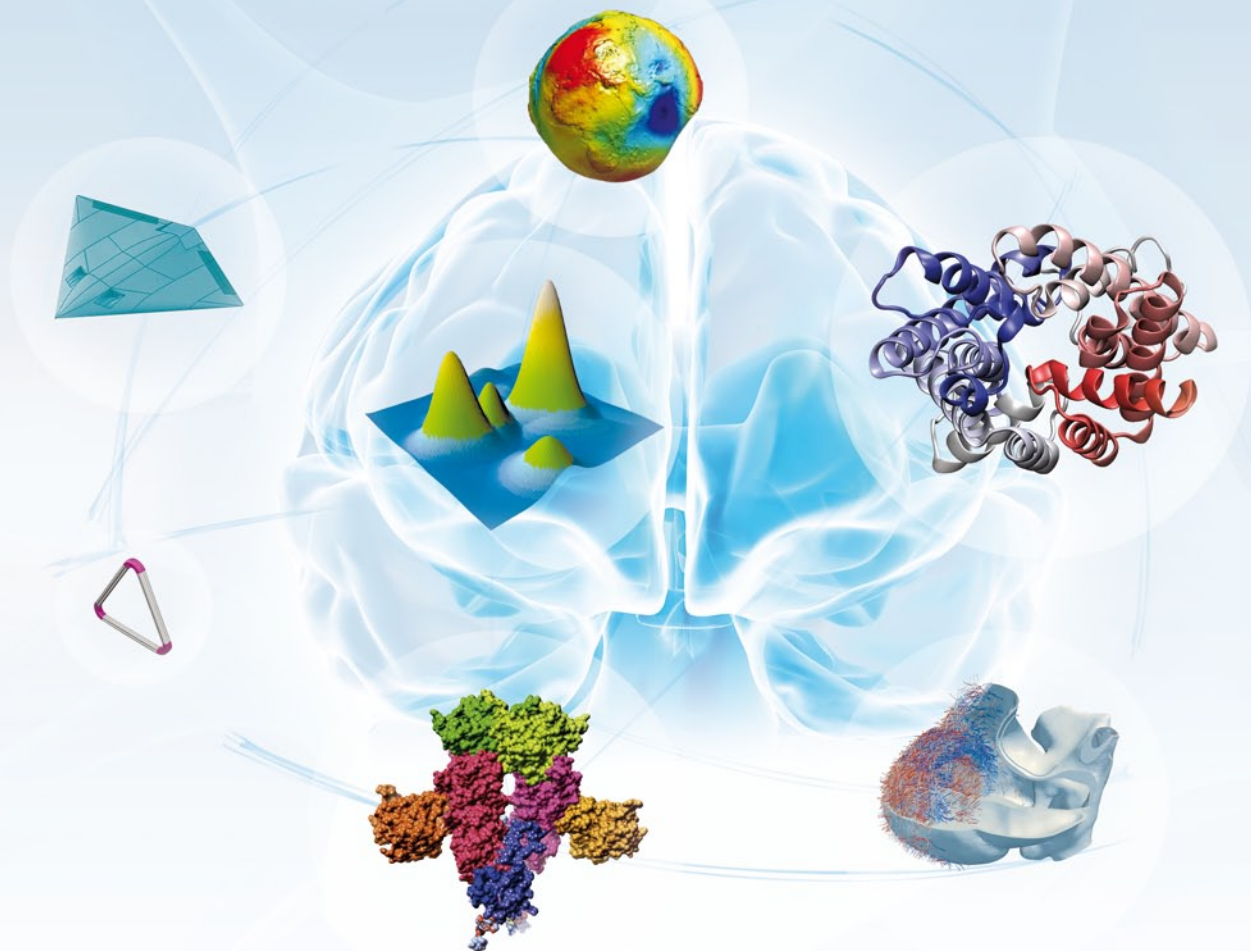# Annual Report

Technische Universität München

Institute for Advanced Study

2011

TUM

Annual Report

Technische Universität München

Institute for Advanced Study

2011

Table of Contents

TUM President's Foreword

For the Technische Universität München as a whole, 2011 was a year that both tested and proved the character of our community. Even while developing multiple proposals for the second program phase of the German Excellence Initiative and simultaneously absorbing an enormous influx of new students, TUM never missed a beat in research, teaching, or engagement with industry and society.

We deliberately approached this round of the Excellence Initiative as a community, particularly with regard to our institutional strategy: "TUM. The Entrepreneurial University." Despite the need to keep details and documents closely restricted, the process itself—a cycle of critical assessment, imaginative design, and pragmatic planning—remained strikingly open and collaborative. The best ideas rose to the top through competition among many excellent ideas. As a result, the future concept that TUM has put forward reflects and belongs to all members of our diverse community.

The TUM Institute for Advanced Study, at the heart of our institutional strategy in the first phase, played a central role in hammering out our vision for the next, not least through the energetic participation and incisive contributions of many TUM-IAS Fellows. The Institute's headquarters building in Garching, completed and donated by the BMW Group in the fall of 2010, served throughout 2011 as both a symbolic and practical hub for this activity.

Of course, the vision we arrived at is more important than the process that got us there. It is still, in the spring of 2012, a bit too soon to reveal much about our vision or the measures we have proposed to bring it, with support from the federal and state governments, fully to life. I can, however, highlight a few emerging themes that will continue to gain in prominence over the coming years:

- TUM is committed to creating internationally competitive career paths for young scientists, in marked contrast to the rigidity of the traditional German system.

- There is no turning back from our drive toward de-compartmentalization of research-oriented teaching, as exemplified by the International Graduate School of Science and Engineering, the TUM Graduate School, and the Munich School of Engineering.

- TUM is intensifying efforts to bring the perspective of humanities and social sciences to technology-oriented science, and to build expertise on the ways society's needs and concerns influence scientific research and technological innovation.

- Beyond embracing and seeking to enhance the diversity of talents in our academic community, TUM is also taking steps to advance understanding of gender and diversity issues on a scientific basis.

In each of these areas, the TUM-IAS can serve as an inspiration, a laboratory for trying new approaches (as for example in the Hans Fischer Tenure Track and Carl von Linde Junior Fellowships), and an active partner in the ongoing transformation of our university.

Behind all of these efforts lies a profound sense of the university's obligation to put its scientific knowledge and technological creativity at the service of society. Even as we continue to strengthen areas of fundamental research, we recognize that the combination of TUM's technological orientation with a uniquely broad research portfolio represents an opportunity, and a duty, to help society and industry address critical challenges of the coming century.

Prof. Wolfgang A. Herrmann
President

TUM-IAS Director's Message
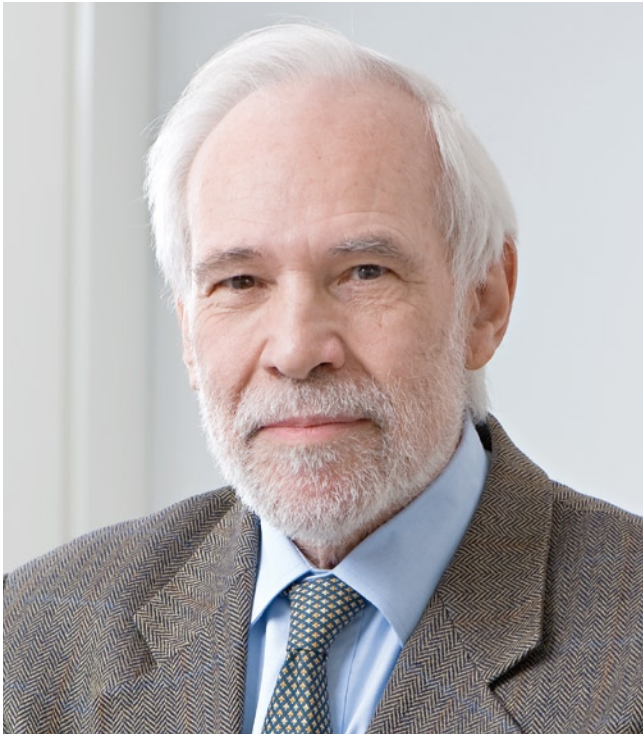
2011 has been an exhilarating year! Since 2010 the Institute is operating at (more than) full capacity, the level of activity has been tremendous, and so have some of the challenges. The Institute can also be proud of a great collection of important results, to be detailed further on in this report (and found on our Web pages). Here I want to concentrate on the main elements that have moved us forward.

2011 was the first full year of operation in our magnificent building in Garching. The atmosphere of light, serenity, enticement to science and comfortable interaction that was promised by its architectural concept has been fully realized, to the delight of all our participating scientists. Very quickly, the building has become a center for scientific events, not only engaging our own Fellows and Focus Groups, but also many bodies in our university community and even outside it. Thanks to its roomy architecture, these events almost never disturbed the serene atmosphere our in-house Fellows need.

In particular, a great number of exploratory workshops, summer schools, and specialized scientific events were held, many in collaboration with other institutions. A complete description is found further on in this report, but I wish to single out the active collaboration with the Peter Wall Institute for Advanced Studies in Vancouver, with whom we organized three timely international exploratory workshops, on bionics, on coherence in ultracold molecules, and on the history of energy sources. Each case involved intense collaboration with other parties as well, respectively the German Aerospace Center (DLR), the Max Planck Institute of Quantum Optics, and the Deutsches Museum. We consider such exploratory workshops to be an important catalyst for new ideas and new proposals.

The main activity of the Institute and its "raison d'être" is of course the original scientific and technological work performed by our Fellows and our Focus Groups. In sheer numbers, the Institute has never been as large and as active scientifically, with a Fellow base that is well balanced between our different target categories: young and experienced, Munich-based and international, and across disciplines.

Did we perform well in 2011? I do not want to succumb to the temptation of citing numbers of publications or number of citations; for the benefit of number crunchers we have put all the performance data on the Web, and it is impressive (see www.tum-ias.de).

The biggest happening in 2011, at least the one that consumed the most energy in the TUM community, was the production of the new Institutional Strategy that we submitted as our contribution to Phase 2 of the Excellence Initiative. (Phase 1 was largely responsible for creating the Institute and providing us with the necessary funds.) Under the inspiring direction of our President, the closely knit TUM community was able to produce a strongly supported vision of its future that we hope will receive a warm reception in Germany, and maybe even worldwide.

In this context, I wish to further highlight one major new element, notwithstanding our permanent strong commitment to scientific and technological innovation. Science and technology have great societal impacts, in several directions and dimensions. We believe in the absolute necessity to *know*, and to know well. That is the prime objective of science. As engineers and applied scientists, we also believe in the absolute necessity to do *things right*. One cannot go without the other (in both directions, new science requires new technology and vice versa), and as our prime goal is scientific and technological innovation, these basic aims are integral to our charter. However, doing things right is in the first place doing things right for society. The huge impact technology has had on almost all fields of endeavor may often be judged positively, as in the case of medical instrumentation, helping social advancement, and making lives more rewarding and productive, but may just as often be judged negatively, for example as needlessly burning fossil fuels, utilizing harmful chemicals, or devising non-sustainable processes.

Quality engineering therefore requires taking societal effects into account in the choice and design process of new technology. We need both scientific knowledge of the effects of our new technology and the incorporation of this knowledge into the design exploration.

"Design technology" is therefore a substantial part of the activities of our Institute (easily about 30% of all). Add to that the scientific activities that go into measuring and modeling, and we can state that at least half of our activities are motivated by societal interest, ranging from environmental science to the design of sustainable mobility and energy systems. Given the need for ever more comprehensive system engineering, societal effects are to become an ever more important component of engineering, and we want to be in the vanguard of this development, making the best possible use of our scientific insights, from statistical analysis to nanoscience.

To conclude this message, I wish to thank very warmly all who have contributed to the success of our Institute in 2011: our Fellows and Hosts for the science they generated in good harmony; the TUM administration and the funding agencies for their much appreciated support; our Board of Trustees and Advisory Council for their guidance and participation in the reviewing processes; also many of our colleagues who have organized workshops, made proposals, and helped out with reviews; the companies that have supported us in various ways, and in particular BMW for the building that we enjoy so much; and our never relenting staff for their strong commitment and much appreciated competence.

Ad multos annos!

Prof. Patrick Dewilde
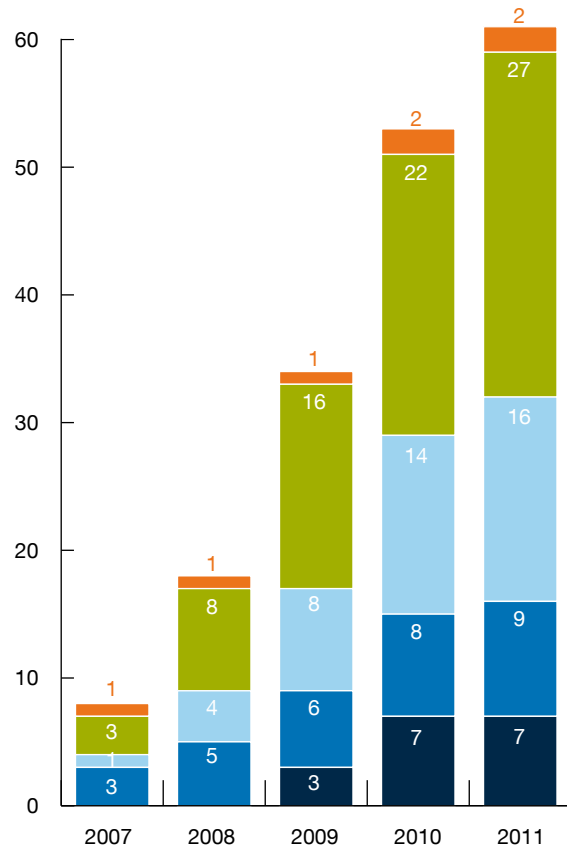Director

2011 Overview

2011 Overview

The TUM-IAS has awarded eight new Fellow-
ships in 2011, among them one Carl von Linde
Senior Fellow, two Carl von Linde Junior Fellows,
and five Hans Fischer Senior Fellows.

The TUM-IAS Fellows come from diverse
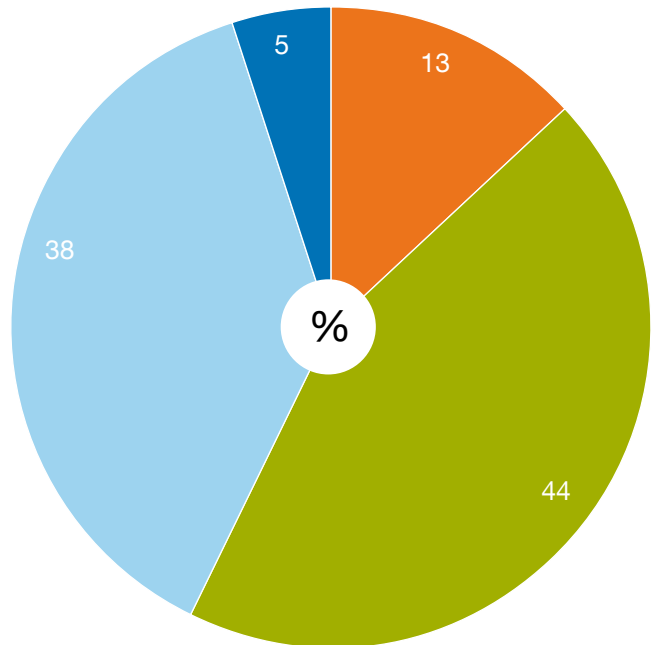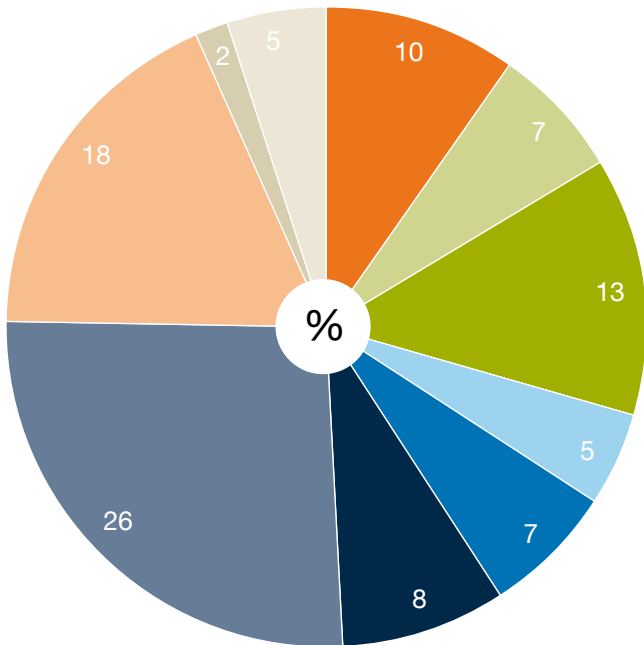disciplines and from 12 different countries.

