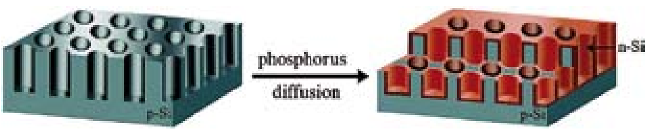
Pioneering scalable solutions in silicon and carbon, from the bottom up

The core of our research is dedicated to addressing major scientific challenges in areas of renewable energy production, biomedical and sensor systems, catalysis, and optoelectronics using functional nanoscale materials. To ensure scalability, and thus maximize the impact of new technologies in these fields, we focus on utilizing naturally abundant materials, such as silicon and carbon, processed at the nanoscale using facile, bottom-up, wet chemical methods. Our approach includes the design of new nanoscale materials, the creation and study of multi-phase interfaces, and the fabrication of state-of-the-art devices. Two exemplary studies, which highlight our approach to integrated nanoscale material design and implementation, are detailed here.

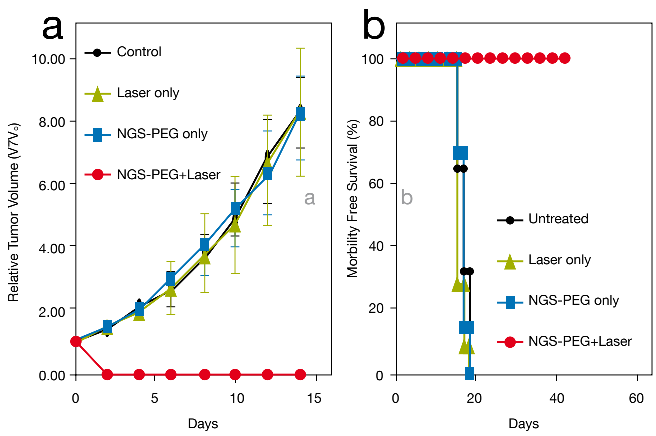
Despite the great potential of photovoltaic solar energy conversion for providing green and sustainable energy, it remains prohibitively expensive for large-scale competition with conventional fossil fuels. One promising approach for increased efficiency is based on core-shell nanowire systems, which greatly enhance the junction area, carrier collection, and light absorption compared to typical planar devices. However, such nanowire devices suffer from mechanical instabilities and significant recombination losses that reduce their efficiencies. Within the last year, we have made significant advancements that increase the efficiency of photovoltaic devices based on silicon nanostructures while simultaneously reducing the complexity and cost of device production. In particular, we have demonstrated a method of producing large-scale arrays of three-dimensional radial p-n junction solar cells with nearly double the efficiencies of comparable nanowire devices. Such structures are mechanically stable and inexpensive to produce, and they hold significant promise for cost-efficient solar energy conversion in the future.

While silicon is dominant for photovoltaic devices, carbon is the clear material of choice for biomedical applications. In recent years, there has been an explosion of interest in sp2 carbon allotropes due to their unique physical and chemical properties. Furthermore, with proper treatment, these materials are biocompatible and can be effectively used for *in vivo* applications. Starting with chemically functionalized, single-walled carbon nanotubes and nanographene sheets, we have undertaken the development of new therapeutic techniques for ultra-efficient tumor ablation. In particular, we have exploited the high tumor uptake of these hybrid nanomaterials and their strong near-infrared optical absorption for selective *in vivo* photothermal therapy. Although significant work remains, these results suggest great promise for future cancer treatments.

1 | Optical images of water-soluble carbon quantum dots of different sizes illuminated with a full spectrum lamp in the visible range (left) and with ultraviolet light (right). By tuning the carbon quantum dot size, the emission wavelength can be continually tuned from the ultraviolet across the visible and into the near-infrared range. These carbon nanomaterials offer great promise for applications ranging from high-efficiency photocatalysis to biological fluorescent markers.



2 | Illustration of the method utilized for fabrication of high-performance Si-based nanohole solar cell devices composed of radial p-n junctions.



3 | Tumor growth curves (a) and survivability curves (b) for different groups of mice after treatment demonstrating that photothermal ablation by near-infrared laser illumination of tumors following the uptake of functionalized nanographene sheets holds great promise for future cancer therapies.

Publications:

[1] H. Li, X. He, Z. Kang, H. Huang, Y. Liu, J. Liu, S. Lian, C. H. A. Tsang, X. Yang, and S.-T. Lee, "Water-soluble fluorescent carbon quantum dots and photocatalyst design," *Angew. Chem. Int. Edit*, vol. 49, no. 26, pp. 4430–4434, 2010.

[2] K.-Q. Peng, X. Wang, L. Li, X.-L. Wu, and S.-T. Lee, "High performance silicon nanohole solar cells," *J Am. Chem. Soc.*, 132, pp. 6872–6873, 2010.

[3] K.-Q. Peng and S.-T. Lee, "Silicon Nanowires for Photovoltaic Solar Energy Conversion," *Ad. Mater.*, vol. 23, no. 2, pp. 198–215, January 2011.

[4] K. Yang, S. Zhang, G. Zhang, X. Sun, S.-T. Lee, and Z. Liu, "Graphene in mice: Ultrahigh *in vivo* tumor uptake and efficient photothermal therapy," *Nano Lett.*, 10, pp. 3318–3323, 2010.

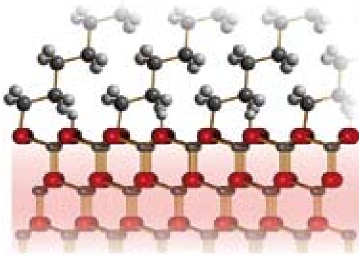
[5] Z. Liu, K. Yang, and S.-T. Lee, "Single-walled Carbon Nanotubes in Biomedical Imaging," *J Mater. Chem.*, 21, pp. 586–598, 2011.

Focus Group **Functional Nanosystems**

Dr. Ian Sharp | Carl von Linde Junior Fellow
Prof. Martin Stutzmann, Experimental Semiconductor Physics, TUM

Ian Sharp

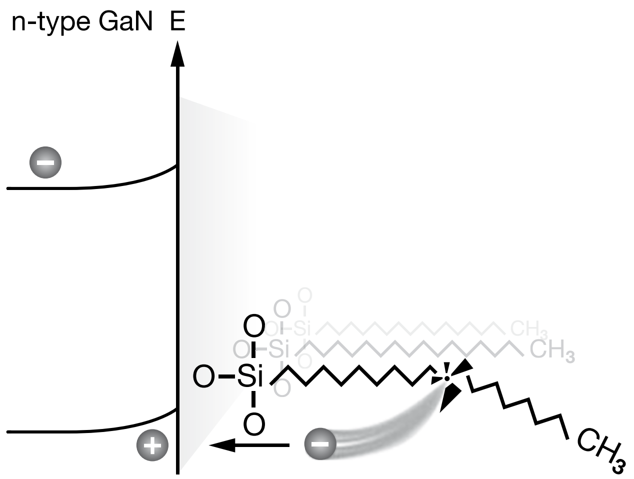
The integration of advanced semiconductors with biomolecular systems offers great potential for applications in artificial photosynthesis, photocatalysis, and biological sensing. To this end, we seek to develop a more complete understanding of electronic processes at bio-inorganic interfaces and to exploit such findings for the formation of functional structures at the nanoscale. Due to the inherent complexity of these hybrid systems, a multi-level approach is required to investigate the energetic alignment and charge transfer pathways between the various components at all stages of construction. Within the last year, we have developed new methods for the chemical functionalization of wide-bandgap semiconductors using both self-assembled monolayers and polymers; we have made significant progress toward understanding the energetic alignment at these interfaces; and we have applied these techniques to graphene, an exciting new two-dimensional material exhibiting a range of unique properties.



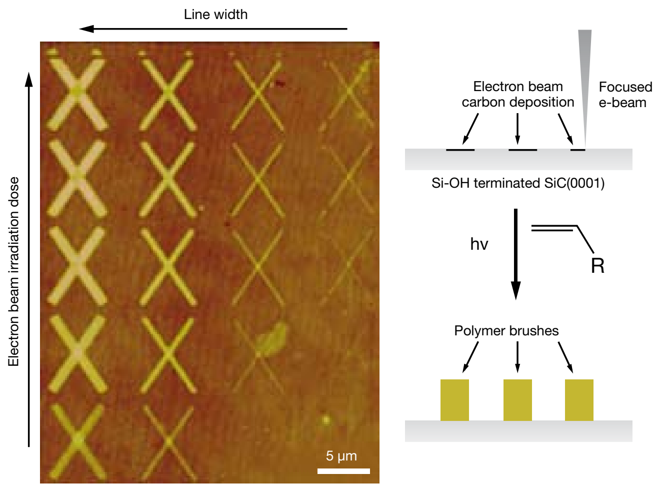
1 | Illustration of an organic self-assembled monolayer on a silicon carbide substrate. The monolayer provides a stable interface for the inorganic material and allows covalent and oriented attachment of complex biomolecules, such as enzymes and photosystems.

An important requirement for heterostructures between biomolecules and semiconductors is the formation of stable and functional organic layers covalently attached to the substrate. These layers act as sites for selective grafting, prevent denaturation of proteins, and function as molecular wires between various components of the system. Therefore, a major focus of our research during the last year was on building a toolkit for the covalent chemical functionalization of wide-bandgap semiconductors and understanding the electronic properties of the resulting interfaces. For example, we developed new photochemical methods for molecular assembly on oxygen-terminated surfaces, such as diamond, silicon carbide, and gallium nitride, and showed that the reactivities and interfacial binding configurations can be tailored by defining surface composition, crystal orientation, and photoexcitation energy. Furthermore, a mechanism for photocatalytic degradation of organic molecules on semiconductor surfaces was identified based on the specific alignment of semiconductor and molecular energy levels. Together, these results greatly enhance our understanding of hybrid material interfaces and provide us with the tools necessary to create increasingly complex and functional systems.

In parallel work, we have greatly expanded our research into graphene, an ideally two-dimensional, zero-bandgap material with exceptional chemical stability, mechanical strength, and ambipolar carrier mobility. This has included the development of a system for state-of-the-art growth of large-area, single-layer graphene by chemical vapor deposition; the characterization of graphene field-effect transistors in electrolyte solutions; and also site-controlled covalent chemical functionalization with both structured and homogeneous polymer brush layers. These advances bring us much closer to realizing advanced graphene-based bioelectronic systems, which are expected to significantly outperform existing devices.



2 | Schematic depiction of charge transfer-induced photocatalytic cleavage of organic molecules on the surface of the wide bandgap semiconductor gallium nitride.



3 | Atomic force micrograph of structured polymer brushes on silicon carbide obtained by local carbon templating with a focused electron beam followed by amplification of the pattern via photopolymerization with styrene.

Publications:

M. Hoeb, M. Auernhammer, S. Schoell, M.S. Brandt, J.A. Garrido, M. Stutzmann, and I.D. Sharp, “Thermally induced alkylation of diamond,” *Langmuir 26*, pp. 18862–18862, 2010.

[1] J. Howgate, S. Schoell, M. Hoeb, W. Steins, B. Baur, S. Hertrich, B. Nickel, I.D. Sharp, M. Stutzmann, and M. Eickhoff, “Photocatalytic cleavage of self-assembled organic monolayers by UV-induced charge transfer from GaN substrates,” *Adv. Mater.* 22, p. 2632.2010.

[2] M. Steenackers, I.D. Sharp, K. Larsson, N.A. Hutter, M. Stutzmann, and R. Jordan, “Structured polymer brushes on silicon carbide,” *Chem. Mater. 22*, p. 272, 2010.

Focus Group **Nanoimprint and Nanotransfer**

Prof. Khaled Karrai | Rudolf Diesel Industry Fellow
Prof. Wolfgang Porod | Hans Fischer Senior Fellow
Prof. Paolo Lugli, Nanoelectronics, TUM

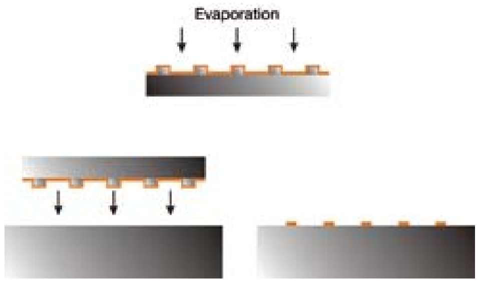
Wolfgang Porod

Khaled Karrai

Toward economical production of novel nanoscale devices

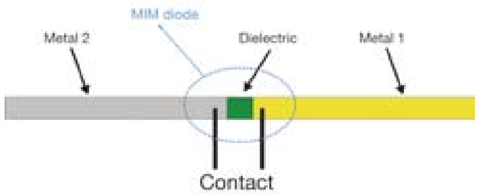
Nanotransfer printing of nanoantenna arrays for absorption of infrared light

Infrared detectors are already important devices. Far infrared light (terahertz radiation) can be used for safety or medical applications. Detectors for these wavelengths are expensive and difficult to fabricate. Our goal is the design of a new, low-cost and fast way to produce an array of nanoantennas using nano-transfer printing (nTP). In this technique, metals are evaporated onto a structured surface (stamp), and metal structures are directly transfered by pressing the stamp on a substrate. Afterwards the stamp can be reused several times. Furthermore, the stamp can be duplicated in the cheap and easy nanoimprint lithography (NIL) process. Therefore, fabrication using nTP and NIL processes could enable high-volume, low-cost production of devices with structural sizes in the nanometer regime.



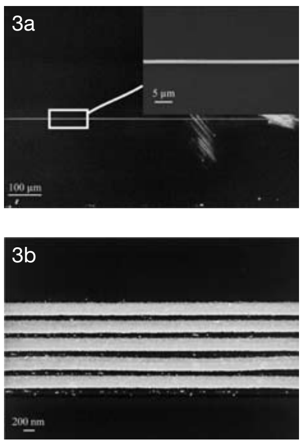
1 | Schematic of the metal transfer process from a stamp to a substrate

For fabricating nanoantennas that are able to detect infrared radiation in the THz range, a rectifier must be implemented in the antenna structure. A metal-insulator-metal (MIM) tunneling diode will be used for this purpose, implemented directly in the antenna structure.



2 | Schematic of a nano-antenna with an integrated MIM tunneling diode

Great progress was achieved in printing arrays of MIM-diodes. A process for fabricating a very thin (~3.6 nm) dielectric was designed, and aluminum-aluminum oxide-gold diodes were printed. Electrical measurements proved a tunnel current in the expected current range. Furthermore, long and thin lines of gold and aluminum were transfered and characterized electrically. These lines will serve as the detecting antennas. The resistivity was in the same range as in bulk material, which proves the suitability of the nTP process of fabricating nanoantennas with a high aspect ratio.

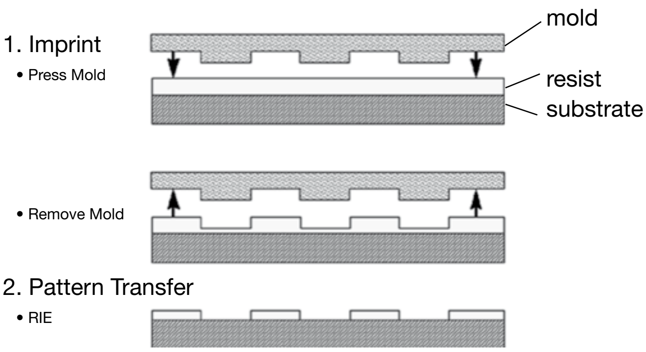


3 a/b | SEM images of transferred Au lines

So far, the MIM-diodes and the antenna have been transfered independently. In the future work, we will focus on transfering complete nanoantenna structures and further decreasing antenna size.

Fabrication of nanochannels on a silicon substrate using the NIL process

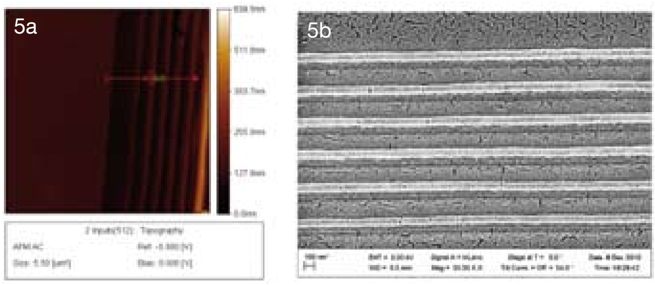
There is great interest in nanochannels for nanofluidics experiments. The use of nanofluidic devices has been reported widely in many areas, including ion transport and DNA analysis. The fabrication of a narrow yet continuous channel at the precise location was a key challenge until now, particularly due to the traditional nanofabrication methods used, e.g., writing and etching nanostructures. Our goal is to fabricate these nanochannels on LED/OPD devices using the nanoimprint lithography method. NIL is an unconventional lithographic technique for patterning of polymer nanostructures at a very low cost with high throughout. It has two basic steps as shown in fig 4.



4 | NIL process

The first is the imprint step, in which a mold with nanostructures on its surface is pressed into a thin resist spin-coated onto a substrate at a temperature higher than the glass transition temperature, followed by removal of the mold - thus creating an impression of the nanostructures on the mold in the substrate. The second step involves an anisotropic etching process such as reactive ion etching (RIE), to remove the residual resist in the compressed area.

In order to fabricate nanochannels, AlGaAs structures produced through molecular beam epitaxy were used as stamps. The structures on the stamp were 6 horizontal lines, each 200x200 nm. The stamps were etched in a citric acid solution to etch the gallium arsenide before the imprint, and a self-assembled monolayer was grown on top. The silicon substrates were subjected to a piranha clean in order to be hydrophilic. An imprint recipe was designed to optimize the reproducible process. AFM (5a) and SEM (5b) measurements of the corresponding imprints showed clear channels in the polymer with a height of approx. 100 nm and a width of 200 nm.



5 a/b | AFM and SEM images of imprinted 200x100nm channels

So far, we have succeeded in fabricating the nanochannels using the NIL on a silicon substrate. Future work will include characterizing these nanochannels as nanofluidic channels and integrating them onto LED/OPD devices. Apart from this, collaborative work with the Walter Schottky Institute (WSI) on the growth of GaAs and InAs nanotubes using NIL is also going on. Furthermore, research on an X-ray source based on field emission from silicon tips using the NIL is under way with the Universität der Bundeswehr, München.

Fabrication of nanomagnets

Nanomagnets have been used for manufacturing high-density memory devices, and they are now being used for fabricating logic devices based on their magnetic interaction when placed closely together. Simulation work has demonstrated their feasibility as a promising option for electronic computation in the future.

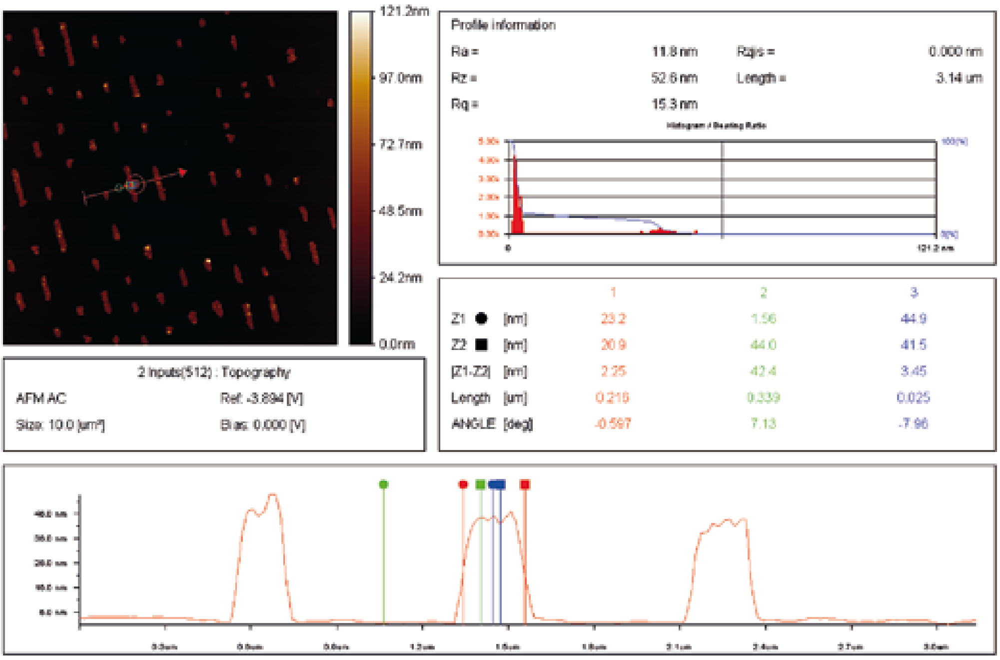
Various techniques are used for their fabrication. Nanotransfer printing is one such technique. A stamp with nanostructures on top is covered with a metal layer. This stamp is then pressed under high pressure and temperature on top on a substrate to fabricate the desired structures.

A silicon wafer with structures 400 nm wide and 400 nm to 1 µm long was used as a stamp. It was coated first with a metal and then with titanium as a gluing interface. This stamp was then pressed on a silicon substrate wafer that had been functionalized to be very hydrophilic. The applied pressure and temperature were optimized for maximum yield. Gold, aluminum, and permalloy (Ni 80%, Fe 20%) were successfully transfered.

Microscopic images show the extent of the patterns transfered. There were some areas where the transfer was not successful. That is due to defects caused by dust particles. AFM images were taken to see exactly what the transfered structures look like. Measured structures were 200 nm wide and 42 nm high.

6 | Transferred Permalloy

7 | Transferred Al



8 | AFM image of transferred permalloy.

Nanoimprint lithography and electrodeposition can also be used for nanomagnet fabrication. First a substrate is coated with a seeding layer to aid in electrodeposition. Then the surface is covered with a polymer. The polymer surface is structured using nanoimprint lithography. After removal of the residual layer, the substrate is put in an electrobath and electrodeposition of the required metal is done. Lift-off is performed to remove the polymer, and the desired structures are obtained.

Focus Group **Biochemistry**

Prof. Horst Kessler | Carl von Linde Senior Fellow
Organic Chemistry and Biochemistry, TUM

Highlights and Achievements

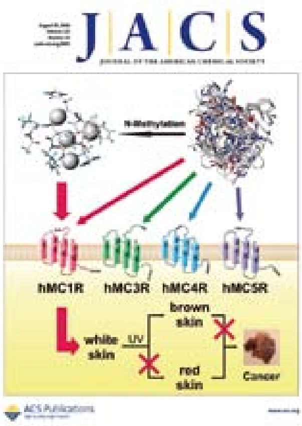
Horst Kessler

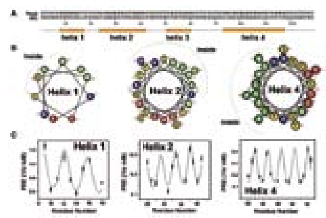
Discoveries with impact, from drug development to biologically inspired materials

In 2010, the Kessler group published 13 manuscripts with a total impact factor of 114.7. Three highlights are presented below.

Nature uses flexible molecules to target multiple receptor subtypes optimized for different functions in biological systems. A library of 31 multiply *N*-methylated products of the α-MSH-derived peptide MT-II yielded an inflexible, potent, and selective agonist of human melanocortin receptor subtype one. To the best of our knowledge, this is the first selective ligand for this receptor. Targeting individual G-Protein Coupled Receptor (GPCR) subtypes is of key importance in drug development.

[1] L. Doedens, F. Opperer, M. Cai, J. G. Beck, M. Dedek, E. Palmer, V. J. Hruby, and H. Kessler, "Multiple N-methylation of MT-II backbone amide bonds leads to melanocortin receptor subtype hMC1R selectivity; pharmacological and conformational studies," *J. Amer. Chem. Soc.*, 132 (23), pp. 8115–8128, 2010.





The heat shock protein Hsp12 of S. cerevisiae is up-regulated several hundred-fold in response to stress. We showed that this protein is important for cell survival under a variety of stress conditions. We observed changes in cell morphology under stress conditions. Surprisingly, Hsp12 exists in the cell either as a soluble cytosolic protein or in association with the plasma membrane. Our NMR analysis revealed that Hsp12, unlike all other Hsps studied so far, is intrinsically unfolded; however, in the presence of certain lipids, it adopts a helical structure. The presence of Hsp12 does not alter the overall lipid composition of the plasma membrane but increases membrane stability.

[2] S. Welker, B. Rudolph, E. Frenzel, F. Hagn, G. Liebisch, G. Schmitz, J. Scheuring, A. Kerth, A. Blume, S. Weinkauf, M. Haslbeck, H. Kessler, and J. Buchner; "Hsp12 is an Intrinsically Unstructured Stress Protein which folds upon Membrane Association and Modulates Membrane Function," *Mol. Cell., 39* (4), pp. 507–520, 2010.

In 2009, we were able to demonstrate the importance of partial defolding of the C-terminal domain of the major ampullate protein of the spider silk "spidroin" that regulates controlled silk fiber assembly. In 2010, the role of the other end of the spidroin was elucidated in our research group. The so-called N-terminal domain of the black widow is monomeric when stored under pH 7.2. In the spinning duct, the pH drops down to 6.0 and the N-terminal domain forms head-to-tail dimers that allow multimeric aggregation. Our study explains, for the first time, the splendorous stability of spider silk.

[3] F. Hagn, C. Thamm, T. Scheibel, and H. Kessler, "pH Dependent Dimerisation and Salt Dependent Stabilisation of the N-terminal Domain of Spider Dragline Silk - Implications for Fibre Formation," *Angew. Chem. Int. Ed.*, 50, pp. 310–313, 2011.

Prof. Axel Haase | Carl von Linde Senior Fellow
Prof. Markus Schwaiger, Clinic for Nuclear Medicine, TUM

Axel Haase

Challenging the limits of magnetic resonance imaging and spectroscopy

Magnetic resonance (MR) is an important tool, with MR spectroscopy helping to determine the structure and dynamics of biomolecules and MR imaging helping to detect many diseases. Various experiments have shown that the structure, function and metabolism of living organisms can be measured by noninvasive and non-destructive MR techniques. Compared to other imaging modalities, however, the measuring time is longer and the spatial resolution is limited due to the inherent low sensitivity of MR. We have worked with various methods and technical advances in order to increase the sensitivity.

One way is to use very high magnetic fields. At 17.6 tesla, a magnetic field that is a factor of 10 higher than normal clinical MRI units, we could apply MRI for cardiac and brain studies in animal experiments [1, 2] with an increased spatial resolution. Hyperpolarization of ^{13}C-labeled substances is another way to increase the sensitivity of MRI. Using dynamic nuclear polarization (DNP), the signal can be increased by a factor of up to 10,000 for selected substances. We have used hyperpolarized [1-^{13}C] pyruvate, which was injected into rats. The substance is metabolized and the downstream metabolites alanine, acetate, lactate, and bicarbonate can easily be identified with their respective MR resonance lines. Unfortunately the high level of signal decays with a relaxation time constant of approximately 30 seconds. Improving the signal-to-noise ratio is therefore an urgent need. We have applied a new 4-channel phased array coil (developed together with RAPID Biomedical GmbH) for the detection of the ^{13}C MR signal *in vivo* (fig. 1). We were able to demonstrate the characteristic features of the phased array coil (3) and will now apply it in our future projects (fig. 2). These experiments are part of the cooperation project with the GE Global Research Laboratory, Garching (Dr. Marion Menzel, Dr. Rolf Schulte) and the TUM (Prof. Markus Schwaiger, Clinic for Nuclear Medicine; Prof. Horst Kessler, TUM-IAS; Prof. Steffen Glaser, Organic Chemistry).

Publications:

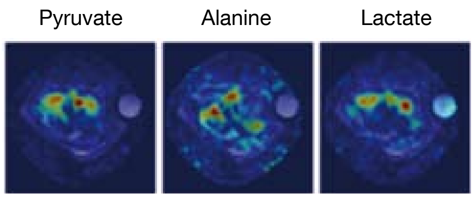
[1] M. J Schmidt, H. A. Oelschläger, D. Haddad, A. Purea, A. Haase, and M. Kramer, “Visualizing premature brain using 17.6 Tesla magnetic resonance imaging (magnetic resonance microscopy),” *Veterinary Journal*, vol. 182, no. 2, pp. 215–222, 2009.

[2] V. Herold, J. Wellen, CH. Ziener, T. Weber, K. H. Hiller, P. Nordbeck, E. Rommel, A. Haase, W. R. Bauer, P. M. Jakob, and S. K. Sarkar, “In vivo comparison of atherosclerotic plaque progression with vessel wall strain and blood flow velocity in apoE-/- mice with MR microscopy at 17.6 T,” *MAGMA*, vol. 22, no. 3, pp. 159–166, 2009.

[3] R. F. Schulte, J. I. Sperl, A. Haase, M. Irkens, M. Manglberger, E. Weidl, G. Kudielka, M. Schwaiger, and F. Wiesinger, „Advanced Parallel Imaging Techniques for Metabolic Imaging with Hyperpolarized ^{13}C,” Proc. of International Society of Magnetic Resonance in Medicine, 2725 (2011).

1a | 4-channel ^{13}C-phased array coil: part of the coil

1b | 4-channel ^{13}C-phased array coil: phased-array coil with housing



2 | Transaxial ^{13}C MRI cross-section of the abdomen of a rat measured at a 3T whole body scanner at GE Global Research Laboratory. The images show high signal (in red and green) of ^{13}C-labelled hyperpolarized pyruvate, alanine and lactate in both kidneys (see ref. 3).

Dr. Marco Punta | Carl von Linde Junior Fellow
Prof. Burkhard Rost, Bioinformatics, TUM

Enhancing a protein "pipeline" from both ends, target selection and analysis

Marco Punta

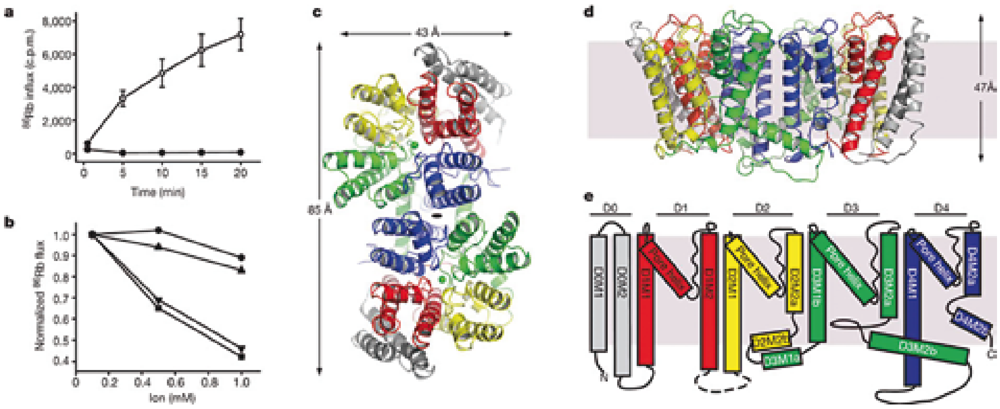
Through 2010, I continued my collaboration with the New York Consortium on Membrane Protein Structure (NYCOMPS). The ultimate goal of NYCOMPS is increasing knowledge of the membrane protein structural universe. Toward this end, we have established a membrane protein production pipeline, based at the New York Structural Biology Center, for cloning, expressing, purifying, and screening (for detergent stability) prokaryotic membrane proteins. Best-performing targets from the pipeline are then distributed to individual NYCOMPS structural biology labs for crystallization trials. This strategy has led in the past two years to determination of a number of novel membrane protein structures.

My role at NYCOMPS has been in target selection, i.e., the first step in the protein production pipeline, as well as in post-production data analysis. Analyzed data includes both expression-purification experiment outcomes and protein structures. In this context, I supervised a number of students working with scientific-assistant or collaboration contracts. Expression data analysis allowed us to identify a number of low-performance genomes together with a number of protein features that correlate with expression [Li et al., in preparation]. This information should be useful to improve our target selection criteria. We could find no correlation between predicted presence of N-terminal signal peptides and protein expression assessed via N-terminal purification tags. This may be explained by one or more of the following: 1) foreign signal peptides are not recognized by E. *coli* signal peptidase; 2) N-terminal tags interfere with cleavage; 3) predictions are not accurate. We noticed that most methods predict a relatively large number of signal peptides in bacterial membrane proteins, while we could only find a handful of known cases in the literature. This may suggest caution in interpreting the results when using such prediction methods on bacterial membrane proteins [Boidol et al., in preparation]. Finally, a combination of structural information, sequence conservation, and correlated mutation analysis led us to predict a number of residues that may be key to separate functional subfamilies of bacterial potassium transporters [Bader et al. in preparation].