Support for the TUM-IAS Fellows includes
funding of around 60 doctoral candidates and
10 postdoctoral researchers, who collaborate
closely with them.

Total Number of TUM-IAS Fellows

Legend:
- Hans Fischer Tenure Track
- Hans Fischer Senior Fellow
- Carl von Linde Junior Fellow
- Carl von Linde Senior Fellow
- Rudolf Diesel Industry Fellow

Distribution According to Faculties

%	Faculty
10	Informatics
7	Chemistry
13	Medicine
5	Mathematics
7	Mechanical Engineering
8	Civil Engineering
26	Physics
18	Electrical Engineering
2	Architecture
5	Center of Life and Food Sciences Weihenstephan

Distribution According to Main Scientific Fields

%	Field
13	Medicine
44	Engineering
38	Natural Sciences
5	Life Sciences

Start-up Funding

ERC Grants by TUM-IAS Members

12 **Summer Camp on Computational Design Synthesis**
Prof. Matthew Campbell | University of Texas
Host: Prof. Kristina Shea | Product Development, TUM

Symposium on Metropolis Nonformal
Prof. Christian Werthmann | Harvard University

Workshop on Advances in Photovoltaics and Photocatalysis
Host: Prof. Paolo Lugli | Nanoelectronics, TUM

Workshop on Frontiers on Functional Interfaces
Dr. Ian Sharp | Experimental Semiconductor Physics, TUM
Prof. Gerhard Abstreiter | Experimental Semiconductor Physics, TUM

Workshop on L1 Adaptive Control and Its Transition to Practice
Dr. Matthias Heller | CASSIDIAN, EADS Deutschland GmbH
Host: Prof. Florian Holzapfel | Flight System Dynamics, TUM

Symposium on Cardiovascular Prevention in Childhood
Prof. Renate Oberhoffer | Preventive Pediatrics, TUM

Starting Grants

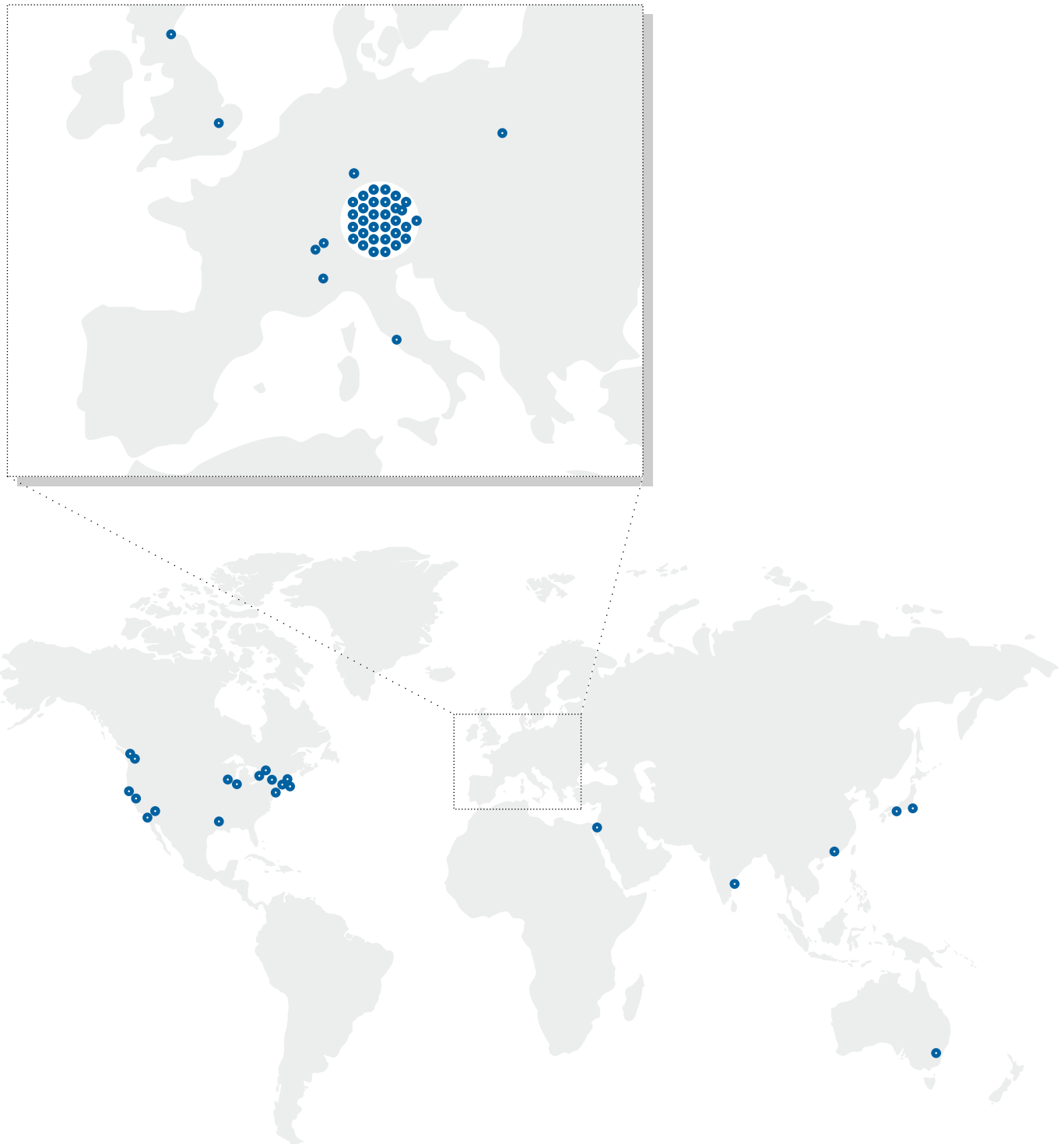Prof. Andreas Bausch | Molecular and Cellular Biophysics, TUM
Project: CompNet

Prof. Annette Menzel | Ecoclimatology, TUM
Project: E3

Advanced Grants

Prof. Martin Buss | Automatic Control Engineering, TUM
Project: SHRINE

Prof. Rüdiger Westermann | Computer Graphics and Visualization, TUM
Project: SaferVis

Where do the TUM-IAS Fellows come from?

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
PhD: Andreas Nagler
Host: Prof. Wolfgang A. Wall | Computational Mechanics, TUM

Advanced Computation
Prof. Matthew Campbell | University of Texas
PhD: Amir Hooshmand, Corinna Königseder
Host: Prof. Kristina Shea | Product Development, TUM

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

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

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

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

Biochemistry
Prof. Horst Kessler | Chemistry, TUM

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

Prof. Walter Kucharczyk | University of Toronto
PhD: Marika Kuschan
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
PhD: Thomas Gerling, Heinrich Grabmayr
Host: Prof. Andreas Bausch | Molecular and Cellular Biophysics, TUM

Clinical Cell Processing and Purification
Prof. Stanley Riddell | University of Seattle
Dr. Christian Stemberger | TUM
PhD: Jeannette Bet, Paulina Paszkiewicz
Postdoc: Dr. Stefan Dreher
Host: Prof. Dirk Busch | Medical Microbiology, Immunology and Hygiene, TUM

Cognitive Technology
Prof. Dongheui Lee | TUM
Dr. Alexandra Kirsch | TUM
Dr. Kolja Kühnlenz | TUM
Dr. Angelika Peer | TUM
Prof. Mandayam A. Srinivasan | MIT
Dr. Georg von Wichert | Siemens, Munich
Dr. Dirk Wollherr | TUM
PhD: Barbara Gonsior, Michael Karg, Christina Lichtenthäler, Andreas Schmid, Bernhard Weber, Liu Ziyuan
Host: Prof. Martin Buss | Automatic Control Engineering, TUM; Prof. Michael Beetz | Computer Science, TUM

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

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

C-H Activation Chemistry
Prof. Polly Arnold | University of Edinburgh
Host: Prof. Fritz Kühn | Molecular Catalysis, TUM

Fiber-Optic Communication and Information Theory
Prof. Frank Kschischang | University of Toronto
Host: Prof. Gerhard Kramer | Communications Engineering, TUM

Fundamental Physics
Dr. Martin Gorbahn | TUM
Prof. Gino Isidori | Frascati National Laboratories
Prof. Stefan Pokorski | University of Warsaw
PhD: Emmanuel Stamou
Postdoc: Dr. Luca Merlo, Dr. Robert Ziegler
Host: Prof. Andrzej Buras | Theoretical Elementary Particle Physics, TUM

Global Change
Prof. Tim Sparks | Coventry University, Cambridge
PhD: Anna Bock, Julia Laube
Postdoc: Dr. Nicole Estrella, Dr. Christian Zang
Host: Prof. Annette Menzel | Ecoclimatology, TUM

High-Performance Computing (HPC)
Prof. Markus Hegland | Australian National University
Dr. Miriam Mehl | TUM
PhD: Christoph Kowitz, Valeriy Khakhutskyy
Postdoc: Dr. Dirk Pflüger
Host: Prof. Hans-Joachim Bungartz | Scientific Computing, TUM

Metropolis Nonformal
Prof. Christian Werthmann | Harvard University
Host: Prof. Regine Keller | Landscape Architecture and Public Space, TUM

Molecular Imaging
Prof. Silvio Aime | University of Torino
Host: Prof. Markus Schwaiger | Clinic for Nuclear Medicine, TUM

Networked Dynamical Systems
Prof. Anuradha M. Annaswamy | MIT
Dr. Dragan Obradovic | Siemens, Munich
PhD: Arman Kiani, Herbert Mangesius, Harald Voit
Host: Prof. Sandra Hirche | Automatic Control Engineering, TUM

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

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

Soil Architecture
Prof. Ingrid Kögel-Knabner | Soil Science, TUM
Postdoc: Dr. Geertje Pronk

Statistical and Quantitative Genomics
Prof. Daniel Gianola | University of Wisconsin-Madison
Host: Prof. Chris-Carolin Schön | Plant Breeding, TUM

Risk Analysis

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

Risk Analysis and Stochastic Modeling
Prof. Richard A. Davis | Columbia University
Dr. Robert Stelzer | TUM
PhD: Martin Moser, Oliver Pfaffel, Eckhard Schlemm, Christina Steinkohl, Florian Ueltzhöfer
Postdoc: Dr. Codina Cotar
Host: Prof. Claudia Klüppelberg | Mathematical Statistics, TUM

Energy and Electromobility

Diesel Reloaded
Prof. Gernot Spiegelberg | Siemens, Munich
PhD: Claudia Buitkamp, Ljubo Mercep, Hauke Stähle
Host: Prof. Alois Knoll | Robotics and Embedded Systems, TUM

Molecular Aspects in Interface Science
Dr. Julia Kunze-Liebhäuser | TUM
PhD: Norbert Kluy, Celine Rüdiger, Christoph Traunsteiner
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
PhD: Matthias Sachsenhauser, Sebastian Schöll
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
PhD: Edgar-Otto Albert, Mario Bareiß, Armin Exner, Qingqing Gong, Muhammad Imtaar, Klaus Thurner, Anandi Yadav
Host: Prof. Paolo Lugli | Nanoelectronics, TUM

Nanophotonics
Prof. Yasuhiko Arakawa | University of Tokyo
Dr. Ulrich Rant | TUM
PhD: Matthias Firnkes, Stephan Funk, Norman Hauke, Markus Schuster, Alexander Schwemer, Thomas Zabel
Postdoc: Dr. Ilaria Zardo
Host: Prof. Gerhard Abstreiter | Experimental Semiconductor Physics, TUM

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

Nonequilibrium Statistical Mechanics at the Nanoscale
Dr. Vladimir García Morales | TUM
PhD: Lennart Schmidt
Host: Prof. Katharina Krischer | Nonequilibrium Chemical Physics, TUM

Resources and Data

In this section a brief survey of the financial data is given. All expenditures of the TUM-IAS are covered by the current "third funding line" of the Excellence Initiative. In 2011 we maintained approximately the same level of expenditures as in the previous year, continuing a steady state at the full capacity of the Institute with 61 Fellows.
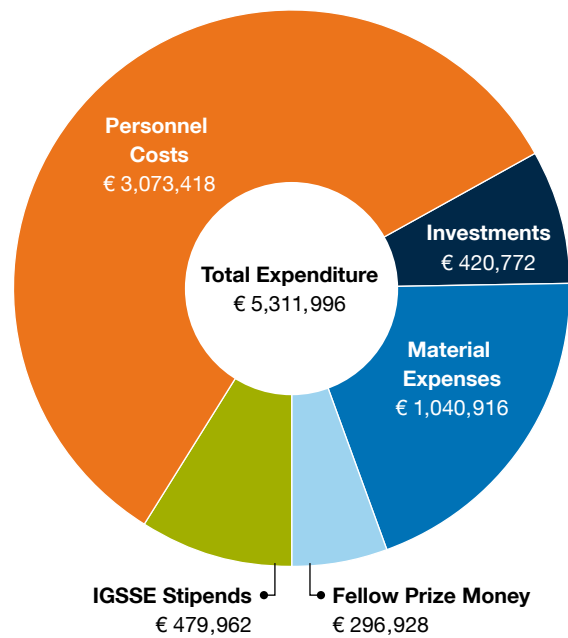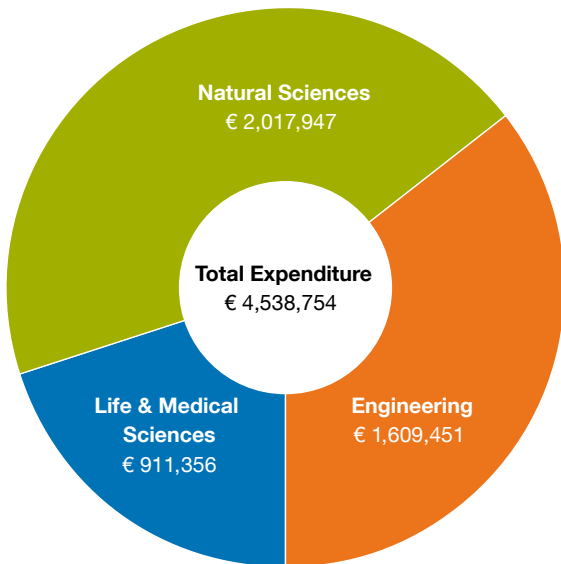
Expenditures per Fellowship Category in 2011

Carl von Linde Junior
€ 895,599

Hans Fischer Senior
€ 1,291,255

Total Expenditure
€ 3,554,461

Carl von Linde Senior
€ 697,364

Rudolf Diesel Industry
€ 320,401

Hans Fischer Tenure Track
€ 349,842
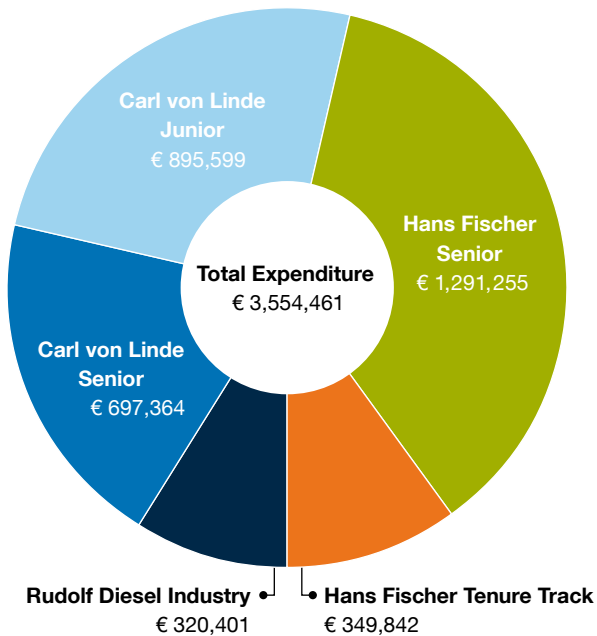
The first chart shows the allocation of expenditures in 2011 according to the different Fellowship categories. Once more the contribution to the internationalization of TUM is quite visible, as the TUM-IAS Fellowship that dominates the program in costs is the Hans Fischer Senior category. These Fellowships 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.