Characterization of a bacterial lipoprotein via a multi-institute collaborative effort

The other main research project I undertook in the last year has been the *in silico* annotation of a protein structure from *B. subtilis* [Wu, Punta et al., in preparation]. This work started as a small collaboration with Prof. Thomas Szyperski at the University of Buffalo (N.Y., USA) and it has now developed into a full project additionally involving Prof. Arne Skerra at TUM and Dr. Marco De Vivo at the Italian Institute of Technology in Genova (Italy).

That project's goal is functional characterization of protein YxeF, a bacterial lipoprotein from *B. subtilis*, the structure of which has been NMR-solved by



Crystal structure of a potassium ion transporter, Nature (2011) doi:10.1038/nature09731

the NorthEast Structural Genomics consortium in the USA. Initial *in silico* analysis showed that YxeF shared several sequence and structural features with members of the lipocalin family. Lipocalins are proteins generally known to bind and transport small hydrophobic compounds, and they have attracted a lot of attention as putative scaffolds for design of novel antibody mimetics (called anticalins). While sharing important similarities with lipocalins, YxeF lacked a signature C-terminal alpha-helix known to be important for lipocalin stability. Two-dimensional [^{15}N,^{1}H] heteronuclear single-quantum coherence (HSQC) spectra from Prof. Szyperski's lab showed that YxeF is stable at least up to temperatures of 50oC. Our current hypothesis is that YxeF may represent the first example of a lipocalin in Gram+ bacteria, although this requires defining a novel structural theme within the lipocalin family, a theme that may be specific to these organisms.

Lipocalin function in bacteria is not well-understood. Available data suggest that they might be involved in lipid and membrane metabolism. In collaboration with the Italian Institute of Technology, we are now performing *in silico* ligand screening in an attempt to identify putative functional ligands for YxeF. Top-scoring molecules will then be tested in the laboratories of Prof. Szyperski and Prof. Skerra. We hope that YxeF will be key to a better understanding of lipocalin function in bacteria, and that it may possibly give important indications on how to design new anticalins featuring a minimal scaffold.

Publications:

[1] A. Schlessinger, C. Schaefer, E. Vicedo, M. Schmidberger, M. Punta, and B. Rost, "Protein disorder - a breakthrough invention of evolution?," *Current Opinion in Structural Biology* [accepted]

[2] W. Shi, M. Punta, J. Bohon, J. M. Sauder, R. D'Mello, M. Sullivan, J. Toomey, D. Abel, M. Lippi, A. Passerini, P. Frasconi, S. K. Burley, B. Rost and M. R. Chance, "Characterization of Metalloproteins by High-Throughput X-ray Absorption Spectroscopy," *Genome Research* [accepted]

[3] Y. Cao, X. Jin, H. Huang, M. G. Derebe, E. J. Levin, V. Kabaleeswaran, Y. Pan, M. Punta, J. Love, J. Weng, M. Quick, S. Ye, B. Kloss, R. Bruni, E. Martinez-Hackert, W. A. Hendrickson, B. Rost, J. A. Javitch, K. R. Rajashankar, Y. Jiang, and M. Zhou, "Crystal structure of a potassium ion transporter, TrkH," *Nature* vol. 471, no. 7338, pp. 336–340, 2011.

[4] Y. H. Chen, L. Hu, M. Punta, R. Bruni, B. Hillerich, B. Kloss, B. Rost, J. Love, S. A. Siegelbaum, and W. A. Hendrickson, "Homologue structure of the SLAC1 anion channel for closing stomata in leaves," *Nature*, vol. 467, no. 7319, pp. 1074–1080, 2010.

[5] J. Love, F. Mancia, L. Shapiro, M. Punta, B. Rost, M. Girvin, D. N. Wang, M. Zhou, J. F. Hunt, T. Szyperski, E. Gouaux, R. MacKinnon, A. McDermott, B. Honig, M. Inouye, G. Montelione, and W. A. Hendrickson, "The New York Consortium on Membrane Protein Structure (NYCOMPS): a high-throughput platform for structural genomics of integral membrane proteins," *J Struct Funct Genomic*, vol. 11, no. 3, pp. 191–199, 2010.

[6] K. K. Singarapu, J. L. Mills, R. Xiao, T. Acton, M. Punta, M. Fischer, B. Honig, B. Rost, G. T. Montelione, and T. Szyperski, "Solution NMR structures of proteins VPA0419 from Vibrio parahaemolyticus and yiiS from Shigella flexneri provide structural coverage for protein domain family PFAM 04175," *Proteins*, vol. 78, no. 3, pp. 779–784, 2010.

[7] Cao Y, Jin X, Levin EJ, Huang H, Zong Y, Quick M, Weng J, Pan Y, Love J, Punta M, Rost B, Hendrickson WA, Javitch JA, Rajashankar KR & Zhou M. "Crystal structure of a phosphorylation-coupled saccharide transporter." *Nature* [accepted]

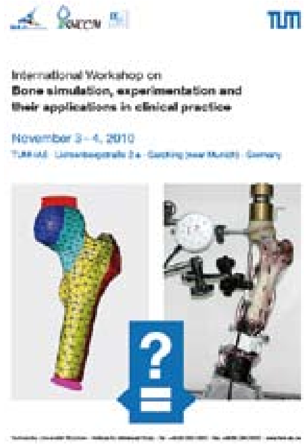
Focus Group **Computational Biomechanics**

Prof. Zohar Yosibash | Hans Fischer Senior Fellow
Prof. Ernst Rank, Computation in Engineering, TUM

Steps toward clinical applications of bone simulation

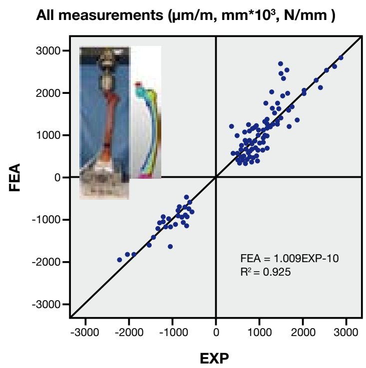
Zohar Yosibash

In the effort to investigate the mechanical response of the human femur and develop a reliable simulation tool based on high-order finite element/cell methods for use in clinical practice, the year 2010 was very fruitful and enjoyable at the same time. I had the pleasure of visiting Prof. Ernst Rank's Group at TUM for a six-month period (Aug. 2010 to Jan. 2011). Together we organized an international workshop (fig. 1) with the generous support of the TUM-IAS, attended by many senior scientists from diverse disciplines – orthopedics, statistics, bio-mechanics, and numerical analysis – and involving equal numbers of junior scientists and doctoral candidates. This intensive, two-day meeting was held in the new TUM-IAS building in an informal, cozy, and very productive atmosphere. These sessions resulted in new collaborations between TUM Professors Daniel Straub and Donna Ankerst and Prof. Joyce Keyak of UC Irvine, with the aim of quantifying the uncertainty associated with bone tissue properties. In this respect, we also enhanced our collaboration with Dr. Rainer Burgkart's group at the TUM university hospital Klinikum rechts der Isar, and we are in the process of analyzing problems of clinical relevance.



1 | Announcement to the international workshop held on Nov 3-4, 2010 in the new TUM-IAS building.

During the past year, we also finalized and summarized a one-year project in collaboration with Prof. Peter Augat at the Murnau Hospital, where we demonstrated the predictive capabilities of our simulation by a double-blind approach on a large cohort of 12 fresh-frozen femurs. Using our novel high-order finite element methods, we predicted the response of the femurs tested by Prof. Augat's group. Our two groups compared results only after our individual sets of tests and analyses were complete (fig. 2), in order to maintain a non-biased perspective. This comparison demonstrates the high quality of our simulation capabilities.



2 | Comparison of displacements, strains and stiffness between the FE predictions and Experimental observations.

Toward the quantification of bone material uncertainties, we first enhanced the newly developed finite cell method from Prof. Rank's Group for simulating bone mechanics. Research on this was successfully started by Hagen Wille, a new doctoral candidate supported by the TUM-IAS, resulting in a manuscript to be submitted for publication in 2011. Several talks on the topic, including keynote lectures, were presented at various conferences. Three papers were submitted for publication.

Publications:

[1] Trabelsi N., Yosibash Z., Wutte C., Augat P. and Eberle S., "Patient-specific finite element analysis of the human femur - a double-blinded biomechanical validation," *Journal of Biomechanics*, In print, 2011.

[2] Trabelsi N. and Yosibash Z., "Patient-specific FE analyses of the proximal femur with orthotropic material properties validated by experiments," *Journal of Biomechanical Engineering*, In print, 2011.

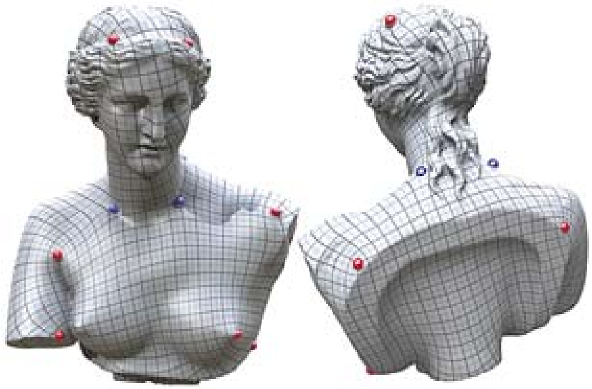
[3] Ruess M., Tal D., Trabelsi N., Yosibash Z. and Rank E., "The finite cell method for bone simulations: Verification and validation," *J. Biomechanics and Modelling in Mechanobiology*, The revised manuscript is under review, 2011.

Prof. Peter Schröder | Hans Fischer Senior Fellow
Prof. Rüdiger Westermann, Computer Graphics and Visualization, TUM

Highlights and Achievements

Digital geometry processing makes connections: between theory and practice, and between disciplines

Peter Schröder



During the first half of 2010, Prof. Peter Schröder continued his residence at TUM and taught a class on his specialty, digital geometry processing, for the Department of Computer Science. This time also marked the beginning of a number of new collaborations. With his Host Prof. Rüdiger Westermann, he started a new project with the goal of constructing so-called multigrid numerical solvers for problems with highly inhomogeneous material properties. Recent advances in homogenization theory provide new ideas to overcome the lack of smoothness in these settings. A former student and present postdoctoral researcher is now continuing this work under joint supervision and took the opportunity to visit the California Institute of Technology (Caltech) during the fall of 2010. During the winter, another of Prof. Westermann's students visited Caltech for an extended time in order to deepen the ongoing collaborations between the two institutions.

Working with Prof. Tim Hoffmann of the Mathematics Department at TUM, Prof. Schröder explored some initial ideas for the construction of planar quad surfaces. These are relevant for architectural structures (glass and steel-free form surfaces), for example. A bachelor thesis was awarded to determine how well these theoretical ideas play out in practice. The first half of 2010 also marked the arrival of a new graduate student co-supervised with Prof. Daniel Cremers of the Computer Science Department. He focuses on the interface between Prof. Cremers's interest in convex optimization algorithms in computer vision and Prof. Schröder's expertise in digital geometry processing.

During his time in Germany, Prof. Schröder was also able to start new projects with other researchers in Germany, most notably at the TU Berlin Math Department. These continue apace, and Prof. Schröder is looking forward to new developments in 2011.

Publications:

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[2] K. Crane, M. Desbrun, and P. Schröder, "Trivial Connections on Discrete Surfaces," *Comput. Graph. Forum*, vol. 29, no. 5, pp. 1525-1533, 2010.

Focus Group **Risk Analysis and Stochastic Modeling**

Prof. Richard Davis | Hans Fischer Senior Fellow
Prof. Claudia Klüppelberg | Carl von Linde Senior Fellow
Dr. Robert Stelzer | Carl von Linde Junior Fellow
Prof. Claudia Klüppelberg, Mathematical Statistics, TUM

Claudia Klüppelberg

Robert Stelzer

Richard Davis

From financial and electricity markets to wind speed and thermodynamics

The past year was another exciting and very fruitful year for our Focus Group, with several noteworthy events. The TUM-IAS Workshop on Statistical Models and Methods on February 1, 2010 brought together TUM researchers from the majority of faculties. The exchange was lively and triggered joint interdisciplinary research ventures in some cases. The “Risks, Crises, and Catastrophes” Symposium (a joint venture of the TUM-IAS, the Carl von Linde-Akademie of TUM, and the Deutsches Museum) took place at the Deutsches Museum on November 18. The symposium was dedicated to the modeling and quantification of extreme events and entailed presentations in front of the full Ehrensaal, the Hall of Fame. The topics ranged from the safety problems of technical systems in coping with natural catastrophes to financial market risks, and even included methodological talks. The general audience waited patiently until the end of the roundtable discussion, and questions from the audience were also addressed. Several long-term visitors contributed to the success of the Focus Group, including Hans Fischer Senior Fellow Prof. Richard A. Davis and Humboldt Research Awardee Prof. Jean Jacod.

Team Klüppelberg
The team has made substantial progress in understanding the fundamental properties of non-Gaussian Lévy-driven processes, one-dimensional and multivariate, including models with short- and long-term memory.

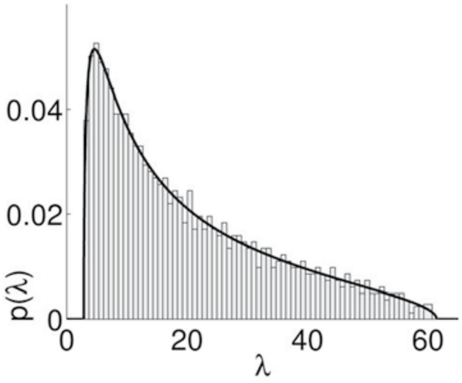
The two doctoral candidates in the Focus Group are making good progress. Florian Ueltzhöfer and Prof. Claudia Klüppelberg estimated a Lévy measure of arbitrary dimension from high-frequency data. Florian Ueltzhöfer is co-advised by Prof. Jacod and spent several weeks in Paris making excellent progress. Christina Steinkohl, Prof. Davis, and Prof. Klüppelberg advanced their investigation of extreme wind fields. Extreme space-time models are in the development stage, and simulation tools and statistical estimation methods are well on their way. Collaboration with the Risø DTU Technical University of Denmark was established, and in spring 2011 Christina Steinkohl and Prof. Klüppelberg will spend one month each at the Danish institute. The TUM-IAS postdoctoral researcher Dr. Codina Cotar and Prof. Klüppelberg are working together on two different projects. In one project, they suggest and develop optimal transport methods for exchange-correlation functionals used in density functional theory. They show that, in the case of two electrons and in the semi-classical limit, the famous Hohenberg-Kohn functional reduces to a particular functional of optimal transport origin, which they explicitly solve. In a second project, they develope spatial risk measures motivated by methods from statistical mechanics and aimed at the modeling of systemic risk in financial and electricity markets. In a separate project, Dr. Cotar is studying macroscopic systems of statistical physics and characterizing their properties in thermodynamic equilibrium.

Prof. Klüppelberg also worked successfully on other projects with several collaborators and doctoral candidates. The dynamic structure of electricity spot prices was well modeled by stationary, stable, non-Gaussian continuous-time linear models (CARMA models). The development of statistical estimation methods for such models also requires the investigation of probabilistic and statistical properties of such processes. Another PhD project was dedicated to the modeling and statistical estimation of dependence between the components of a multivariate Lévy process. Moreover, long-term memory, Lévy-driven processes have been investigated and applied in order to model stochastic hazard. Statistical modeling and first statistical analyses of turbulent wind speed present dynamic mean flow as a stochastic integral over a memory function, which we have estimated from turbulence data with high Reynolds numbers. Numerous publications are concerned with financial risk modeling and risk assessment. For financial data, it is commonly believed that the volatility (variance) is stochastic. Moreover, there is an ongoing debate on whether volatility exhibits jumps. We have also contributed to this discussion by various deep statistical analyses.

Team Stelzer

In the past year, a new project on high-dimensional statistics using random matrix theory was initiated together with Hans Fischer Senior Fellow Prof. Davis. Substantial progress has been made. In random matrix theory, one considers the limiting distributions for eigenvalues of square matrices, whose entries are stochastic, as the dimension approaches infinity. These results are used especially in connection with the estimation of covariance matrices (or some of their properties) when the number of observations is comparable to the number of dimensions. So far, the case of independent identically distributed (iid) entries is well understood in the literature. However, for dependent entries, which often occur in applications, the available results are rather limited thus far. Oliver Pfaffel and Eckhard Schlemm have shown limit results for eigenvalue distributions when the matrix entries are given by linear random processes, obtaining more explicit expressions for the limiting distribution than previously attained. Moreover, Prof. Davis, Oliver Pfaffel, and Dr. Stelzer have developed a new approach for obtaining limiting results for random matrices with heavy-tailed iid entries when the entries have an infinite variance. They are currently working on extending this approach to the dependent case.

Other major research projects have been furthering the understanding of infinitely divisible stochastic processes (Florian Fuchs, Martin Moser, and Dr. Stelzer) and the estimation of Lévy-driven CARMA processes (Florian Fuchs, Eckhard Schlemm, and Dr. Stelzer). During a long-term stay at Colorado State University (Fort Collins, USA), Prof. Peter Brockwell and Eckhard Schlemm made important progress on estimating the driving Lévy



Histogram of the eigenvalues and limiting spectral density $\lambda \mapsto p(\lambda)$ of $\frac{1}{p}XX^T$ when the rows of the $p \times n$ matrix X are given by ARMA(1,1) processes of the form $Y_1 = 0.5Y_{1-1} + Z_1 + Z_{1-1}$ for $y = \frac{n}{p} = 5$ and $p = 1000$.

process of a CARMA process. Finally, Martin Moser investigated the tail behavior of random walks with dependent increments together with Thomas Mikosch during a long-term visit to the University of Copenhagen (Denmark).

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[1] O. E. Barndorff-Nielsen, J. Bertoin, J. Jacod, and C. Klüppelberg, eds. *Lévy Matters I. A Subseries on Lévy Processes*. Springer, Lecture Notes in Mathematics, vol. 2001, 2010.

[2] S. Asmussen , V. Fasen, and C. Klüppelberg. “Heavy tails in insurance.” In *Encyclopedia of Quantitative Finance*, edited by R. Cont, 873–875. Chichester: Wiley, 2010.

[3] K. Böcker and C. Klüppelberg. “Multivariate models for operational risk.” *Quantitative Finance* 10, no. 8 (October 2010): 855–869. PRMIA Award 2007 “New Frontiers in Risk Management.”

[4] E. Brodin and C. Klüppelberg. “Modelling, Estimation and Visualization of Multivariate Dependence for High-frequency Data.” In *Statistical Modelling and Regression Structures Festschrift in Honour of Ludwig Fahrmeir*, edited by Thomas Kneib and Gerhard Tutz, 267300. Heidelberg: Physica-Verlag, 2010.

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[6] H. Esmaeili and C. Klüppelberg, “Parameter estimation of a bivariate compound Poisson process,” *Insurance: Mathematics and Economics*, vol. 47, no. 2, pp. 224-233, October 2010.

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[9] C. Klüppelberg, T. Meyer-Brandis, and A. Schmidt, “Electricity spot price modelling with a view towards extreme spike risk,” *Quantitative Finance*, vol. 10, no. 9, pp. 963–974, 2010.

[10] R. Stelzer, “Multivariate COGARCH(1,1) Processes,” *Bernoulli*, vol. 16, no. 1, pp. 80–115, 2010.

Focus Group **Networked Dynamical Systems**

Prof. Anuradha M. Annaswamy | Hans Fischer Senior Fellow
Prof. Martin Buss, Automatic Control Engineering, TUM

Anuradha M. Annaswamy

Publications:

[1] A. Kiani and A. Annaswamy, "Wholesale Energy Market in a Smart Grid: Dynamic modeling, and stability," submitted to the IEEE Conference on Decision and Control (CDC), Orlando, Florida, USA, Dec. 2011.

[2] H. Voit, R. Schneider, D. Goswami, A. Annaswamy, and S. Chakraborty, "Optimizing hierarchical schedules for improved control performance," presented at the IEEE Symposium on Industrial Embedded Systems (SIES), Trento, Italy, July 7–9, 2010.

[3] H. Voit, R. Schneider, D. Goswami, A. Annaswamy, and S. Chakraborty, "Adaptive controllers for multi-mode cyber-physical systems with modeling uncertainties," submitted to the International Conference on Embedded Software (EMSOFT), Taipei, Taiwan, October 2011.

Groundwork for smart management of sustainable power systems

With our ultimate research goal being the analysis of smart technical systems and their synthesis with energy system applications, we investigated in the past year:

- the dynamics of wholesale energy markets in "smart grids" and the effect of renewable energy sources;
- state estimation in distributed power systems;
- the realization of high control performance in complex embedded systems.

The area of smart grid research is of significant interest due to the recent paradigm shift in energy systems driven by several factors: the need to integrate renewable energy sources, the availability of information via advanced metering and communication, and an emerging demand structure policy intertwined with pricing. Our efforts during 2010 focused on the development of a fundamental dynamic model capturing the interactions among generation, demand, pricing, and congestion. This dynamic model also lays the foundation for the analysis and design of a robust energy market and enables the study of the effects of intermittency in renewable energy resources (RERs), the mitigation of the integration cost of RERs using the notion of demand response, and the role of information obtained using smart meters with a delay. Our next step is to explore how control can be integrated into this framework.

While the presence of RERs leads to better sustainability, it can also pose stability problems for system operation. Distributed state estimation is a central tool for alleviating such stability problems. We began to develop a novel method allowing for a better estimate of the system state and therefore a better management of overall distribution management systems in a power grid.

All physical systems with a rudimentary level of complexity involve some sort of cyberstructure interaction that helps, monitors, predicts, or manages their functions. As the level of complexity increases, the interaction between the cyber and physical components needs to be kept specific, systematic, nuanced, and robust. Our focus is on one such cyber-physical system where the objective is to realize high control performance in applications with distributed embedded systems. We are developing a novel co-design of control and communication architectures combining adaptive switching controllers together with a multi-modal, real-time system; this has yielded promising results. Our next steps are to develop formal methods, combining control in engineering and real-time systems in computer science, and to validate our approach through placement in an automotive system, which is a typical example of a distributed embedded system.

Dr. Dragan Obradovic | Rudolf Diesel Industry Fellow
Prof. Sandra Hirche, Automatic Control Engineering, TUM

Highlights and Achievements

Dragan Obradovic

Building out a collaborative network for smart grid research

Most of Dr. Dragan Obradovic's TUM-IAS activities in 2010 were focused on establishing new domestic and international cooperation contacts related to the research interests of the Networked Dynamical Systems Focus Group and to presenting research results.

In April 2010, Dr. Obradovic visited Prof. Antonello Monti of the E.ON Research Center at RWTH Aachen. There is ongoing discussion about the the idea of establishing joint cooperation between TUM, RWTH, and possibly Siemens AG. The collaboration with Prof. Monti resulted in joint conference publications and a journal submission.

Based on an invitation from Dr. Obradovic, Prof. Sanjoy Mitter of MIT gave an TUM-IAS lecture at TUM in November 2010 entitled "Systems Theory: A Retrospective and Prospective Look." Visits from Prof. Mitter and Dr. Roozbehani of MIT to the laboratory of Prof. Martin Buss and Prof. Sandra Hirche were also organized.

Prof. Claudia Klüppelberg visited Siemens Wind Power in Denmark together with Dr. Obradovic in November 2010. A cooperation project between Prof. Klüppelberg and Siemens Wind Power is expected in 2011.

Contact with the group of Prof. Birgit Vogel-Heuser was established in 2010 with the goal of designing a real-time control demonstrator using Siemens control equipment.

Dr. Obradovic's presented a talk titled "Networked Control Systems (NCS) and their Selected Applications in Automation Systems and Power Grids" at the TUM-IAS General Assembly in April 2010. In June, he presented "Selected Control Problems in Grids with High Percentage of Renewable Energy" at the TUM-IAS seminar workshop "Information-based Analysis and Design of Networked Control Systems." A common venture called "Networked Control for Smart Grids" was presented by Prof. Hirche and Dr. Obradovic at the TUM-IAS Symposium "Energy and Electromobility – Exploring the Fundamental Research Challenges" in October.

Some 2010 activities looked ahead to potential future events, such as a workshop on the distributed control of electric grids.

In addition, we are glad to report that Herbert Mangesius, a PhD student financed by the Rudolf Diesel Industry Fellowship of Dr. Obradovic, started his doctoral studies in the summer of 2010 at the TUM Institute of Automatic Control Engineering.

Focus Group **Cognitive Technology**

Prof. Mandayam A. Srinivasan | Hans Fischer Senior Fellow
Prof. Martin Buss, Automatic Control Engineering, TUM

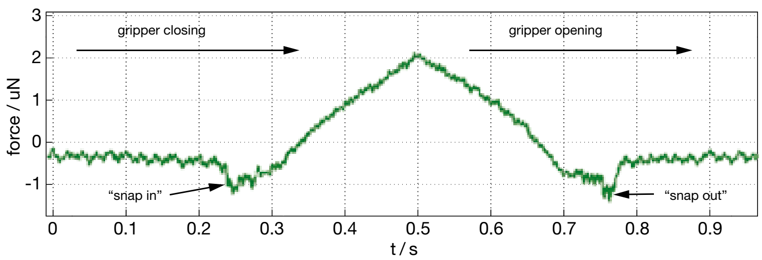
Mandayam A. Srinivasan

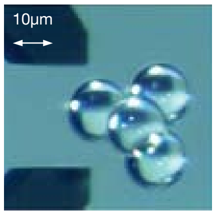
Extending the human touch: Telehaptics for micro/nanoassembly

How can human touch be extended to enable manual exploration and manipulation of microstructures and even nanostructures? This is one of the key questions driving our research. Since the start of the project, we have been developing tools and methods to manipulate microparticles as easily and as intuitively as possible.

Over the past year, two core topics have been addressed:

- Adhesion forces arising in microenvironments are a major obstacle in the precise and intuitive manipulation of objects. To gain a better understanding of the phenomenon itself and the associated factors, studies on surface treatments and electric potentials have been carried out (Fig. 1).
- After succeeding in our first manipulation task, the stacking of microbeads into a pyramid using our newly developed haptic microgripper (Fig. 2), we have made progress in controlling an atomic force microscope (AFM) with the same haptic interface.





1 | Effects of adhesion on the gripping process.

2 | A pyramid of polystyrene microbeads stacked manually using the telehaptic system. Microgripper arms are also shown.

All of the experimental steps are carried out in close collaboration with Dr. Stefan Thalhammer's Group at the Helmholtz Center Munich and the Institute of Automatic Control Engineering at TUM. The two project leaders supervise the TUM-IAS-funded doctoral candidate Andreas Schmid.


peter
MADE IN GERMANY

New Fellows and Research Plans

Nanoscience

- Nanophotonics
- Nanoscale Control of Quantum Materials
- Nonequilibrium Statistical Mechanics at the Nanoscale
- Molecular Aspects of Interface Science

Biophysics

Clinical Cell Processing and Purification

Advanced Cardiac Mechanics Emulator

High-Performance Computing (HPC)

Advanced Computation

Advanced Construction Chemicals and Materials

Advanced Stability Analysis

Aircraft Stability and Control

Cognitive Technology

Diesel Reloaded

Global Change

Introduction

With great pride and pleasure TUM-IAS welcomes its new 2010 Fellows and their Hosts. They present themselves in this section. The total number of honored proposals has been nothing short of astounding (two Carl von Linde Senior Fellows, six Carl von Linde Junior Fellows, six Hans Fischer Senior Fellows, one Hans Fischer Tenure Track Fellow, and four Rudolf Diesel Industry Fellows), and this, needless to say, from a much larger collection of very worthy proposals.

First, we are extremely happy with the new Rudolf Diesel Industry Fellows in our midst. This category was definitely underrepresented in our past program and has now been effectively brought up to par. Each of the new Rudolf Diesel Industry Fellows brings a very unique quality to TUM-IAS, besides a very much appreciated relationship with an innovative, research-oriented company. Dr. Tsuyoshi Hirata is known worldwide for his invention of special concrete additives and is our first Diesel Fellow from Japan; also, he is spending a full year as a researcher at TUM-IAS, another first. Dr. Matthias Heller brings in invaluable expertise in the area of aircraft control and a very active mind, always searching for the best new method, not eschewing the most advanced approaches. Prof. Gernot Spiegelberg is the electrifying motor behind a project called “Diesel Reloaded” that will redefine electromobility. All three are not only excellent scientists, but also accomplished engineers, bringing a new dimension into TUM-IAS.

With the nomination of six new Carl von Linde Junior Fellows and one Hans Fischer Tenure Track Fellow, TUM-IAS is fulfilling its role in rejuvenating research at TUM, not only in terms of age, but also in terms of new ideas and topics. For the concrete plans of these new Fellows we happily refer to their respective pages further on; let it be noted here that the competition for this category of Fellows has been very tough. We had to reject an equal number of proposals, although many of them still ranked pretty high in the evaluation. For this category of Fellows, we use an orthodox Delphi ranking procedure – for a description of this keen selection method see our web site – which results in a blind (and statistically relevant) ranking by a jury. Selected proposals all ranked better than 1.5.

As usual, TUM-IAS received a number of very impressive nominations for Hans Fischer Senior Fellow. These proposals are not subjected to a Delphi procedure, but are presented directly to our Advisory Council, together with an assessment or a recommendation by one of our top scientists. In most cases the quality of the nomination, both in terms of the person proposed and her or his plan, is overwhelming. Our Hans Fischer Senior Fellows are truly exceptional, internationally recognized researchers with great plans for research innovation in close collaboration with one of the most outstanding research groups at TUM. The Fellowship is awarded in due recognition of these facts, honoring both the Fellow and her or his Host professor.

TUM-IAS has also been very fortunate to be able to nominate two Carl von Linde Senior Fellows, in recognition of their great leadership at TUM, allowing them to put a crown on their impressive scientific oeuvre. It needs no explanation why Prof. Gerhard Abstreiter, director of the Walter Schottky Institute and creator of the new ZNN (Center for Nanotechnology and Nanomaterials) and Prof. Ulrich Stimming, a driving force behind the renewal of research in sustainable energy at TUM, received the award.

Most of the time, our Fellows do not operate in isolation, but are part of very active communities of researchers, often with several Fellows and Fellows in different categories working together. We certainly recognize the strengthening of our main "Research Areas" – collaborations that largely exceed single groups. In the present batch we have several new Fellows in Nanoscience, Knowledge Engineering, Medical Instrumentation, and Advanced Computation. Such concentrations of Fellows are not intentional, but happen almost through natural selection, enhanced by the presence of Clusters of Excellence. No doubt, quality seeks quality. Nonetheless, and true to our mission, we remain open for any excellent proposal, without any political forethought or afterthought.

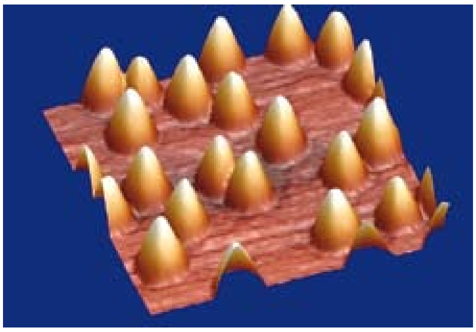
Focus Group **Nanophotonics**

Prof. Gerhard Abstreiter | Carl von Linde Senior Fellow
Host: Experimental Semiconductor Physics, TUM

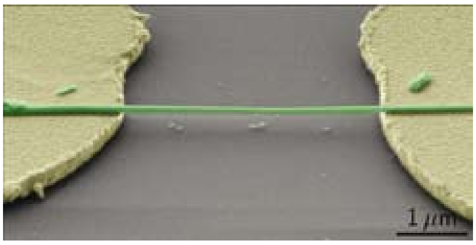
Nanotechnology aims to control matter on an atomic scale and make use of the altered physical and chemical properties of nanostructures for novel applications. We concentrate our research on semiconductor nanostructures fabricated both with so-called “top-down” and “bottom-up” techniques and aim to create novel nanoelectronic and nanophotonic devices for information and communication technology, efficient energy conversion, and biochemical sensing for medical applications. Our more basic studies in quantum science and nanoscience deal with fundamental investigations of the quantum mechanical properties of nanoscale objects. Our goal in this direction is the coherent control of single charges, spins, and photons in semiconductor quantum dots and nanowires as a basis for quantum information technology and sensing.

In 2010, we established the new Center for Nanotechnology and Nanomaterials (ZNN) as an extension of the Walter Schottky Institute on the Garching Research Campus, where state-of-the-art nanotechnology and nanoanalytic facilities are now available. The planned projects will be conducted in close collaboration with the research groups of Prof. Alexander Holleitner, Prof. Jonathan Finley, and Hans Fischer Senior Fellow Prof. Yasuhiko Arakawa of the University of Tokyo.

1 | High purity molecular beam epitaxy system for fabrication of semiconductor quantum dots and nanowires



2 | Atomic force microscope image of InAs quantum dots on GaAs



3 | Scanning electron microscope image of a GaAs nanowire device for measuring thermoelectric properties

Publications:

[1] M. Soini, I. Zardo, E. Uccelli, S. Funk, G. Koblmüller, A. Fontcuberta i Morral, and G. Abstreiter, “Thermal conductivity of GaAs nanowires studied by micro-Raman spectroscopy combined with laser heating,” *Applied Physics Letters*, vol. 97, no. 26, 263107, 2010.

[2] G. Koblmüller, S. Hertenberger, K. Vizbaras, M. Bichler, F. Bao, J.-P. Zhang, and G. Abstreiter, “Self-induced growth of vertical free-standing InAs nanowires on Si(111) by molecular beam epitaxy,” *Nanotechnology*, vol. 21, no. 36, 365602, 2010.

[3] S. Hertenberger, D. Rudolph, M. Bichler, J. Finley, G. Abstreiter, and G. Koblmüller, “Growth kinetics in position-controlled and catalyst-free InAs nanowire arrays on Si(111) grown by selective area molecular beam epitaxy,” *J. Appl. Phys.*, vol. 108, no. 11, pp. 114316–114317, 2010.

Gerhard Abstreiter
graduated in physics from TUM in 1973 and received his doctorate in 1975 working on cyclotron resonance in silicon inversion layers. From 1975 until 1979, he was a postdoctoral researcher and staff scientist at Max Planck Institut für Festkörperforschung in Stuttgart and Grenoble. He returned to the TUM Physics Department as a group leader in 1979. In 1987, he became a full professor and the Director of the newly founded Walter Schottky Institute. He was elected a Fellow of the American Physical Society in 1992, a member of the Bavarian Academy of Sciences in 2007, and a member of acatech in 2009.

Focus Group **Nanoscale Control of Quantum Materials**

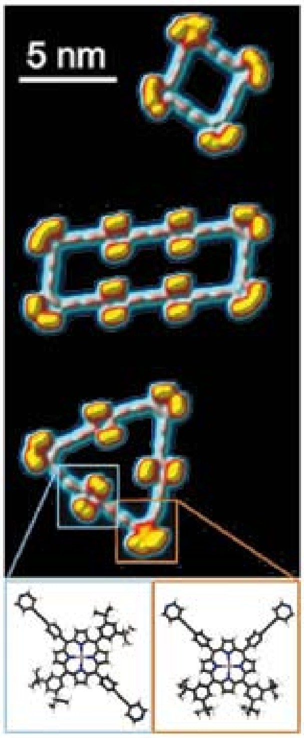
Dr. Wilhelm Auwärter | Carl von Linde Junior Fellow
Prof. Johannes Barth, Molecular Nanoscience and Chemical Physics of Interfaces, TUM

Functional molecular architectures on surfaces

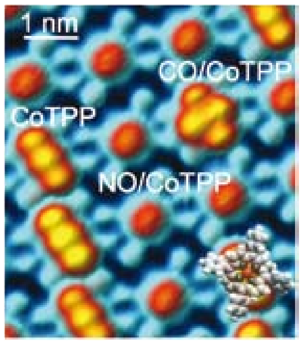
Our research focuses on the comprehensive characterization and engineering of low-dimensional nanostructures on surfaces. Specifically, we construct molecular architectures on well-defined substrates, applying self-assembly protocols inspired by supramolecular chemistry. The interplay between molecular building blocks and support is intimately related to the functionality of the surface-anchored molecular structure.

During the past year, we developed and refined strategies to build specific, well-defined molecular architectures on silver and copper surfaces including open-pore chiral networks, cyclic supramolecules, and one-dimensional coordination polymers. To this end, we implemented the so-called bottom-up approach, relying on individual atoms and functional molecules as building blocks and applying powerful surface science techniques, such as scanning tunneling microscopy (STM) and spectroscopy (STS), to characterize the resulting low-dimensional nanostructures on the atomic scale. We put particular emphasis on systems based on porphyrin molecules interacting via metal-ligand bonds. Given their intriguing variety of functional properties, which are exploited in both biological and artificial systems, these versatile species are ideally suited as building blocks for surface-anchored nanostructures.

For example, the binding of small gas molecules to the metal center in porphyrins is crucial for oxygen-breathing organisms. Accordingly, it plays an important role in catalysis or in the implementation of chemical sensors. We performed comparative studies on the binding mechanism of carbon monoxide and nitrogen monoxide to iron and cobalt porphyrins on a metal support. The very different reaction of the porphyrins to these gases was observed at the single-molecule level, allowing us to decipher the underlying binding mechanism.



1 | STM image of cyclic supramolecules assembled by combining two programmed porphyrin building blocks on a Cu(111) surface.



2 | STM image of a metalloporphyrin (CoTPP) array on a Ag(111) surface exposed to a mixture of carbon monoxide and nitrogen monoxide gases. Three different species (bare CoTPP, NO/CoTPP, and CO/CoTPP) can be clearly identified.

Future work will include more complex substrates, specifically, ultra-thin insulating films and semimetals, but also transition metal oxides. This approach aims at tuning the molecule-substrate interaction and thus controlling system properties such as chemical reactivity and conformational deformation. By combining the unusual electronic and magnetic properties of such complex surfaces with the inherent functionality of porphyrins and organic or biomolecular building blocks in general, we attempt to achieve the desired functionalities of surface-anchored nanostructures.

For the realization of these experiments, we currently set up a novel high-end scanning tunneling microscope reaching temperatures in the 1 K-range. This instrumentation will allow for high-resolution topographic imaging and spectroscopic characterization of the target oxide and semimetal samples functionalized with molecular species and architectures.

Publications:

[1] D. Heim, K. Seufert, W. Auwärter, C. Aurisicchio, Ch. Fabbro, D. Bonifazi, and J. V. Barth, "Surface-Assisted Assembly of Discrete Porphyrin-Based Cyclic Supramolecules," Nano Lett., vol. 10, no.1, pp. 122 – 128, 2010. doi: 10.1021/nl9029994.

[2] D. Heim, D. Ecija, K. Seufert, W. Auwärter, C. Aurisicchio, Ch. Fabbro, D. Bonifazi, and J. V. Barth, "Self-Assembly of Flexible One-Dimensional Coordination Polymers on Metal Surfaces," J. Am. Chem. Soc., vol. 132, no.19, pp. 6783 – 6790, 2010. doi: 10.1021/ja1010527.

[3] K. Seufert, W. Auwärter, and J. V. Barth, "Discriminative Response of Surface-Confined Metalloporphyrin Molecules to Carbon and Nitrogen Monoxide," J. Am. Chem. Soc., vol. 132, no. 51, pp. 18141 – 18146, 2010. doi: 10.1021/ja1054884.

Wilhelm Auwärter

From 1993 – 1999, Wilhelm (Willi) Auwärter studied physics at the University of Zurich (Switzerland). After completing his diploma, he started his doctoral research in 1999 and received his doctorate from the University of Zurich in 2003. Subsequently, he stayed as postdoctoral Fellow at the University of British Columbia (Canada) and at the École Polytechnique Fédérale de Lausanne (Switzerland). Today, he works as a research associate at TUM.

Focus Group **Nonequilibrium Statistical Mechanics at the Nanoscale**

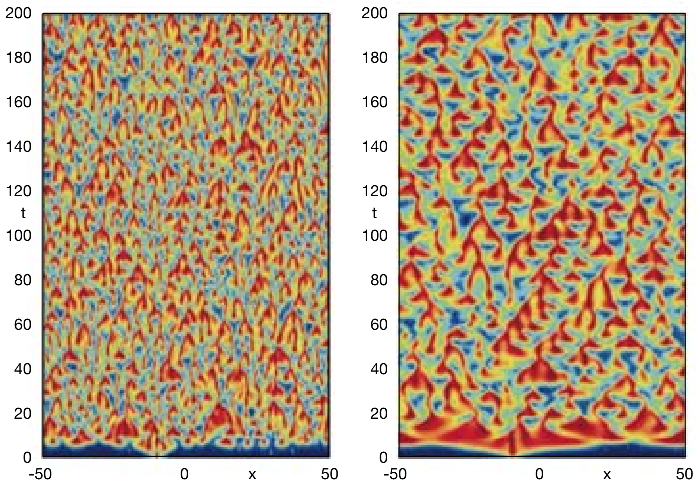
Dr. Vladimir García Morales | Carl von Linde Junior Fellow
Prof. Katharina Krischer, Interfaces and Nonlinear Dynamics, TUM

Our research focuses on nonequilibrium statistical mechanics of nonlinear and nanoscale systems. These systems exhibit memory, nonlocal interactions, and dynamical correlations that render the standard formalism of Boltzmann-Gibbs thermostatistics inapplicable. One of the biggest challenges in the field of statistical mechanics is the development of nanodevices and Brownian motors and understanding of the role of complexity and self-organization on system collective dynamics with many degrees of freedom. The aim of our research is to develop a theory that allows for complex spatiotemporal dynamics in order to extract the dynamical behavior of macroscopic observables from the microscopic description. Another closely related goal is to find appropriate measures of ordered states far from equilibrium.

During 2010, in collaboration with Prof. Katharina Krischer, we discovered a new effect at the nanoscale coming from complex interactions in need of statistical description: fluctuation-enhanced electrochemical reaction rates. Several interesting questions were answered and challenging new research projects were initiated.

We developed a theory that allows for the rigorous description of electrochemical reactions on nanoelectrodes. A new electrochemical master equation was introduced, a general simulation algorithm was established, and a surprising effect was discovered and substantiated through simulations and analytical results in the weak noise limit. We found that all electrochemical reaction steps occur faster at the nanoscale and that rare reaction events are favored because of molecular fluctuations that affect the electrode potential on which the rate constant explicitly depends. We then realized that nanoscale electrochemical systems obey new kinds of statistics because of the non-Markovian properties of their stochastic kinetics. Work is currently being carried out to connect these results to a new formalism of nonequilibrium statistical mechanics, which we are currently developing. Collaborations with experimentalists from other universities are being set up to measure all of these exciting theoretical predictions, which may have a profound impact on the design of nanodevices.

We also studied the behavior of spatially extended oscillatory systems under nonlinear global coupling. Different kinds of states of order grown out of turbulence, such as standing waves and subharmonic cluster patterns, were discovered and elucidated theoretically. We also discovered a new kind of turbulence originating from nonlocal interactions, and we are working toward its characterization using statistical mechanics tools. Experiments are also being carried out in our group to find new states of order and to prove, as our theory indicates, the role of nonlocal interactions on the emergence of order far from equilibrium.



Electrochemical turbulence

Publications:

[1] V. Garcia-Morales, and K. Krischer, “Fluctuation enhanced electrochemical kinetics at the nanoscale,” *Proc. Natl. Acad. Sci.* USA, vol. 107, no. 10, pp. 4528–4532, March 2010.

[2] V. García-Morales, J. Cervera, and J. A. Manzanares, “Nanothermodynamics,” in *Handbook of Nanophysics Vol. 1, Principles and Methods*, K. Sattler, Ed., New York: Taylor & Francis, pp. 15-1 – 15-22, 2010.

[3] V. Garcia-Morales, A. Orlov, and K. Krischer, “Subharmonic phase clusters in the complex Ginzburg-Landau equation with nonlinear global coupling,” *Phys. Rev. E* 82, 065202(R), 2010.

Vladimir García Morales

studied physics at the University of Valencia (Spain) where he received his Master of Science in 2001. There, he was also awarded a doctoral degree in 2005 with a dissertation on nanothermodynamics and ion transport properties of interfacial nanostructures. During these years, he collaborated with chemists at the Universities of Porto (Portugal) and Helsinki (Finland) and worked as a teaching assistant at the University of Valencia. After obtaining his doctoral degree, he was awarded a DAAD scholarship, which enabled him to collaborate with Prof. Katharina Krischer’s group in the TUM Physics Department. Later, he joined this group as a postdoctoral researcher and teaching assistant, where he worked on establishing general models for the dynamics of oscillatory electrochemical systems as well as models for the stochastic dynamics of such systems on nanoelectrodes.

Prof. Ulrich Stimming | Carl von Linde Senior Fellow
Interfaces and Energy Conversion, TUM

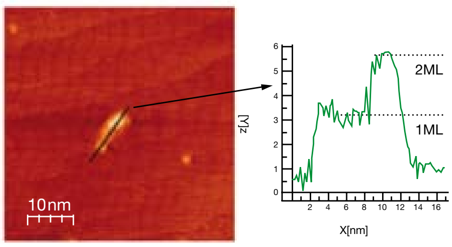
Charge transfer at the nanoscale for energy storage and conversion

Our research focuses on charge transfer reactions at the solid-liquid interface in fundamental as well as applied energy storage and energy conversion systems, such as batteries and fuel cells. This involves fundamental research on single nanoparticles using different microscopy and electrochemical techniques in order to acquire information about their chemical, catalytic, electro-catalytic, or physical properties. The aim of the applied fuel cell research is the development of "the complete pathway" starting from the synthesis and preparation of new catalysts and support materials to their application in real fuel cell systems. During the last few years, aspects of electro-catalytic reactions in biological systems were also investigated.

Selected topics in the research group:

Nanostructured systems for electro-catalysis

Nanostructured electrodes were used in order to separate the different parameters influencing the electro-catalytic activity for various reactions. These parameters are particle size, interparticle distance, influence of the support, and chemical composition of the active material. Experiments dealing with single nanoparticles (Fig. 1) and large nanostructured surfaces produced with different techniques allow a distinct separation of the above-mentioned effects. In collaboration with theoretical groups, we developed new models to describe the unique behavior of metallic nanoparticles on various substrates in terms of their extraordinary electro-catalytic behavior. This approach provides guidance for the development of highly efficient catalyst systems.



1 | Left: single Pt particle on Au(111); Right: cross section of single particle

Preparation of catalytically active nanoparticles

Catalytically active nanoparticles are the basis of efficient and selective catalysts in electrochemical energy conversion processes. High surface-to-volume ratios are as important as the specific electro-catalytic activity. These requirements can be achieved by chemical as well as physical preparation techniques that allow the production of monometallic, alloy or core shell particles in the nanometer range. In most cases noble metals such as platinum and palladium are used. Thus, increasing catalyst performance (at given costs) is an important goal for nanoparticle synthesis.

Advanced fuel cell technology

Fuel cells directly convert chemical energy into electrical energy, offering potentially high efficiencies due to a direct conversion as compared to heat cycle-based systems, which are limited by Carnot cycle efficiency. Existing fuel cell systems are based on hydrogen as fuel for low-temperature applications, and high-temperature systems use natural gas or biogas as fuel; such systems are available but still need optimization. Fuel cells should be able to directly convert as many fuels as possible; therefore, approaches using a direct conversion of ethanol and carbon in fuel cells are currently investigated in the group. Ethanol, which can be produced from biomass (e.g. cellulose which is not part of the food chain), is an alternative fuel that requires operating temperatures of 150°C to 250°C. Current research on the direct oxidation of carbon aims at operating temperatures well below 800°C, so that CO formation according to the Boudouard equilibrium can be avoided. Using carbon based on biomass with an easy capture of CO_2 at the anode (and further sequestration), a negative CO_2 effect is possible; i.e., while producing electricity CO_2 is removed from the atmosphere. Under these reaction conditions, expensive precious-metal catalysts may be avoided when compared to the hydrogen/oxygen fuel cell running at temperatures less than 100°C.

Publications:

[1] L. Wang, U. Stimming, M. Eikerling, "Kinetic Model of Hydrogen Evolution at an Array of Au- Supported Catalyst Nanoparticles," *Electrocatalysis*, 1, 60, 2010.

[2] H. Wolfschmidt, O. Paschos, U. Stimming; "Hydrogen Reactions on Nanostructured Surfaces," in *Fuel Cell Science: Theory, Fundamentals, and Biocatalysis*, A. Wieckowski and J. K. Nørskov, Eds., New York, 2010, 1.

[3] H. Wolfschmidt, D. Weingarth, U. Stimming, "Enhanced reactivity for hydrogen reactions at Pt nanoislands on Au(111)," *ChemPhysChem,* 11, 1533, 2010.

Ulrich Stimming

received his diploma in chemistry in 1974 and was awarded his doctoral degree in physical chemistry in 1979 from the Freie Universität Berlin. In 1982, Prof. Stimming joined the IBM Watson Research Center (New York, USA) before he became a member of the faculty of Columbia University, New York (1983 to 1991). In 1991, he was appointed Head of the Institute of Energy Process Engineering at the Research Center Jülich (Germany) and became a full professor of physical chemistry at the University of Bonn. Since 1997, he has held the Chair of Technical Physics at TUM and is the Scientific Head of Division 1 of the Bavarian Center for Applied Energy Research (ZAE Bayern). In 2004, he became the Director of the Center for Nanotechnology and Nanomaterials (nanoTUM) and also a permanent visiting professor at the University of Yamanashi (Japan). Since 2010, Prof. Stimming has been the Co-Director of the Joint "Institute for Advanced Power Sources" (IAPS) of TUM and Tsinghua University (Beijing, China).

Focus Group **Biophysics**

Prof. Hendrik Dietz | Hans Fischer Tenure Track Fellow
Prof. Andreas Bausch, Molecular and Cellular Biophysics, TUM

Bending DNA to new ends

By folding into intriguing molecular shapes, biological macromolecules, such as proteins, are able to carry out all kinds of wondrous functions in our cells. Proteins zigzag around in our cells, catalyze the manufacture of new molecules, chew up others, relay signals, and act according to the latest genomic digest. Many of these processes rely fundamentally on the complex shapes of macromolecules, but they also rely on their relative position and orientation. It is notoriously difficult to observe, let alone control, the shape, position, and orientation of biomolecules because of their ultra-small size and their constant thermal fluctuations in solution.

Advanced molecular self-assembly with “DNA origami” [1–3] offers a unique route for building custom shaped, high-complexity objects that are commensurate in size to biological macromolecules. DNA origami objects can be used as platforms for placing, orienting, and even manipulating biological molecules in user-defined ways. Thus, DNA origami objects can not only help to improve existing experimental methods in the molecular biosciences, but they also can open completely new avenues of exploration.

In our laboratory, we have set out to develop custom “nano” instrumentation based on DNA origami that interfaces with state-of-the-art, single-molecule-level methods for observing and manipulating biological macromolecules. Among other goals, we seek to enable the study of adhesive interactions between biomolecules that are fundamental to processes such as gene regulation in unprecedented detail, and we plan to explore the conformational dynamics of proteins at work in novel ways. More long term, we hope to take important steps toward creating a biologically inspired nanotechnology that may become relevant for everyday human purposes.

References:

[1] P. Rothemund, “Folding DNA to create nanoscale shapes and patterns,” *Nature*, 440, pp. 297–302, March 2006.

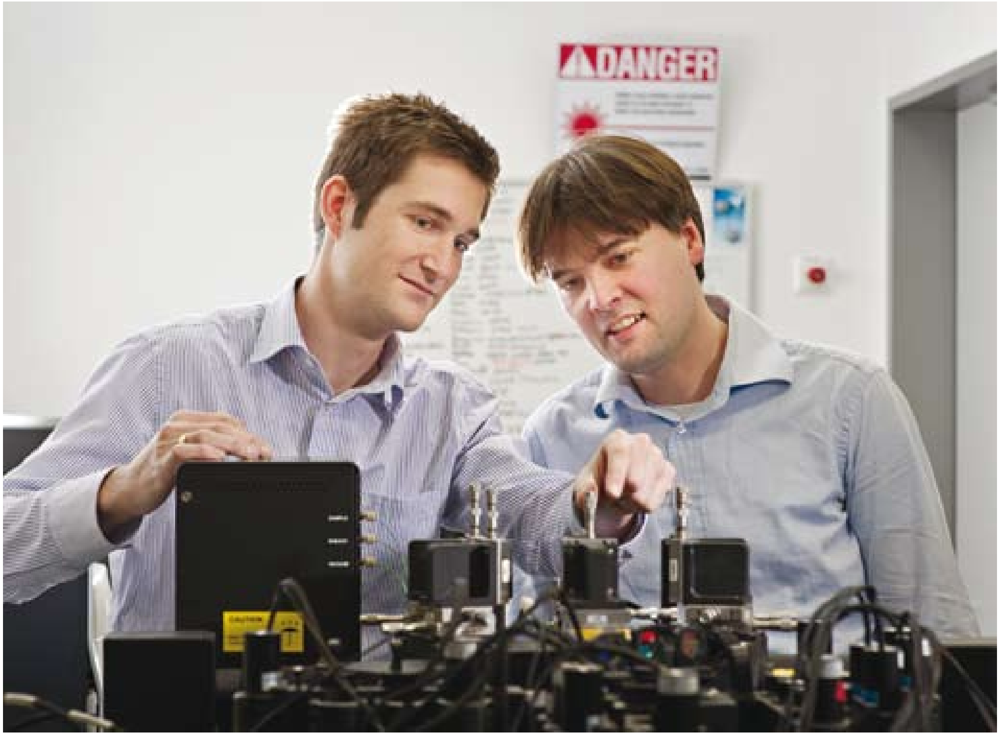
[2] S. Douglas et al, “Self-assembly of DNA into nanoscale three-dimensional shapes,” *Nature*, 459, pp. 414–418, May 2009.

[3] H. Dietz et al, “Folding DNA into Twisted and Curved Nanoscale Shapes,” *Science*, vol. 325, no. 5941, pp. 725–730, August 2009.

Hendrik Dietz
studied physics at the University of Paderborn (Germany), the Universidad de Zaragoza (Spain), and Ludwig-Maximilians-Universität München (LMU). He received a physics diploma in 2004. In early 2007, he was awarded a doctoral degree from the Physics Department of TUM for his work on the development and application of novel single-molecule methods for the mechanical and structural analysis of protein molecules. Prof. Dietz then turned from proteins to DNA and joined a team of nanotechnology enthusiasts located at the Dana-Farber Cancer Institute at Harvard Medical School (Boston) in order to conduct postdoctoral research. In June 2009, he returned to the Physics Department at TUM as an assistant professor for biological physics and established the Laboratory for Biomolecular Nanotechnology.

Focus Group **Clinical Cell Processing and Purification**

Prof. Stanley Riddell | Hans Fischer Senior Fellow
Dr. Christian Stemberger | Carl von Linde Junior Fellow
Prof. Dirk Busch, Medical Microbiology, Immunology and Hygiene, TUM



Enabling cell-based therapies for personalized medicine

The Focus Group Clinical Cell Processing and Purification is dedicated to the development of cellular therapeutics that can be used clinically in the treatment of infections, certain forms of cancer, and other immunologically related diseases. The core interests of our research are the identification, targeting, and isolation of precisely defined cells for use in adoptive cell transfers. Our main goal is to set up a fully integrated cell processing platform to facilitate the clinical preparation of highly functional and minimally manipulated therapeutic cells for highly individualized medical care.

Our research is focused on the identification and evaluation of appropriate target cells, such as different types of T cells, NK cells, and/or (hematopoietic) stem cells. For adoptive transfer, both the identification of clinically relevant target T-cell antigens on infected and malignant cells and the unraveling of genetic programming for distinct memory T-cell subsets – those that enable long-term survival and rapid immune reconstitution – are of great interest.

Besides defining appropriate targets, we develop new molecular methods that allow for highly specific and reversible targeting of desired cells. So far, clinical cell preparations are typically obtained by rather imprecise isolation techniques, often resulting in very limited purities. This general problem often causes substantial variability in the quality of cell products and might account for negative side effects due to unwanted contaminants. Highly pure populations can best be obtained using positive selection, where the target cells are selected by direct labeling via cell-specific surface markers. For clinical applicability, however, each marker has to be extensively tested and approved by regulatory authorities. In addition, the labeling reagents by themselves can severely affect the functionality and viability of selected cells.

To overcome these general problems, we have developed multimeric protein reagents – so-called "*Strep*tamers" – based on the multimerization of either MHC class I or low-affinity, antibody-derived Fab-fragments. The latter, in particular, can be generated for virtually any antigen and can be used in combination – simultaneously or successively – for multiparameter cell handling. Subsequently, all single components can be completely removed from the enriched cells, providing a minimally manipulated, unaltered cell product for all relevant therapeutic settings. We have already succeeded in generating a first set of reversible reagents that is in principle ready for use in clinical applications. We are currently transfering our selection protocols to conform to Good Manufacturing Practices (GMP) conditions, which we hope can be introduced by 2012 in the newly built GMP facility at the campus of TUM's university hospital, Klinikum rechts der Isar.

Our future vision is that with the combination of reversible cell staining and the *de novo* development of technically advanced flow cytometric cell sorting techniques, we can one day generate currently unattainable quality in cellular therapeutic products.

Stanley Riddell
received his M.D. from the University of Manitoba in Winnipeg, Canada. He trained in Medical Oncology and Immunology at the Fred Hutchinson Cancer Research Center and the University of Washington from 1985–1990. He subsequently joined the faculty at these institutions, and is currently Member and Associate Program Head of the Program in Immunology at the Fred Hutchinson Cancer Research Center and Professor, Department of Medicine at the University of Washington.

Christian Stemberger
studied Biology and received his Diploma (in Molecular Biology and Biochemistry) in 2004 from TUM. From 2004 to 2008 he performed his PhD thesis work in immunology at TUM (dissertation: Origin of CD8+ T cell subsets; Thesis Advisor Prof. Dirk Busch). After finishing his thesis he continued working as a postdoctorate at the Institute for Medical Microbiology, Immunology and Hygiene.

Focus Group **Advanced Cardiac Mechanics Emulator**

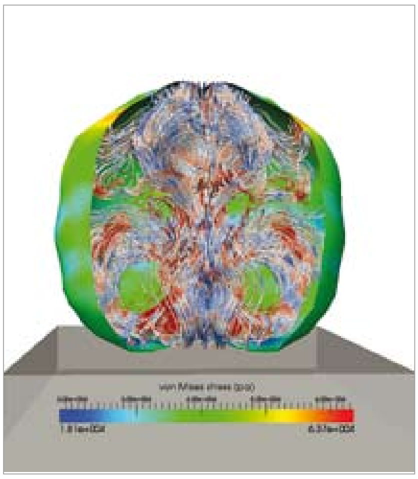
Prof. Michael Ortiz | Hans Fischer Senior Fellow
Prof. Wolfgang A. Wall, Computational Mechanics, TUM

Toward a medically reliable model of the human heart in action

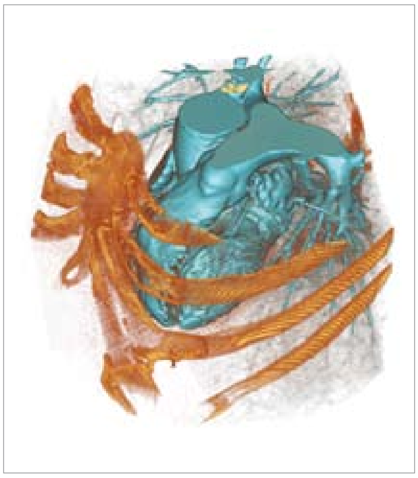
The predictive simulation of cardiac function from biomechanical models of muscle tissue, hemodynamics, and electrophysiology, coupled to our current knowledge of myocardial structure, remains a grand challenge of our time. Given that heart failure is a leading cause of non-accidental death in developed countries, advances in computational cardiac mechanics have the potential for high societal impact.

Toward that end TUM, UCLA, and Caltech have a collaborative effort currently under way, partly under the auspices of the Institute for Advanced Study. The chief objective is the development of a complete computational model of the human heart, the Advanced Cardiac Mechanics Emulator (ACME), which will enable detailed and high-fidelity predictions of cardiac function in both healthy and diseased individuals. ACME combines the most advanced biomechanical models to date of myocardial tissue, hemodynamics, and the electrophysiological response of the heart with the latest advances in high-performance and extreme computing.

The core computational engine underlying ACME is the optimal transportation meshfree (OTM) method, developed at Caltech under the direction of Prof. Michael Ortiz. OTM combines techniques from optimal transportation theory, information theory, and discrete Lagrangian mechanics in a manner that facilitates the simulation of fluid flows interacting with highly-deformable soft tissue (Fig. 1). The hemomechanical model is closed through the use of inlet and outlet boundary conditions derived from reduced-order models of the entire cardiovascular system. ACME achieves a high degree of anatomical correctness by drawing on high-resolution electrocardio-triggered CT images in order to generate high-fidelity geometrical models of the myocardium (Fig. 2), an effort led by Prof. Wolfgang A. Wall at TUM. Close collaboration with physicians and radiologists from the TUM university hospital Klinikum rechts der Isar, ensures the anatomical and physiological correctness of all geometric modeling assumptions. The UCLA team, led by Prof. William Klug, has successfully developed a micro-anatomically accurate model of the electrophysiological response of the heart. High-resolution diffusion tensor DT-MRI imaging data is segmented to produce finite element meshes that describe the geometry of the anisotropic tissue microstructure.



1 | Complex vorticity patterns in bouncing air-filled balloon (Li, B., Habbal, F. and Ortiz, M., *Int. J. Numer. Meth. Eng.*, 83: 1541-1579, 2010)



2 | Geometrical model generated from high-resolution electrocardio-triggered CT image during systolic phase.

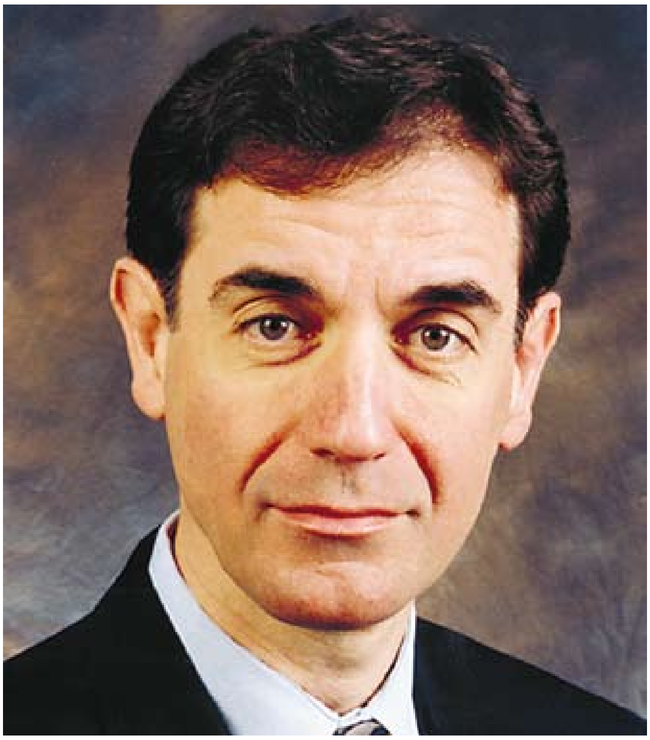
3 | Muscle fiber directions from high resolution diffusion tensor DT-MRI image data.