In the Rudolf Diesel Industry category we have now six times more expenditures than in the previous year, as the nominations of 2010 have become now fully active and operational.

The Carl von Linde Senior Fellowship shows less expenditures in comparison to the past year, in part because some Fellows terminated their tenure in 2010; the change also reflects the fact that from 2010 on only one Fellow per year is to be nominated in this category. The Carl von Linde Junior category (less cost-intensive than the senior category) registered an increase in expenditures in comparison with the previous year, underlining the emphasis that the TUM-IAS places on funding very promising young scientists, giving them the opportunity to develop their own ideas and research independently. Not accounted for in the chart are the positions of the doctoral candidates coached by the Junior Fellows, as they are financed by the Start-up Fund.

Natural Sciences
€ 2,017,947

Total Expenditure
€ 4,538,754

Life & Medical Sciences
€ 911,356

Engineering
€ 1,609,451

Personnel Costs
€ 3,073,418

Total Expenditure
€ 5,311,996

Investments
€ 420,772

Material Expenses
€ 1,040,916

IGSSE Stipends
€ 479,962

Fellow Prize Money
€ 296,928

This chart shows the expenditures of the different Fellowships grouped into the TUM scientific fields, as well as the expenditures from the start-up program according to scientific fields. Interdisciplinary projects were considered as long as a dominant field could be established. The natural sciences are still the strongest represented field at the TUM-IAS (especially physics with 17 Fellows), but there was growth in the life sciences and medicine as well as engineering from 2010 to 2011, reflecting the Institute's efforts to cover the different areas of expertise at TUM.

The total expenditures maintained approximately the same level as in 2010, as already then the Institute was operating at full capacity. It has become the policy of the Institute to offer to doctoral candidates only working contracts, and this is reflected in an increase in personnel costs and a decrease in expenditures for PhD stipends.

TUM-IAS Fellows and their Research

Introduction

2011 was the most active year of the Institute so far, according to possibly all characteristics: number of Fellows, number of Focus Groups, number of workshops, and number of publications – a detailed account on numbers can be found on the TUM-IAS Web site, both for 2011 and the whole first five years of the Institute (2006-2011). But numbers are not the most important thing; they may be indicative, but they cannot replace what could be called genuine "effects" and "results," with a special emphasis on the first item: "effects."

TUM has created the Institute to foster research innovation and creativity, especially in applied sciences. Although the Institute is fully committed to excellence, its prime objective is the creation of an advanced knowledge and expertise environment to incubate the new ideas and facilitate their development. In this section, our Focus Groups present the highlights of their research output in 2011. This gives a lot of specific results and highlights, in the many areas in which the Institute is active. Just as important is how the Focus Groups have been able to create the desired knowledge environment.

Last year, we accounted for our results in a "bottom up" fashion, starting from our program in fundamental particle physics, and then moving up the dimension scale to nanophysics, electronics, biophysics, molecular engineering, working with and understanding cells, medical instrumentation, modeling processes, control and design, telecommunications, high-performance computing, statistics, system engineering, energy and mobility, earth science and ecology. This year we present our results in the opposite order, starting from large-scale systems and ending with the fundamental particles, reporting original results in all these areas.

But the fields do not stand isolated. The strength of our knowledge environment lies in the cross-connections, not only those that are made between TUM and the many participating and outstanding research units elsewhere, but especially between the disciplines themselves. From all the accounts a number of crucial cross-fertilizations between the fields emerge, which have highly conditioned some of the excellent results obtained. Here are some pertinent examples that do not claim completeness, and might even be thought motivated by appealing modern issues – but that is the nature of applied research.

Energy and mobility are not only central themes in our modern society, but they also form a strong bond between a number of research areas, all of which contribute major new ideas. Although the future of electromobility may still be thought uncertain due to the many remaining unsolved problems, the TUM-IAS Focus Group "Diesel Reloaded" has been moving full speed toward gauging how global electromobility could be realized. This has tentacles to robotics, smart grids, and networked dynamical systems as represented in the Focus Groups around CoTeSys, and beyond robotics to control, signal processing, and overall system design.

If we want to move to a full e-world, the whole system environment has to be made more distributed and hence more intelligent, from anticipation of driver behavior through adapted supply of electrical energy to clever use of local supplies. In a parallel technological development, TUM's very extensive expertise in catalysis is being combined with new ideas in nanotechnology to devise a novel generation of batteries, energy storage devices, and energy generation systems, as vividly exemplified by the results of the Focus Group on Molecular Aspects of Interface Science.

Our interest in non-conventional or "fat tail" statistics may be thought to go in a very different direction, but it has mobilized massive cooperation within the Institute, mixing mathematicians with practitioners to handle not only regular statistical problems, but also very risky, even catastrophic issues. Amazing is the similarity of methods used in telecommunications, DNA phenotyping, immunology, and preventive medicine, and how the various groups teach each other their approaches. One step further is the development of advanced statistical theory for more realistic analysis of potential catastrophes by our Focus Group on Risk Analysis and Stochastic Modeling, and applications thereof in ground pollution management, water management (Focus Group Engineering Risk Analysis), wind farms, and energy distribution.

Real physical processes are difficult to model sensibly, and the models become very hard to compute at a reasonable level of complexity. Such issues appear in many of our Focus Groups, where the sharing of expertise is almost a question of life and death.

In this area we do report major results, resulting from multidisciplinary collaborations between physicists and engineers and/or medical doctors (depending on the case). One goal is to develop a complete computational model of the human heart enabling cardiac emulation; current models are shown by the Focus Group Advanced Cardiac Mechanics Emulator. The Focus Group Computational Biomechanics focuses on a similar issue, but now concerning bones, and already can claim models of unheard-of accuracy and efficiency. A third direction concerns the combination between combustion problems and statistical mechanics, with a major breakthrough claimed by the Focus Group Nonequilibrium Statistical Mechanics at the Nanoscale concerning the emergence of complexity in nature and how to model it. All these pointed efforts have in the background an internationally very active Focus Group on High-Performance Computing, with new ideas and results in combining strategies from multiple physical domains and handling the complexity of higher dimensions.

The Institute can also boast extensive continuing collaborations between Focus Groups on which it reported before, in particular the groups in Nanoscience, in Cognitive Technology, in Neurophysiology, in Biochemistry, in Medical Instrumentation and in Fundamental Particle Physics – too many to give details. Multidisciplinarity is a hallmark of excellence in technological research. Without it microelectronics, NMR, mobility, energy distribution, security, and sustainable system design would not even have been conceivable.

Systems, Design and Control

Diesel Reloaded

Molecular Aspects in Interface Science

Risk Analysis and Stochastic Modeling

Aircraft Stability and Control

Cognitive Technology

Advanced Computation

Networked Dynamical Systems

Fiber-Optic Communication
and Information Theory

Discrete Optimization

Focus Group **Diesel Reloaded**

Prof. Gernot Spiegelberg | Rudolf Diesel Industry Fellow
Claudia Buitkamp, Ljubo Mercep, Hauke Stähle | Doctoral Candidates
◎ Prof. Alois Knoll, Robotics and Embedded Systems, TUM

Gernot Spiegelberg

Demonstration of Innotruck

Driving into the future

The goal of our project is to implement a holistic approach to electromobility, taking into account the complex interconnections between the vehicle, the infrastructure, and the user's habits.

During 2011 the demonstrator "Innotruck" was being built up, breathing in life to a heavily streamlined vision from the German designer Luigi Colani. Low wind resistance is complemented by a flat vehicle base for a high level of fuel economy. A standard truck with a combustion engine was taken as the basis. Complex modifications to the vehicle chassis, interior, and power network were incrementally introduced with the help of a growing list of industry sponsors. Driving safety is improved with an unconventional high-performance braking system and adaptation to road conditions.

Cooperation with various industrial and academic partners was established in order to yield additional value from common interests. At the Technische Universität München, the Innotruck is a subject of research at the Chair for Automotive Technology (FTM), the Chair for Industrial Design, and the Chair for Robotics and Embedded Systems.

Conception and …

… Construction of the Innotruck Project.
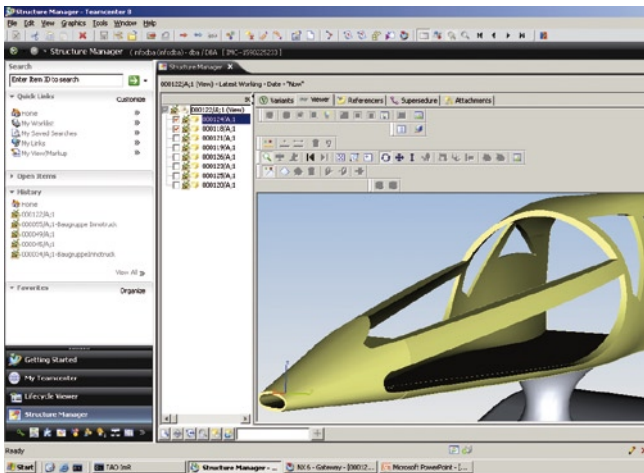
The project was presented to a broad public at the Hannover Messe, the Trade Fair for Commercial Vehicles (Nutzfahrzeugmesse) in Karlsruhe, the Michelin Challenge Bibendum in Berlin, and the International Consumer Electronics Fair (IFA) in Berlin. The Innotruck also took part in the World Advanced Vehicle Expedition Race (WAVE Europe). These public appearances aroused a lot of interest in the research behind the extraordinary design.

Three doctoral candidates performed preliminary research in their respective areas and proposed first implementations on the demonstrator, with emphasis on system architecture, energy management, and the human-machine interface.

The centralized system architecture achieves optimal information flow between all functional units and stands in contrast to the heterogeneous, distributed approach to be found in present-day vehicles. Additional key points include reducing and handling complexity, as well as concepts for safety-critical systems and data fusion.

Energy management and distribution are interwoven with optimal driving strategy. Total energy flow is managed from the very beginning by harnessing solar and wind energy while recouping energy with regenerative brakes and reusing it as long as technically feasible. Electricity is now the Innotruck's primary energy form.

The human-machine interface accepts the driver's wishes in an adaptive and intuitive way. In the first phase we selected redundant sidesticks as the primary input solution. In every consecutive phase we will approach a step closer to the driver's thought pattern, turning a command-executing machine into a mobility partner.

In 2012, the project team will deepen their research and expand the project horizon with interested partners. The work on the demonstrator will enter its final phase, and the first drive-by-wire electrical truck will enter the roads of Germany.

Dr. Julia Kunze-Liebhäuser | Carl von Linde Junior Fellow
Celine Rüdiger, Christoph Traunsteiner | Doctoral Candidates
◉ Prof. Ulrich Stimming, Interfaces and Energy Conversion, TUM

Julia Kunze-Liebhäuser

Electrochemistry research in energy conversion and storage – from fundamentals to nanotechnology applications

Our research focuses on interface science, where we investigate the properties of two adjacent condensed phases. Such properties are important in materials science, energy conversion and storage, catalysis and electrocatalysis as well as for medical applications. Two selected topics are described in detail below.

1. Novel material systems for electrocatalysis and energy storage

Conductive titanium oxycarbide (TiO_xC_y) is studied as a support for catalyst nanoparticles and as an anode material for Li ion intercalation.

Conversion of compact TiO_2 to TiO_xC_y substrates for use in electrocatalysis
In electrocatalysis it is of interest to develop and study stable support materials that can replace carbon supports. A detailed investigation of the carbothermal reduction process in acetylene/argon atmosphere was performed by studying different annealing temperatures between 750 and 1050°C for the conversion of compact TiO_2 films to TiO_xC_y [1]. An increase in charge transfer resistance of the ferri-/ferrocyanide redox couple was observed with increasing annealing temperature. First hydrogen evolution reaction (HER) studies on TiO_xC_y indicate that the electrocatalytic properties directly depend on the chemical, structural, and electronic properties of the surface, since the overpotential of the HER shifts to higher values with increasing annealing temperature [1]. This finding is of great importance for the investigation of conductive and electrochemically stable flat TiO_xC_y films as model supports for electrocatalysis studies.

**Ethanol oxidation on TiO_xC_y–supported Pt nanoparticles**
We studied the electrocatalytic activity of Pt nanoparticles supported on planar TiO_xC_y films toward the ethanol oxidation reaction (EOR) in a half cell electrochemical setup. After EOR, their morphology and activity remain unaltered on TiO_xC_y annealed at 750°C (Pt/TOC750), while the activity undergoes changes on TiO_xC_y annealed at 850°C and higher. Our experiments showed that the electrocatalytic activity of Pt deposited on TiO_xC_y is strongly dependent on the substrate preparation conditions and can be directly related to the conductivity of the support. Pt/TOC750 possessed higher activity compared to Pt deposited on glassy carbon. These findings demonstrate that TiO_xC_y is a potential candidate to replace carbon as a support for use in direct ethanol fuel cells.

TiO$_2$ and TiO$_x$C$_y$–based anode material for lithium ion intercalation

In this case, flat as well as nanotubular films of TiO$_2$ and TiO$_x$C$_y$ were used as anode materials for Li ion intercalation. Fundamental insights into the Li intercalation process were obtained by combining electrochemical experiments with structural, morphological, and chemical characterization of the anode material. Our preliminary Li intercalation experiments conducted on amorphous as well as crystalline TiO$_2$ and TiO$_x$C$_y$ nanotubes revealed very promising storage capacities: reversible charging and discharging capacities of 300 mAh/g and 253 mAh/g, respectively, with capacity retention over 91% between cycles 20 and 100. These findings are very promising, and a more detailed investigation is under way.