Fig. 3 shows the surface of one such mesh superposed over a section of glyphs indicating the local muscle fiber directions. This fiber data is essential for defining both the anisotropic electrophysiology of the heart as well as its mechanical contraction. Established connections between the Centers for radiology, nuclear medicine and vascular surgery, and the Institute for Computational Mechanics at TUM, provide the multidisciplinary framework essential for the success of the ACME project.

The ACME project is also expected to benefit from close interactions with the newly founded Munich Heart Alliance and the German Heart Center in Munich. The patient-specific heart models supplied by ACME, will contribute to the study and clinical treatment of a number of healthy and diseased conditions of the human heart such as those resulting from myocardial infarction, valvular cardiomyopathy, dilated cardiomyopathy, and others.

Publications:

[1] B. Li, F. Habbal, and M. Ortiz, “Optimal transportation meshfree approximation schemes for fluid and plastic flows,” *International Journal for Numerical Methods in Engineering*, vol. 83, no. 12, pp. 1541–1579, 2010.



Michael Ortiz
received a Bachelor of Science in civil engineering from the Polytechnic University of Madrid (Spain) and master's and doctoral degrees in civil engineering from the University of California at Berkeley. From 1984 to 1995, he held a faculty position in the Division of Engineering at Brown University (Rhode Island). He is currently the Dotty and Dick Hayman Professor of Aeronautics and Mechanical Engineering at the California Institute of Technology (Caltech). He has been a faculty member at Caltech since 1995 and currently serves as the Director of the DoE/PSAAP Center on High-Energy Density Dynamics of Materials. Prof. Ortiz has been a Fulbright Scholar, a Sherman Fairchild Distinguished Scholar at Caltech, and an elected Fellow of the American Academy of Arts and Sciences.

Focus Group **High-Performance Computing (HPC)**

Prof. Markus Hegland | Hans Fischer Senior Fellow
Prof. Hans-Joachim Bungartz, Scientific Computing, TUM

Computational mathematics

Computational science has had a lasting impact on society. It is a major driver of technological development, scientific exploration, and data analysis. The availability of faster computers, most recently of large multi-core clusters, enables us to tackle increasingly large and complex problems. Within the High-Performance Computing (HPC) Focus Group, we are exploring the frontier of computational science relating to high-dimensional and inverse problems. These problems are a challenge for even the fastest computers, and their solution requires special numerical techniques.

High-dimensional problems occur in the study of complex gene-regulatory networks in molecular biology and in the exploration of data with large attribute numbers. Plasma physics is a particularly rich source of high-dimensional problems. This includes the analysis of huge amounts of magnetic time series data on the one hand, and of kinetic plasma models using the Vlasov equations on the other. These equations are not only six-dimensional partial differential equations, but they also feature a complex geometrical domain in addition to multi-physics modeling of both kinetic and electrodynamic effects. Our work will build on the leading work by Prof. F. Jenko and his group. It will investigate methods that are able to deal with complex simulations arising in the ITER project.

To address the “curse of dimensionality,” which is endemic when solving high-dimensional problems, we will use technology based on work done at TUM, beginning 20 years ago with the introduction of sparse grids by Prof. C. Zenger. In order to achieve regular data access, which is important for multi-core clusters, we use the sparse grid combination technique, which extrapolates a sparse grid approximation from many smaller non-isotropic grids. As was demonstrated by J. Garcke in his thesis, this extrapolation can be unstable. We have subsequently stabilized the original combination technique in the Opticom method.

The complex geometric domain requires adaptive solution methods. We will consider the “dimension adaptive” approach introduced by the author, which can be seen to be particularly effective when joined with the combination technique. Wavelets will be applied for both implementation and theory.

Arguably, the ultimate challenge in this area is inverse high-dimensional problems. In addition to the curse of dimensionality, one has to deal with ill-posedness. New methods to solve this problem will be developed. These methods are based on the theoretical advances of the investigator.

Publications:

[1] M. Griebel and M. Hegland, “A finite element method for density estimation with Gaussian process priors,” *SIAM J. Numer. Anal.*, vol. 47, no. 6, pp. 4759–4792, 2010.

[2] M. Hegland, “Error bounds for spectral enhancement which are based on variable Hilbert scale inequalities,” *J. Integral Equations Appl.*, vol. 22, no. 2, pp. 285–312, 2010.

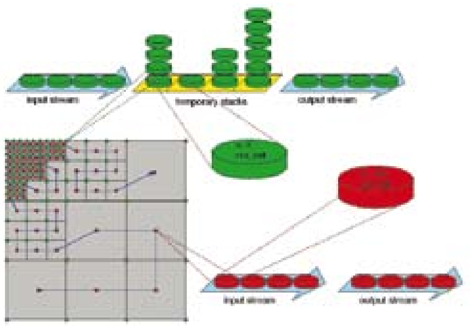
Markus Hegland
is a member of the Computational Mathematics Group at the Institute of Advanced Studies of the Australian National University (ANU). In 2011 he became the Acting Head of the ANU Centre for Mathematics and its Applications. He received his doctoral degree at the ETH Zurich in 1988. Afterwards and until 1991, he worked as a researcher and support staff under Prof. Martin Gutknecht at the Interdisciplinary Project Centre for Supercomputing (IPS) of the ETH Zurich. In 1992, Prof. Hegland joined an HPC group at the Australian National University (ANU) where he worked on algorithms for Fujitsu's VPP and AP series. He also continued research on the solution of ill-posed problems. In the late 1990s, he established the first data mining course at the ANU and acted as leader of a data mining group. In recent years, Prof. Hegland has been a chief investigator in the ARC (Australian Research Council) Centre of Excellence in Bioinformatics.

Focus Group **High-Performance Computing (HPC)**

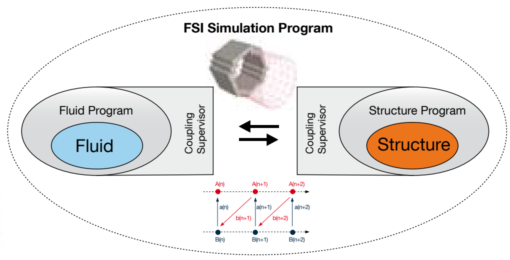
Dr. Miriam Mehl | Carl von Linde Junior Fellow
Prof. Hans-Joachim Bungartz, Scientific Computing, TUM

Tackling the multi-physics challenge

Our research concerns the development of efficient methods for numerical simulation of multi-physics applications. The term "multi-physics" has to be interpreted from a macroscopic view, where relevant physical effects in applications from science and engineering are described by different mathematical models. As an example, think of the interaction of rigid particles (Newton's law of motion) and a surrounding fluid (Navier-Stokes equations).



1 | Stream- and stack-based data handling of the flow solver Peano for cell- and vertex-centered data in an adaptively refined tree-structured Cartesian grid.

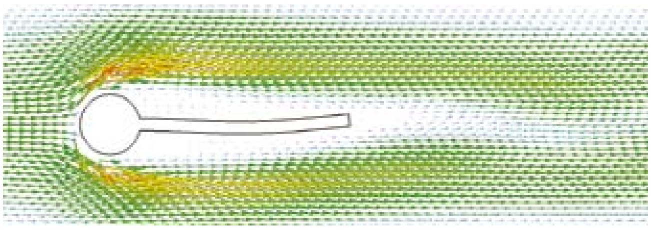


2 | Modular simulation concept for multi-physics applications using the coupling tool preCICE as a coupling supervisor (source: Bernhard Gatzhammer).

The large variety and high complexity of multi-physics applications requires simulation environments that are flexible (in terms of exchanging models and solvers), robust, and very efficient (in terms of numerics and hardware usage). To fulfill these mathematical and computer science requirements, our vision is to develop partial differential equation solvers and a coupling unit combining single-physics solvers in a multi-physics environment.

As a showcase, we consider fluid-structure interactions (fsi) that are relevant in many fields, such as biomedical science, biomechanics, automotive and aerospace engineering, and ship design. At the same time, fsi are highly challenging with regard to computational complexity and numerics, because we have to tackle a full three-dimensional model, complex and changing geometries, high accuracy requirements, and stability problems evolving from physical conservation laws.

Our flow solver in the in-house framework Peano is based on a memory-optimized data concept that allows the running of a Navier-Stokes or Lattice-Boltzmann solver using only streams and stacks as data structures. This minimizes data access times by optimally exploiting the cache hierarchy. In 2010, we could prove the correctness of the underlying algorithm, which was until then only assumed due to experience with the implementation in Peano (SIAM SISC, submitted).



3 | Simulation of a fluid-structure interaction benchmark scenario (Turek/Hron, 2006) using the in-house codes Peano and preCICE.

Within the Project B7 (PDE Toolbox) of the Munich Center of Advanced Computing (MAC, www.mac.tum.de), various methods are currently implemented and evaluated in the Sundance Toolbox (Sandia National Labs, USA) for accurate boundary treatment of complex geometries using Cartesian grids. Our coupling tool "preCICE," whose prototype was developed in the Research Group FOR498 (2004–2010) of the German Research Foundation (DFG), was enhanced by adding additional numerical coupling methods with improved robustness and efficiency. The preCICE tool has been applied in benchmark problems as well as in the simulation of very large floating structures (TUM IGSSE, Project 3.10).

Publications:

[1] H.-J. Bungartz, J. Benk, B. Gatzhammer, M. Mehl, and T. Neckel, "Partitioned Simulation of Fluid-Structure Interaction on Cartesian Grids," in *Fluid-Structure Interaction - Modelling, Simulation, Optimisation*, part II, volume 73 of LNCSE, H.-J. Bungartz, M. Mehl, and M. Schäfer, Eds., Berlin, Heidelberg: Springer, 2010, pp. 255–284.

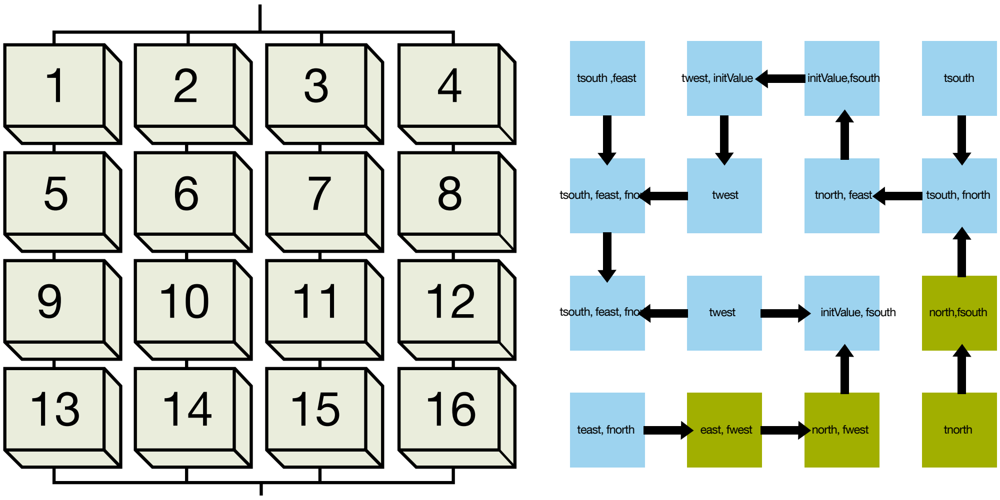
[2] H.-J. Bungartz, M. Mehl, T. Neckel, and T. Weinzierl, "The PDE framework Peano applied to fluid dynamics: an efficient implementation of a parallel multiscale fluid dynamics solver on octree-like adaptive Cartesian grids," *Computational Mechanics*, vol. 46, no. 1, pp. 103–114, June 2010.

Miriam Mehl

After receiving her diploma in mathematics from TUM in 1997, Dr. Miriam Mehl completed her doctorate in the interdisciplinary area of biological wastewater treatment in 2001. She finished her habilitation in the TUM Department of Computer Science in summer 2010, and is involved in several projects in the fields of computational fluid dynamics (CFD), simulation of fluid-structure interactions, and high-performance computing. Since 2002, she has been heading the CFD Group at the Department for Scientific Computing in Computer Science at TUM. This group works with a strong focus on numerically and hardware-efficient algorithms for PDE solvers on high-performance computing architectures.

Prof. Matthew Campbell | Hans Fischer Senior Fellow
Prof. Kristina Shea, Product Development, TUM

Making the computer a more capable partner in product design



A typical human-designed solar panel (on the left) follows a logical and simple set of parallel and series connections, but the computer-generated solution on the right is optimized for a set of common direction shading conditions.

Prof. Matthew Campbell's research is focused on the computational challenges in automating engineering design. While the concept of a computer independently designing real artifacts may seem altogether ultramodern, formidable, and intractable, many practical benefits come from automating difficult and tedious design decisions in tandem with human designers. The research projects initiated at TUM focus on synthesizing complex networks and three-dimensional shapes for common, challenging engineering problems. In 2010, Prof. Campbell spent 28 weeks at TUM to initiate this project and hired two research assistants within TUM's Institute of Product Development within the Faculty of Mechanical Engineering.

One ongoing project at TUM involves determining the optimal network of solar panels to maximize power under a variety of sunlight conditions. The most obvious networks – connecting all of the modules in parallel or in series – are often not the most robust when the array is partially shaded. A more complex and perhaps asymmetric solution may be best. To outfit the computer with abilities to design new networks, we borrow from a wide variety of research fields: mechanical and electrical engineering, artificial intelligence, discrete mathematics, and even linguistics. Clearly, the engineering fields are necessary in defining the simulation so that it can predict power from a candidate network. The combination of disciplines culminates in research on generative grammars. As originally defined by Noam Chomsky, generative grammars can be extended beyond the original linguistic goals to represent languages for real artifacts like solar panels.

The researchers conjecture that simple grammar rules can be defined by humans to represent key design heuristics that a computer can then utilize in building its own design alternatives. In an upcoming conference and journal paper, the use of generative grammar is shown to greatly improve computer-designable networks compared to conventional stochastic optimization methods.

In a second project recently initiated through the Fellowship, a flexible three-dimensional shape grammar is explored for solving or finding optimal shapes for challenging engineering problems, such as wheel-spoke design, heat fins, and load-bearing supports. Even though there are other approaches to three-dimensional shape optimization, all existing approaches require a predefined mesh of blocks or points. Our new work will ensure that generated solutions conform to the limitations of conventional fabrication processes.

In the coming years, Prof. Campbell plans to return to TUM during the summer months. He and his Host, Prof. Kristina Shea, are coordinating a week-long international workshop on computational design synthesis, to take place at TUM-IAS in August 2011.

Publications:

[1] T. Kurtoglu, A. Swantner, M. I. Campbell, “Automating the Conceptual Design Process: From Black Box to Component Selection,” *AI EDAM*, 24, 01, pp. 49–62, 2010.

[2] D. Agu M. I. Campbell, “Automated Analysis of Product Disassembly to Determine Environmental Impact,” *International Journal of Sustainable Design*, vol. 1, no. 3, 2010.

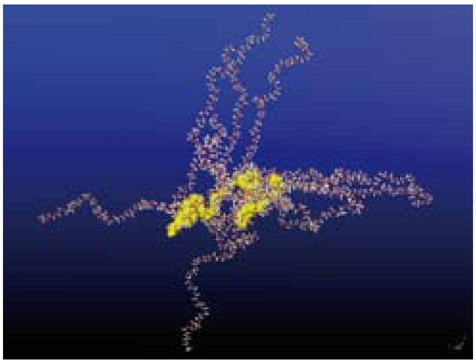
[3] P. Radhakrishnan M. I. Campbell, “A graph grammar based scheme for generating and evaluating planar mechanisms,” *Design Computing and Cognition*, 10, 2010. DOI: 10.1007/978-94-007-0510-4_35.

Matthew Campbell
received his Bachelor and Master of Science in mechanical engineering from Carnegie Mellon University (Pittsburgh, USA) in 1995 and 1997 respectively. In 2000, he was awarded his doctoral degree from Carnegie Mellon University. Prof. Campbell joined the Manufacturing and Design Program of the Mechanical Engineering Department at the University of Texas (Austin) as an assistant professor in the same year and there founded the Automated Design Lab. Since 2006, he has been working as an associate professor and William J. Murray Jr. Fellow for the Department of Mechanical Engineering.

Focus Group **Advanced Construction Chemicals and Materials**

Dr. Tsuyoshi Hirata | Rudolf Diesel Industry Fellow
Prof. Johann Plank, Construction Chemicals,TUM

Fundamental research on superplasticizers could produce concrete results



Polymer molecule structure of a typical PCE, gray: carbon atom, white: hydrogen atom, red: oxygen atom, yellow: oxygen atom in a main chain.

We aim to clarify the working mechanisms of superplasticizers in concrete on the basis of nanoscience, from a viewpoint combining cement chemistry, computer simulation, and statistical analysis.

Our larger goal is to build up the most suitable molecular structure for superplasticizers with adaptability against external factors, such as a variation in cement composition. The dosage to obtain a given initial fluidity should not increase excessively, but should always show both excellent performance and good economy against any manufacturing conditions of concrete, such as differences in cement ingredients, new concrete materials, and temperature changes.

Polycarboxylate-type superplasticizers with polyethylene glycol pendants (PCEs), which were invented three decades ago in Japan by Nippon Shokubai Co., Ltd., have been used widely all over the world because of their excellent cement-dispersing capability. PCEs have played a part in the development of highly durable products such as ultra-high strength concrete and self-compacting concrete.

However, the required dosage of PCE is sensitive to the above-mentioned external factors. Furthermore, PCE introduces a certain amount of air voids into concrete, which are required for freeze-thaw resistance but reduce the concrete's final strength. To balance these two factors, the amount of PCE-introduced air voids should always be kept constant. The basics of cement chemistry must be reviewed in order to propose an adaptable polymer molecule structure beyond conventional PCE superplasticizers.

Cement is a complex system consisting of four clinker phases and calcium sulfates. It generates many hydration minerals by reacting with water, making it harden. It is well-known that PCE superplasticizers adsorb onto cement and disperse cement particles by steric repulsion originating from polyethylene glycol side chains. However, there are many questions remaining, such as:

- How does the polymer conformation of PCE change in cement pore solution?
- How does the surface of cement change by the hydration reaction?
- Which part of the hydration products does PCE adsorb onto over time?
- What is the adsorbed conformation of PCE on the surface of cement particles over time?
- How does this adsorption conformation of PCE affect its dispersing force?
- Which factors reduce the dispersing effect of PCE in some types of cement?

The worldwide production volume of cement for 2009 was 2.8 billion tons. (About half of the world's cement, by volume, is produced in China.) Thus, cement represents the largest industrially made product in the world. Our aim is to allow better use of cements.

Publications:

[1] T. Hirata and T. Nawa, "On Entraining Air of Polycarboxylate Type Water Reducer." *J. Struct. Constr. Eng., AIJ* 75, no. 648 (2010): 231 – 240.

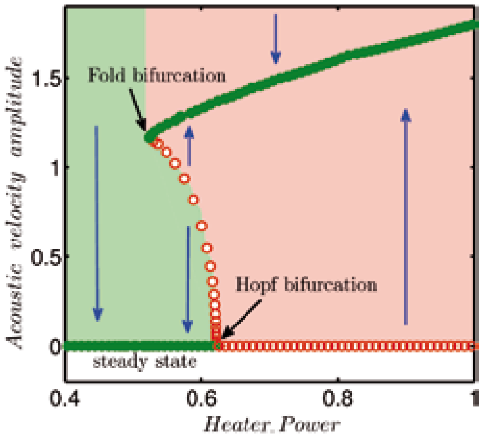
[2] T. Hirata, "Design of Polycarboxylate-type Superplasticizer for Concrete Based on Its Working Mechanisms." PhD thesis, Hokkaido University, 2010.

Tsuyoshi Hirata
received his Bachelor and Master of Science in chemistry from Nagoya Institute of Technology (Japan) in 1979 and 1981 respectively. Since 1981, he has been performing research on water-soluble polymers at Nippon Shokubai Co., Ltd. (Japan). Compared to conventional polymers (the main ingredients of concrete superplasticizer), polymers from the Hirata Research Group show high water-reducing performance and excellent flow retentive ability and have been applied in the development and expansion of new technologies in the construction industry. In early 2010, he was awarded his doctoral degree from Hokkaido University (Japan) for his study on the design of polycarboxylate-type superplasticizer for concrete based on its working mechanisms.

Focus Group **Advanced Stability Analysis**

Prof. Raman I. Sujith | Hans Fischer Senior Fellow
Prof. Wolfgang Polifke, Thermodynamics, TUM

Burning questions: Investigating combustion instability in a whole new light



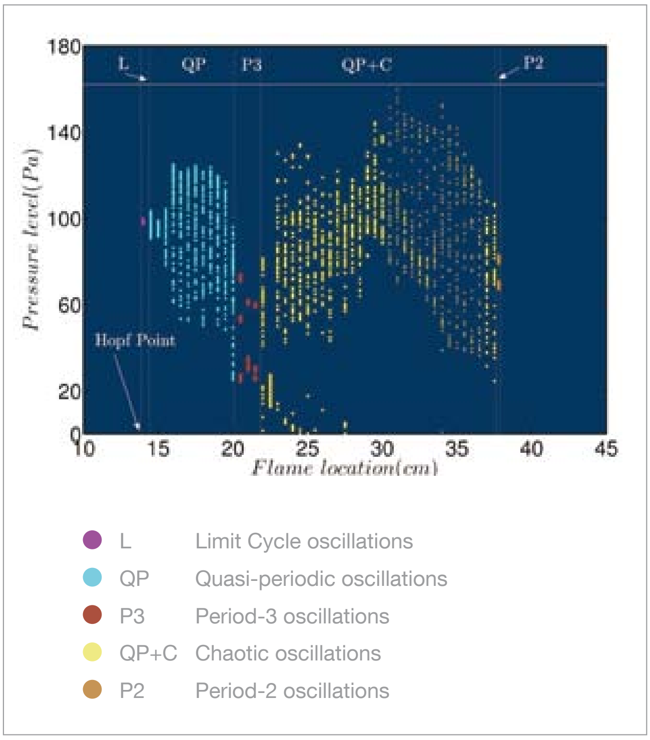
Bifurcation diagram showing sub-critical Hopf bifurcation of a thermoacoustic system obtained using continuation method

The occurrence of thermoacoustic instability (also known as combustion instability) has been a plaguing problem in the development of combustors for rockets, jet engines, and power-generating gas turbines. Predicting and controlling thermoacoustic instability requires an understanding of the interactions between the combustion process and the acoustic waves.

Much work has been performed over the last 50 years, mostly in the framework of classical linear stability analysis of normal modes. We have recently discovered the non-normal nature of thermoacoustic interactions, leading to a paradigm shift in the way thermoacoustic systems are analyzed. Non-normality can lead to transient growth of oscillations in a system even when the eigenvalues indicate linear stability. In a linear system, this transient growth will be followed by asymptotic decay. However, there could be situations where the short-term growth of fluctuations lead to significant amplitudes, where nonlinear effects could cause "nonlinear driving," eventually leading to a limit cycle. Thus, non-normality and nonlinearity together can lead to subcritical transition to instability (triggering), from small but finite amplitude initial conditions.

Traditionally, the asymptotic state of a thermoacoustic system was believed to be a limit cycle. We have recently observed that other states, such as quasi-periodic, frequency-locked, and chaotic, are possible even for ducted burners with simple laminar flames. The Ruelle - Takens' route to chaos was observed in our experiments. These chaotic oscillations are much more detrimental to the combustor hardware than constant amplitude limit-cycle oscillations.

Together with Prof. Katharina Krischer and Dr. Vladimir García Morales, we are studying non-normal and nonlinear effects in thermoacoustic systems both experimentally and theoretically. We are following a two-step approach. In the first step, we investigate problems involving laminar flames, which are relatively easy to model when compared to turbulent flames. We have established a mathematically rigorous framework based on asymptotic analysis for coupling heat release and acoustic processes that occur at different length scales but on the same time scale. Further we have used adjoint looping for determining the most dangerous initial condition (one that leads to maximum growth in energy). We have used continuation algorithms to obtain the bifurcation diagram for thermoacoustic systems. We are working on linear and nonlinear system identification techniques that will capture both the non-normal and the nonlinear effects. Having enjoyed success with the first step, we are now moving toward the study of these phenomena in practical burners that have turbulent flow.



Non-normal and nonlinear stability analyses are well-established in the applied mathematics community, but have yet to be translated to the thermoacoustic community. Our vision is that the framework that we construct to perform thermoacoustic analysis and the tools that we adapt from applied mathematics will become part of a suite of standard tools in future proprietary and non-proprietary stability analysis packages. Prof. Peter Schmid, LadHyx, Ecole Polytechnique, France, and Dr. Matthew Juniper, Department of Engineering, Cambridge University, UK, will be joining the Focus Group as TUM-IAS Visiting Fellows in the summer of 2011.

Publications:

[1] S. Mariappan, and R. I. Sujith, "Thermoacoustic instability in a solid rocket motor: non-normality and nonlinear instabilities", *Journal of Fluid Mechanics*, 653, pp. 1–33, 2010.

[2] P. Subramanian, S. Mariappan, R. I. Sujith & P. Wahi, "Bifurcation analysis of thermoacoustic instability in a horizontal Rijke tube," *International Journal of Spray and Combustion Dynamics*, vol. 2, no. 4, pp. 325–356, 2010.

Raman I. Sujith

In 1988, Prof. Raman I. Sujith graduated with a Bachelor of Technology in aerospace engineering from the Institute of Technology Madras (India) with first rank. He completed his Master of Science (1990) and doctorate (1994) with Prof. Ben Zinn at the Georgia Institute of Technology (Atlanta, USA). After graduation, he worked as a postdoctoral Fellow at the Georgia Institute of Technology until he joined the Institute of Technology Madras in 1995 as a lecturer. Since 2006, Prof. Sujith has been working as a full professor. As a Humboldt Fellow, Prof. Sujith worked at DLR Goettingen (2000 to 2001) and at TUM (2004). He is a Fellow of the Indian National Academy of Engineering.

Focus Group **Aircraft Stability and Control**

Dr. Matthias Heller | Rudolf Diesel Industry Fellow
Prof. Florian Holzapfel, Flight System Dynamics, TUM

Guiding unmanned flight technology toward civil aviation

Established in December 2010, the TUM-IAS Focus Group on Aircraft Stability and Control is a dedicated research collaboration between CASSIDIAN Air Systems and TUM. Rudolf Diesel Industry Fellow Dr. Matthias Heller is an expert advisor on flight mechanics for CASSIDIAN, responsible for the flight dynamics clearance recommendations for the Tornado aircraft. The focus of his three-year Fellowship is the investigation of new techniques in the dynamics, performance, stability, and control of innovative autonomous flight systems. The project exploits synergies of expertise and know-how between CASSIDIAN and the TUM Institute of Flight System Dynamics.

The vision of autonomous flying vehicles as valuable assets in diverse applications has come closer to reality with the advent of miniaturized sensors, actuators, and computer systems, along with advances in propulsion efficiency (fossil and electrical) and energy storage. Without a human pilot on board, many limitations related to weight, size, and load factors vanish, and a new freedom in configuration design arises. Unconstrained by conventional approaches, designers have new options for optimizing mission performance.

In recent years, many highly visible successes in flight demonstrations – conducted by universities, research institutions, and industry – have created the impression that autonomous flying systems have already matured to a level that makes innovative applications practical. This impression is, however, misleading. Although illustrative, most of the demonstrated approaches are practical dead-ends. They have been developed mainly by institutions with no aerospace background and tailored for specific, limited functions. They have not been designed to satisfy the aerospace industry's rigid requirements in safety, accuracy, reliability, and integrity. Yet these are the requirements that will matter most, if an unmanned flying system is to be used in normal (civil) airspace, and, thus above urban or populated areas and in the same airspace as manned aircraft.

A key objective of the TUM-IAS Fellowship is to account for these issues that have often been neglected in fundamental research but represent the basis for the real industrial application of unmanned flying systems, especially for civil applications. The research is not to be limited to conventional configurations. The aim is rather to develop, implement, and demonstrate methods that increase the level of automation, in computing and optimizing safety and certification-relevant characteristics of autonomous flight systems – especially flight control system performance, stability, and survivability.

1 | TUM (FSD) unmanned flying testbeds for Innovative Autonomous Flight Control

Activities with unmanned flying vehicles began a few years ago at the Institute of Flight System Dynamics with the goals of demonstrating the application of modern control theory and algorithms to real flying

2 | Joint Research Demonstrator "Sagitta" representing a 1:4 scaled Innovative Autonomous Flight System

testbeds and investigating the potential of innovative autonomous flight systems (Fig. 1). A research collaboration between CASSIDIAN and the Institute of Flight System Dynamics was established involving diploma and doctoral students active at both university and company sites. The Fellowship will enhance this cooperation, particularly in tight teamwork on an unmanned aerial vehicle project called "SAGITTA – Open Innovation" (Fig. 2). The scope of cooperation will expand to teaching activities at the Institute of Flight System Dynamics, and in the outreach program of TUM-IAS. A main focus of the Fellowship is the merger of scientific and engineering excellence. Hence, the Fellowship will strongly support Munich Aerospace's lead project "Autonomous Flying" and will help to ensure continuity in the joint research efforts between Munich Aerospace and CASSIDIAN.

Matthias Heller
studied aerospace engineering at TUM and graduated in 1992. He received his doctoral degree from TUM in 1999. Thereafter, he started working with EADS CASSIDIAN Air Systems, first as a research and development engineer within the Department of Flight Mechanics and Flight Guidance and then, from 2002 to 2007, as a lecturer responsible for control theory, flight mechanics, and flight control at the Joanneum Graz within the Austrian EFA Offset. In 2007, he was appointed Expert Advisor for Flight Mechanics for the entire BU CASSIDIAN Air Systems, in the Department of Flight Control and Navigation Systems. Since 2009, he has been a regular lecturer at the TUM Institute for Flight System Dynamics on the subject of flight dynamics design challenges of highly augmented aircraft.

Focus Group **Cognitive Technology**

Dr. Dirk Wollherr | Carl von Linde Junior Fellow
Prof. Martin Buss, Automatic Control Engineering, TUM

Robot action and interaction in human environments

Today, there are a number of robotic systems assisting people in everyday tasks such as vacuum cleaning and lawn mowing. These systems still have very limited capabilities, however, tailored to their specific purposes. A long-standing vision in the field of autonomous robotics has been to create systems that are capable of assisting humans in intelligent and versatile ways. This requires sophisticated cognitive abilities that incorporate perception, decision-making, and learning as well as the ability to interact with humans and inquire after information.

In general, we assume that robotic systems that assist humans in cognitive ways will not possess all the information required to fulfill their tasks. Thus the ability to retrieve information through interactions is a central aspect of intelligent autonomous behavior. Therefore, a highly desirable yet missing feature of today's robots is the ability to assess gaps in knowledge and retrieve missing information from other agents, including humans, whenever possible.

As a first step toward generic information acquisition from humans, we focus on the interaction in retrieving route descriptions and reasoning about them. While other factors, e.g., how to approach people and establish contact, play an important role, human-robot communication plays the central part in the retrieval of information required to complete a task. A dialogue system, employing instruction-based learning, handles the communication. The dialogue has to be natural and intuitive for the human user, without any prior instructions. Central abilities of the dialogue system are the identification of missing information and the capacity to guide the human to provide it by posing follow-up inquiries. Structured interaction patterns allow reactions to human input in order to clarify ambiguities.

Our project has an inversion of initiative, as compared to most existing human-robot interaction paradigms. We investigate interaction scenarios in which it is the robot that initiates communication and seeks to retrieve information from human partners. It is therefore essential for the robot to maintain the human partner's interest and facilitate communication by providing intuitive and natural communication capabilities.

Natural language is often vague or ambiguous and, thus hard for technical systems to interpret. To enable robotic systems to correctly interpret natural-language expressions, we need to incorporate findings from human-human communication into the dialogue systems of robots. We transfer theories from linguistics research and deduce rules for human-robot interaction. Furthermore, analysis of human-human communication patterns has uncovered human strategies for avoiding misunderstandings and detecting erroneous interpretation of information, which show remarkable similarities to controlled engineering approaches.

Publications:

[1] B. Gonsior, D. Wollherr, M. Buss, “Towards a Dialog Strategy for Handling Miscommunication in Human-Robot Dialog,” *IEEE International Symposium on Robot and Human Interactive Communication* , pp. 284–289, 2010.

[2] A. Weiss, J. Igelsböck, M. Tscheligi, A. Bauer, K. Kühnlenz, D. Wollherr, M. Buss , “Robots Asking for Directions: The Willingness of Passers-by to Support Robots,” *International Conference on Human-Robot Interaction*, pp. 23–30, 2010.

[3] G. Bätz, A. Yaqub, H. Wu, K. Kühnlenz, D. Wollherr, M. Buss, “Dynamic Manipulation: Nonprehensile Ball Catching,” *Proc. 18th IEEE Mediterranean Conference on Control and Automation*, 2010.

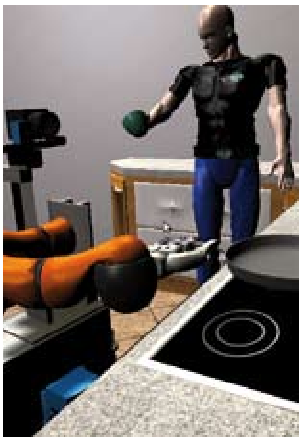
[4] U. Mettin, A. S. Shiriaev, G. Bätz, D. Wollherr, “Ball Dribbling with an Underactuated Continuous-Time Control Phase,” *Proc. IEEE International Conference on Robotics and Automation ICRA 2010*, 2010.

Dirk Wollherr
is currently a senior researcher and lecturer for the Institute of Automatic Control Engineering in the TUM Faculty of Electrical Engineering and Information Technology. He received a diploma degree in electrical engineering in 2000 and a doctorate in electrical engineering in 2005 from TUM. From 2001 to 2004, he was a research assistant in the Control Systems Group, Technische Universität Berlin. In 2004, he was granted a research Fellowship from the Japanese Society for the Promotion of Science (JSPS) at the Yoshihiko-Nakamura-Lab, University of Tokyo. From 2006 to 2008, Dr. Wollherr acted as General Manager of the Excellence Cluster Cognition for Technical Systems (CoTeSys). Since 2005, he has served as a principal investigator, independent junior research group leader, and research area leader in CoTeSys.

Dr. Alexandra Kirsch | Carl von Linde Junior Fellow
Prof. Michael Beetz, Computer Science, TUM

Household and kitchen as testbeds for intelligent autonomous systems

Robots for personal use have entered the homes of millions of users in the form of autonomous household appliances, entertainment robots, and assistive technology for elderly or handicapped people, as well as in the forms of home security and surveillance. These systems are gradually improving with respect to functionality, physical strength, and dexterity. While these developments enable more powerful products for personal use, they also imply additional risks for users with respect to safety, privacy, and personal comfort.



1a |

1b | Vision of a household robot that knows the abilities and preferences of its user and adapts its behavior accordingly.

The main problem underlying these risks is the inability of developers to foresee all possible situations which a personal robot might encounter in an ordinary household. Even though current robots can identify and handle some kinds of failures, a robot can only appropriately react to the situations programmers have anticipated. We explore the concept of "expectations" to formulate general knowledge about how things would normally happen in the world, taking into account human actions and the robot's own. Using such knowledge allows the robot to recognize failures in a more general way. Failure cases potentially exist in situations where the robot's expectations are not met.

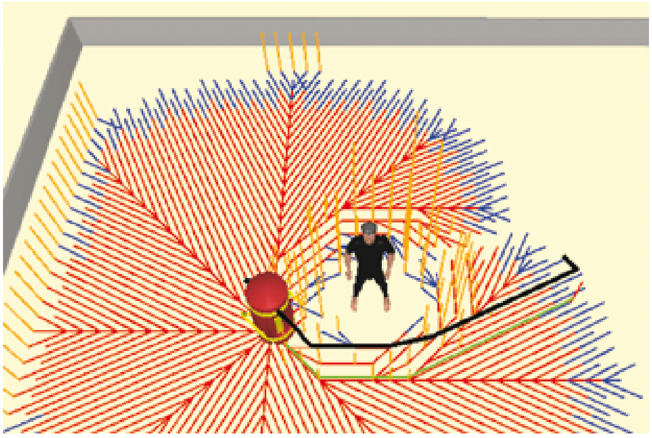
One central question is how to represent expectations generally. We want to be able to express facts and temporal relations about:

- basic mechanisms of the world (e.g., if an object has no reason to move, it is expected to stay at its position);
- the effect of robot actions (e.g., if the robot has performed actions to grip an object, it expects this object to be in its gripper thereafter and stay put); and
- ordinary human behavior and the specific habits of a user (e.g., the need of an elderly person to use a walking aid).

Another important problem is how to acquire specific data for the representation of a specific houshold and the users living there. We explore learning mechanisms to observe the effects of robot actions and learn about the abilities, habits, and preferences of users.

These learning tasks are particularly challenging because:

- robot perception is “noisy” and can lead to ambiguous or inconsistent data;
- not all relevant information can be recognized with current technology (e.g., the activity of a person in preparing a meal); and
- state-of-the-art learning algorithms require large sets of data, which cannot realistically be acquired through normal interaction with a user.



2 | Human-aware cost model for spatial reasoning.

We explore the representation of expectations, their use for action selection, and the automatic acquisition of individual instantiations for specific environments in the context of a household robot performing kitchen work together with a human.

Publications:

[1] Alexandra Kirsch, Thibault Kruse, E. Akin Sisbot, Rachid Alami, Martin Lawitzky, Dražen Brščić, Sandra Hirche, Patrizia Basili, and Stefan Glasauer, “Plan-based control of joint human-robot activities.” *Künstliche Intelligenz*, 24, 3, pp. 223–231, 2010.

[2] Thibault Kruse and Alexandra Kirsch, “Towards opportunistic action selection in human-robot cooperation,” in *33rd Annual German Conference on Artificial Intelligence*, LNAI, Springer, 2010.

[3] Thibault Kruse, Alexandra Kirsch, E. Akin Sisbot, and Rachid Alami, “Dynamic generation and execution of human aware navigation plans,” in *Proceedings of the Ninth International Conference on Autonomous Agents and Multiagent Systems (AAMAS)*, 2010.

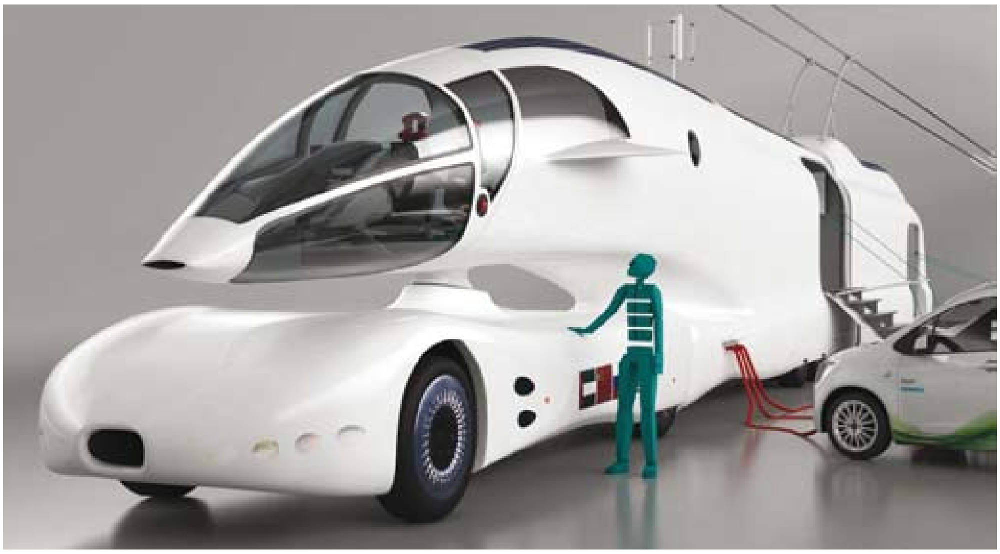
Alexandra Kirsch
is a senior research scientist for the Intelligent Autonomous Systems Group in the TUM Faculty of Informatics and a leader of the independent Junior Research Group “Planning for Adaptive Robot Assistance” in the Excellence Cluster Cognition for Technical Systems (CoTeSys). She received her diploma in computer science from TUM in 2003. She worked as a research and teaching assistant at TUM between 2003 and 2007 and received her doctoral degree. Afterwards, she worked as a management consultant at Booz & Co. She returned to TUM as a senior researcher in 2008 and since then has been establishing her own research group in the area of plan-based human-robot collaboration.

Focus Group **Diesel Reloaded**

Prof. Gernot Spiegelberg | Rudolf Diesel Industry Fellow
◎ Prof. Alois Knoll, Robotics and Embedded Systems, TUM

Taking a holistic approach to electromobility, and taking it on the road

Globally, efforts to develop electric vehicles have grown so numerous and diverse that they are now difficult to overlook. However, most of them focus almost



"Diesel Reloaded" represents a holistic concept of electric-powered individual mobility using the latest technologies of mechatronics and energy technology, developed in the context of a Rudolf Diesel Industry Fellowship at TUM–IAS.

exclusively on vehicle development and only marginally consider the complex interactions among vehicles, infrastructure, and user behavior.

The objective of our project is to pursue a holistic approach to the study of electromobility. On the one hand, the technology will be a focal point – reflected in the development of a new diesel-electric truck. Parallel to this, however, there will be great emphasis placed on the external presentation of activities and results, signifying the importance of the electromobility research field for TUM. In this regard, a road show is planned in which the model vehicle will itself carry and demonstrate the technology on a large-scale national or international tour. Thereby, the vehicle will be both subject and object of development.

The activities are being carried out through the involvement of three doctoral researchers with distinct yet interrelated research tasks:

- electric power train and energy management;
- electronic system architecture of all interconnected functions; and
- development of a novel human-machine interface with side stick controller.

Additionally, under the guidance of a postdoctoral researcher, a basic concept will first be implemented from which the final, innovative, revolutionary solutions will be derived.

In Part 1, an innovative vehicle (Science eMobile) is being built as a diesel-electric serial hybrid based on the latest technology. Its electronic system architecture will be based on a new structure consisting of five functional modules. In this special vehicle, the functional areas will be divided from one another in a way that allows both better presentation and optimized data flow. This can be better illustrated in a truck than in a car, due to the availability of more physical space. In addition, the vehicle will be equipped with the latest technology, such as drive-by-wire systems and new human-machine interfaces, and it will be controllable by a side stick. In total, this technology will offer new scope for longer-term cost reduction and ergonomics, as well as functionality for meeting future global megatrends such as demographic change, urbanization, and increasing environmental awareness.

In Part 2 of the project, the "Science eMobile" is expected to go on the road as a presentation platform (Science eShow) for the whole chain of electromobility topics, including energy generation, transport, and distribution as well as metering and billing. A demonstration drive is planned as part of the project "Zero Emission Race" (http://www.zero-race.com/).

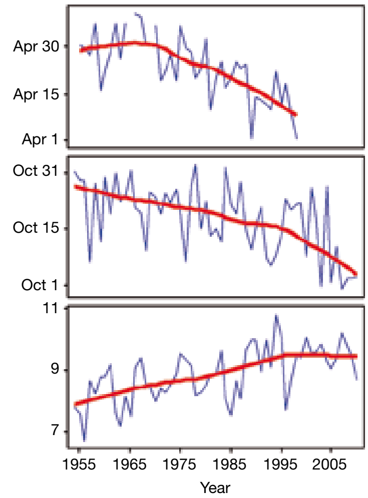
The total project "Diesel Reloaded" will end after three years.

Gernot Spiegelberg
studied mechanical engineering at the University of Siegen and at the RWTH Aachen. After having successfully passed his diploma in 1986, he worked as an assistant at the Institute for Gear Technology and Dynamics of Machines (RWTH Aachen). From 1989 to 1997, he worked on the development of DC-Unimog and LKW in Gaggenau. In 1998, he became the Head of Department, Systems and Technology DC-Powersystems, for drive-by-wire technologies in Stuttgart. Prof. Spiegelberg completed his doctorate at the TU Karlsruhe in 2002 followed by a lectureship for Intelligent Automotive Systems at TU Budapest (Hungary) in 2004, for which he was awarded the Honorary Professorship. From 2006 to 2008, he acted as the Executive Vice President for Group Strategy/Technology at Siemens VDO Automotive AG in Regensburg. Thereafter, he transfered to the Corporate Technology Department and since then has been working on the Technology and Business Model for the Introduction of Electric Vehicles.

Focus Group **Global Change**

Prof. Tim Sparks | Hans Fischer Senior Fellow
Prof. Annette Menzel, Ecoclimatology, TUM

Analyzing overlooked observations of climate and biosphere change



Trends in (top) hop wiring dates (1954-1998), (middle) grapevine harvest dates (1954-2010) and (bottom) the annual mean temperature (°C) recorded at Nürnberg (1954-2010). The red lines show underlying trends as determined by a distance-weighted smoother. (data collected by Anna Bock)

We need to understand more about how our natural environment is changing and the consequences of these changes in climate and the biosphere. This requires the use of long-term data from a wide variety of sources and on a broad range of subject areas. We use data from wherever we can find them, from tree rings and archives to natural gradients and experiments. Rarely were our sources compiled for their present-day purposes.

Change is a fascinating subject. Our environment is constantly changing, not only in mean values but also in variability. But how aware are we of such changes? Human memory tends to be quite short-term, unreliable, and not particularly suited to an objective assessment of change.

Consequently, we rely on recorded evidence to assess environmental change and its often time-lagged impacts. Many measurements of the environment (whether they record pollution, climate, or biodiversity) are highly variable. Therefore, we often require data sets of 20 years or longer in order to reliably detect that changes are happening and to assess their velocity, variability, and drivers. This time frame is typically longer than dependable human memory.

There is now no doubt that the Earth's climate is warming and very little doubt that this is attributable to human pollution of the environment by so-called greenhouse gases. Without a spare planet or two to experiment with, we have to rely on computer simulations to forecast the Earth's climate in the coming century. Results from these simulations vary according to scenario, global climate model, and starting condition, but they consistently predict further warming, sea level rise, more extreme weather events, and changes in precipitation patterns.

So, there is an urgent need to understand what the consequences of these changes may be. Sadly, we often lack data in the areas we wish to investigate. We could and should start to collect such data now, but we may have to wait two decades to fully understand what is happening. Exploiting existing data must now be a priority, and time spent scouring all sorts of archives for further data is time well spent.

As an example of our work with a focus on local culture and economics – considering that the Institute is based in a region that produces one-quarter of the world's hops – the graphs presented here show substantial change in the timing of Bavarian hops and wine cultivation. They also demonstrate contemporary climate warming. Prof. Tim Sparks's Fellowship started in the forgotten heat wave of June 2010 and continued through the recent and unforgettable periods of uncharacteristic snowfall. He has integrated into the TUM ecoclimatology group, within which a diverse mixture of graduate and postdoctoral researchers undertake a diverse range of projects. Two TUM-IAS-supported doctoral candidates and a post-doctoral researcher in dendroecology help contribute to the Focus Group's diversity.

Further research is planned on the timing of natural events. Determining the limits of phenological change is of particular interest, as is discovering more about what drives the timing of events in autumn. These drivers are much more complex than those in spring and likely include the effects of day length, frost, storms, and rainfall as well as temperature. This natural end of the growing season could be hugely important for understanding future changes affecting changes as varied as timber production, pest control, crop production, and tourism.

Publications:

[1] Lehikoinen, E. and Sparks, T.H., "Changes in migration," in: *Effects of climate change on birds*, Moller, A.P. Fiedler, W. & Berthold, P. (Eds), Oxford University Press, Oxford, 2010, pp. 89–112.

[2] Thackeray, S.J., Sparks, T.H., Frederiksen, M., Burthe, S., Bacon, P.J., Bell, J.R., Botham, M.S., Brereton, T.M., Bright, P.W., Carvalho, L., Clutton-Brock, T., Dawson, A., Edwards, M., Elliott, J.M., Harrington, R., Johns, D., Jones, I.D., Jones, J.T., Leech, D.I., Roy, D.B., Scott, W.A., Smith, M., Smithers, R.J., Winfield, I.J. & Wanless S., "Trophic level asynchrony in rates of phenological change for marine, freshwater and terrestrial environments," *Global Change Biology*, 16, pp. 3304–3313, 2010.

[3] Askeyev, O.V., Sparks, T.H., Askeyev, I.V., Tishin, D.V. & Tryjanowski, P., "East versus West: contrasts in phenological patterns?" *Global Ecology and Biogeography*, 19, pp. 783–793, 2010.

Tim Sparks
received his doctoral degree in environmental sciences from Sheffield Hallam University (England) following earlier master's degrees in applied statistics and operational research. In 1998, he founded the UK Phenology Network. He represents the UK in collaborative research programs in phenology. Prof. Sparks is a visiting professor at the Poznań University of Life Sciences (Poland) and at the University of Liverpool (England) and was a contributing author to the most recent IPCC report. Immediately prior to starting his TUM-IAS Fellowship, he worked on biodiversity indicators at the University of Cambridge (England).

Start-up Funding

Biaxial Tension Test Machine

Energy Conversion and Storage

Nanomagnetic Computing

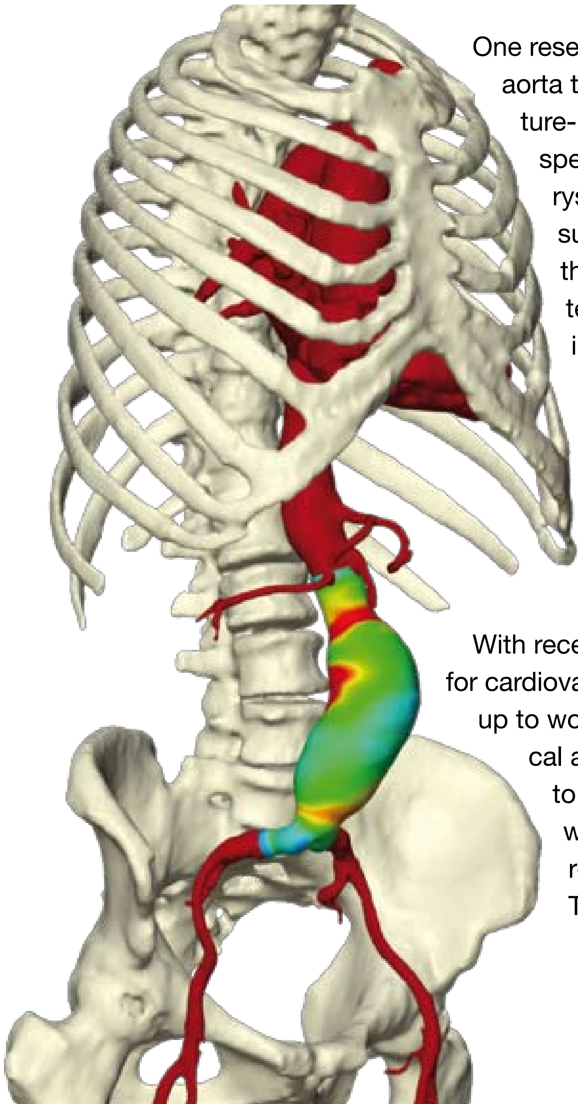
Protein Folding in a Cellular Environment

Biaxial Tension Test Machine

Prof. Wolfgang A. Wall | Computational Mechanics, TUM

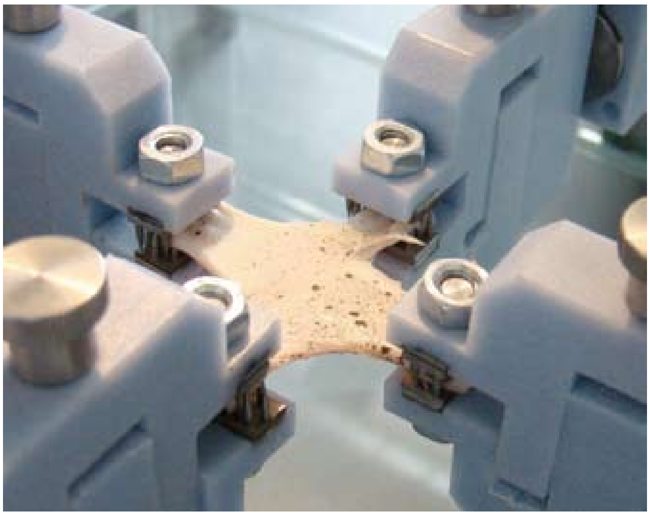
Cardiovascular diseases are on the rise. Diagnoses of such diseases are often easy and cheap; however, meaningful risk assessment for clinical decision making is missing, and in most cases surgical treatments are costly and sometimes more dangerous for the patient than the disease itself. The aim of a joint project of the TUM Institute for Computational Mechanics and the Clinic for Vascular Surgery at the university hospital Klinikum rechts der Isar is to understand the pathological processes in the human cardiovascular system, to properly measure, describe and quantify the mechanical changes of the affected tissue, and to enable identification of high-risk patients and improve clinical treatment.

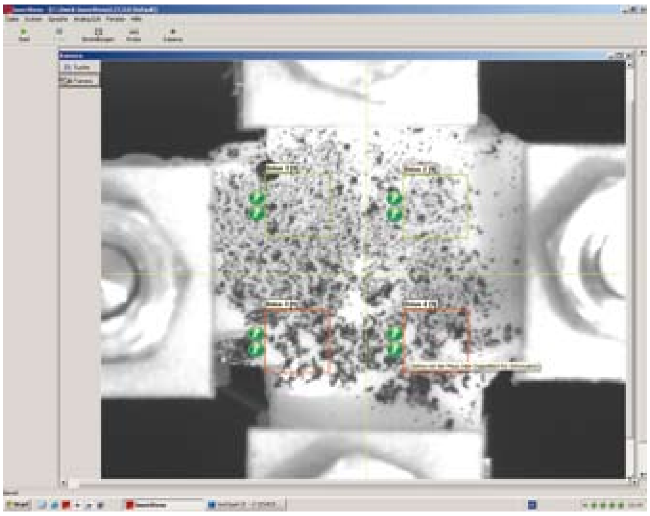
Start-up Funding by TUM-IAS made it possible to acquire a biaxial tension test machine (Zwick GmbH & Co. KG, Ulm, Germany) specially customized for mechanical characterization of human tissue. Each of the four linear actuators provides a stroke of 50mm at a resolution of 0.1µm and can be positioned independently to stretch tissue specimens using displacement- or load-control. Resulting forces are measured by four 100N-load cells with a resolution of 0.1mN. A video system mounted to the top of the machine is used for non-contacting optical tracking of the specimen deformation in all directions. Compared to uniaxial test rigs, the new biaxial tension test machine allows for measuring anisotropic behavior of human tissue that is due to the orientation of different fiber components in the tissue microstructure.



One research target of the project group is the aortic aneurysm, a dilation of the aorta that is potentially fatal in case of rupture. To identify patients with rupture-prone aneurysms, biaxial testing results were used to create patient-specific models for the mechanical properties of the tissue and the aneurysm rupture probability. First, tissue specimens were harvested during surgical aneurysm treatment. The elastic behavior of the specimens and the tissue strength were then measured in biaxial tension tests. Finally, testing results were correlated with non-invasively measurable clinical indicators to create statistical models for preoperative assessment of tissue properties. The findings were used in finite-element simulations of patient-specific aneurysms. A first study on patient control groups with unruptured and ruptured aneurysms revealed that this new approach bears the potential to more reliably identify high-risk patients and to reduce the number of unnecessary operative aneurysm treatments by more than 50%.

With recent advances in tissue testing and improvement in modeling techniques for cardiovascular applications, the interdisciplinary TUM project group has moved up to world-class in the highly competitive international field of biomechanical and cardiovascular research. The work of the group has already led to several publications in both medical and biomechanical journals, as well as keynote speeches at renowned international conferences. More recently, the work evolved into a DFG grant that will further support the TUM project group, ultimately for the benefit of the patient.





Electrochemistry Research in Energy Conversion and Storage

Dr. Julia Kunze-Liebhäuser | Carl von Linde Junior Fellow
Host: Prof. Ulrich Stimming, Interfaces and Energy Conversion, TUM


Julia Kunze-Liebhäuser

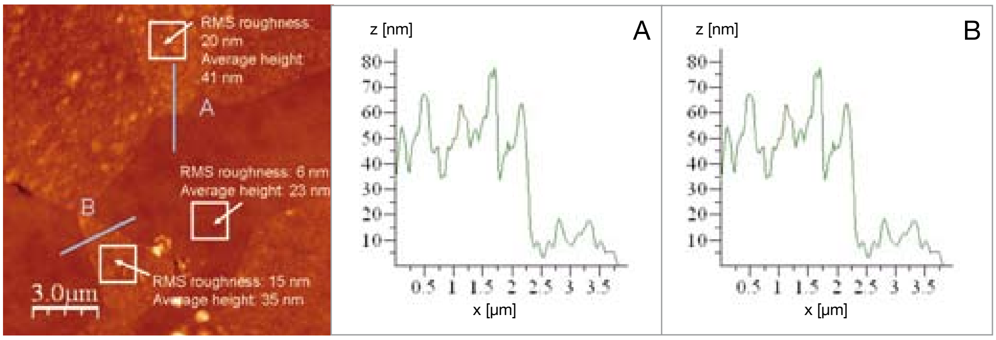
Our research focuses on interface science, where we investigate the properties of two adjacent condensed phases. We fabricate nanostructured surfaces and characterize them in terms of their catalytic activity and their use in the respective applications. We employ scanning probe microscopy (SPM), electrochemical techniques, and surface analysis tools for detailed investigations of the systems.
Of the SPM techniques, atomic force microscopy (AFM) in particular has been applied in the project until now, in order to image the surface morphologies of TiO_2 (semiconductive) and TiO_xC_y (conductive). AFM is well suited to study surfaces that are not conductive and not atomically smooth. It shows the surface topography in very great detail, as shown in figure 1, where the root-mean-squared roughness (rms-roughness) and the topography have been determined. The rms and cross-section data show clearly that the oxide grown on differently oriented grains of titanium has different morphologies; thus the morphology of the oxide depends on the orientation of the underlying substrate.

Figure 2 depicts the morphologies of an amorphous TiO_2 film and an annealed TiO_xC_y film in comparison. The detailed evaluation of the AFM micrographs reveals that the morphology changes from a rather rough surface to a regular, smoother appearance characterized by a lamellar structure.

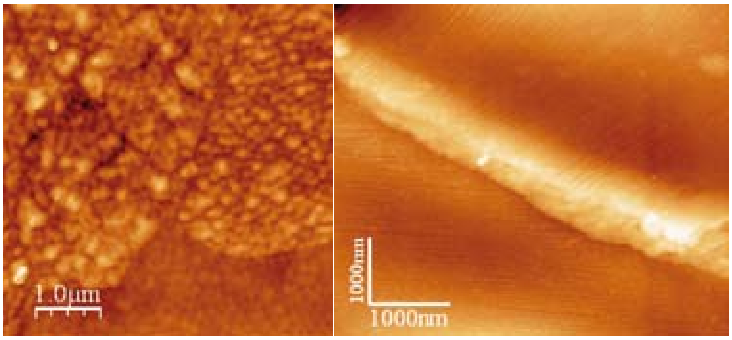
We are currently investigating the interdependence of the conductivity on the grain orientation with tunneling AFM (TUNA), a method in which electric current is allowed to flow through the AFM tip. These investigations will reveal important information for further analysis of the electrocatalytic properties of the surfaces after decoration with Pt. Figure 3 depicts a topographic AFM image (left) and its corresponding current image (right) of an annealed TiO_2 surface. The cross section of the morphology image clearly shows the grain boundary as the highest elevation of the surface, whereas the current image reveals a uniform conductivity. The absolute value of the conductivity can be determined with the help of force distance curves. We are currently correlating the data obtained with this new method and data measured with classical electrochemical impedance spectroscopy.

The morphology of TiO_2 nanotubes covered with a so-called capping layer after the production in fluoride containing glycerol-based electrolytes has also been investigated (Fig. 4). The AFM micrographs of this nanostructured surface deliver important additional information on the topography that scanning electron microscopy (SEM) cannot deliver, such as the topographic profiles shown in panels A and B of figure 4.

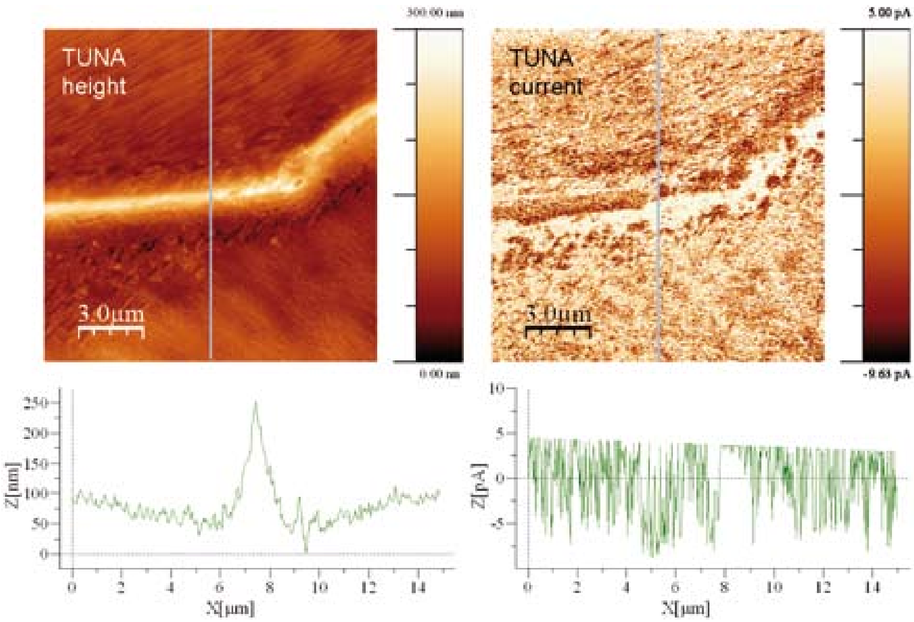
We are currently working on well resolved electrochemical scanning tunneling microscopy (EC-STM) and scanning electrochemical potential microscopy (SECPM) images of enzymes immobilized on thiol covered Au(111) surfaces. These images will be presented in the next progress report.



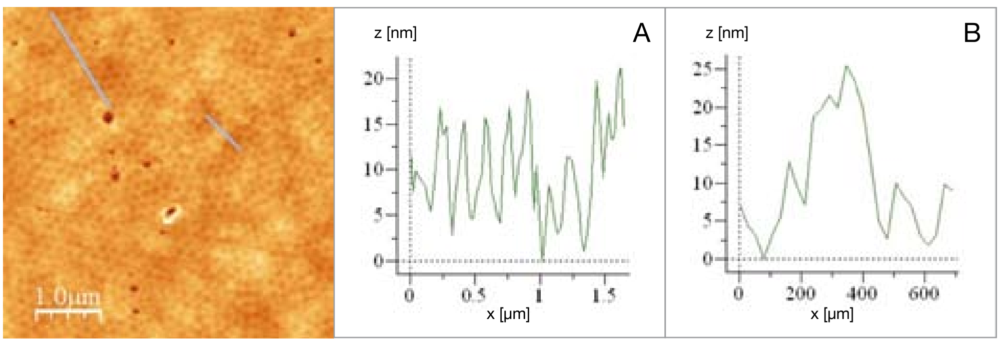
1 | AFM micrographs of amorphous TiO_2 compact films, grown on polycrystalline Ti, with cross sections and values for the roughness of different grains.



2 | AFM micrographs of TiO_2 compact films prior to (A) and after reduction at 850°C (B).



3 | AFM (left) and TUNA (right) micrograph with the corresponding cross sections.



4 | AFM micrograph of nanotubular TiO_2 covered with a capping layer and corresponding cross-sections.