2. Self-organized anodic titania nanotubes – fundamentals and applications

Self-organized formation of TiO$_2$ nanotubes on titanium can be induced by a simple electrochemical anodization technique.
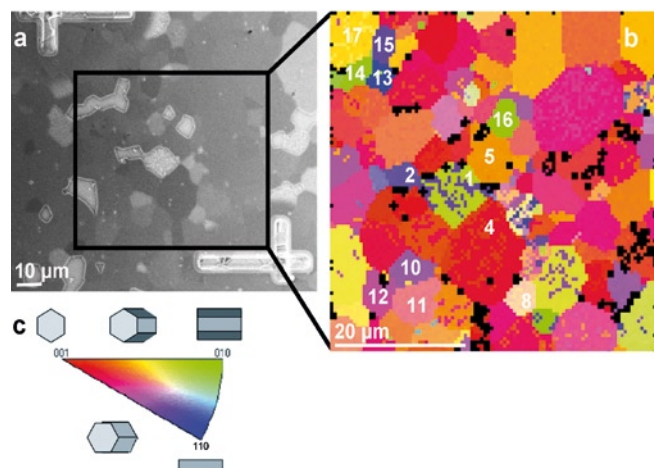
(a) SEM micrograph of the area chosen for EBSD investigations;
(b) Inverse pole figure of the area between the markers shown in
(a); (c) Color legend for (b).

Interdependence of substrate grain orientation and growth characteristics

The influence of the crystallographic orientation of the underlying Ti substrate grains on the growth characteristics of anodic, self-organized TiO$_2$ nanotubes was investigated on electropolished polycrystalline titanium [2]. The preferred formation site for self-organized, amorphous TiO$_2$ nanotubes is Ti(111), whereas no nanotube growth was observed on Ti(001) oriented grains. Instead, a compact oxide film was formed on Ti(001), exhibiting a mixed anatase and rutile nanocrystalline character with a large degree of structural disorder. As an intermediate case, on Ti(010) and Ti(110) oriented grains, nanotubes form but are capped by a strongly chemically etched overlayer. It has been observed that TiO$_2$ nanotubes exclusively form on grains with an orientation that allows for the formation of a thick valve metal oxide. This insight will enable controlled and effective growth over large areas of nanotubular films on titanium and, presumably, on other transition metals that have not shown growth of nanotubular oxides before [2].

Selected Publications:

[1] C. Rüdiger, F. Maglia, S. Leonardi, I.D. Sharp, O. Paschos, and J. Kunze, "Surface Analytical Study of Carbothermally Reduced Titania Films for Electrocatalysis Application," accepted in Electrochim. Acta, February 2012.

[2] S. Leonardi, A. Li Bassi, V. Russo, F. Di Fonzo, O. Paschos, T.M. Murray, H. Efstathiadis, and J. Kunze, "TiO$_2$ nanotubes – interdependence of substrate grain orientation and growth characteristics," *J. Phys. Chem.C*, vol. 116, no. 1, pp. 384–392, 2012.

Focus Group **Molecular Aspects in Interface Science**

Prof. Ulrich Stimming | Carl von Linde Senior Fellow
Norbert Kluy | Doctoral Candidate
◎ Interfaces and Energy Conversion, TUM

Ulrich Stimming

ORR current density
normalized on gold
surface versus nano-
particle size.

Fundamental and applied fuel cell research

The research interest of the group of Prof. Ulrich Stimming is in the field of electro-chemical energy conversion and storage, with a focus on the physics and chemistry at the solid-liquid interface. The different projects range from basic research to the development of suitable membranes for novel fuel cell systems [1].

The use of model catalyst systems can improve the understanding of the influence of different structural, chemical, and morphological properties on catalytic activity by individual variation of single parameters. Gold and platinum nanoparticles with sizes down to ~1 nm were prepared on different planar carbon substrates using electrochemical methods. The catalytic activity toward hydrogen oxidation and evolution reaction did not show any influence of the particle size on the activity [2] – no losses are therefore expected for the use of small nanoparticles in technical applications. In contrast, the oxygen reduction reaction (ORR) on gold nanoparticles was found to be strongly dependent on particle sizes; the activity increases with decreasing particle size (see figure).
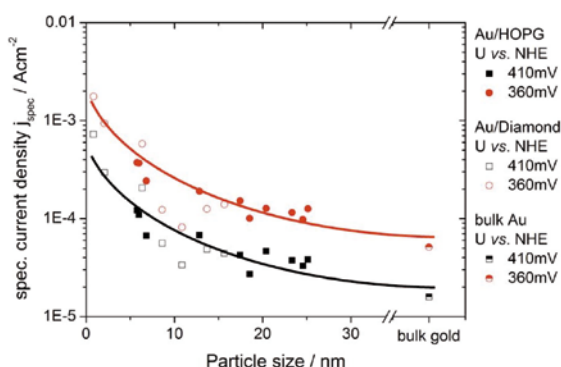
Since electrochemical deposition methods yield randomly distributed nanoparticles with varying size and spacing, the preparation and investigation of ordered nanostructures for efficient electrochemical systems remains a highly challenging task. Therefore, a project linking nanostructuring techniques to electrocatalysis was recently started to quantify the influence of electrode geometry on electrode activity.

On the applied side, direct alcohol fuel cells are moving into the focus of fuel cell research, with bioethanol as a particularly interesting fuel, as it shows the potential to be obtained from renewable sources and provides storage and distribution advantages due to its liquid form. The efficiency that can be reached with the usual low-temperature approach is still too low for commercial application. Higher efficiency can be reached for higher temperatures above 200° C; however, new membrane materials are needed to operate fuel cells at these temperatures. Toward this end, we fabricated and tested novel electrode material based on ammonium polyphosphate (APP).

Selected Publications:

[1] O. Paschos, J. Kunze, U. Stimming, and F. Maglia, "A review on phosphate based, solid state, protonic conductors for intermediate temperature fuel cells," *Journal of Physics – Condensed Matter*, vol. 23, no. 23, 234110, 2011.

[2] T. Brülle, W. Ju, P. Niedermayr, A. Denisenko, O. Paschos, O. Schneider, and U. Stimming, "Size-dependent electrocatalytic activity of gold nanoparticles on HOPG and highly boron-doped diamond surfaces," *Molecules*, vol. 16, no. 12, pp. 10059–10077, 2011.

Focus Group **Risk Analysis and Stochastic Modeling**

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

Claudia Klüppelberg

Robert Stelzer

Richard A. Davis

Mathematical models, turbulence, wind energy, and finance

In the third year of the Focus Group, the first doctoral candidate, Eckhard Schlemm, finished with an excellent thesis consisting of six papers (four of them already accepted for publication in journals) on the estimation of continuous-time linear time series models (see the first issue of TUM-IAS Primary Sources for an overview) and random matrix theory. Moreover, a second doctoral candidate, Martin Moser, submitted a very interesting thesis consisting of three papers (one already published) on extreme value theory results for stochastic processes, which are of high importance for risk modeling. One major achievement is that for the first time conditions have been given so that the powerful concept of functional regular variation can be brought to bear on a certain class of processes heavily used in applications, in particular for certain models describing financial markets. Another important change in the personnel was the appointment of Carl von Linde Junior Fellow Dr. Robert Stelzer, who finished his habilitation in February, 2011, to a full professorship in mathematical finance at Ulm University. Although starting in Ulm on April 1st, Prof. Robert Stelzer remained an active member of the Focus Group.

All doctoral candidates in the Focus Group have been making excellent progress. Florian Ueltzhöfer, advised by Prof. Jean Jacod and Prof. Claudia Klüppelberg, has spent several weeks in Paris working on non-parametric estimation of the semimartingale characteristics from high-frequency data. Such stochastic processes, which are solutions of stochastic differential equations, are of foremost importance in finance, and the new research will have influence on the solution of pricing and hedging problems. Christina Steinkohl made an enjoyable and fruitful three-month visit to Columbia University. Together with Prof. Richard A. Davis and Prof. Claudia Klüppelberg, she has proceeded with the investigation of extreme space-time models. For these models, simulation tools have been developed and statistical estimation methods based on pairwise likelihood theory have been implemented and shown to have nice properties like consistency and asymptotic normality. During Oliver Pfaffel's three-month visit to Columbia University and Hans Fischer Senior Fellow Prof. Richard A. Davis's summer visit to TUM, significant progress was made on the analysis of random matrices with heavy-tailed and dependent entries. The first resulting paper, dealing with the limiting distribution of the eigenvalues of sample covariance matrices when the underlying observations are very heavy-tailed and have a certain non-trivial dependence structure, was submitted. Such results are very helpful in high-dimensional settings where the number of observations is often comparable to the dimensionality and thus traditional statistical approaches fail. Moreover, scientists are confronted with data being heavy-tailed and dependent in many applications, including financial or energy markets and natural disasters.

TUM-IAS postdoctoral researcher Dr. Codina Cotar and Prof. Claudia Klüppelberg have continued to work on two very different projects. In one joint project with Prof. Gero Friesecke (Mathematics Department, TUM), they suggest and develop optimal transport methods for exchange-correlation functionals used in density functional theory.

Martin Moser, Oliver Pfaffel, Eckhard Schlemm Christina Steinkohl, Florian Ueltzhöfer | Doctoral Candidates
Dr. Codina Cotar | Postdoctoral Researcher

They have extended the case of two electrons to an arbitrary number and solved in the semiclassical limit the corresponding optimal transport problem. In their second, ongoing project, Codina and Claudia (jointly with Prof. Hans Föllmer, Emeritus of the Humboldt University Berlin) have been developing spatial risk measures, motivated by statistical mechanics methods and aiming at the modeling of systemic risk.

In cooperation with several collaborators and doctoral candidates, Prof. Claudia Klüppelberg also worked successfully on other projects. The dynamic structure of electricity spot prices is very well modeled by stationary stable non-Gaussian continuous-time linear models (CARMA models). This price model was extended to a market model also including futures, which are traded on the market. Three doctoral candidate projects were completed. The first one was dedicated to the modeling and statistical estimation of dependence between the components of multivariate Lévy processes. Another one solved pricing and hedging problems in electricity markets by combining stochastic models with numerical analysis tools. The third investigated long-memory Lévy-driven processes and their application to model defaultable bonds. In an ongoing doctoral candidate project, stochastic turbulence models with relevance to wind energy production are being investigated. Several data sets of wind speed data at high Reynolds numbers have been analyzed; the analysis supports the new model.

A special highlight was the visit of Prof. Victor Pérez-Abreu, who delivered an excellent short course on Random Matrices and Free Probability that was very well attended by people from many different backgrounds. He gave a detailed introduction into the mathematical theory and the applications, particularly high-dimensional statistics and signal processing (especially in wireless communication networks). During this time he and Prof. Robert Stelzer also finished their work on defining and analyzing a matrix-valued infinitely divisible distribution that has many desirable properties and should be potentially very useful in applications.

Selected Publications: 33

[1] O.E. Barndorff-Nielsen, and R. Stelzer, "Multivariate supOU processes," *Annals of Applied Probability*, vol. 21, no. 1, pp. 140–182, 2011.

[2] M. Moser, and R. Stelzer, "Tail behavior of multivariate Lévy-driven mixed moving average processes and supOU stochastic volatility models," *Advances in Applied Probability*, vol. 43 no. 4, pp. 1109–1135, 2011.

[3] H. Fink, and C. Klüppelberg, "Fractional Lévy driven Ornstein-Uhlenbeck processes and stochastic differential equations," *Bernoulli*, vol. 17 no. 1, pp. 484–506, 2011.

[4] F. Ueltzhöfer, and C. Klüppelberg, "An oracle inequality for penalised projection estimation of Lévy densities from high-frequency observations," *Journal of Nonparametric Statistics*, vol. 23, no. 4, pp. 967–989, 2011.

[5] R.A Davis, and C-Y Yau, "Comments on Pairwise Likelihood in Time Series Models," *Statistica Sinica*, vol. 21, no. 1, pp. 255–277, 2011.

[6] R.A Davis, and L. Song, "Functional Convergence of Stochastic Integrals with Application to Statistical Inference," *Stochastic Processes and Their Applications*, vol. 122, no. issue 3, pp. 725–757, 2012.
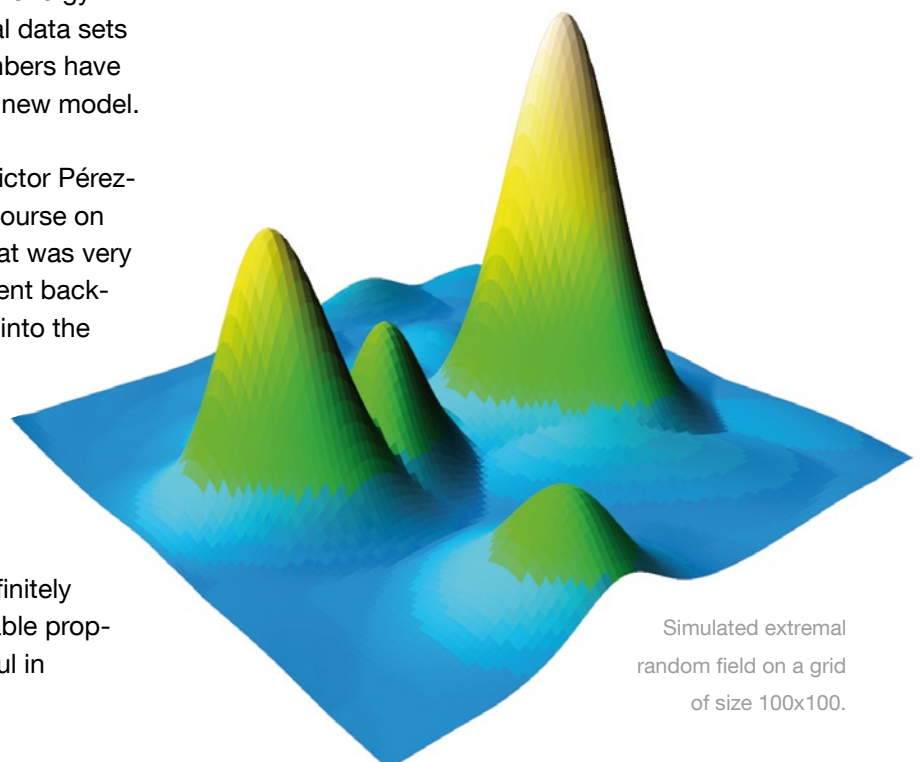
Simulated extremal random field on a grid of size 100x100.

Focus Group **Aircraft Stability and Control**

Dr. Matthias Heller | Rudolf Diesel Industry Fellow
Markus Geiser | Doctoral Candidate
◉ Prof. Florian Holzapfel, Flight System Dynamics, TUM

Matthias Heller

## Steps guiding autonomous flying systems toward civil applications

The main objective of the TUM-IAS Focus Group Aircraft Stability and Control is to investigate new techniques in the field of dynamics, performance, stability, and control of innovative autonomous flight systems. Within the effort to realize the vision of autonomously flying unmanned aerial vehicles (UAVs) as valuable assets for a broad range of applications, new degrees of freedom for configuration designs enabled by the absence of a human pilot can be utilized to optimize the mission profiles and performance.

However, due to complex high-level objectives, the resulting configurations pose novel challenges, especially regarding the flight control system. When operating such an UAV in normal (civil) airspace, certifiable control systems featuring guaranteed stability, robustness, and performance properties represent a key technology and consequently have to satisfy the rigid requirements on safety, accuracy, availability, and survivability that are common in aviation.

The dedicated lead project *SAGITTA* will culminate in 2014 in the maiden flight of an advanced multidisciplinary research demonstrator, a low observability flying wing UAV (see figure 1). This project embodies the vision described above and creates a fruitful and close research collaboration between CASSIDIAN and TUM-IAS involving a broad range of additional outstanding partners.

In contrast to the majority of current aircraft, the *SAGITTA* demonstrator configuration exhibits serious inherent stability and control deficiencies, which pose manifold challenges. In order to cope with these characteristics and in particular to ensure the stabilization and maneuvering capability as a major premise for the design freeze and subsequent control system development, sophisticated flight dynamics studies (w.r.t. stabilization and controllability) were conducted. One key issue, a novel assessment technique of the lateral-directional stabilization capability in early design stages, is depicted in figure 2. Respective results form the fundamental basis for the crucial control surface and actuator sizing.