Nanomagnetic Computing

Prof. Doris Schmitt-Landsiedel | Technical Electronics, TUM

When approaching nanometer scales, new physical phenomena become accessible for use in electronic devices and systems. This enables alternative ways for high-performance data and signal processing, e.g., for image and voice recognition. One of these ways is nanomagnetic computing, which exploits the dipolar interaction of nanomagnetic domains. Devices and circuits for this particular concept of field-coupled computing, also known as "magnetic quantum cellular automata" (MQCA) and co-invented by Hans Fischer Senior Fellow Prof. Wolfgang Porod, are investigated at LTE in collaboration with the TUM-IAS Focus Group Nanoimprint and Nanotransfer.

Our devices are made from perpendicularly magnetized ultra-thin films that are patterned by means of focused ion beams. This concept was invented by Prof. György Csaba, a former postdoctoral researcher at the TUM Institute for Nanoelectronics, and it has already achieved a distinct level of maturity. We demonstrated the basic computing elements and also the electrical input and output. These are indispensable for integrating all-magnetic computing schemes with standard electronic systems.

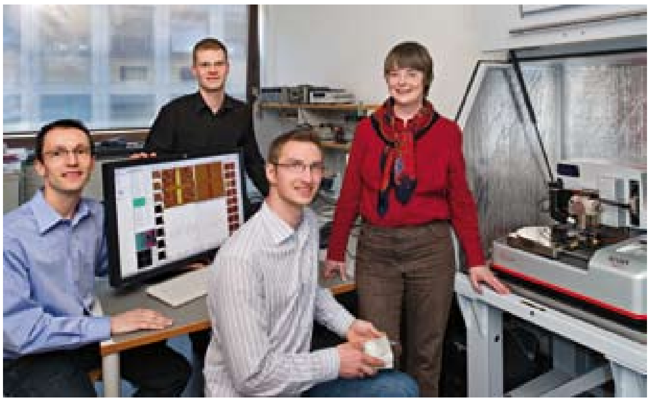
As a first step, enabled by TUM-IAS Start-up Funding, we aim to investigate the feasibility and performance of a complete magnetic computing system. With a recently purchased, state-of-the-art magnetic force microscope, we will develop a customized setup allowing us to stimulate the device under in-situ testing by electrical input and magnetic fields. We have already started to design, fabricate, and test pole pieces for the generation of 3-dimensionally variable magnetic fields tailored for mounting into the scanning magnetic microscope. In order to avoid unwanted perturbation, the challenge is to find a balance between applied magnetic fields, the stray field of the probe tip, and the magnetization state of the device under test. With this unique measurement tool, we will be able to directly observe the computing characteristics, notably magnetic switching events and domain wall movement, in our magnetic logic devices and gates. This will provide the information required to understand these events, calibrate the simulations, and develop complete systems beyond single logic gates.

This new measurement tool will also be accessible to all other interested TUM groups. Special care will be taken to make it user-friendly and to allow long-term access for experiments with elaborate, personalized measurement setups.

In the second part of the nanomagnetic computing project, we want to invent and design larger processing units beyond basic inverters and majority gates. For such arrangements, there are many possibilities for positioning a larger number of dots and for activation schemes. This has never before been investigated, and it can provide undiscovered opportunities for the application of nanomagnetic computing. This part includes the investigation of a novel low-power clocking scheme invented recently in our group, with a patent pending. It solves the general problem of efficient on-chip magnetic field generation by highly localized fringing fields of mobile domain walls. We believe that this is not an incremental improvement in the field of nanomagnetic devices but rather an innovation paving the way for magnetic logic to become a mainstream family in computing circuits.

1 | Close-up view of the MFM scanning head above the 3D field-generator.

2 | Assembling the microscope with the device under test.



3 | Research Group for Nanomagnetic Computing at LTE: Markus Becherer, Josef Kiermaier, Stephan Breitkreutz, and Doris Schmitt-Landsiedel (from left).

Watching a Single Protein Molecule Fold in a Cellular Environment

Prof. Matthias Rief | Biophysics, TUM

Proteins are the basic molecular building blocks in a living cell and are constantly synthesized in our body. In order to perform their vital functions *in vivo*, they must self-organize and fold into complex 3-dimensional structures. So far, our understanding of the folding of protein molecules has been largely based on observations in isolated artificial environments. However, the folding and functioning of proteins occurs in a crowded cellular environment. Hence, it is critical to investigate protein folding in the presence of crowding agents. Although the importance of crowding has been recognized for a number of years in the context of biophysical processes, molecular models have only recently been proposed to examine crowding-induced changes in stability, kinetics of proteins, and RNA.

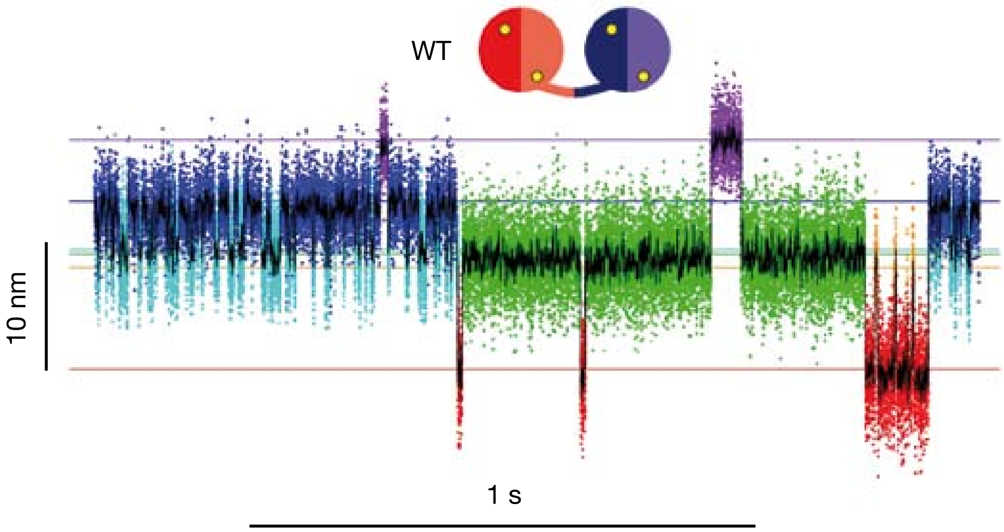
Together with Prof. Dave Thirumalai, Humboldt awardee and TUM-IAS associate, we will initiate research in this unexplored field by combining his unique theoretical expertise with the cutting-edge technology of our TUM biophysics laboratory. Together, we have already demonstrated that a combined theoretical and experimental approach can lead to new understanding of the folding of a complex protein structure *in vitro* (1).

In our Start-up project, we will carry out a series of single-molecule experiments in combination with molecular simulations to probe the crowding effects of cellular environments on the folding and mechanical stability of proteins. The new experimental challenges will require the development of ultrastable and sensitive optical tweezer technology. We have recently demonstrated that it is, in principle, feasible to observe folding/unfolding transitions in an individual molecule over minutes under *in vitro* conditions (see Fig.1).

We need to establish well defined model environments in order to obtain a fundamental understanding of the complex processes caused by the interaction of a protein with, e.g., ribosomes and cytoskeletal structures as well as lipids and other macromolecules that occupy a substantial amount of the accessible space in the folding molecule. To this end, we will follow a systematic strategy, starting from a model environment and increasing its complexity gradually to the complexity of the full cellular environment. A molecular interpretation of these experiments will critically depend on the development of theory and molecular simulations.

Note

[1] M. Mickler, R. I. Dima, H. Dietz, C. Hyeon, D. Thirumalai and M. Rief, “Revealing the bifurcation in the unfolding pathways of GFP by using single-molecule experiments and simulations,” *Proc. Natl. Acad. Sci. USA* 104, no. 51 (December 2007): 20268–20273.



1 | Online recordings of the folding/unfolding fluctuations of a single protein molecule.

Industry Program

Industry Program

The activities of TUM-IAS toward industrial collaboration have shown three main facets: our Rudolf Diesel Industry Fellowship Program, activities toward enhancing "technology push" in the general effort of TUM to foster entrepreneurship, and the organization of joint events. We give a short account of each of them.

Our main vehicle for industrial cooperation is through our Rudolf Diesel Industry Fellowship program, very much in line with the general objectives of the TUM-IAS Fellow-oriented program. We have been happy to welcome four new Diesel Fellows in 2010. These Fellows and their programs are presented in the "New Fellows and Research Plans" section in this report.

We have two main reasons to reward top researchers from industry with a Rudolf Diesel Industry Fellowship. One is to promote a strong and effective collaboration between a TUM research group and an outstanding researcher from industry, for mutual benefit. The other is to allow such an outstanding industrial researcher to develop a new idea, unconstrained by the immediate needs of his company but, of course, in full agreement with it. Often the two goals coexist, whereby the facilities offered by TUM and TUM-IAS allow our Fellow to develop his novel concept effectively. We also have a special bias toward technology-oriented research, in particular toward the creation of a not yet existing type of "product," through technical exploration and experimentation. This is not an easy proposition, which may require almost superhuman effort to bring all the elements together that make a technical realization possible.

In this spirit, both Prof. Gernot Spiegelberg from Siemens and Dr. Matthias Heller from CASSIDIAN Air Systems, EADS, have started their Diesel Fellowship in 2010, the first with the goal to develop a new concept of electromobility (called "Diesel Reloaded") and the other a new concept in advanced aircraft control. In both cases the extensive collaboration networks these Fellows are developing within the university are remarkable, and we are especially happy to see such collaboration even extend to our former international Fellows, in particular, with Prof. Anuradha M. Annaswamy for the aircraft control project. A new international dimension has been added to our Diesel Fellowship program, with Dr. Tsuyoshi Hirata from Nippon Shokubai and Dr. Chin Mok, from AMEC in Oakland, California, joining the program. Dr. Hirata is known worldwide for contributing new types of concrete with very special properties through the addition of special polymers. He has developed a close collaboration with the group of Prof. Johann Plank at TUM and the German industrial giant BASF, and he is our first Diesel Fellow to spend a full year sabbatical in our midst. Dr. Mok is joining the new group of Prof. Daniel Straub and TUM-IAS in 2011, reinforcing our research on climate change and risk management.

We have also been active in trying to develop the “technology push” concept further, in close collaboration with UnternehmerTUM and the furtherance of the EXIST program toward EXIST-IV. As TUM-IAS is very much geared toward promoting new ideas and original concepts, we would also very much like to see these find their way toward new economic or industrial activity. There are many roadblocks on the way, not the least of which is the financing of the all-important development phase between the invention and the first industrially or economically feasible prototype or system. This critical phase is pre-entrepreneurial, and is typically considered “post-research” by research supporting agencies. All studies on the economic trajectory of a new idea toward a product indicate that the cost for such early development normally exceeds the cost of research by a factor three to five. We believe that a so-called “linear model” whereby one does the research first, then moves to entrepreneurship and development is erroneous and does not lead to success. The research and the development have to be done in parallel and in a mutually reinforcing fashion – that is the path technological research has to follow. That means that at an early, not yet economically feasible stage, a close collaboration between researchers and future developers has to be established, leading toward gradual transfer but also mutual reinforcement.

A new idea often requires further exploration – deepening the scientific aspect, but also extensive testing – and both require the availability of prototypes and an environment where the experimentation can be done. Often, the whole original idea has to be scuttled and an alternative approach, discovered while trying, has to be initiated. Our efforts in 2010 have been directed toward setting up such a system; we have had a number of discussions on how to attack the problem, developing models, studying the economics, and exploring the feasibility. We hope these ideas will come to fruition in 2011.

The third component of our industry-oriented activities has been the organization of some joint exploratory workshops. Prominent was our inaugural symposium on the theme "Energy and Electromobility," which saw a strong participation of industry, especially on the theme of electromobility. Our emphasis is on "sustainability," and a number of interesting and fundamental research issues coalesce and bring the two topics together. A very interesting one has to do with the future of fuel cells and batteries, the importance of which for the future of the automobile industry can hardly be overestimated. One of the factors limiting the use of fuel cells is their present reliance on platinum as a catalyst.

We think much better can be done, e.g., by developing "bio-inspired" catalysts. The whole field of electrochemistry is in a state of renaissance, and we believe that we can contribute excellent science here with a strong and direct economic impact. TUM-IAS likes to stake its strong Research Areas on contributing industrially feasible solutions based on fundamental insights and knowledge.

Good examples are provided by the efforts of our Carl von Linde Senior Fellow Prof. Claudia Klüppelberg and her doctoral student Christina Steinkohl toward predicting the performance of wind farms based on advanced statistical models, and by the collaboration between our Diesel Fellow Dr. Dragan Obradovic and his Host, Prof. Sandra Hirche in developing distributed control for smart grids.

We intend to expand these programs in the future. In particular, we intend to create a new kind of Diesel Fellowship dedicated to combining research and development efforts toward enhancing technology push in critically feasible topics. We shall also expand our program of joint exploratory workshops with industry, not only to enhance mutual understanding but also to define new research challenges based on pertinent innovation needs. True to the central policy of our Institute, we shall accept proposals with high potential in any (technological or scientific) field or direction that we can accommodate at TUM, but shall also be proactive in motivating potential applications based on our strong current Research Areas. Collaborating with industry and enhancing entrepreneurship are gradually becoming natural and cherished dimensions of the TUM-IAS program.

In Focus: Group Interviews

In Focus **Global Change**

Excerpts from an interview on February 15, 2011

Patrick Regan

Tim Sparks, Annette Menzel

I can't recall a single interview (out of thousands over the years) more generously peppered with laughter than my session with five members of the TUM-IAS Global Change Focus Group: Hans Fischer Senior Fellow ***Tim Sparks*** *(TS), his Host Professor* ***Annette Menzel*** *(AM), postdoctoral researchers* ***Nicole Estrella*** *(NE) and* ***Christian Zang*** *(CZ), and doctoral candidate* ***Anna Bock*** *(AB). More often than not, the explosion of laughter would have been set off by the aptly named Sparks, who himself sat quietly at the epicenter, looking innocent. But this lively group is dead serious about climate research. On that subject they expressed not only a feeling of urgency, but also what they called a sense of duty. (PR)*

PR: Is it getting warmer? The measurements say yes. Is human activity making it get warmer faster? The evidence seems overwhelming. There are open scientific questions about the speed of global warming, about where the tipping points might be, about the degree of human influence – but you are focusing mainly on potential impacts and responses. Why?

TS: Too many people don't see climate change as a threat. I don't think there's anything being proposed to try to lessen the effects of climate change that is going to damage the planet in any way, shape, or form – reducing CO_2, reducing travel, making things more sustainable, none of those are going to be damaging. So I can't understand the resistance to change. You can imagine a situation some years down the road, where someone, maybe your grandchild, says, "Why didn't you do more?" And that I think is quite humbling. There's an urgent need to know more about what's going to happen.

AM: I like your first two points. First they doubted that it was getting warmer. Now they have to believe it. Second, they doubted the human influence, and now it seems clear that there is a very strong human influence. And now they say: OK, it's getting warmer, maybe even because of human influence – but it's nice. Don't you like warm summers? And if you look in long paleoclimate data, the warmer periods have been linked to periods of higher biodiversity. Or look at the planet itself. We have tropical regions with high biodiversity. Or think about the contrast between living conditions in the warmer periods of medieval times and the cold, dark times of barbarian migration. These are the kinds of arguments coming up now, to say that getting warmer is not all bad. And now we come on the scene to say, have you seen these impacts, those reductions in growth in the course of the European summer heat wave of 2003, for example, that might be a very good idea of what might happen in a hundred years? Or have you seen farmers changing this or that habit? We know – as Nicole showed in one paper – that farmers are not reacting as appropriately as the plants are. So I think this is more or less our duty at the moment.

Patrick Regan

TS: Duty is a good word.

NE: And you have to keep in mind that the face of change is different, compared to former times. We have now around seven billion people living in the world, and many areas that have something to fear from climate change are heavily populated. And there is something we don't even know from the paleo records: What happened to animals directly while it was changing? Not when it was nice, when it was warm, but the transition times. We don't know much about it, and therefore you have to be careful – especially if climate critics state, oh well, warming might be nice. What about the rest of the world?

AM: It's also the speed we have to care about. Here's a local example. Our university is part of a consortium that operates the environmental research station Schneefernerhaus just below the Zugspitze. We recently took a look at vegetation below the station, which will have to move upwards 500 meters when it's three degrees warmer. You can imagine beautiful green alpine meadows – but the reality will be landslides, rock falls, permafrost melting, and no vegetation, because there is no soil, and there won't be any soil in a hundred years.

PR: Your approach to investigating climate change and its likely impacts contrasts sharply with computer modeling, which necessarily deals with global averages and abstract representations of physical processes. Here you are looking at phenology, events in the life cycles of plants over time, on a regional or even local level – such as the timing of Bavarian hops and grapevine cultivation. What does this add to our ability to understand what's happening globally, and to plan for the future?

TS: We need to exploit every little bit of information that we can get hold of. I have someone in Scotland that Annette laughs about because he recorded, I think since 1983, every time he cut his lawn. So you get from that the first cut dates, last cut dates, the cutting season, and the number of cuts. And there's a remarkable linkage with temperature. I see a great need to look at existing data sets, and these are data that people can associate with. I think it's something that has a public face to it. About sixteen years ago, I was working as a statistician in ecological research, and I came across a strange box, which contained a strange graph. And it became apparent from this graph someone had left when he retired that the U.K. had something in the order of two hundred years' worth of data on the leafing dates of trees, which seemed to be forgotten. It had been published in 1926 and forgotten about subsequently. So to me it was very obvious that those data could be used to look at how leafing varied with the weather of that particular year. It turned out that the family had continued to record this data; it had been recorded by a single family from 1736. They carried on recording until at least 1958, in the same village, generation after generation recording the same events. And we ended up with a very long time series of data, collected in the same way, to the same formula if you like, and I published that in about 1995 – at roughly the same time Annette published a Nature paper on trees across Europe.

PR: Does your collaboration go back to that time?

AM: During my first visit to the U.K., Tim did show me this famous village with its famous family, and the graveyard where they were buried. We began writing papers on phenology together a bit later, about 2000. And when I served as a lead author for the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, both Tim and Nicole were contributing authors. Within the working group that focused on impacts, adaptation, and vulnerability, we were among others responsible for the assessment of observed changes and responses in natural and managed systems, the so-called fingerprint of climate change. We wrote about changes all over the world, during the previous four decades, that could be attributed to climate change. I was a member of the German delegation in Brussels when the Fourth Assessment Report of IPCC was adopted in April 2007. A few nations disliked the idea of saying it was "very likely" that these changes in nature could be attributed to human influence and increasing greenhouse gases.

PR: Do you see your TUM-IAS Focus Group as a framework for extending that collaboration, or as something new entirely.

TS: It's going to intensify it. There's no doubt about that. This is the first time it's put it on a concrete basis,

Tim Sparks

Annette Menzel, Christian Zang

that research collaboration. So I'm anticipating a lot more research jointly between us. There's such a diverse group of people, working on lots of different things, and I'm just sticking my nose in everywhere.

AM: We are covering a wide range of different research questions, all of which address atmosphere-biosphere interactions. So we are always looking at interdisciplinary questions. And they are mostly related to impacts, how to detect them, what's statistically significant, what's due to climate change, what can be attributed and what might have other causes like invasive species, pollution, too much nitrogen and so on. Then we have another branch of interest that is related to extreme events, because it's not only the change in mean values, a rise of one degree Celsius in temperature, that matters, but especially the effects of extreme events. This is the second one. These investigations range from phenology to changes in wild forest fires, for example, and forest fire regimes in the alpine region, as well as questions of influences of photosynthetically active radiation and radiation indices on competition in mixed forests. Nicole has worked in both areas.

NE: First I started with phenological observations and connections to temperature, and now I have switched more to the extreme side of it. I try to find the connection between the climate and the environmental reactions of plants. For example, I took photographs of trees in autumn and spring, and I want to connect the phenological observations to the LAI, the leaf area index, and then connect it with the climatological parameters. To do that I use both existing data sets and outputs of regional climate simulation models.

AM: We are also working with the medicine faculty here, on questions related to pollen and human health. Now with this Focus Group we want to settle up these research topics. And we have broadened our interest further to dendro-ecology questions by hiring Christian, working in more paleoclimatological issues.

PR: So you're using tree rings to put contemporary or recent data into the context of a longer timeline?

CZ: In tree rings we have very long time series and large data sets to be explored, with annual resolution. One project will be to sample data from a historic wooden building in the Berchtesgaden Alps and do a local climate reconstruction from late medieval times, maybe 1200 or so, to the present, just to get an idea about how tree growth recently changed.

AM: You might get the idea that we are doing tiny little things on a regional scale, but it has global implications. And one research focus is the timeline. We are not working on ice cores, so the 800,000 years in Antarctica are out of our scope. But even the question of the climate in the past thousand years is a very interesting one, with the discussion of the warm medieval ages. Christian's tree ring research gives us a handle on a topic called the divergence effect. If we calibrate our tree ring reconstructions with temperature data and pretend we are not measuring temperature now but just ask the trees about the temperature, we would fail to get these current warm temperatures. And this is called divergence. Knowing this fact you have then some doubts: What about the warm medieval ages reconstructed by different proxy data? Because there were no measurements, we can only rely on

Nicole Estrella

phenological data and historical data, as well as dendroclimatological data.

CZ: I encountered some shortcomings of dendroecological research during my PhD work, namely the need for recalibration of data. I was focusing on tree growth subject to climate, looking at extremes, but also at mean values as well. The background was that foresters need to know which species of trees to plant in the future. And I worked mostly on how droughts and other extreme climate events influence tree growth, and which species are more susceptible than others. In order to make some climate reconstructions, I had to calibrate recent tree growth with recent climatic conditions and transfer it into the past. Now I want to focus on improving these relations between climate and tree growth. Dendroscience is a lot about methods, but most of them date back to the sixties or seventies and haven't improved much since that time.

PR: So this could be an opening for you to create tools for the whole field?

CZ: Of course it is.

AM: And we want to find out more about this divergence effect. What's behind that? Is it connected to some other factor being now at a minimum – not temperature, but maybe not enough precipitation – or could it be there's a statistical, methodological reason behind the divergence?

PR: Are there other questions that have a direct bearing on the reliability of predictions?

AM: When we talk about whether the trees have green leaves or not, this might seem like a tiny thing. But it's a very important question. It's one of the boundary conditions of the climate models. As soon as vegetation is in leaf, more latent heat and less sensible heat is transferring energy. Whether there is green vegetation doing photosynthesis, whether it is acting as a sink or a source for carbon, the leaf area changes biogeochemical cycles and the energy budget of the atmosphere. And a longer growing season could, for example, give more competitive force to those species that might be able to take advantage of it. Everything is related to changes in the growing season.

PR: One of the biggest advances ever in climate studies was coupling ocean and atmosphere models. Is the biosphere the next frontier?

AM: It's done, coupling atmosphere-ocean models to dynamical global vegetation models. We had a look at their procedures and sub-models to get the growing season.

NE: Of course these kinds of models are definitely needed, and they are useful. But there's work to be done. If you take for example Germany, or the temperate climate zone, then you always have a problem with the broadleaf trees in autumn. The models need an ending of the growing season, but if you try to trigger it by climatic parameters, it's hard. They're not taking into account the temperature of the foregoing month or anything like that, because leaf senescence might

Anna Bock, Tim Sparks, Annette Menzel, Patrick Regan, Christian Zang

integrate all the climate over the whole year. And it's not only climate but eventually pollution or the competition situation among the trees, and then the appropriate data might be something like the life span of the leaves. It's not possible, so far, to accurately model leaf coloring or falling of leaves in these regions. But of course the models need these dates. So they either simplify it or do some kinds of calculations.

TS: For leafing out of trees in spring, we are looking at extremely good models just on temperature alone, across a whole range of tree species. It does vary from area to area, but that seems to be the major controlling influence. Trying to predict leaf fall, as Nicole is saying, is much more difficult. You know, it could be a single frost event, it could be gales, it could be heavy rainfall, it could be a mixture of those; it could be drought in the summer that influences it. But the end of the season can be quite important for how much carbon is being stored in trees. It can be quite important for fungal activity at the forest floor level, because the fungi are basically cycling basic elements in the plant food if you like.

PR: Do you mean the mycorrhizal communities among the roots?

TS: Basically the mycorrhiza but also the fungal fruiting bodies, the above-ground bits. That is what becomes active when the trees stop being active. And that's all very interesting, that interaction, and we know so little about autumn. We've got much more data on spring. The timing of it, as Nicole said, could be critical to a lot of these models of what's going on, how the atmosphere and the biosphere are interacting. We need to know what's driving it, and how it will change in the future.

AM: There is more. Now we are focusing more in the middle of this vegetation period, the summer vegetation period. We know of a huge treasure of notes since 1934 about seed quality changes, for around thirty different species of trees, which could tell us a lot about flowering and fruiting regimes. This matters. It is not only the vegetative period but also the regeneration – how fast, how often and how successful – which drives natural regeneration, adaptation, and shifting of species ranges. Also, we have the suspicion that the amount of pollen in the air in Europe is increasing, and it took us some time just to work out whether we could find any relationship to climate.

This too depends on finding good data sets. Tree rings can tell us something more about water, and water use efficiency. There is more in the air than temperature! The Focus Group on Global Change gives us a good framework for broadening our research, and for pulling these separate strands of evidence together.

PR: How do the doctoral candidates' research projects fit into the big picture?

AB: My project is to find data sets, long-term data sets – well, strange data sets. The idea is to find the footprint of climate change in things that have not been analyzed yet. One example is grape phenology, harvest dates, and composition. I already have a book of wine yields covering a period from 1804 to 1904. From the cultivation of hops, I have data from 1924 to 1998. There's another idea about bee data, such as swarming dates and the yield of honey.

TS: I'm going to take Anna back to Cambridge so she can go through some old German manuscripts in the library there, which I can't cope with. So we're hoping that there's something there as well. I see Anna as more of a historian, looking at past data sets and seeing what they can tell us, whereas Julia Laube, our other TUM-IAS-supported PhD candidate, will be generating and analyzing new data. Julia is a botanist, and she will be manipulating environments or, for example, looking at altitudinal transects and how things vary with environment going up a mountain slope, as well as what's happening with alien or invasive species.

PR: Do you see advantages in doing this research as part of the TUM-IAS, as opposed to some other arrangement?

TS: The TUM-IAS funding makes this collaboration possible, including the two PhD studentships and Christian's postdoc position. I don't think it would have happened otherwise, or it would have been much harder.

CZ: For me it's quite attractive because I am free to do what I want. I'm free to develop my own focus within the Focus Group.

NE: That is a real advantage, that the research areas are open, so that you are really free in choosing your own direction. But there is also this amazing interdisciplinarity. At TUM-IAS workshops, for example, it's always very interesting to see how other people are handling data, and to consider adapting techniques from one field to totally different types of data sets. Of course there's literature, and other ways of finding things out, but if you're taking part in these workshops, it's a totally different atmosphere and a great way of working.

AM: I would go even farther. It's a pity to admit, but I think it's our only chance to work in such an interdisciplinary cross-faculty way. In typical department meetings you're much more likely to find people talking about funding issues or structural problems than about research topics. And if you want to see something beyond your own interests – especially if your interests are already very broad – you would never attend any congress in math or theoretical physics. Nobody would pay you to go there, and you wouldn't understand a thing. But here you have people who are trying to get their message across in a way that can help someone from a different field really understand the broad ideas. And I have no other idea where to go to get this same kind of information.

Tim Sparks, Annette Menzel

In Focus **Clinical Cell Processing and Purification**

Excerpts from an interview on March 18, 2011

Patrick Regan

Patrick Regan, Dirk Busch, Christian Stemberger, Stanley Riddell

*Although Hans Fischer Senior Fellow **Stanley Riddell** (SR) had flown in from the Pacific Northwest just a couple of days earlier, he already was so engaged with life at TUM that he had to be pulled away from a student journal club for our interview. His Host, Professor **Dirk Busch** (DB), explained that big-screen video conferencing has helped in developing a close-knit collaboration between Munich and Seattle but can't begin to substitute for time spent in each other's institutes. The exchange goes both ways and is transforming both labs. Busch, Riddell, and Carl von Linde Junior Fellow **Christian Stemberger** (CS) form the core of the Focus Group on Clinical Cell Processing and Purification – a name in which, as I was reminded repeatedly, every word has deep significance. Within the Focus Group, the TUM-IAS also supports two doctoral candidates, Jeannette Bet and Paulina Paszkiewicz, and postdoctoral researcher Stefan Dreher. Riddell is a pioneer in cell therapy, often relying on* in vitro *culture steps before suitable cells can be used for clinical applications; Busch and Stemberger have been pushing the limits of what can be achieved without culturing cells. Together, they are creating a technology platform that they expect will enable revolutionary advances: in cell-based therapies against cancers and infections, in regenerative medicine, and in fundamental biological research. (PR)*

PR: To provide a rough map of the area where your research interests meet, could you sketch out the state of the art in the therapeutic use of cells, its limitations, and its promise?

SR: Cellular therapies have been used for many years, for example the use of bone marrow transplantation for leukemia or various blood cancers. My early training in the 1980s was in bone marrow transplantation, and the process for transplantation really has not changed in 30 years. Bone marrow or peripheral blood stem cell preparations, which are now commonly used, are actually a complex mixture of cells, some of which are essential for the success of the procedure and some of which cause serious complications.

This Focus Group is looking at ways of being able to select out particular cells to rigorous purity so that you may improve the clinical outcome. So rather than giving a mixture of uncharacterized cells, some of which you know are necessary, you can purify each of the subsets that are in that mixture to make a better therapeutic.

The importance of cell purification for bone marrow transplantation is one example, but this extends into another field that we're all interested in, which is immunotherapy for infections or cancers, where selecting particular immune cells for therapy is critical to the success of the procedure.

What attracted me to this opportunity here in Munich is that the group at the Technical University is at the forefront of developing new technical procedures that would allow rigorous cell purifications to be achieved. There are very few places in the world where you could even contemplate simultaneously making critical technical advances and moving the work to clinical therapy. The purities that are achieved with the methodology that is being developed are extraordinary. It's not uncommon to have a selection where it's 99 percent pure, very close to 100 percent pure because you're looking at very, very low levels of contamination. That level of cell purity is something that I think will be very important for clinical applications.

PR: Is increasing the "yield" of a particular type of cell from a given sample a primary goal, or are other characteristics more important?

DB: I think the right term is quality. Yield is important, because you have a starting point, a mixture of cells, and of course what you can do with it will depend somewhat on how many cells I can purify out of it. But the fascinating thing is that there are examples where you can even titrate it down to a single cell, *if you have the right cell,* and you can still measure a therapeutic effect in a mouse and we think, potentially, also in a patient as well.

CS: It's such a broad field. We started with a focus on T cell-based immunotherapies especially, but the same rules apply to other cell types, for example also to stem cells. You have to make sure that you get exactly those cells that are best suited for a specific therapeutic application, or that science tells us are the best, and to dissect them from potentially harmful cells.

SR: We have a lot of evidence that the clinical applications will be better if we can do this. But there's also a lot to be learned about cell behavior, by being able to work with defined subsets of cells. The experiment that Dirk referred to, where essentially a single cell was able to mediate a major therapeutic effect, is teaching us a lot about the biology of individual cells and how they can respond, proliferate, and self-renew. But in order to be able to study these questions, either experimentally in animals or in the clinic, you have to be able to purify the cells at the highest level. And that's what the technology being developed is going to allow us to do.

PR: Let's focus in more closely on the technology itself. What are the key technical challenges, and what is distinctive about your approach?

CS: The challenges occur on many levels. The first level is that we are dealing with mixtures of cells. If you simply draw some blood, there is not only a single cell type in there, but there are, let's say ten major subtypes, and you want to have only, in the best case, one. And this needs to be precisely defined. To do this, a single marker – so let's say a surface protein in the

cell membrane, a receptor that can serve as a marker – in almost all cases is not sufficient. So you often need more than one marker.

DB: And you need to have methods that allow you to transfer these types of protocols not only to highest purity, but also to the clinic, which is a very different area from pre-clinical experimental studies.

PR: Because here we're getting into regulatory regimes?

DB: Absolutely.

SR: We must be prepared to deal with the regulatory aspects for clinical translation.

PR: Is that also a reason you in the Munich group have put such an emphasis on processing and purification without resorting to cell culture?

DB: As soon as a cell is kept in culture or changed from the way it was before, then the regulatory hurdles that you have to overcome are much higher. So this helps us, at least for certain applications, to process a cell in such a way that it stays "minimally manipulated," to make it easily accessible to bring it back into a patient, and also to make it meet the requirements of the regulatory process.

CS: I should add that it makes sense not only in the regulatory view, but it also in a biological view. If the labeled surface marker is, for example, a receptor that is essential for the function of the cell, even though the marker-binding itself might not directly harm the cells, the label still could block the receptor – and if you switch off its function, that is obviously not good for the cell.

PR: So how do you do it?

CS: We invented a technology that allows us to label the cells in a population of interest according to one or multiple markers, and afterwards we can retrieve the labels completely so at the end of the day we only have a cell without anything that's bound to the surface.

PR: That practically sounds like magic.

CS: It's been described as the painless fish hook.

SR: A very good description.

PR: How does it work?

CS: The way this functions is not that complicated. For instance, the cell type you are interested in purifying shares the same surface marker with another cell type that you don't want, but it also expresses an additional marker, and the combination of both markers is unique to the target cell population. So this shows us that for purifying the cells of interest out of this mixture, you need at least two markers. If you go in with the first marker, you fish both marker-positive populations out, and then after disengaging the first marker, you go fishing again with the second marker to home in on the desired cell type.

With the reagents we use to do this, we have one ligand that actually binds to the cell; the interaction is extremely weak. So if you only have a single one,

Christian Stemberger

you won't get a stable binding of that ligand to the cell. The trick now is, you take not only one of those weak binding ligands, but a few of them. And by doing that you increase the binding strength. So let's say if one goes away, there are still two or more bound to the cell, and that way you keep contact. This is called multimerization. You increase what we call avidity, the total binding strength, by multiplying weak interactions.

DB: It's a biological principle, which is used in many biological interactions to modify the strength of the binding. We learn from nature.

CS: So you can multimerize the ligands by using a kind of backbone molecule, and you can label the backbone molecule, for example with a fluorescence molecule or a magnetic particle that enables us to tear the cells out of the mixture. The multimer binds stably to the cell, but you can easily disrupt the binding to the backbone and break the whole complex apart.

DB: And that goes incredibly fast.

CS: Super fast.

SR: Less than a few minutes.

CS: Basically you just wash the cells, wait a couple of minutes, and the cell label will simply dissociate off. And that's how the cells lose not only the backbone but everything that you've bound to them. So this is the basic principle of our technology.

SR: Because you can now re-suspend the cells and come back in with a second (or third) reagent, the advantage is that you can do this sequentially, and very rapidly. There's no other technology that allows you to bind something and have it fall off so quickly that you can then come in right away with a second selection step.

CS: In basic experimental research, you could envision sorting target cell populations different ways, but it is not possible to transfer these strategies to the requirements of clinical cell processing.

PR: Is the problem the nature of the reagents?

CS: Well, yes and no. Yes, because conventionally available reagents simply stick to the cell and stay there.

Patrick Regan

SR: They would go back into the patient, and especially if you are using multiple reagents, you don't want to administer those back to the patient.

DB: Transferring a marker into a patient brings up a lot of regulatory hurdles. You have to show that the marker is not doing anything else, other than just pulling out the cell.

PR: If you can prove that your technique doesn't leave a marker, then, could that make it easier to get approval for use with patients?

DB: That's a very important issue. We are currently using this type of technology already in a first clinical trial, where we treat patients who are suffering from a chronic virus infection, specifically Cytomegalovirus (CMV) infection, after allogeneic bone marrow transplantation. We use one marker to pull out CMV-specific T-cell populations from the bone marrow donor. And indeed, because we were able to demonstrate to the regulatory authorities that we could completely eliminate the label for cell purification, they recognized the cell product as being "minimally manipulated," which at least for some applications is very advantageous.

An aspect of the technology that is very important is that we keep everything we are doing at relatively low temperatures. At physiological temperatures, for example 37 degrees C., a reagent that is bound to a cell can stimulate the cell, and potentially could transfer a signal to it. We can avoid this by keeping the temperature below 10 degrees, and preferably at 4 degrees.

SR: You want to take the cell from the blood and do the purification in such a way that in the end, the cell is unchanged. And you can do that by keeping the cells metabolically inactive through the whole process, then warming them up.

PR: That gives us at least the broad outlines of the innovation here, a purification or "positive enrichment" process that is extremely precise and reversible. Could you explain more about the range of clinical applications this technology could address, and the research challenges posed by different applications?

SR: There are many clinical applications. The potential here for human cell therapy is very broad. Right now the focus for us is primarily diseases that can be treated with T cells, because that builds on our collective scientific expertise.

DB: The immune system has mechanisms for developing specificity to an invader, such as an infectious agent or also some cancers. Besides antibodies, which are made by B cells, T cells are an important component of adaptive immunity. Those are cells that carry receptors that recognize a specific invader and have active functions that we are very interested in, such as destroying cells that are infected with a virus. Compared to antibodies, T cells have the major advantage of longevity, something we call immunological memory.

SR: Assuming you were vaccinated against the smallpox virus, for example, that will have induced specific T cells that recognize smallpox antigens, which are degraded components of the smallpox virus. Some of those smallpox-specific T cells will be in your body for the rest of your life, and will provide immune memory for the virus.

Stanley Riddell

DB: It is possible to do therapy with antibodies, and that is a very big area of research at the moment. But such antibodies have a relatively short half-life. This might be good in one situation but problematic in others. One of the major advantages of T cells, compared to a small-molecule drug or an antibody, is that they have this capacity to maintain themselves over extremely long periods of time. A lot of research, including our own, is aimed at better understanding the mechanisms of memory. But we are thinking mainly about how it can be used for therapy.

PR: How does this relate, for example, to the clinical trial that you mentioned earlier?

DB: In treating leukemia, because the cancer is sitting right within the immune system itself, you may get to the point where you eliminate the immune system, together with the cancer, and then build up a new one by giving a bone marrow transplantation. But within the time window of immune reconstitution, there's a serious threat that viruses that the patient's immune system normally keeps in check, especially members of the so-called herpes virus family, will cause very complicated clinical infections. If the bone marrow donor is positive for the same virus, then he will also have a population of virus-specific T cells, and those could be used to protect the patient. But in the peripheral blood of the donor you have a mixture of cells, with a small subpopulation of cells that is extremely useful for the patient and many others that could be harmful for the patient – for example, causing something called graft-versus-host disease, where T cells from the donor attack the tissue and organs of the patient.

SR: So by purifying the virus-specific T cells from the donor's blood and transferring them, you can protect the patient.

PR: Are there hybrid scenarios in which this approach to cell processing and purification would be combined with cell culture?

SR: Let's say you have a cancer. Suppose we take a memory cell out of your own blood – maybe it's specific for a virus – and then we engineer that cell to have a receptor that sees your cancer, and we put it back into your body. And because the T cell has the potential to be long-lived, to be able to proliferate,

Dirk Busch

it should work as long as there's a cancer cell there, until the last cancer cell is gone, and then it would enter a resting state – and survive even longer. One of our first clinical trials will test precisely this approach. That's a case where short-term culture comes in, because we can now introduce tumor-targeting receptors very rapidly. Because of the rigorous purity that you can get, you don't have to culture out the cell you care about; it's there to start with, and you can very rapidly manipulate it.

PR: And to what extent have you expanded your research beyond T cells?

SR: The group has developed reagents for selecting cells that have stem cell properties, so you could think of potentially purifying cells that you may want to use for transplantation, making highly pure products for example from umbilical cord blood. You could extend this even further and think about regenerative medicine, where we're talking now about stem cells that have the potential to become different tissues – again, being able to use markers for selection that may define the cells' ability to differentiate to a certain tissue.

CS: It was hard work, but we found a way to transfer the basic principle we learned from T cells to virtually any cell type that you can imagine being potentially useful for cell-therapeutic applications. The underlying principle of the broad extension of the technology is based on antibodies, or parts of antibodies that are called Fab fragments. Fabs are the parts of an antibody that recognize the target structure, or antigen, on the cells of interest.

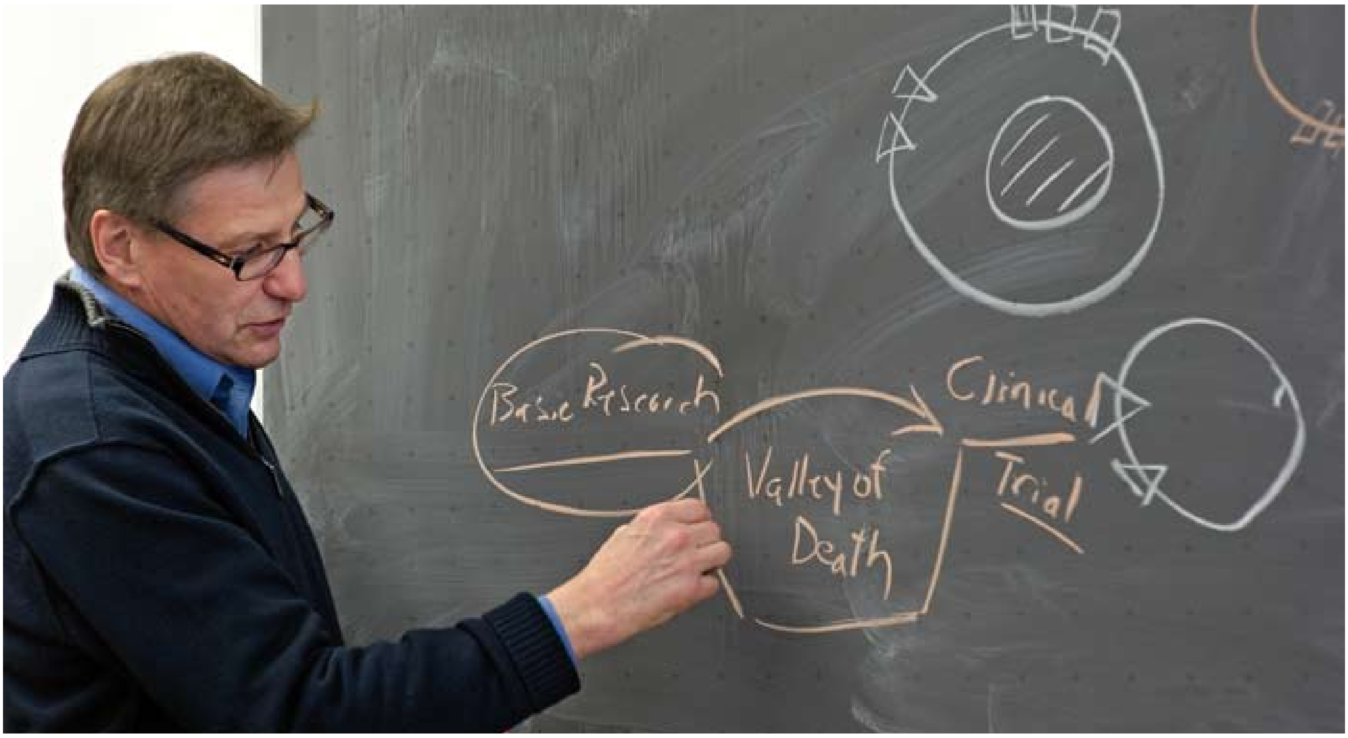
SR: In a normal antibody, the Fabs are always present in a multimeric form, either as a dimer or as a more complex multimer. But for our approach we engineer the Fab in a monomeric form.

DB: The basic principle.

CS: An antibody looks like a Y-shaped molecule; we are only using one of the arms. What we are doing is isolating the structure of the Fab fragment from nature and then engineering it to fit into a multimeric complex. But there is an important challenge. The most basic principle of our reversible agents is of course reversibility in order to eliminate the cell-selection reagent after purification from the cell, but by nature, antibodies are designed exactly the other way. They are often designed to bind extremely strongly. So we now have to go back to the bench and engineer or modify the molecule in such a way that it binds substantially more weakly to its antigen. Already, we have succeeded with fifteen different Fabs to engineer fully reversible Fab-multimers, and we would actually argue that we can succeed with any antigen for which we have an antibody sequence to start with – though Stan might laugh because he knows details about a really tough one.

PR: Is that a typical kind of interaction in this collaboration?

SR: The interactions can be contentious, but are meant to facilitate both the practical and scientific applications of the approach. Right now we have a GMP facility in Seattle, meaning "Good Manufacturing Practices," and we are doing clinical trials, and have expertise in the kinds of things necessary to perform a procedure for purifying cells that is compliant with that kind of facility. Here in Munich, they have the reversible multimer technology for cell selection but are just beginning to build a GMP facility. So I often find myself saying, that's wonderful, but how are we going to move it toward a clinical application?



Stanley Riddell

DB: Our Focus Group is more than collaboration, it's translation. In most cases scientists are talking about translation, but they are far away from ever doing it. And we are entering here an interface that not many researchers really reach. I can't emphasize strongly enough that Stan Riddell is a real pioneer. He was doing the first adoptive T-cell therapies with great success. And yet it's frustrating that although it was so successful, this treatment has not ended up in a commonly performed procedure. And this is the gap we have to close with our Focus Group.

SR: Right. We did the first cell transfer in 1990, but after 20 years it's not an approved product that patients can routinely get. In clinical translation, we often talk about a Valley of Death. I can draw it on the board – over on this side is basic research, which we all do, either to understand a biological process or some fundamental aspects of how human biology works; across here on the other side, we'd like to be able to apply that knowledge in a clinical application. And the gap from here to there is enormous, often for technical reasons. And what the TUM-IAS program is actually allowing us to do is essentially to make this leap across the Valley of Death, because we're developing technologies that have come from basic research and our understanding of how cells work, and being able to use this technology to move things into the clinic. You can spend your entire career on one side or the other, but to be able to bridge the gap is something special. I am very confident, even after just the first year of this Focus Group, that we will actually be using some of the technologies that Christian is working on in the clinic, before our program is finished.

PR: That's fast.

SR: That's incredibly fast. And I think it will include purified T cells that are cultured for brief periods of time to endow them with unique activities.

DB: We will both benefit in a couple of years in that we can set up a technology platform that allows us to do this clinical cell processing and purification jointly and in a similar manner.

SR: The idea is that this will eventually come together with platforms that are not just going to be useful for Munich and Seattle. We hope and believe that these will be adopted widely in the immunotherapy community in many countries. And Dirk is working with other groups as well, as are we. But someone has to make the commitment to the technology development, and that's what our group is doing.

PR: "Platform" is a concept I understand intuitively. But getting down to the nitty-gritty, what will it mean practically?

DB: The idea is really to have on one side the mixture – you draw blood from the patient, or you have a cell sample – and you decide I need this or that population. We believe the simplicity of the basic concept even will make it possible to automate this process.

SR: We haven't worked through all of the steps, but my lab has experience with doing the genetic modification of cells and expanding them. Dirk and Christian have the experience in doing the cell selection. What we have to do now is combine these in a sequence of manufacturing processes. And it may mean having an instrument – one of the things being worked on is an instrument where the blood would go in and the desired cells would come out at the end.

DB: Whatever cell you want.

PR: It seems to me that papers about cell biology often include a section of statistics, basically to reassure you that the researchers probably were looking at the cells that they say they were looking at. And here it seems you have an answer to that, so that biologists would have a new way of being confident that the cells they are observing are exactly and only what they want to be studying. Would you like to see your platform become a tool for basic research as well as therapy and medical research?

DB: The basic principle that we're describing here, to find ways to purify, to isolate, a very defined cell population in a minimally manipulating manner, is something that could be incredibly valuable for basic research as well. Many data that are out there in the field have been generated in conventional ways where it's difficult really to purify cells. So you might be able to address very important questions in a much more sensitive way than we could do before. There are a lot of basic research applications that we currently envision.

Dirk Busch

New Headquarters in Garching

TUM-IAS Headquarters in Garching
A home for visionary research – with a view

On a clear day, you can see the Alps from the new TUM-IAS headquarters on the Garching Research Campus, around 20 kilometers north of Munich. Any day, in any kind of weather, you may see the future.

Ever since its official opening on October 21, 2010, the building has been bustling with exactly the kinds of activity it was designed to promote. This is a place that sets the stage for exchange of ideas on every scale, from one-on-one to a symposium, and on every level: from the ground floor, which offers a 140-seat auditorium, up to the top floor with its Faculty Club, fireside lounge, and panoramic views.

On the middle levels, central meeting areas – a mix of formal and informal, private and open – are surrounded by ample office space for Fellows, visiting scientists, and staff. Walking the wood-paneled hallways, one is never more than a few steps from a whiteboard or some kind of "room for thought" such as a library, a reading room, or a so-called Think Tank – a one-person cockpit for concentration just this side of sensory deprivation.

TUM alumni Rüdiger Leo Fritsch and Aslan Tschaidse were responsible for the architectural design. To build it, the BMW Group provided ten million euros and its own impressive competence – not so widely known as its automotive engineering prowess – in construction. After completing this complex project on time and within budget, the BMW Group donated the TUM-IAS headquarters to the Technische Universität München.

“Not only has BMW created a building that is a model of ecology,” TUM-IAS Director Patrick Dewilde asserts, “with its special climatic installations that make the building react intelligently to outside conditions, it also has achieved an artistic masterpiece, making the center of the Garching Campus an aesthetic experience on a par with its scientific mission.”

Artwork for the building’s interior was created by students of Prof. Hermann Pitz at the Akademie der Bildenden Künste München. The jury selected works by the following artists: Wona Cho, Gerald Demetz, Peter Guberina, Stefan Hutton, Agnes Jänsch, Florian Lechner, Tobias Ollert, Kathrin Partelli, and Susanne Wagner.

Like most official events at TUM, the opening ceremony began with music. Violinist Hans-Joachim Bungartz – also known as Professor Bungartz, Chair of Scientific Computing – played an allemanda by J. S. Bach, a solo piece that evokes “missing” harmonies in the listener’s head. What followed was more like a chorus, with explicit harmonies in the messages of the industry, government, and university leaders who spoke.

BMW Group CEO Norbert Reithofer:

“This building is a good investment in the future. Here, young scientists and engineers are carrying out fundamental research and working on future topics that concern us all. Industry and research – both can profit if they are closely interlinked.”

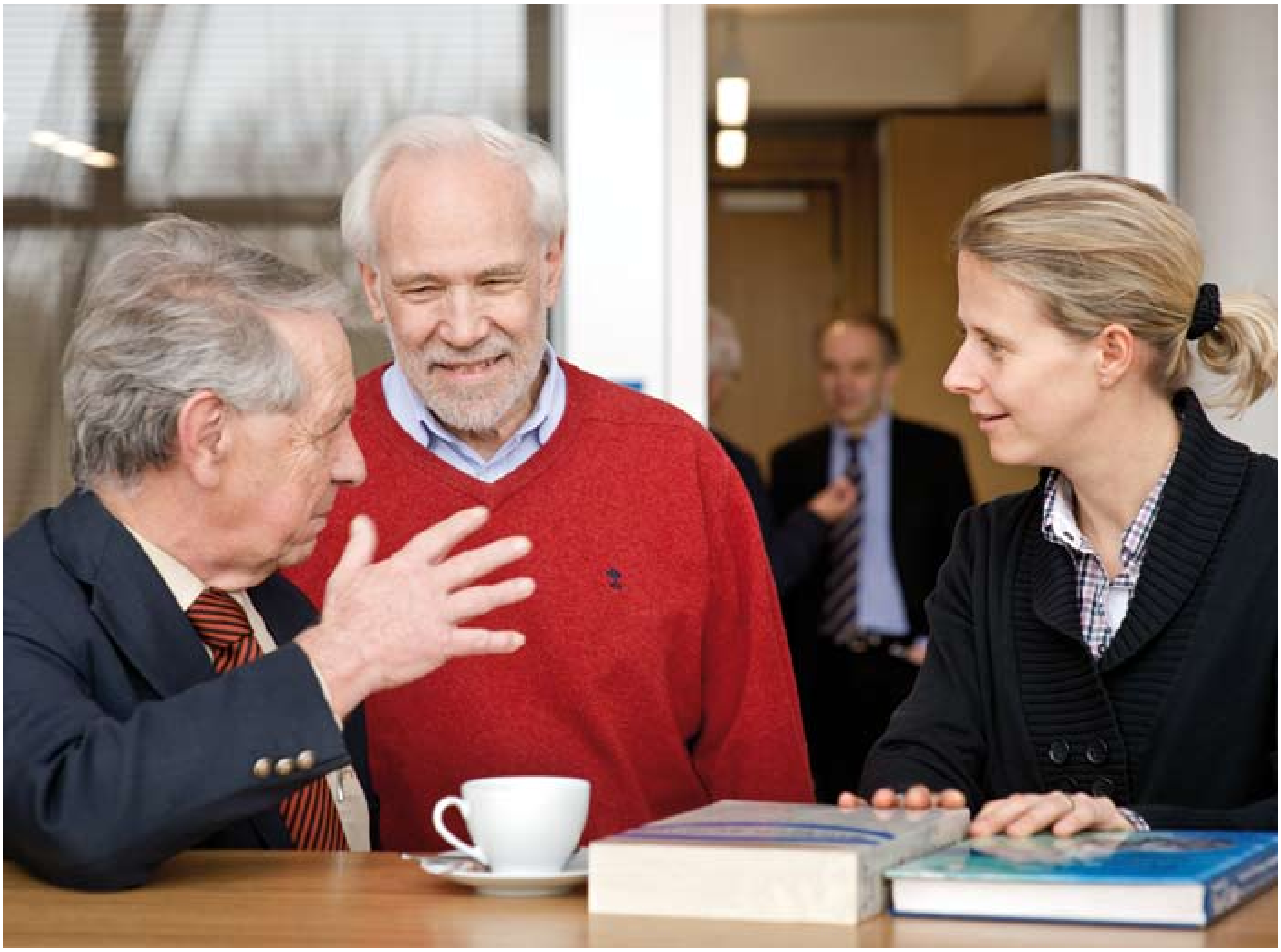
Bavarian Science Minister Wolfgang Heubisch:

“With the construction of the new TUM Institute for Advanced Study, BMW has set new benchmarks in terms of corporate support for science and research. There is no doubt in my mind that the state-of-the-art new building will lend wings to the work of the TUM-IAS and will reinforce the Institute’s presence and image.”

TUM President Wolfgang Herrmann:

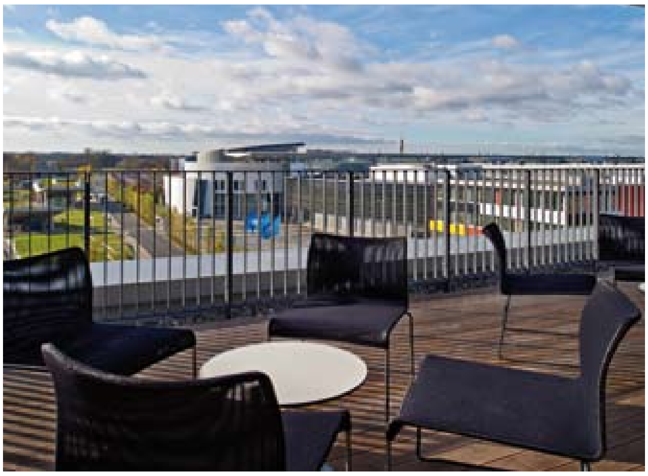
“BMW has set a laudable example as patron, which testifies to the company’s great confidence in the potential of our university. This building radiates entrepreneurial spirit, and intellectual creativity is set to unfold within its walls.”

A demonstration of that potential capped off the opening celebration. Christina Steinkohl, a TUM-IAS-sponsored doctoral candidate, explained how stochastic modeling of air flows through wind farms could help to optimize their production of electric power.



And by the next morning, the first major conference hosted here was under way. “Energy and Electromobility: Exploring the Fundamental Research Challenges” covered topics ranging from big-picture issues – such as technical and economic questions raised by the prospect of transforming energy and transportation systems for a “low-carbon” future – to specific cutting-edge research problems in energy conversion, storage, and control.

Prof. Martin Greiner of Aarhus University kicked off the program with a talk on “Fully Renewable Energy Systems for Europe 2050.” Among the other featured speakers were industrial R&D leaders from BMW, Daimler, General Motors, E.ON Energie, and Siemens; the energy and transport director of DLR, the German Aerospace Center; and the head of the climate center at Munich RE. TUM physicists, chemists, and engineers outlined energy and electromobility challenges from their research perspectives. A discussion of market considerations focused on a specific case: the TUM initiative to show that an affordable electric car for a large customer base could be manufactured now, by uniting available and novel components in a visionary design.



Reaching out to the next generation of innovators, an "Ideas Market" gave selected TUM master's degree students and doctoral candidates a chance to present their own proposed solutions. Symposium participants endorsed what they considered the most promising ideas by giving out symbolic money, which the TUM-IAS would convert into a real investment in the very best proposals. And in a nod to the Institute's openness to creativity and surprise, the program closed with a mock-serious research talk that quickly morphed into a thought-provoking and hilarious magic show.

Since that strong start, the new building has hosted a nearly constant stream of activities. Naturally, it's home to TUM-IAS events, but that's just the beginning. For a growing number of TUM faculties, academic-industrial collaborations, and partners such as the Munich School of Engineering, this is a preferred place for exploring ideas and tackling important problems.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Think Tank


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Institute Activities

Fellows’ Lunches

Every month during the academic year, TUM-IAS organizes a lunch meeting to which all Fellows of the Institute, along with their Hosts, the members of the Advisory Council, and the Humboldt Prize winners are invited. Typically, a Fellows’ Lunch is organized around the discussion of a research theme of general interest to the members of the Institute, with the express goal of fostering a multidisciplinary approach.

Themes that were tackled in 2010 include, for example, “Genome Analysis” (Prof. Chris-Carolin Schön), “Nanotechnology and Nanomaterials” (Prof. Gerhard Abstreiter), “The Nano-haptics Project” (Andreas Schmid), “Nanoimprint Technology” (Prof. Paolo Lugli), “MRI and the Future” (Prof. Axel Haase), “Radiation Treatment of Cancer - toward Laser-driven Particle Beams” (Prof. Fridtjof Nüsslin), “Global change and changing baselines” (Prof. Tim Sparks), as well as “Mass: a mystery?” (Prof. Stefan Pokorski).

Some lunches have been dedicated to presentations of new research topics by Fellows of the Institute. Participants have also dealt with summaries of recent workshops and their import for the various fields the Institute is covering, as well as important themes and research areas for the Institute’s future.

Advisory Council Meetings

TUM-IAS established its Advisory Council at the end of 2008, consisting of the main leaders of Research Areas in the Institute, leaders of other university-wide scientific initiatives, and some members who were closely involved in setting up the Institute (12 in total). The TUM-IAS Advisory Council functions as a standing advisory board to the TUM-IAS Director and his Management Team. One of its prime functions is advising on the suitability and ranking of nominations of Fellows in the various categories the Institute awards. (This function is, in accordance with the decision of the Board of Trustees, not to be directly engaged in the Fellows nomination process, leaving this decision making to a well qualified and appropriate body). In addition, the Council advises on the scientific and technological course of the Institute, on the basis of an assessment of the potential and needs of the University. The Advisory Council meets regularly, typically once every two months.

Fundamental Physics

Speakers: Prof. Andrzej Buras | Carl von Linde Senior Fellow
Dr. Martin Gorbahn | Carl von Linde Junior Fellow
Prof. Gino Isidori | Hans Fischer Senior Fellow
Prof. Stefan Pokorski | Hans Fischer Senior Fellow
Particle Physics, TUM

Prof. Andrzej Buras – *Grand View of the Focus Group: Fundamental Physics*

Prof. Stefan Pokorski – *A Turning Point in the Physics of Elementary Interactions*

Abstract: Dr. Martin Gorbahn – *Beauty, Strangeness and Precision: Tests of Elementary Interactions*
With high-precision experiments elementary interactions can be tested at the smallest accessible distances. This talk showed that decays of strange and bottom quarks provide an ideal framework for these tests: New short-distance interactions can alter their decay rate significantly from the Standard Model expectation. With our precise calculations we can disentangle the contributions of new physics from the standard model background.

Abstract: Prof. Gino Isidori – *The Flavor Puzzle*
According to the Standard Model (SM) of particle physics the basic constituents of matter are three “families” (or “flavors”) of quarks and leptons. In the last decade huge progress in experimentally measuring and theoretically understanding the mechanism of quark-flavor mixing has been achieved. No evidence for physics beyond the SM has been established. Consequently, strong constraints on new physics at high scale applied. In particular, the flavor structure of new physics at the TeV scale is strongly constrained. These constraints were reviewed and future prospects were discussed to better understand the flavor structure of physics beyond the Standard Model.

Tackling the Multi-Challenge - Multi-Physics

Speaker: Dr. Miriam Mehl | Carl von Linde Junior Fellow
Department of Computer Science, TUM

Abstract: Multiphysics simulations, that is simulation scenarios involving physical effects described by different mathematical models such as fluid flow, structural mechanics, acoustics, thermodynamics, or chemical reactions are crucial to tackle current engineering problems with sufficient accuracy. The computational challenges are the required flexibility in exchanging or adding involved phenomena and choosing solver codes, the high computational costs induced by high spatial and time resolutions, ill-conditioned system matrices, and multiscale properties of the application scenarios as well as the higher complexity regarding domain decomposition and load balancing strategies. We use a partitioned approach combining existing single-physics solver codes to a multiphysics simulation environment

using a suitable 'glue' or coupling unit represented by a separate software code and show some of the numerical and implementational issues induced by this approach for the example of fluid-structure interactions (FSI) with incompressible fluids together with possible solution strategies. FSI with incompressible fluids are particularly demanding in terms of stability of the overall simulation due to the strict incompressibility constraint.

Estimating Structural Breaks in Time Series

Speaker: Prof. Richard A. Davis | Hans Fischer Senior Fellow
Department of Statistics, Columbia University

Abstract: Many time series from diverse fields such as engineering, finance, biomedicine, and environmental science possess structural breaks. The program AutoPARM, which fuses ideas from statistics, information theory, and stochastic optimization, was developed to detect structural breaks in a time series arising from a level shift or a change in spectrum. The ideas behind AutoPARM were discussed and its use was illustrated in a range of applications (This was joint work with Thomas Lee and Gabriel Rodriguez-Yam).

Infinite Divisible Stochastic Processes

Speaker: Prof. Jan Rosinski | Visiting Fellow
Department of Mathematics, University of Tennessee

Abstract: Infinitely divisible processes are one of the simplest models incorporating jumps in random evolution of systems. Their most natural and best understood examples are Lévy processes, which are continuous-time random walks. Lévy processes are also building blocks of more complicated infinitely divisible processes exhibiting long-range dependence, stationarity, and high variability. The understanding of such processes depends on interaction with several areas of mathematics, economics, and natural sciences. This talk outlined some basics of the theory and applications.

Challenges and Structure of Multidimensional Problems

Speaker: Prof. Markus Hegland | Hans Fischer Senior Fellow
Mathematical Sciences Institute, Australian National University, Canberra

Abstract: Most traditional techniques like the finite element method have been derived from two and three-dimensional problems. It is well known that many of these techniques, when generalized to multidimensional problems, start to become infeasible for relatively small numbers of dimensions. This observation is well known in the computational science community under the name "curse of dimension." Even highly parallel and very fast computers would only allow the solution of very low-dimensional problems. Around 20 years ago, Prof. Zenger and his collaborators from TUM introduced the sparse grid method, which pushes the dimension of feasible problems to over 10.

It is less known that the theoretical framework used in finite elements (based on classical Sobolev spaces) also breaks down in high dimensions. The type of regularity required for sparse grid methods, for example, is no longer a consequence of simple regularity theory for partial differential equations. The theory of higher dimensional problems uses ideas from statistics like the

ANOVA decomposition in addition to lower-dimensional manifolds, dimension-weighted Sobolev spaces, function spaces based on tensor products and the concentration of measure.