However, the mere stabilization capability is not sufficient for safe operation of the UAV. Rather, the aircraft actually has to be stabilized and guided along its mission by a suitable controller to perform safely and successfully also in the case of faults and failures. One promising approach to design a safe and robust flight controller is represented by the innovative L1 adaptive control theory, which is one of the alternatives to be considered by the Focus Group for the *SAGITTA* demonstrator. This control approach is qualified to cope with model uncertainties and, even more important, with faults or damages of the aircraft in a deterministic and robust way. Hence, it is assured that failures of the airframe will only result in graceful degradations of the flight performance and thus allow finishing the mission safely as long as the configuration is physically controllable and aerodynamically capable to fly.

SAGITTA Demonstrator: Basic Characteristic Data

Mass: 100 kg
Wingspan: 3 m
Range: 300 km
Endurance: 90 min
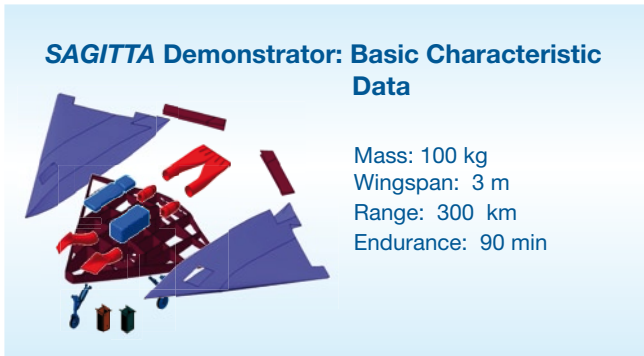
1 | Multidisciplinary *SAGITTA* research demonstrator representing a low observability flying wing (UAV).
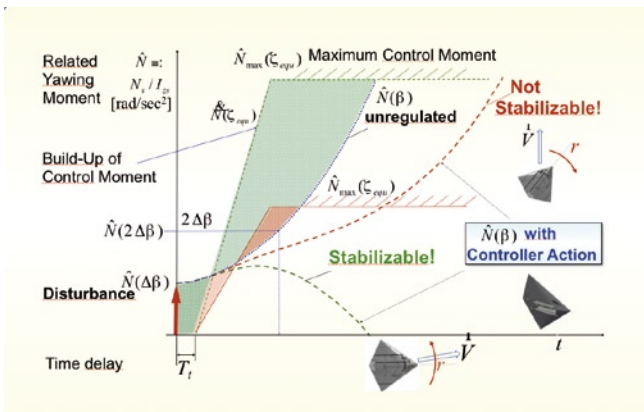
2 | Assessment technique for lateral-directional stabilization capability in early design phases; applied to *SAGITTA* demonstrator.

Control System Design, Analysis & Safety Assessment
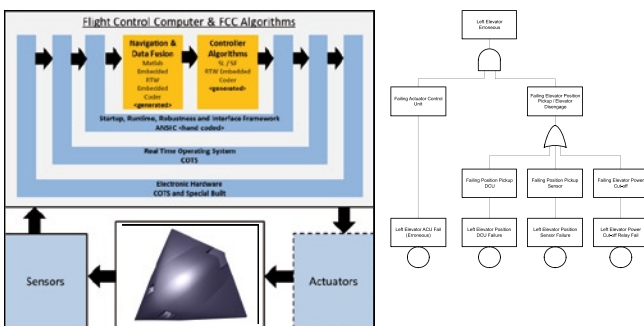
3 | Preliminary (complex) multidisciplinary control system design accompanied by associated safety assessment accomplished for *SAGITTA* demonstrator.

The complex multidisciplinary system synthesis of the flight management system comprising the sophisticated overall autonomous flight guidance, navigation, and control algorithms developed for the *SAGITTA* demonstrator is a further challenge of the Focus Group. To provide a basis for implementing the innovative control algorithms we have developed, a preliminary (hardware) system design, together with the associated safety assessment, was accomplished (figure 3).

Furthermore, in order to strengthen networking and to support exchange of outstanding knowledge, two very interesting and well appreciated international workshops were organized by the Focus Group in summer 2011: the TUM-IAS workshop on "L1 Adaptive Control and its Transition in Practice," held by Dr. Naira Hovakimyan (University of Illinois at Urbana-Champaign), and the workshop on "Handling Qualities Research in Russia," featuring Prof. Alexander Efremov from the Moscow Aviation Institute (MAI).

Selected Publications:

[1] M. Heller, F. Schuck, L. Peter and F. Holzapfel, "Hybrid Control System for a Future Small Aircraft," in *AIAA Guidance, Navigation, and Control Conf.*, Portland, OR, pp. 7324–7341, 2011.

[2] M. Geiser, E. Xargay, N. Hovakimyan, T. Bierling, and F. Holzapfel, "L1 Adaptive Augmented Dynamic Inversion Controller for a High Agility UAV," in *AIAA Guidance, Navigation, and Control Conf.*, Portland, OR, 2011.

Focus Group **Cognitive Technology**

Dr. Alexandra Kirsch | Carl von Linde Junior Fellow
Dr. Kolja Kühnlenz | Carl von Linde Junior Fellow
Prof. Dongheui Lee | Carl von Linde Junior Fellow
Dr. Angelika Peer | Carl von Linde Junior Fellow

Alexandra Kirsch

Kolja Kühnlenz

Dongheui Lee

Readying robots for interactive roles in human environments

Our Focus Group aims to enable interactive robots for real-world applications, capable of autonomous action and close (co-)operation in human-centered environments. For this purpose we do research on various levels, from fundamental interdisciplinary aspects in visual perception and human factors to action planning and control strategies, complex integrated systems, and application scenarios. Significant progress was made in the following areas.

To master the complexity of the real world, artificial cognitive systems need to understand and reason about the world in abstract terms. This requires the capability to abstract from raw sensor readings, to construct abstracted models, and to map abstract plans to concrete control actions. In our work we aim to provide these capabilities, for example, to robots that need to understand the structural properties of their operating environment. To explicitly address the uncertainty inherent in real application scenarios, we employ probabilistic models and reasoning methods. On the basis of these models and methods, our robots now represent their possibly partial understanding of, e.g., an indoor floor plan as a belief distribution over possible semantic interpretations of their sensor readings. Besides being a mandatory prerequisite for robust operation under realistic conditions, this capability is also highly valuable for human-robot communication.

Humans tend to interact socially with technology. As robots are gradually entering our daily lives, an essential issue is to make robots aware of this human factor. In order to make communication between humans and robots more natural and intuitive, we are designing mathematical models of social interaction in collaboration with psychologists. Results are quantitative and dynamic descriptions of socially relevant parameters such as autonomy, security, and emotions, which we use for the design of control mechanisms steering the interaction to mutually acceptable social and task-related goals. This way we could achieve a higher subjective performance as well as empathy toward the robots. Such advances could bring the benefits of more fluent and easy interaction into our cooperation with robots in daily life.

Moving through the world is a basic task for assistive robots. Situations in which humans move in the same environment are particularly challenging, not only to guarantee safety, but also to move in a way that is intuitively understood by users. In an interdisciplinary effort we compared human strategies for avoiding other moving humans with the navigation behavior of robots. It turns out that humans seem to employ completely different strategies. Moreover, the behavior is difficult to explain with global optimization strategies and thus seems to be highly context-dependent. We have proposed a robot navigation strategy that imitates human behavior and are developing evaluation metrics to ensure that the robot behavior will be well understood and accepted.
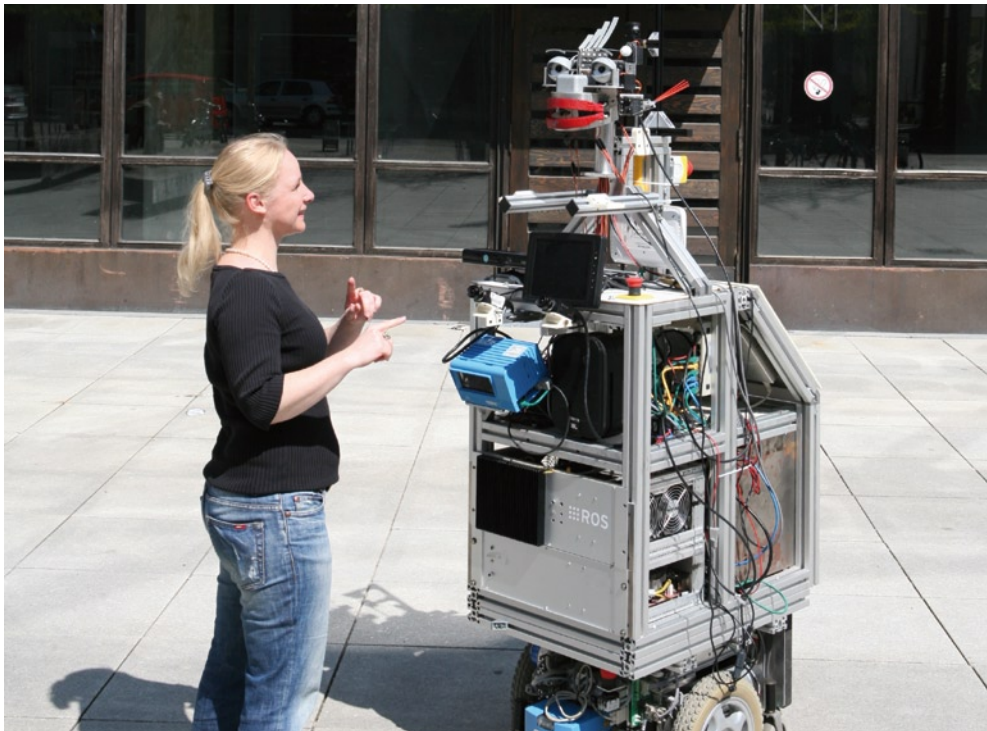
Dr. Georg von Wichert | Rudolf Diesel Industry Fellow
Dr. Dirk Wollherr | Carl von Linde Junior Fellow
Barbara Gonsior, Michael Karg, Christina Lichtenthäler, Bernhard Weber, Liu Ziyuan | Doctoral Candidates
◎ Prof. Martin Buss, Automatic Control Engineering, TUM
◎ Prof. Michael Beetz, Computer Science, TUM

Researcher Barbara Gonsior communicates socially with the Interactive Urban Robot (IURO).

Angelika Peer

Georg von Wichert

Dirk Wollherr

Natural and intuitive physical interaction is considered one prerequisite for future robotic systems that are supposed to share their working space with humans and closely collaborate with them. Typical application fields range from physical assistance to skill training, rehabilitation, and social interaction. Algorithms for intention recognition, joint decision making, path planning, and adaptation are required to develop an interactive and proactive haptic interaction partner. To realize such behavior, we adopted an experimentally driven approach that uses human-human interaction as a reference, analyzes and models observed behavior, and finally transfers gained knowledge to human-robot interaction. In line with this approach, our investigations were oriented to two main targets: computational models underlying haptic coordination and haptic shared decision making, and large-area, multi-point haptic interactions.

Programming by demonstration provides an efficient way for a robot to learn new skills through human guidance, potentially saving time and reducing costs. The inference mechanism of imitation learning can be applied not only to the robot's free body motion, but also to manipulation tasks (including grasping skills) and human-robot cooperation tasks. In the context of autonomous robotic learning, unsupervised incremental learning techniques for segmentation and clustering

are applied to enhance human-robot cooperation tasks over time, with the special focus on predicting the human partner's behavior. Iterative on-line learning can further improve the learned skills via kinesthetic coaching, which leads to eliminating kinematic mapping errors and learning synchronized whole body motions.

Systems that are to assist humans will not always possess all the information required to fulfill their tasks. A highly desirable yet missing feature of today's robots is the ability to assess their own knowledge with regard to gaps and to retrieve missing information from other agents, including humans. As a first step toward generic information acquisition from humans, we are focusing on interaction with humans to retrieve route descriptions and reason about them. While other factors, such as approaching people and establishing contact, play an important role, the actual human-robot communication is the central aspect of retrieving the missing information. 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. A central ability of the dialogue system is to identify missing information and pose follow-up inquiries, guiding the human to provide the missing information. Structured interaction patterns allow the robot to react to human input in order to clarify ambiguities in human-provided information.

Selected Publications:

[1] D. Lee and C. Ott, "Incremental Kinesthetic Teaching of Motion Primitives Using the Motion Refinement Tube," *Autonomous Robots*, vol. 31, no. 2, pp. 115–131, 2011.

[2] J.R. Medina Hernández, M. Lawitzky, A. Mörtl, D. Lee, and S. Hirche, "An Experience-Driven Robotic Assistant Acquiring Human Knowledge to Improve Haptic Cooperation," in *IEEE/RSJ International Conference on Intelligent Robots and Systems*, San Francisco, CA, pp. 2416–2422, 2011.

[3] C. Lichtenthäler, T. Lorenz, and A. Kirsch, "Towards a Legibility Metric: How to Measure the Perceived Value of a Robot," in *International Conf. on Social Robotics, Work-In-Progress-Track*, Amsterdam, Netherlands, 2011.

[4] Z. Liu, D. Chen, and G. von Wichert, "Online Semantic Exploration of Indoor Maps," in *IEEE International Conference on Robotics and Automation* (ICRA), 2012, to be published.

[5] B. Gonsior, S. Sosnowski, C. Mayer, J. Blume, B. Radig, D. Wollherr and K. Kühnlenz, "Improving Aspects of Empathy and Subjective Performance for HRI through Mirroring Facial Expressions," in *20th IEEE International Symp. on Robot and Human Interactive Communication (RO-MAN)*, Atlanta, GA, pp. 350–356, 2011.

[6] B. Gonsior, C. Landsiedel, N. Mirnig, S. Sosnowski , E. Strasser, J. Złotowski, M. Buss, K. Kühnlenz, M. Tscheligi, A. Weiss, and D. Wollherr, "Impacts of Multimodal Feedback on Efficiency of Proactive Information Retrieval from Task-Related HRI," *Journal of Advanced Computational Intelligence and Intelligent Informatics*, 2012, to be published.

Focus Group **Cognitive Technology**

Prof. Mandayam A. Srinivasan | Hans Fischer Senior Fellow
Andreas Schmid | Doctoral Candidate
◎ Prof. Martin Buss, Automatic Control Engineering, TUM

Telehaptics for micro/nanoassembly

Mandayam A. Srinivasan

Since the beginning of the project, our goal has been to develop tools and methods that enable human operators to interact with microstructures as easily and intuitively as possible through the inclusion of touch feedback. Over the last year, we were able to achieve progress on three fronts:

Examination of Volvox colony with microforce probe and suction pipette.

Increasing usability and functionality through hardware extension: Our haptic-controlled micromanipulation system now features bimanual operation in the usage of force-reflecting grippers and probes. This allows intuitive examination and characterization of micron-scale structures by pulling, pushing, and squeezing in three dimensions.

Cell characterization: Using our manipulation setup we are able to capture, fix, and probe single cells or small cell aggregates. Our recent focus has been on probing Volvox, a colony-forming green alga (figure).

Virtual reality interfaces: Physical interaction with micron-sized objects significantly differs from that on a macroscopic scale, since surface and short distance forces dominate as mass decreases with shrinking object size. The modeling of the relevant forces and their exploration with interactive virtual reality techniques help us to better understand scaling effects and to predict micro-object behavior. This tool can also serve educational and training purposes.

We thank Dr. Stefan Thalhammer's group at the Helmholtz Center Munich and the Institute of Automatic Control Engineering at TUM for continued cooperation and support.

Selected Publication:

[1] A. Schmid, R. Yechangunja, S. Thalhammer, and M.A. Srinivasan, "Human-operated 3D micro-manipulator with haptic feedback," *Proceedings of the IEEE Haptics Symposium,* Vancouver, Canada, pp. 517-522, 2012.

Focus Group **Advanced Computation**

Prof. Matthew Campbell | Hans Fischer Senior Fellow
Amir Hooshmand, Corinna Königseder | Doctoral Candidates
◎ Prof. Kristina Shea, Product Development, TUM

Matthew Campbell

Automatically generated designs through generative grammars

Numerical optimization requires that a user specify the problem as a fixed set of variables to be solved. What if the number of variables is unknown? What if the basic shape or configuration to be designed is unknown? The approach taken by Prof. Matthew Campbell's research group is to encode the basic constraints and building blocks of the design problem in question as a set of generative grammar rules. Through such rules, a computational system can explore a wider variety of solutions to problems that are too complex or tedious for humans to solve. The team developed the generative grammar concept and has applied it to three domains: photovoltaic (PV) solar arrays, gear train design, and general shape optimization.

In the photovoltaic solar array problem, the computer is tasked with designing an optimal network of solar panels to maximize power under a variety of sunlight conditions. The engineering knowledge is represented using a graph to describe the design of the PV array and a small set of graph grammar rules (e.g., to add, delete, or connect solar cells on a grid) that define how the graph can be altered. The layout of the PV array is changed through automatic selection and application of these rules. Each candidate array is then evaluated in terms of its efficiency under various lighting conditions. We compared candidate solutions to those generated by a multi-objective genetic algorithm. We found that while the two approaches produced comparable results, encoding the correct connectivity constraints for the PV array was much more complex in the genetic algorithm than in the grammar rules. Current efforts are focused on making search with the grammar rules more efficient by learning beneficial combinations of rules.

The second problem the team addressed is automated synthesis of gear trains. Designing a gear train can be a very time-consuming task that has various tedious steps, such as calculating gear stresses. As a result, the problem domain is an excellent candidate for automated synthesis. In order to define a generative grammar for gear train design, a graph formalism is defined to represent the shafts and gears as well as their connections. Graph grammar rules have been implemented to add, delete, or change this graph both topologically (e.g., number of gears and connectivity) and parametrically (e.g., number of gear teeth and positions). Current research is investigating how to organize the search among these topological and parametrical changes.

Finally, the team concentrates on combining shape grammars with conventional simulation and analysis methods. Existing shape optimization methods require thousands of design variables to define even simple two-dimensional shapes, yet user-defined engineering parts are defined by small sets of control points that define smooth and manufacturable surfaces (i.e., are defined as boundary representations). Therefore, the team is seeking a novel approach to optimal shape synthesis that takes advantage of the variety and ease of adding constraints within a shape grammar, with the ability to optimize designs for such criteria as heat transfer or stress analysis.

Selected Publications:

[1] C. Königseder, K. Shea, and M. I. Campbell, "Comparing A Graph-Grammar Approach To Genetic Algorithms For Computational Synthesis Of PV Arrays," in *22nd CIRP Design Conf.*, Bangalore, India, 2012.

[2] M. Kumar, M. I. Campbell, C. Königseder, and K. Shea, "Rule Based Stochastic Tree Search," in *Fifth Int. Conf. on Design Computing and Cognition,* College Station*, Texas, 2012, submitted for publication.
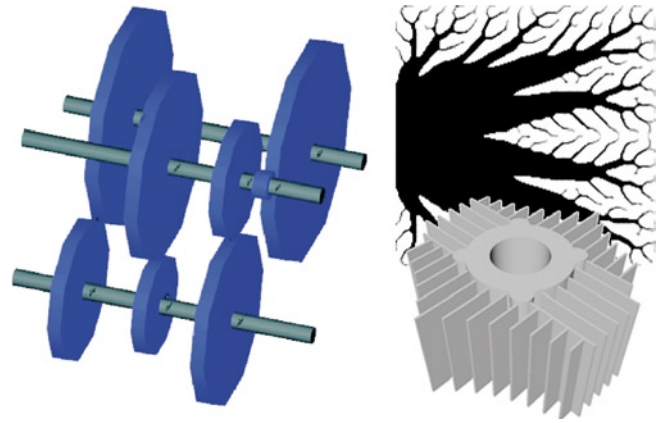
A gear train is shown on the left that has been automatically synthesized using a graph grammar technique. On the upper right a heat fin is defined using traditional topology optimization techniques, which require thousands of design variables and can produce a shape too complex for manufacturing. The picture on the bottom right shows a heat fin that is defined by a shape grammar.
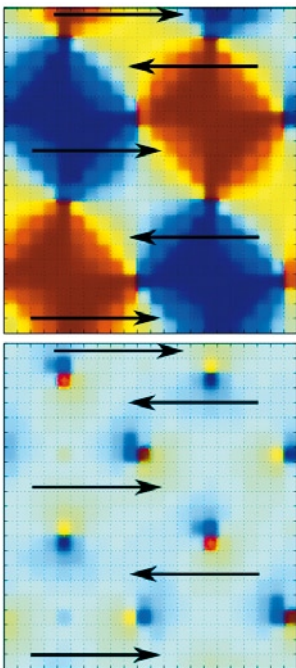
Focus Group **Networked Dynamical Systems**

Dr. Dragan Obradovic | Rudolf Diesel Industry Fellow
Herbert Mangesius | Doctoral Candidate
◎ Prof. Sandra Hirche, Automatic Control Engineering, TUM

Dragan Obradovic

Novel model for the dynamics of the power grid: A Kuramoto-type system with spatial embedding

The non-stationary behavior of the electric power grid is still not fully understood but has a tremendous influence on its operation; in worst-case scenarios, this behavior may cause blackouts. Without appropriate control measures, detrimental effects are expected to become even worse in future power grids with a high penetration of renewables. Therefore it is important to understand the dynamics of the power grid and the factors that influence it. The dynamics of the grid primarily consists of the dynamics of the generators, which are coupled through the transmission lines. The stability of local variables such as voltages, or of global variables such as frequency in the AC networks, is obtained by applying local control actions at the generators. The resulting closed-loop system exhibits both temporal and spatial dynamic phenomena resulting in traveling wave fronts. The interaction of local control with global coupling can cause dynamically induced instabilities as a matter of resonance between spatial and temporal waveforms. We have developed a novel model based on classic coupled oscillator models of Kuramoto-type, with an additional spatial embedding via a state-dependent coupling kernel capable of reproducing such effects [1]. Such models are of high importance not only because of their explanatory power and for the analysis of influential factors, but also for the design of novel distributed control mechanisms for the future electric power grid. As a next step, we are targeting the quantitative characterization of the equilibrium state and the transient behavior.

Illustration of the temporal-spatial dynamics of the Kuramoto-type model with spatial embedding: oscillator phases (top) and local coupling strength (bottom); arrows indicate the direction of traveling waves.

Selected Publications:

[1] H. Mangesius, S. Hirche, D. Obradovic, "On Signaling and Invariance Principles Determining Global Solution Properties of Oscillator Networks and its Approximations Illustrated on Electric Power Grid Dynamics," *American Control Conference*, 2012, to be published.

[2] M. Roozbehani, M. Rinehart, M. A. Dahleh, S. K. Mitter, D. Obradovic, H. Mangesius, "Analysis of Competitive Electricity Markets under a New Model of Real-Time Retail Pricing," *8th International Conference on the European Energy Market*, 2011.

Focus Group **Networked Dynamical Systems**

Prof. Anuradha M. Annaswamy | Hans Fischer Senior Fellow
Arman Kiani, Harald Voit | Doctoral Candidates
◎ Prof. Sandra Hirche, Automatic Control Engineering, TUM

Research toward smarter systems for energy applications

Anuradha M. Annaswamy

Our ultimate research goal is the analysis and synthesis of smart technical systems with applications to energy systems. During the past year, we investigated (i) the dynamics of wholesale energy markets in smart grids and the effect of renewable energy sources, (ii) state estimation in distributed power systems, and (iii) 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 the need to integrate renewable energy sources, the availability of information via advanced metering and communication, and an emerging policy of a demand structure that is intertwined with pricing. Our effort during 2011 focused on development of a fundamental dynamic model that captures the interactions between generation, demand, pricing, and congestion [1]. This dynamic model also lays the foundation for analysis and design of a robust energy market and enables the study of the effects of intermittency in renewable energy resources (RERs), mitigation of the integration cost of the RERs using the notion of demand desponse, and the role of information, obtained using smart meters, with a delay. Integration of the market framework into automatic generation control, a common procedure used in power systems, is proposed using a novel hierarchical strategy.

While the presence of RERs leads to better sustainability, they can also pose stability problems in system operation. Distributed state estimation is a central tool in alleviating such stability problems. We have proposed a new method of observability that allows a better estimate of the system state and therefore better management of the overall distribution management systems in a power grid [1].

Any physical system with a rudimentary level of complexity includes interaction with a cyber structure that helps, monitors, predicts, or manages its function. As the level of complexity increases, this interaction between the cyber and physical components needs to be 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 that combines adaptive switching controllers with a multimodal real-time system, and this effort has yielded promising results [2]. Our next set of steps is developing formal methods that combine control in engineering and real-time systems in computer science with validation in an automotive system, which is a typical example of a distributed embedded system.

Selected Publications:

[1] A. Kiani and A.M. Annaswamy, "Wholesale Energy Market in a Smart Grid: Dynamic modeling, and stability," in *IEEE Conference on Decision and Control (CDC)*, Orlando, FL, 2011.

[2] H. Voit, A.M. Annaswamy, R. Schneider, D. Goswami, and S. Chakraborty, "Adaptive Switching Controllers for Systems with Hybrid Communication Protocols," in *American Control Conference*, Montreal, Canada, 2012, to be published.

Focus Group Fiber-Optic Communication and Information Theory

Prof. Frank Kschischang | Hans Fischer Senior Fellow
◉ Prof. Gerhard Kramer, Communications Engineering, TUM

## Powerful error-correcting codes for fiber channels

Advances in physics – leading to the invention of the laser, low-loss optical fiber, and the optical amplifier – have driven rapid growth in worldwide data communications. Yet traffic demand continues to grow year after year because of data-hungry technologies such as, for example, smart phones and on-line video games. As a result, industry needs to push optical technology to its limits, to maximize energy and spectral efficiency and to minimize cost. System designers have started to use the most advanced techniques from information and coding theory, in particular long and powerful error-correcting codes.

The ITU Telecommunication Standardization Sector (ITU-T) has standardized several powerful codes for optical networks. One of the most successful approaches is called a "product code" because of the way it combines two basic codes to extract excellent performance with reasonable encoding and decoding complexity. In our work, we have developed a new class of energy-efficient error-correcting codes called staircase codes, whose construction combines ideas from product codes and the newest research breakthroughs on "coupled codes." In particular, a basic product code is copied many times and connected in a staircase-like fashion to further improve the error-correction performance without sacrificing encoding and decoding simplicity. We use this idea to propose an ITU-T standard-compatible staircase code. Our analysis and simulations show that this code has an extremely low "error floor" with a bit-error probability of 4×10^{-21}. Hardware-based simulations show that the code requires 10 times less energy than systems without coding, and that the code improves on the best ITU-T codes by a reasonable margin. The code operates very close to the ultimate "Shannon limit," so that little further improvement is possible.

The above work is indicative of the type of research that we plan for my Fellowship at the TUM-IAS. We plan to investigate the capacity of new fiber structures, understand what types of signal-processing algorithms are needed to approach the capacity, and design codes of reasonable complexity that are well suited for optical transmission. An important requirement for making progress in this work is to take an interdisciplinary approach, by working together with optical physicists who understand how light propagates in optical fibers.

Selected Publications:

[1] B. P. Smith, A. Farhood, A. Hunt, F. R. Kschischang, and J. Lodge, "Staircase Codes: FEC for 100 Gb/s OTN," *IEEE/OSA J. of Lightwave Technology*, vol. 30, no. 1, pp. 110–117, 2012.

[2] B. P. Smith and F. R. Kschischang, "A Pragmatic Coded Modulation Scheme for High-Spectral-Efficiency Fiber-Optic Communications," *IEEE/OSA J. Lightwave Techn.*, to be published.
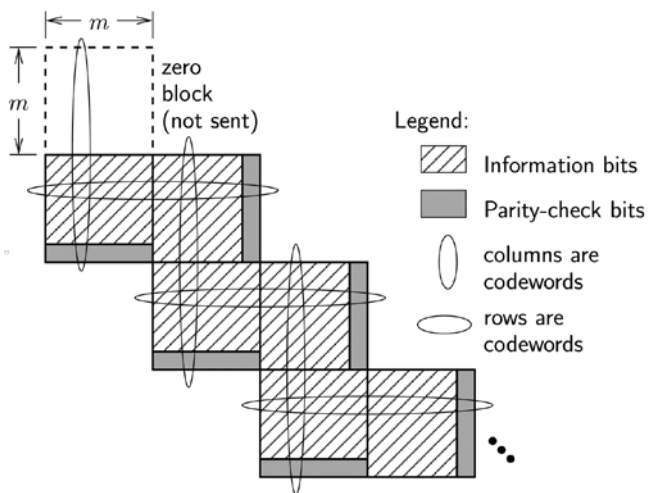
The "staircase" visualization of staircase codes. The squares are m x m binary matrices whose rows and columns indicate which bits are included in parity checks.

Frank Kschischang

is a Professor of Electrical and Computer Engineering at the University of Toronto, where he has been a faculty member since 1991. During 1997-98, he was a visiting scientist at MIT, Cambridge, MA, and in 2005 he was a visiting professor at the ETH, Zurich. His research interests are focused primarily on the area of channel coding techniques, applied to wireline, wireless, and optical communication systems and networks. In 1999 he was a recipient of the Ontario Premier's Excellence Research Award and in 2001 (renewed in 2008) he was awarded the Tier I Canada Research Chair in Communication Algorithms at the University of Toronto. In 2010 he was awarded the Killam Research Fellowship by the Canada Council for the Arts, and the University of Toronto Faculty Award of Excellence.

Jointly with Ralf Koetter he received the 2010 Communications Society and Information Theory Society Joint Paper Award. Prof. Kschischang has received a number of teaching awards at the University of Toronto, including the Applied Science and Engineering Faculty Teaching Award. He is a Fellow of IEEE and of the Engineering Institute of Canada. During 1997–2000, he served as an Associate Editor for Coding Theory for the IEEE Transactions on Information Theory. He also served as technical program co-chair for the 2004 IEEE International Symposium on Information Theory (ISIT), Chicago, and as general co-chair for ISIT 2008, Toronto. He served as the 2010 President of the IEEE Information Theory Society.

Focus Group **Discrete Optimization**

Prof. Andreas S. Schulz | Honorary Hans Fischer Senior Fellow, Alexander von Humboldt Awardee

◎ Prof. Peter Gritzmann, Applied Geometry and Discrete Mathematics, TUM

Discrete Optimization

Andreas S. Schulz

I had the privilege of visiting the TUM-IAS for five months in 2011, at the kind invitation of Prof. Gritzmann. Thanks to the extraordinarily helpful and dedicated staff at TUM-IAS, the unique atmosphere of the building that is conducive to intensive research, and the countless discussions with Prof. Gritzmann and the members of his group, I had an exceptionally pleasant, productive and interesting stay. Below is a summary of two projects that I worked on while I was visiting the TUM-IAS, which are exemplary of my research interests.
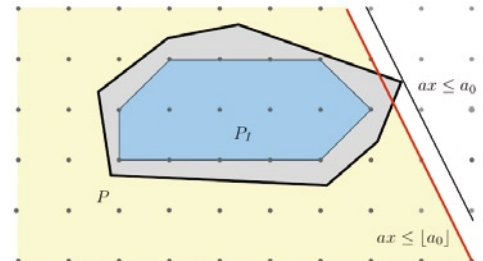
Illustration of a Gomory-Chvátal cut $ax \leq \lfloor a_0 \rfloor$ which helps to define a tighter approximation of the convex hull P_I of integer points inside P than that given by the polyhedron P itself.