This talk illustrated the challenges posed by multi-dimensions with a few examples including interpolation, density estimation, and the solution of partial differential equations that arise, for example, in plasma physics and molecular biology. Both computational and theoretical questions were covered. The focus was on the structure of the problems, which admits computational approximation and compares this structure to the regularity structure used in lower dimensions. Also discussed were variants of the sparse grid combination technique that are both adaptive and suitable for parallel implementation, and which address a potential instability of the original combination technique. These techniques naturally fit in with the multi-core and multi-physics questions and thus into the TUM-IAS Focus Group HPC – Tackling the Multi-Challenge.

Clinical Cell Processing

Speakers: Prof. Dirk Busch | Host
Prof. Stanley Riddell | Hans Fischer Senior Fellow
Dr. Christian Stemberger | Carl von Linde Junior Fellow
Medical Microbiology, Immunology and Hygiene, TUM

Abstract: Prof. Dirk Busch – *Clinical Cell Processing and Purification*
Cell therapy provides promising perspectives for future developments of more effective therapies for a wide spectrum of human diseases. However, a major bottleneck in the field is that clinical cell preparations are often characterized by limited purity. This general problem causes substantial variability in the quality of cell products and might be responsible for negative side effects due to unwanted contaminants. The TUM-IAS Focus Group has been trying to establish technologies to overcome these current limitations.

Abstract: Prof. Stanley Riddell – *Novel Perspectives in Adoptive Immunotherapy*
The T-cell adaptive immune system can distinguish diseased from normal cells based on recognition of antigens by diverse receptors that result from somatic rearrangement of distinct gene segments. T cells also differentiate into distinct subsets that are genetically programmed to provide long-lived immune memory. The specificity and durability of T-cell recognition was exploited to treat potentially fatal viral infections and advanced malignancies in humans with some success. However, the broader application of adoptive T-cell transfer to establish therapeutic immunity would require the rapid identification or engineering of rare T cells of defined specificity and function, and for amplifying these cells *in vitro* (or *in vivo*).

Abstract: Dr. Christian Stemberger – *New Technologies in Clinical Cell Purification*
Highly pure populations can best be obtained using positive selection and multiple selection markers. However, for clinical cell sorting, each marker has to be extensively tested and approved by regulatory authorities. In addition, the labeling reagents themselves could affect the functionality and viability of sorted cells. The group has developed a fully reversible staining method based on the multimerization of low-affinity antibody-derived Fab-fragments. Such reagents could be generated for virtually any antigen and could be used in combination – simultaneously or successively – for multiparameter cell handling.

Modeling Product Architecture with Graph Theory and Graph Transformation

Speaker: Prof. Matthew Campbell | Hans Fischer Senior Fellow
Department of Mechanical Engineering, University of Texas at Austin

Abstract: Flowcharts, electric circuits, exploded views, and process flow diagrams are a few examples of the way graphs are used in engineering design and analysis. In fact, graphs, along with written text and illustrations, encompass all engineering knowledge. This talk addressed questions such as what the common elements of graphs are, and how graphs can best be stored and communicated in engineering design.

The presentation started with an introduction on the basics of graph theory and a rudimentary look at their common computer implementations. It then explored how graph transformation methods may be employed in engineering design. Graph transformation or graph rewriting has traditionally been a mathematical field focused on ways to properly represent rules that change the graph. Like English or German grammar, which dictates the proper ways to form valid statements, one can create graph grammars that form valid graphs of electric circuits, gear trains, or bulk-machining processes. Such grammars could be useful in educating engineers about a particular field. But such rules may also be viewed as antagonistic to real creativity. Also, grammar rules may outfit the computer with abilities to design or improve on new engineering systems, and that was the focus of the author's following seminar. This seminar was intended to lead participants to a better understanding of graphs and their implications in engineering.

Magnetic Resonance Imaging Physics: Where will the future take us?

Speaker: Prof. Axel Haase | Carl von Linde Senior Fellow
IMETUM (Zentralinstitut für Medizintechnik), TUM

Abstract: During the last three decades, magnetic resonance imaging (MRI) has become an important tool for medical diagnosis and biomedical research. The method has an excellent soft tissue contrast with a high spatial resolution and can be applied for functional and metabolic studies. MRI is non-invasive and non-destructive due to the application of low-energy electromagnetic waves and static magnetic fields. Compared to other imaging modalities, however, MRI is insensitive.

New technologies under development could dramatically increase the sensitivity of MRI. This is especially the case with new MRI phased-array coils, parallel imaging, and the application of high magnetic fields. In special cases, the magnetic resonance signal could be further enhanced using hyperpolarization. These technologies were described in the lecture, and experiments were shown using a portable MRI system.

Calender of Events 2010

February

February 1 Workshop Statistical Methods and Models

Organizers:
Prof. Claudia Klüppelberg | Carl von Linde Senior Fellow
Prof. Chris-Carolin Schön
Dr. Stephan Haug

The Workshop on Statistical Methods and Models was directed at TUM scientists whose research requires statistical methods and models, and its aim was getting acquainted, networking, and planning for future joint actions and events. The lectures were given by experts from various scientific fields such as computer science (Prof. Javier Esparza), electrical engineering (Prof. Sandra Hirche and Prof. Wolfgang Uschick), life sciences (Prof. Jutta Roosen and Prof. Annette Menzel), mathematics (Prof. Silke Rolles), and civil engineering (Prof. Daniel Straub).

March

March 24 The Algebra of Fast Transforms: Banded Matrices with Banded Inverses

Keynote speaker: Prof. Gilbert Strang (Massachusetts Institute of Technology, USA), Visiting Fellow

March 25 Ohm Lecture

Keynote speaker: Prof. Gilbert Strang (Massachusetts Institute of Technology, USA), Visiting Fellow

April

April 8 Peptides as Drugs

Keynote speakers:
Prof. Chaim Gilon (Hebrew University Jerusalem, Israel) on “Conversion of Peptides and Active Regions in Proteins into Drug Leads”
Prof. Victor J. Hruby (University of Arizona, Tucson, USA) on “The Chemistry of Human Behavior”

April 11 – 13 TUM-IAS General Assembly

The second TUM-IAS General Assembly took place at Hotel Schloss Berg at Lake Starnberg and brought together the TUM-IAS community including TUM-IAS Fellows, Board of Trustees members, the Advisory Council, TUM-IAS host professors, and doctoral candidates directly connected to the activities of the Institute.











The TUM-IAS wants to foster an active community of scientists based on dialogue and communication. By organizing the General Assembly TUM-IAS gives its members the possibility to meet, to exchange ideas and to learn about each others' research. Fellows of the Institute presented their research projects, with an emphasis on what they viewed as the main research issues in their respective fields. Great talks were given by the Focus Groups Clinical Cell Processing and Purification, Cognitive Technology, Computational Biology, Computational Biomechanics, Biophysics, Control of Quantum Materials, Fundamental Physics, Nanoscience, Neuroscience, Risk Analysis and Stochastic Modeling, Satellite Geodesy.

On the last day three keynote lectures were given: Hans Fischer Senior Fellow Prof. Walter Kucharczyk presented "Novel Imaging Guidance Methods for Excisionless Tumor Diagnosis and Treatment"; Carl von Linde Junior Fellow Dr. Julia Kunze-Liebhäuser informed the TUM-IAS community about "Electrochemistry Research in Energy Conversion and Storage – from Fundamentals to Nanotechnology Applications"; and Hans Fischer Senior Fellow Prof. Peter Schröder talked about "Geometric Modeling: From Entertainment to Engineering." The TUM-IAS General Assembly was concluded by the Board of Trustees meeting in the afternoon.

May

May 3–5 Waiting for the LHC: Electroweak and Flavour Dynamics

Organizer: TUM-IAS Focus Group Fundamental Physics

June

June 18 – 19 Synapses Twenty Ten

Organizer: Prof. Arthur Konnerth | Carl von Linde Senior Fellow

Symposium on the occasion of Prof. Josef Dudel's 80th birthday

June 23 Conference on Earth System Engineering: Methods for Sustainable Solutions of Global Crisis

Organizers: Carl von Linde-Akademie, International Expert Group on Earth System Preservation (IESP), TUM Institute for Advanced Study
Location: Bayerische Akademie der Wissenschaften

This conference focused on the causes of the current global crisis, as well as on methods to address both causes and impacts. Recommendations on how our economy and politicians should act were discussed: Global crises were only to be tackled in their entirety and complexity, and through a holistic approach. The presentations explained how acting in a responsible manner would be in the best interest of the whole.

June 28 Workshop Information-Based Analysis and Design of Networked Control Systems

Organizers: DFG funded priority program SPP1305,
TUM-IAS Focus Group Networked Dynamical Systems
Keynote speakers:
Prof. Koji Tsumura (University Tokyo, Japan)
Dr. Maben Rabi (University of Cambridge, United Kingdom)

June 30 – July 4 Jacques-Monod-Conference on Imaging Brain Circuits in Health and Disease

Chairman: Prof. Arthur Konnerth | Carl von Linde Senior Fellow
Location: Roscoff, France

July 19 – 23 TÜV Süd Stiftung Student-Workshop

Organizer: Prof. Steven D. Glaser (University of California, Berkeley, USA), TÜV Süd Stiftung Visiting Professor

Understanding the use of seismic methods for acoustic imaging of structural behavior involves finding unseen faults and detecting structural damages as well as learning to non-destructively evaluate the status of structures. Furthermore, it requires becoming acquainted with advanced methods of quality evaluation. In this respect, a lot of hands-on exercises including techniques such as acoustic emission, ultrasound, and radar were carried out.

July 21 – 22 TUM-IAS Summer Seminars

Speaker: Prof. Leon O. Chua (University of California, Berkeley, USA), Visiting Fellow

“Memristor Brains and Minds”

Abstract: The first part was a self-contained introduction to memristors for those who did not know what a memristor was. The second part was on memristor applications to neurobiology, learning, and associative memory developed from an information theoretic perspective. It was also shown that brains are made of memristors.

“Nonlinear Dyamics: Perspective on Wolfram’s New Kind of Science”

Abstract: This subject consisted of rigorous mathematical developed theories and was completely original, and quite fundamental, with relevance to nonlinear dynamics and group-theoretic physics.

September

September 8 – 9 International Symposium on Frontiers of Nanoelectronics

Organizers: Fraunhofer Research Institution for Modular Solid State Technologies (EMFT) (Prof. Karlheinz Bock), TUM Institute for Advanced Study, TUM Institute for Nanoelectronics (Prof. Paolo Lugli, Prof. Peter Russer)
Cosponsored by: GAUSS Instruments, Excellent Cluster Nanosystem Initiative Munich (NIM), Siemens AG

The symposium was part of the project “Nanoelectronics in Germany” conducted by acatech (German Academy for Science and Engineering). It focused on the long-term potential and challenges of nanoelectronics.

September 16 Pattern-Based Control - Basic Ideas and Application to Power Systems for Dynamic Learning Control of Unknown Systems via Partial Models Learned in Prior Experiences

Keynote speaker: Prof. David J. Hill (Australian National University), Visiting Fellow

Abstract: This talk provided an introduction to the recently developed deterministic learning theory for nonlinear dynamical systems. Deterministic learning emphasizes learning from “experiences” in uncertain dynamic environments. The associated information and control used could be stored for later use to give fast-response control. The main topics are knowledge acquisition, representation, and utilization in unknown dynamic environments. Referred to as “deterministic learning” to distinguish it from the celebrated “statistical learning,” the new learning theory is developed utilizing concepts and tools of adaptive control and dynamical systems. It provides the potential for design approaches for nonlinear system identification, temporal/dynamical pattern recognition, and pattern-based intelligent control of nonlinear systems in uncertain dynamical environments. An illustration of using the basic ideas in power systems control was given.

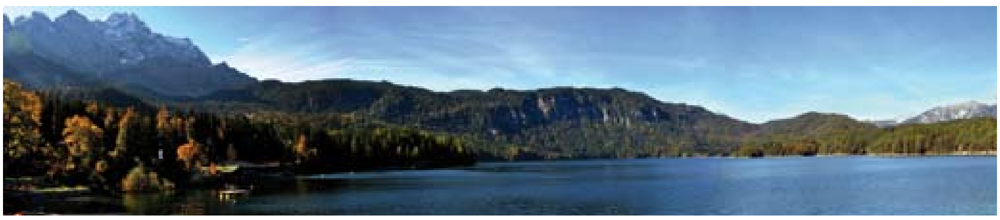
September 17 Theory of Force-Induced Ligand-Receptor Unbinding

Keynote speaker: Prof. Robijn Bruinsma | Hans Fischer Senior Fellow
University of California, Los Angeles, USA

October

October 3 – 6 3rd International Workshop on Cellular and Molecular Mechanisms of Axon Degeneration

In parallel to the experimental efforts to better understand axon injury, the Neuroscience Group also organized a major international meeting on the mechanisms of axon degeneration. Together with Prof. Martin Kerschensteiner, their collaboration partner at LMU, the group succeeded in bringing the world’s leading researchers in the field of axon degeneration to Bavaria. The third installment of the “International Workshop on Cellular and Molecular Mechanisms of Axon Degeneration” was held at Eibsee in October 2010. The TUM-IAS provided



key sponsoring and administrative support for organizing this event, with 20 international speakers and over one hundred scientists from around the world. Among the numerous topics that were discussed, two keynote lectures stood out: One, delivered by Prof. Jeff Lichtman of Harvard University, focused on new, large-scale efforts to reconstruct entire neuronal circuits ("connectomics") using transgenic mouse technology and automated electron microscopy. The second keynote lecture was given by Prof. Marc Tessier-Lavigne, President of Rockefeller University, on a recently discovered molecular pathway that links Alzheimer's disease to local axon degeneration. Further sessions addressed the molecular mechanisms of posttraumatic injury, the neuroinflammatory processes that lead to axon injury, the role of physiological axon dismantling during development, and emerging technologies that are becoming available to study degenerating axons using light and electrons.

October 5 Annual Meeting Synbreed Open Science Session

Speakers: Prof. David Balding (University College London, United Kingdom) on "Statistical Methods for Genetic Association Analyses in the Resequencing Era" Prof. Theo Meuwissen (Norwegian University of Life Sciences) on "Prediction of Genetic Value using Whole Genome Sequence Data."

October 7–9 Flavor Physics: Strong Dynamics, Rare Decays and New Phenomena

Location: Hotel Schloss Berg, Lake Starnberg

This symposium, organized by Prof. Andrzej Buras (Carl von Linde Senior Fellow), Prof. Gerhard Buchalla (LMU) and Sigrid Wagner (TUM-IAS), gathered around 80 experts in flavor physics. In addition to the Hans Fischer Senior Fellows Prof. Gino Isidori and Prof. Stefan Pokorski and Carl von Linde Junior Fellow Dr. Martin Gorbahn, a number of leading flavor physicists from Europe, the USA, and Canada presented their recent results on rare decays and CP violation, both in the framework of the Standard Model of particle physics and in its various extensions such as supersymmetry, models with extra dimensions and new strong dynamics. In Scientific stars including Prof. William Bardeen (Fermilab, USA), Prof. Andrzej Czarnecki (University of Alberta, Canada), Prof. Konrad Kleinknecht (LMU), Prof. Roberto Peccei (UCLA), Prof. Chris Quigg (Fermilab, USA), Prof. Chris Sachrajda (University of Southampton, England) and Dr. Luca Silvestrini (Sapienza University of Rome), as well as a large number of young postdocs, predominantly former PhD students of Prof. Andrzej Buras, presented their most recent results, which were discussed intensively during the full duration of the workshop. The symposium demonstrated in an impressive manner the potential of flavor physics in the search for new phenomena, providing a very optimistic outlook for the years to come.

October 12 Quantum Dots with Photonic Crystal Nanocavity for Nanophotonic Application

Speaker: Prof. Yasuhiko Arakawa | Hans Fischer Senior Fellow
University of Tokyo, Japan

October 13 Robots and the Human

Speaker: Prof. Oussama Khatib (Stanford University, USA), Visiting Fellow

October 21 TUM-IAS Building Opening Celebration






October 22 Energy and Electromobility – Exploring the Fundamental Research Challenges

Industrial R&D leaders joined university researchers – including the next generation of scientists and engineers – for an intensive look at hurdles in the path to a "low-carbon" future.












October 25 – 26 International Symposium on Advances in Nanoscience

Organizers: Nanosystems Initiative Munich (NIM), TUM Institute for Advanced Study, Center for Nanotechnolgy and Nanomaterials (ZNN; Walter Schottky Institute)

Session 1: Quantum- and Nanosystems
Session 2: Hybrid Nanosystems
Session 3: Nano and Energy
Session 4: Bio-Nanoscience

November

November, 3 – 4 Bone Simulations, Experimentations and their Applications in Clinical Practice

Organizers: TUM-IAS Focus Group Computational Biomechanics
Prof. Ernst Rank (TUM), Host
Prof. Zohar Yosibash | Hans Fischer Senior Fellow
Ben-Gurion University, Israel

November 12 Systems Theory: A Retrospective and Prospective Look

Speaker: Prof. Sanjoy Mitter (Massachusetts Institute of Technology, USA), Visiting Fellow

Abstract: System theory is the transdisciplinary study of systems in general, with the goal of elucidating principles that can be applied to all types of systems in all fields of research. Pioneering works were accomplished in the field of cybernetics by researchers like Norbert Wiener and John von Neumann, who examined complex systems with only pencil and paper using mathematics. Developments in system theory brought up the concepts such as communication and control in living organisms, machines and organizations, focusing on how information is processed, how reaction to information is taken, and how changes could be made to better accomplish the first two tasks. Understanding the emerging behavior from multiple interconnected elements and its evolution is a main challenge in system theory and the key to future technological innovation.

November 18 Risiken, Krisen, Katastrophen: Wie lassen sich Extremereignisse beherrschen?

Organizers: Carl von Linde-Akademie (Prof. Klaus Mainzer), Deutsches Museum, TUM Institute for Advanced Study (Prof. Claudia Klüppelberg)
Location: Deutsches Museum








Extreme occurrences such as climatic catastrophes, pandemics, stock market crashes, and finance and economic crises increasingly determine our lives. To be prepared in a globalized and complex world, one has to learn to analyze and estimate risks and coincidences of rare events. Traditional methods and models of natural phenomena, stock exchanges, and banks can be misleading, as the latest occurrences of climate change and world economic crisis show. This practically oriented symposium illustrated how new mathematical methods would able to properly estimate extreme events and how they could assist us in managing risks, crises, and catastrophes.

November 25 Liesel Beckmann Symposium Gender in Management Studies

Organizers: TUM Gender Center, TUM Institute for Advanced Study
The topic of this annual symposium was “Gender in Management Studies.” The focus of the several lectures and workshops was, apart from gender budgeting and gender marketing, the topic “management.” Prof. Sabine Sczesny of the University Bern talked about the historic change of both “gender stereotypes” and “management styles” and the interplay between them.

Prof. Madeline Heilman of the New York University Psychology Department was persuaded to hold a lecture on the topic “Affirmative Action and its Unintended Consequences for Career Progress.”

December

December 7 Who knew !? Health Advancing Discoveries for Women

Speaker: Prof. Jerilynn Prior (University of British Columbia, Canada), Visiting Fellow

December 10 Zanner Colloquium

A “Surprise Colloquium” was organized to see off TUM-IAS Managing Director Dr. Markus Zanner who started his new job as Chancellor at the University of

Bayreuth in January 2011. The theme of the Zanner Colloquium was “Paths are made by walking,” a reflection on the management of innovation at universities.

People

Fellows

Carl von Linde Senior

2007 Prof. Andrzej Buras, Prof. Arthur Konnerth, Prof. Reiner Rummel
2008 Prof. Horst Kessler, Prof. Claudia Klüppelberg
2009 Prof. Axel Haase
2010 Prof. Gerhard Abstreiter, Prof. Ulrich Stimming

Carl von Linde Junior

2007 Dr. Adrian Jäggi
2008 Dr. Martin Gorbahn, Dr. Ulrich Rant, Dr. Robert Stelzer
2009 Dr. Kolja Kühnlenz, Dr. Julia Kunze-Liebhäuser, Dr. Marco Punta, Dr. Ian Sharp
2010 Dr. Wilhelm Auwärter, Dr. Vladimir García Morales, Dr. Alexandra Kirsch, Dr. Miriam Mehl, Dr. Christian Stemberger, Dr. Dirk Wollherr

Hans Fischer Senior

2007 Prof. Gerhard Beutler, Prof. Walter Kucharczyk, Prof. Bert Sakmann
2008 Prof. Anuradha M. Annaswamy, Prof. Yasuhiko Arakawa, Prof. Douglas Bonn, Prof. Mandayam A. Srinivasan, Prof. David A. Weitz
2009 Prof. Matthew Campbell, Prof. Richard Davis, Prof. Gino Isidori, Prof. Shuit-Tong Lee, Prof. Wolfgang Porod, Prof. Stanley Riddell, Prof. Peter Schröder, Prof. Zohar Yosibash
2010 Prof. Stefan Pokorski, Prof. Michael Ortiz, Prof. Tim Sparks, Prof. Raman I. Sujith, Prof. Markus Hegland, Prof. Robijn Bruinsma

Hans Fischer Tenure Track

2007 Prof. Thomas Misgeld
2010 Prof. Hendrik Dietz

Rudolf Diesel Industry

2009 Prof. Khaled Karrai, Dr. Dragan Obradovic, Dr. Georg von Wichert
2010 Dr. Tsuyoshi Hirata, Prof. Gernot Spiegelberg, Dr. Matthias Heller, Dr. Chin Man Mok

Prof. Brian D.O. Anderson
Research School of Information Sciences and Engineering
The Australian National University
Host: Prof. Sandra Hirche

Prof. Steven N. Blair
Department of Exercise Science
University of South Carolina
Host: Prof. Martin Halle

Prof. Peter J. Brockwell
Department of Statistics
Colorado State University
Host: Prof. Claudia Klüppelberg

Prof. Leon O. Chua
Electrical Engineering and Computer Sciences
University of California, Berkeley
Host: Prof. Klaus Mainzer

Prof. Suh-Urk Chung
Department of Physics
Brookhaven National Laboratory
Host: Prof. Stephan Paul

Prof. Anna Fontcuberta i Morral
Institut des Matériaux
Ecole Polytechnique Fédérale de Lausanne
Host: Prof. Gerhard Abstreiter

Prof. Hassan Foorosh
School of Electrical Engineering and Computer Science
University of Central Florida
Host: Prof. Nassir Navab

Prof. Martin Greiner
Centre for Applied Sciences
Aarhus University
Host: Prof. Claudia Klüppelberg

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Department of Chemistry and Biochemistry
University of California, Santa Barbara
Host: Prof. Steffen Glaser

Prof. Madeline E. Heilman
Department of Psychology
New York University
Host: Prof. Isabell Welpe

Prof. David J. Hill
School of Engineering
The Australian National University
Host: Prof. Sandra Hirche

Dr. Emiko Hiyama
Nuclear Physics Laboratory
RIKEN, Japan
Host: Prof. Wolfram Weise

Prof. Victor J. Hruby
Department of Chemistry and Biochemistry
The University of Arizona
Host: Prof. Horst Kessler

Dr. Tetsuo Hyodo
Department of Physics
Tokyo Institute of Technology
Host: Prof. Wolfram Weise

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Nuclear Physics Laboratory
RIKEN, Japan
Host: Prof. Wolfram Weise

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INRS, Énergie, Matériaux et
Télécommunications, Québec, Canada
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Washington University, St. Louis
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Prof. Oussama Khatib
Department of Computer Science
Stanford University
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Host: Prof. Nassir Navab

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Centro de Investigación en Matemáticas
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The University of British Columbia
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Prof. Jan Rosinski
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University of Tennessee, Knoxville
Host: Prof. Claudia Klüppelberg

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Department of Chemistry
University “La Sapienza”, Rome
Host: Prof. Hubert A. Gasteiger

Prof. Gilbert Strang
Department of Mathematics
Massachusetts Institute of Technology
Host: Prof. Klaus Diepold

Dr. Frederick T. Wagner
General Motors R&D
New York
Host: Prof. Hubert A. Gasteiger

Prof. Elke U. Weber
Department of Psychology
Columbia University
Host: Prof. Isabell M. Welpe

Prof. Yosef Yarom
Director of the Otto Loewi Center for Neurobiology
The Hebrew University of Jerusalem
Host: Prof. Arthur Konnerth

Board of Trustees

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

Members

Appointed in 2011

Advisory Council

The Director is advised by the Advisory Council with regard to recruiting new Fellows and setting the research agenda of the Institute. This body is constituted of members of TUM. The leaders of the TUM-IAS Focus Groups, and the leaders of related bodies in the Excellence Initiative as well as advisors closely connected with the institute, make up this Council.

Members

Prof. Gerhard Abstreiter Experimental Semiconductor Physics 1
Prof. Andrzej Buras Institute for Theoretical Elementary Particle Physics
Prof. Martin Buss Institute of Automatic Control Engineering
Prof. Klaus Diepold Institute for Data Processing
Prof. Joachim Hagenauer Emeritus Chair of Telecommunications Engineering
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Prof. Reiner Rummel Institute for Astronomical and Physical Geodesy
Prof. Peter Wilderer Emeritus Chair of Water Quality Control and Waste Management

Management Office

Our staff situation has been very dynamic, not only because of their enormous dedication and the changes in our operation environment, but also because of some inevitable movements affecting the constitution of the management office. It started with our Associate Managing Director Ms. Margaret Jaeger taking maternity leave and giving birth to her charming boy Noah. Her task as manager of our scientific office was taken over with gusto by Ms. Stefanie Hofmann, very expertly seconded by Ms. Tatjana Steinberger. Stefanie and Tatjana managed the Fellow selection process in 2010. They were assisted by an equally highly motivated secretariat, with Ms. Rebecca Innerhofer and Ms. Sandra Schmidt as its driving forces. Our staff not only took care of the selection process for our Fellows, but also of their needs in terms of housing (e.g., managing our guest house in Schwabing), running their projects, managing the usage of our new office building, welcoming visitors, and many other visible and invisible tasks, in particular during our move from the city to Garching. They were assisted by a good crew of student assistants, to whom the Institute also owns great thanks.

In October, Dr. Ana Santos Kühn joined us as our new Managing Director, to replace Dr. Markus Zanner, who took over the Chancellery of the University of Bayreuth in January 2011. The many achievements of Markus and his contributions to TUM and TUM-IAS were properly celebrated in a festive “Zanner Symposium,” in which innovative university management methods were discussed and illustrated. From the start, Ana has made a great effort in organizing the financial office in Garching and laying the foundations for a sound future financial management.

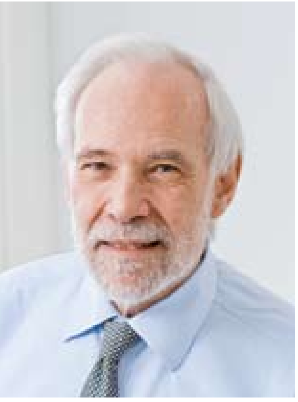
A special word of thanks should go to our Event Manager, Ms. Sigrid Wagner, who put in long hours of organizing the many events that took place at the Institute in 2010, and whose charming presence makes her a perfect host for the Institute. The Institute could not survive without the help of many in the University administration, too many to name here; let me just mention Ms. Melanie Hüttinger and Ms. Nicole Jerouschek, who took care of the bookkeeping.

Toward the end of 2010 one of our partner organizations, the TUM Corporate Communications Center (CCC), generously allowed us to draw one of its members more directly into our team. Patrick Regan, who in CCC is responsible for international press relations and video production, now also serves as a science writer and editor for TUM-IAS.

Finally, let me also thank the many people who have provided services to the Institute, our home caterer Studentenwerk with its staff, our housekeepers, the cleaning services and their staff, the computer services, and many others without whom the Institute could not function properly and who have, without exception, contributed with grace and friendliness.

Patrick Dewilde
Director

Staff



Prof. Patrick Dewilde
Director

Dr. Markus Zanner
Managing Director
(through 2010)

Dr. Ana Santos Kühn
Managing Director
(since 2011)

Margaret Jaeger
Associate Managing Director

Stefanie Hofmann
Program Manager

Tatjana Steinberger
Program Manager

Sigrid Wagner
Event Manager /
Web Coordinator

Sandra Schmidt
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Rebecca Innerhofer
Secretary

Melanie Hüttinger
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Excellence Initiative

Patrick Regan
Science Writer and Editor

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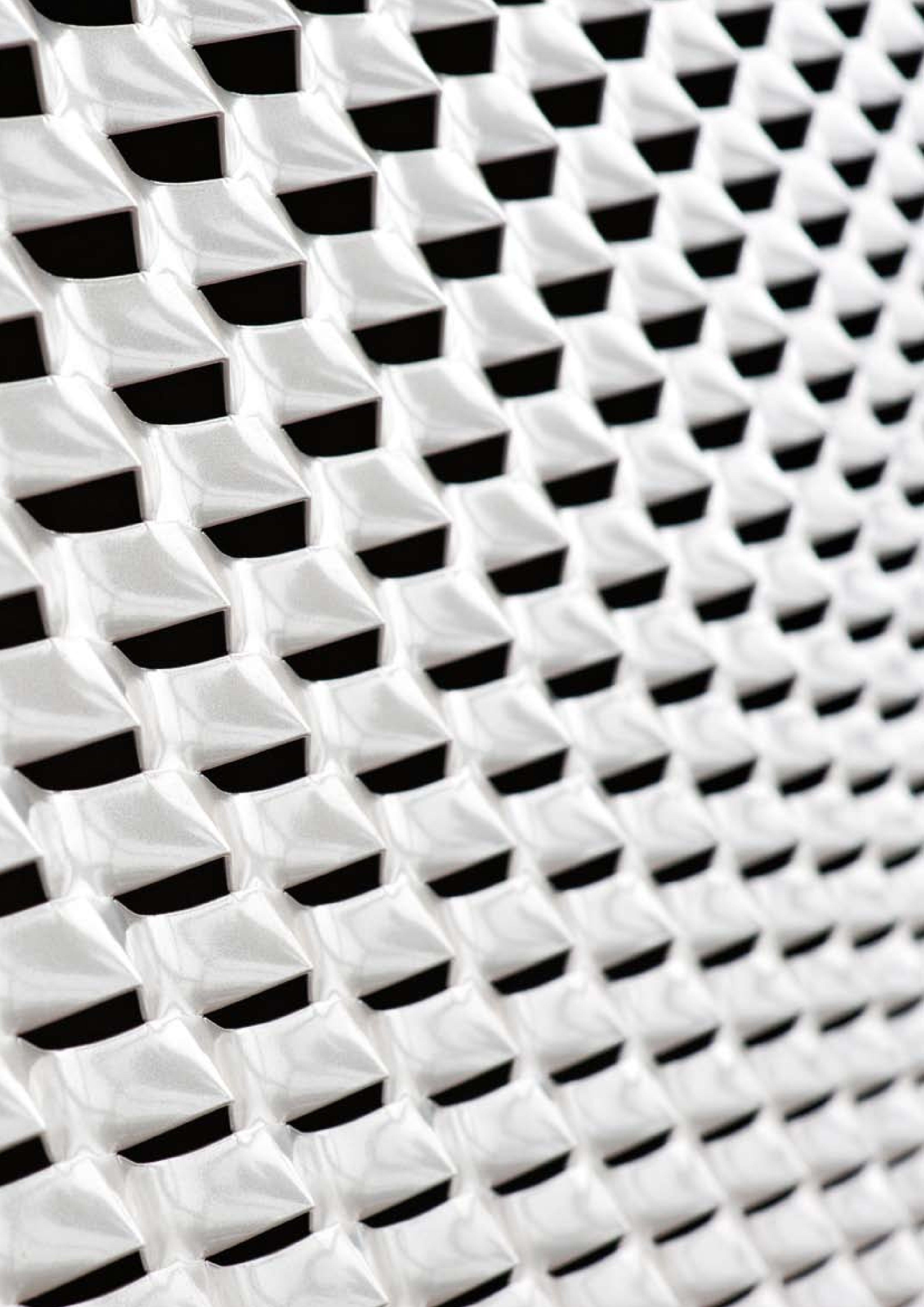

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