Cutting-plane methods are among the most successful techniques for solving discrete optimization problems in practice. Cutting planes also give rise to a rich theory. A Gomory-Chvátal cut for a polyhedron P is an inequality of the form $ax \leq \lfloor a_0 \rfloor$, where a is an integral vector and the half-space defined by $ax \leq a_0$ contains P. The Gomory-Chvátal closure of P is the intersection of all half-spaces defined by such cuts. Even though this closure is defined by an infinite number of half-spaces, some 30 years ago it was shown that the closure of a *rational* polyhedron is again a polyhedron. However, it remained open whether the closure of a *non-rational* polytope is a polytope. J. Dunkel and I proved that this is the case indeed: The closure of a non-rational polytope can be described by a finite set of rational inequalities [1]. Our proof uses ideas from convex analysis, polyhedral theory, and the geometry of numbers.

The joint replenishment problem (JRP) is a widely used model in inventory theory for coordinating the replenishment of a collection of goods so that continuous demand is satisfied at minimum overall ordering and holding costs. The computational complexity of this problem was open for several decades. C. Telha and I showed that finding an optimal replenishment policy is at least as hard as integer factorization, even when demand rates are constant [2]. This result provides the first theoretical evidence that the JRP may have no polynomial-time algorithm. Although integer factorization is unlikely to be NP-hard, it is widely believed to be outside the complexity class P. In fact, this belief supports the hypothesis that RSA and other cryptographic systems are secure. Our result is the first to explain the complexity of any optimization problem in terms of that of integer factorization.

Selected Publications:

[1] J. Dunkel and A. S. Schulz, "The Gomory-Chvátal closure of a non-rational polytope is a rational polytope," *MIT Working Paper*, May 2011.

[2] A. S. Schulz and C. Telha, "Approximation algorithms and hardness results for the joint replenishment problem with constant demands," in *Lecture Notes in Computer Science*, vol. 6942, pp. 628–639, 2011.

New Computing Paradigms

Advanced Cardiac Mechanics Emulator
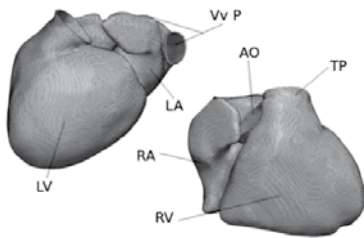
High-Performance Computing

Computational Biomechanics

Advanced Stability Analysis

Nonequilibrium Statistical Mechanics
at the Nanoscale

Advanced Computation

Focus Group **Advanced Cardiac Mechanics Emulator**

Prof. Michael Ortiz | Hans Fischer Senior Fellow
Andreas Nagler | Doctoral Candidate
◉ Prof. Wolfgang A. Wall, Computational Mechanics, TUM

Michael Ortiz

1 | Right and left views of the ACME FE-Grid. (RV: right ventricle; RA: right atrium; TP: truncus pulmonalis; LV: left ventricle; LA: left atrium; AO: aorta: Vv P: vena pulmonalis; cava inferior and superior are not shown).

The advanced cardiac mechanics emulator

The Advanced Cardiac Mechanics Emulator (ACME) is a collaborative effort of TUM, UCLA, and Caltech whose chief objective is the development of a complete computational model of the human heart, enabling 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 computing.

The first challenge in carrying out this program is to model the geometry of the human heart. To date, most heart geometrical modeling has focused solely on ventricular geometry extracted from *ex vivo* data and, consequently, there is a paucity of solid models that account for all four chambers on the basis of *in vivo* data. We have addressed this gap by using *in vivo* ECG-gated computer tomography (CT) to construct a finite-element (FE) discretization. The resulting solid geometry is segmented with the aid of image-processing techniques, and a stereolithography is generated and smoothed in order to eliminate noise and sampling artifacts. The ACME full-heart FE mesh generated to date contains in the order of 850,000 elements (figure 1).

To simulate the physiology of the heart, a model of the myocardium histology, specifically the intricate distribution and orientation of muscle fibers whose coordinated contraction results in the systole of the heart, needs to be overlaid on top of the solid model. We construct our fiber-orientation model from human cardiac diffusion-tensor magnetic resonance imaging (DT-MRI) data. In general, the geometry derived automatically from the MRI data needs to be modified by hand on the basis of expert judgment, to eliminate artifacts and ensure physiologically meaningful geometries. The current ACME fiber-orientation model is shown in figure 2. The geometry and physiology of the human heart valves are particularly complex and require special attention. These valves are: the two atrioventricular (AV) valves, the mitral valve, and the tricuspid valve, which connect the atria and the ventricles; and the two semilunar (SL) valves, the aortic valve, and the pulmonary valve, which connect to the arteries that exit the heart. The present ACME myocardium model is modular and includes geometrically precise attachments for the insertion of individual valve models (figure 3). Ongoing work to model the valves, including the flaps and their fibrous structure, the chordae tendineae and the papillary muscles, relies on ex vivo data and open-literature analytical models.

Other aspects of the project that are in progress at present are the passive constitutive modeling of the heart muscle, the modeling of the electrophysiology of the heart, and the modeling of hemodynamics. We specifically adopt the model of Holzapfel (2009) for purposes of simulating the passive response of the heart muscle. We extend the model to account for active contraction by recourse to the time-honored method of eigendeformations.

2 | Detailed view of ACME
ventricular fiber organization.
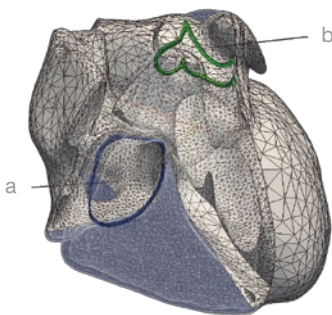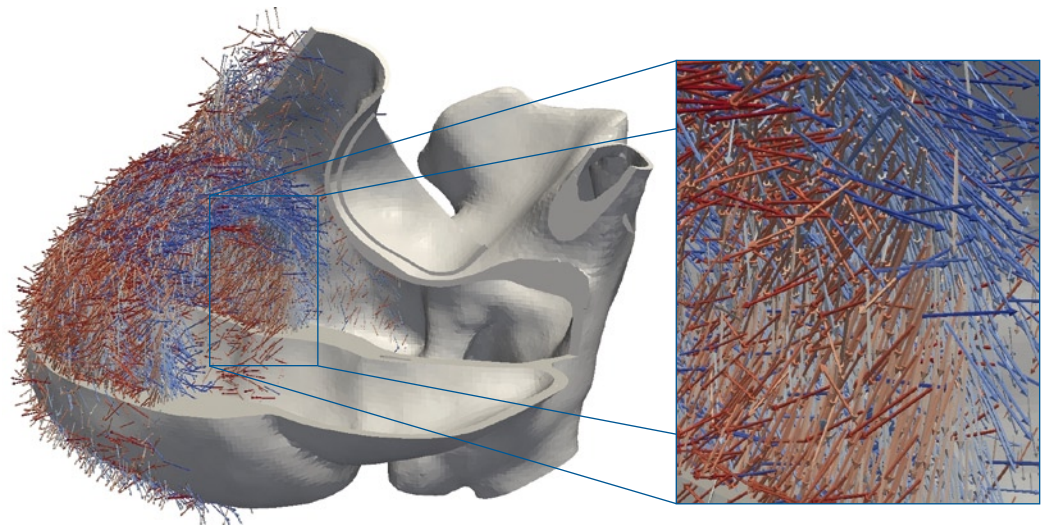
3 | Attachments of pulmonary
and tricuspic valves in ACME
model.
a   tricuspid valve
b   pulmonary valve
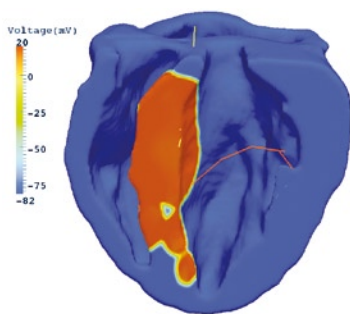
4 | Snapshot of electrical
stimulus predicted by electro-
physiology model.

The eigendeformations represent the deformations of free-standing heart muscle in the absence of constraints; their precise value and time-dependence are supplied by the electrophysiology model. The ACME electrophysiology model ensures the correct description of the cardiac contraction through careful modeling of the conduction system and calculation of excitation wave propagation, by accounting for the anisotropic conductivity values in the fiber and cross-fiber directions, and by modeling the correspondence between electrical stimulus and mechanical response (figure 4). The ACME hemomechanical model is based on optimal transportation techniques to simulate the flow of blood through the chambers and its interaction with the endocardium and the valves. The coupling of the hemomechanical and solid models is presently in progress. Particular attention is being given to the formulation of inlet and outlet conditions that simulate the effect of the remaining cardiovascular system and to the verification and validation of the valve/blood interaction.

Close collaboration with physicians and radiologists from the TUM hospital Klinikum Rechts der Isar ensures the anatomical and physiological correctness of all geometric modeling assumptions. Established connections at TUM between the centers for radiology, nuclear medicine, and vascular surgery and the Institute for Computational Mechanics 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 understanding of the healthy human heart as well as to the study and clinical treatment of a number of disease conditions, such as those resulting from myocardial infarction, valvular cardiomyopathy, and dilated cardiomyopathy.

Selected Publication:

[1] A. Nagler, M. Gee, W. A. Wall, W. S. Klug and M.Ortiz, "Advanced Cardiac Mechanics Emulator
     (ACME): Simulating the beating heart," to be presented at *ECCOMAS 2012, European Congress on
     Computational Methods in Applied Sciences and Engineering*, Vienna, Austria, September 10–14,
     2012.

Focus Group **High-Performance Computing**

Dr. Miriam Mehl | Carl von Linde Junior Fellow
Prof. Markus Hegland | Hans Fischer Senior Fellow
◉ Prof. Hans-Joachim Bungartz, Scientific Computing, TUM

Miriam Mehl

Markus Hegland

Tackling multiple multi-challenges

Today, the task of scientific computing is not just to simulate a physical process but to do this with a high accuracy for a deep understanding of scientific or engineering scenarios and – in the end – an optimization of the underlying processes. This has implications that go far beyond solving a problem with higher resolution on ever more powerful computers: The mathematical models have to be enhanced, for example by including more physical effects leading to multiphysics problems, which can be a combination of several single-physics models or even induce multi-dimensional equations. The potentially higher accuracy of such models can be exploited only with an extremely high grid resolution. To prevent severe performance breakdowns caused by the memory bottleneck and massively parallel structure of today's computing architectures, the development of new algorithms tailored for hybrid multicore architectures is required.

With the current Fellows Prof. Markus Hegland (Australian National University, Canberra) and Dr. Miriam Mehl (TUM), postdoctoral researcher Dr. Dirk Pflüger, and the two doctoral candidates Christoph Kowitz and Valeriy Khakhutskyy, our Focus Group even faces an additional challenge: the multi-hemisphere challenge tackled with several measures in 2011. Prof. Markus Hegland attended the TUM-IAS General Assembly in March and had a longer stay at the TUM-IAS in September, where he organized a very successful workshop on numerics for the Chemical Master Equation. In addition, the multidimensional issue has been a topic at the Ferienakademie in Sarntal. In October, the trans-equatorial exchange continued with Dr. Dirk Pflüger's two-month visit in Canberra. Here, the focus has been on a deeper understanding of efficient methods for high-dimensional data mining (extracting relevant information from collected data) and plasma-physics applications. At the end of the two months, not only were the respective methods working, but we had also gained insight into the deeper mathematical reasons why they are so efficient, a promising basis for further improvements and an obvious proof for the potential of tight cooperation with the ANU.

Christoph Kowitz, Valeriy Khakhutskyy | Doctoral Candidates
Dr. Dirk Pflüger | Postdoctoral Researcher

Sparse grids allow us to tackle high-dimensional problems, e.g., in plasma physics. Complexity is reduced from $O(N^d)$ to $O(N \log N^{d-1})$. Our code SG++ provides a toolbox for various high-dimensional applications (www5.in.tum.de/SGpp).

Fourier Space
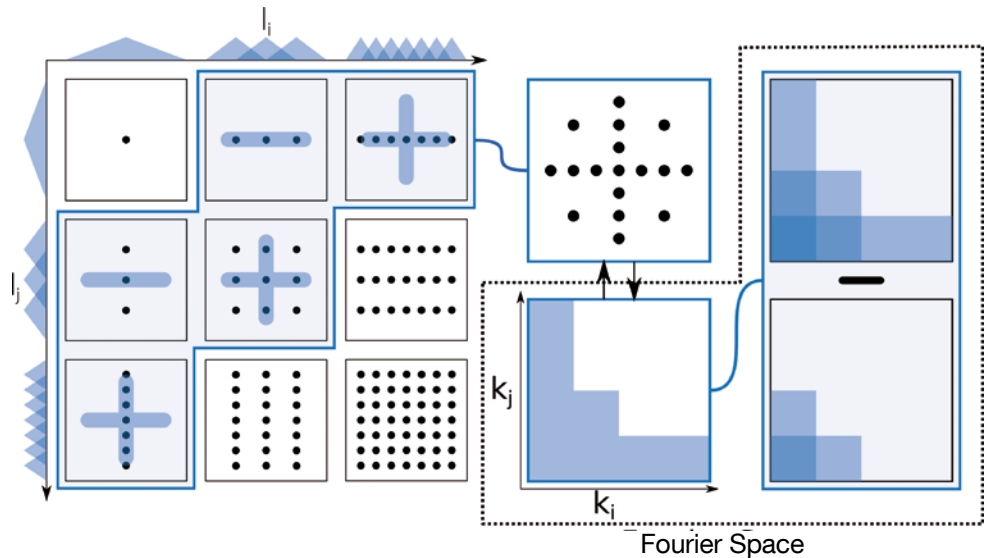
In March, Prof. Frank Jenko, our cooperation partner at the Max Planck institute for Plasma Physics (MPP), gave an invited talk at the ASIM (www.asim-gi.org) workshop in Munich. Plasma physics is the lead application of our Focus Group, as it combines a multi-dimensional (5D to 7D) multiphysics (magneto-hydro-dynamics) application and large computational needs, making the usage of multicore architectures inevitable. The goal is the simulation of the fusion reactor ITER (www.iter.org), a step toward solving the world's future energy problems to a large extent. With GENE, the MPP has a sophisticated high-performance computing code that, however, is reaching its limits and requires the implementation of further optimizations, in particular to weaken the "curse of dimensionality," i.e., the vast amount of data induced by the high dimensionality. The "numerical ITER" is out of reach without such improvements.

Further multiphysics-oriented activities of the Focus Group were the organization of the Munich Multiphysics Meeting as part of the annual summer workshop of the Munich Centre of Advanced Computing (www.mac.tum.de) and the invited participation of Dr. Miriam Mehl at the Multiphysics Summer Workshop of the Institute for Computing in Science of the Argonne National Laboratory (Park City, Utah, August 2011). We also organized minisymposia on multiphysics, fluid-structure interaction, and the interactive handling of large data sets at FEF 2011 (Finite Elements in Fluids, Munich, March 2011), SIAM CSE 2011 (Reno, February 2011), and ICCE 2011 (International Conference of Computational Engineering, Darmstadt, October 2011).

For 2012, we look forward to the stay of Christoph Kowitz at ANU (January through March), the visit of Prof. George Biros (Gordon Bell Prize 2010) at TUM-IAS as a Visiting Fellow in March (which we hope marks the beginning of a longer-term cooperation on the multicore topic), Prof. Markus Hegland's next stay at TUM-IAS (June through September), the International Conference on Parallel and Distributed Computing in June, and the Workshop for Sparse Grids and Applications in July.

Selected Publications:

[1] T. Weinzierl and M. Mehl, "Peano – A Traversal and Storage Scheme for Octree-Like Adaptive Cartesian Multiscale Grids," *SIAM SISC*, vol. 33, no. 5, pp. 2732–2760, 2011.

[2] H.-J. Bungartz, B. Gatzhammer, M. Lieb, M. Mehl, and T. Neckel, "Towards Multi-Phase Flow Simulations in the PDE Framework Peano," *Comp. Mech.*, vol. 48, no. 3, pp. 365–376, 2011.

[3] M. Hegland and J. Garcke, "On the numerical solution of the chemical master equation with sums of rank one tensors," *ANZIAM Journal*, vol. 52, pp. C628–C643, 2011.

[4] M. Hegland and P.C. Leopardi, "The rate of convergence of sparse grid quadrature on the torus," *ANZIAM Journal*, vol. 52, pp. C500–C517, 2011.

Focus Group **Computational Biomechanics**

Prof. Zohar Yosibash | Hans Fischer Senior Fellow
Hagen Wille | Doctoral Candidate
◉ Prof. Ernst Rank, Computation in Engineering, TUM

Activities during second year of fellowship
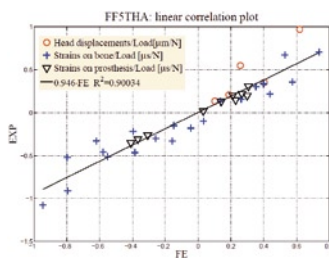

Zohar Yosibash

The aim of the overall project is to develop a patient-specific simulation of the mechanical response of the human femur to be used in clinical practice. In the first year we demonstrated the predictive capabilities of our simulations by a double-blind approach on a large cohort of 12 fresh frozen femurs.
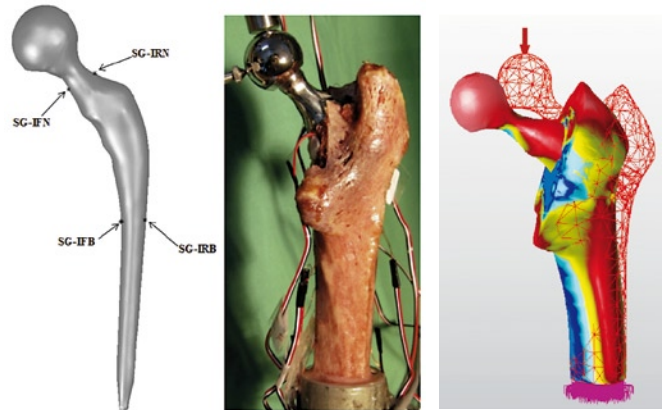
Experiment and FE model.

Using our novel high-order finite element methods, we predicted the response of the femurs, which were tested in another group to maintain an unbiased perspective. The comparison demonstrates unprecedented capabilities.

Comparison between the FE prediction and experimental observations.

Toward the quantification of bone material uncertainties, we first enhanced the newly developed finite cell method in Prof. Ernst Rank's group to handle bone mechanics. We made a strong start toward this aim thanks to TUM-IAS support for doctoral candidate Hagen Wille, who already has published one paper and two conference presentations.

Our simulation capabilities were extended this year to predict the mechanical response of patient-specific fractured human femurs undergoing a total hip replacement using cemented prostheses. A fresh-frozen human femur was loaded until fracture at the neck. The head and neck were removed, and the femur was implanted with a cemented prosthesis and loaded through the prosthesis so that strains and displacements could be measured. High-order FE models mimicking the experiments were generated – the total construction and solution time was about six hours, which means that a good agreement with experiments was achieved ($EXP = 0.946FE + 0.0012$, $R^2 = 0.90$).

Several talks at various conferences were presented on the topic, three papers were published (see two of the papers below), and a grant was awarded. The last year of the project will concentrate on the transition of such simulation capabilities into clinical practice, quantification of uncertainties in loading conditions, and enhancement of the finite cell method to enable simulation of femurs in a fraction of a second.

Selected Publications:

[1] M. Ruess, D. Tal, N. Trabelsi, Z. Yosibash, and E. Rank, "The finite cell method for bone simulations: verification and validation," *Biomechanics and Modeling in Mechanobiology*, vol. 11, no. 3, pp. 425–437, 2012.

[2] H. Wille, E. Rank, and Z. Yosibash, "Prediction of the mechanical response of the femur with uncertain elastic properties," *Journal of Biomechanics*, in press, 2012. doi:10.1016/j.jbiomech.2012.02.006

Focus Group **Advanced Stability Analysis**

Prof. Raman I. Sujith | Hans Fischer Senior Fellow
Ralf Blumenthal, Sebastian Bomberg | Doctoral Candidates
◎ Prof. Wolfgang Polifke, Thermodynamics, TUM

Burning questions about singing flames

Raman I. Sujith

Toward the ultimate goal of predicting and controlling instability in industrial combustors, our Focus Group concentrated in the last year on adopting the dynamical systems approach to analyzing thermoacoustic instability. In the first quarter of 2011, Prof. Wolfgang Polifke and Ralf Blumenthal visited IIT Madras, where Prof. Raman I. Sujith organized an Indo-European workshop on advanced stability analysis. Further, we worked on the dynamics of premixed flames, employing non-modal stability analysis tools. In summer, Prof. Raman I. Sujith visited Munich along with doctoral candidates Priya Subramanian, Sathesh Mariappan, and Lipika Kabiraj. The Focus Group was also augmented by the visits of two short-term Fellows, Prof. Peter Schmid (Ecole Polytechnique) and Dr. Matthew Juniper (University of Cambridge). Prof. Raman I. Sujith delivered pedagogical lectures on the dynamical systems approach to analyzing thermoacoustic instabilities. We also organized a seminar series on thermoacoustics and a mini-workshop on model reduction, together with Prof. Boris Lohmann (TUM) and Dr. Miriam Mehl (TUM-IAS).

The summer at TUM-IAS was an exciting period of three months, with the entire group working in close collaboration. The use of impulse response functions to characterize linear stability bounds of thermoacoustic systems in the time domain was undertaken as a joint effort between TUM and IIT doctoral candidates. Sebastian Bomberg began working on a multiscale multiphysics solver to predict instability.

Emphasis was laid on investigating nonlinear aspects of flame-acoustic interaction. Traditionally, it is believed that when the acoustic driving provided by the flame is balanced by the losses in the system, one attains limit-cycle oscillations. Our recent findings indicate that limit cycle is just one of the possible end states of the system. As demonstrated by the experimental work of Lipika Kabiraj, thermoacoustic systems can undergo further bifurcations and attain states such as quasiperiodic, period-doubling, frequency-locked, and chaotic states. Such states have been observed in both experiments and computations. We have observed both the Ruelle-Takens and the frequency-locking quasiperiodic route to chaos in our experiments. Further, we observed intermittency before the occurrence of flame blowout.

This rich dynamical behavior calls for a theoretical description able to reproduce all the bifurcations. The complex behavior found in the experiments might be reduced to a four-dimensional system consisting only of two coupled nonlinear oscillators, capturing the whole scenario of nonlinear dynamical states. Dr. Vladimir García Morales (TUM-IAS) is working with Prof. Katharina Krischer's group to establish such a theory. In close collaboration with Prof. Raman I. Sujith's group, they expect to gain profound insight on the nonlinear dynamics of thermoacoustic phenomena.
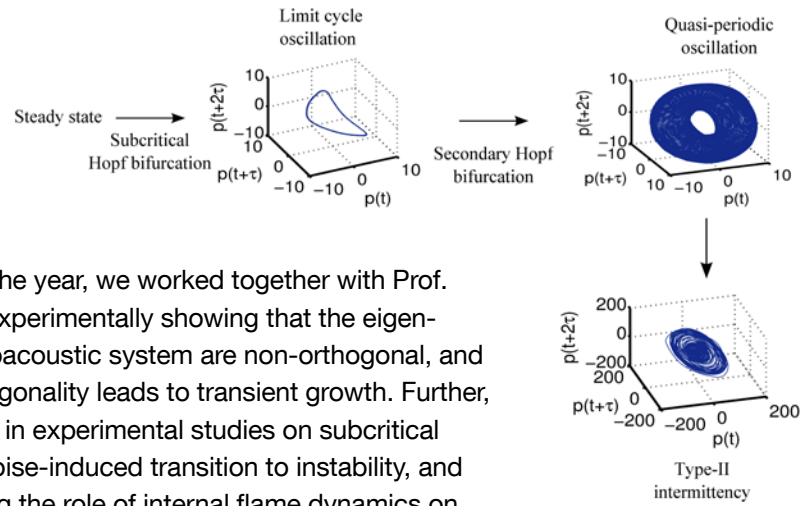
Bifurcation sequence
for thermoacoustic
oscillations of a ducted
premixed flame.

During the rest of the year, we worked together with Prof. Peter Schmid on experimentally showing that the eigen-modes of a thermoacoustic system are non-orthogonal, and that this non-orthogonality leads to transient growth. Further, we made progress in experimental studies on subcritical bifurcations and noise-induced transition to instability, and also on determining the role of internal flame dynamics on the instabilities. We also made progress toward finding a satisfactory answer to the question, "What is the appropriate norm for measuring the disturbance energy?" and toward identification of the heat transfer dynamics for non-modal stability analysis. In the next year our efforts will be focused on (1) establishing a general framework for coupling flow, sound and combustion, exploring both the method of multiple scales and state-space models, and (2) study-ing the dynamics of industrial combustors that have swirling turbulent flow.

Selected Publications:

[1] F. Selimefendigil, R. I. Sujith, and W. Polifke, "Identification of heat transfer dynamics for nonmodal stability analysis of thermoacoustic stability," *Applied Mathematics and Computation*, vol. 207, no. 11, pp. 5134–5150, 2011.

[2] P. Subramanian and R. I. Sujith, "Non-normality and Internal Flame Dynamics in Premixed Flame-Acoustic Interaction," *Journal of Fluid Mechanics*, vol. 679, pp. 315–342, 2011.

Experience Report

Laptop and Lunghi

Laptop and lunghi[1] – just like Bavaria, India is a place where tradition and history meet high-end sciences and technology. Within the framework of Prof. Raman I. Sujith's TUM-IAS Hans Fischer Senior Fellowship, doctoral candidates of the Advanced Stability Analysis Focus Group from Technische Universität München visited the Indian Institute of Technology Madras (IITM) in Chennai, South India, and vice versa.

Organizing the stay in India was not bureaucratic or time-consuming at all, as TUM-IAS provided all the necessary documents for visa applications as well as traveling expenses in plenty of time for the trip. When we arrived in India, transport from the airport to the IITM campus had already been arranged. The local Office of International Relations of IITM and the Indian members of the TUM-IAS Focus Group had planned ahead and provided help and support in all kinds of situations, such as finding accommodations, acquiring Indian SIM cards and mobile phones, and even administrative tasks such as applying at the registration office.

During the stay in India, our group attended a three-day workshop in Mumbai on hydrodynamic and thermo-acoustic instabilities. The workshop included some excellent talks by leading international researchers from renowned institutions such as the University of Cambridge, the Royal Institute of Technology in Stockholm,

[1] Lunghi: Traditional South Indian garment similar to a wrap-around skirt.

and of course the Indian Institutes of Technology in Mumbai, Kolkata, and Kanpur. At the social get-togethers, knowledge exchange and discussions took place. But also we got to know each other a little more over cups of hot chai tea.

Besides the big cities such as Mumbai, there are a number of places near IITM to discover. For example, the famous temples of Mahabalipuram or the Pondicherry area with its French colonial style buildings can be visited in a day's time. The IITM campus itself is definitely an attraction, too, with its chital deer, blackbuck antelopes, and bonnet macaque monkeys. Most students and researchers live on the IITM campus. They come from different parts of India, so English is the language of choice for teaching and work. The Indian colleagues, students, and professors were all very helpful. It takes a foreigner some time and effort to learn how to eat properly with one's hands, as is common practice in India. And without the experience and caution of our colleagues from the lab, more than one chocolate bar would have been snatched by the monkeys.

In summary, the visit to IITM broadened the horizons of everyone involved. Fruitful scientific discussions evolved, and things were seen in a different light. Working with sometimes limited possibilities turned out to be a boost to our creativity. India's historic buildings and beautiful landscapes were deeply impressive. All those friendly, ever-smiling people seemed to say: "Thank you. Visit again."

Ralf Blumenthal and Sebastian Bomberg (TUM)

Summer at TUM-IAS

We had the opportunity to visit the TUM Institute for Advanced Study during the summer of 2011 to be part of the Advanced Stability Analysis Focus Group. Support for our trip and stay from the staff of TUM-IAS had begun long before we landed in Munich with their help in arranging for accommodation. Upon our arrival, we lost no time in setting up our work, thanks again to the very helpful staff at TUM-IAS. The program managers and secretaries made sure that we were fully equipped and informed about the use of the generous and well thought-out amenities available at the Institute. Our stay at TUM-IAS was pleasant and engaging, with numerous opportunities to meet and hold interesting discussions with researchers in varied fields. Experts in fields such as statistical mechanics, information theory, and quantum mechanics were literally as close as a walk down the hall!

The many talks and presentations that took place during our stay were welcome introductions to many new fields and new lines of thought, which we hope to pursue in our research careers. Discussions over different approaches to solving a problem, and sometimes even discussions over languages, were quickly sorted out with small sketches on one of the handy whiteboards. Over talks in the coffee room or the chairs in the common areas, we met and talked with doctoral candidates from TUM. These talks made us see our own research area through a fresh set of eyes. The entire building at TUM-IAS is extremely interesting to work in, and we were able to fully utilize our time. As a result of our stay at TUM-IAS, three joint research papers were written and are currently under review with journals.

With the help of e-bikes available at the Institute, we were able to cycle to the nearest village for groceries or to explore the Isar along its route near the campus. We completely enjoyed our stay at TUM-IAS, and we hope to visit the Institute again as part of a Focus Group or as research fellows in the near future.

Lipika Kabiraj, Sathesh Mariappan, Priya Subramanian (Indian Institute of Technology Madras (IITM))

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

Dr. Vladimir García Morales | Carl von Linde Junior Fellow
Lennart Schmidt | Doctoral Candidate
◎ Prof. Katharina Krischer, Nonequilibrium Chemical Physics, TUM

Vladimir García Morales

Statistical mechanics of electrochemical nanosystems, cellular automata, and complexity

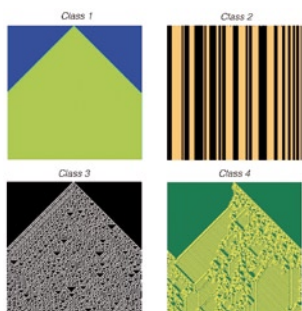Last year we completed our formulation of a theory of statistical mechanics for nanoscale electrochemical systems [1, 2]. It generalizes the standard Boltzmann-Gibbs formalism in a rigorous way and with no further *ad hoc* assumptions. A new entropic form was derived for the enhancement of electrochemical kinetics found in these systems [1]. We found that rare events are enhanced at the nanoscale compared to predictions from the (macroscopic) Second Law of Thermodynamics. Several projects were started to experimentally validate these exciting theoretical results, which may have profound consequences in heterogeneous catalysis at the nanoscale and in the development of nanodevices.

One PhD project was started, funded by the TUM-IAS, to study the emergence of order in oscillatory nonlinear dynamical systems. Nonlocal coupling, as found in electrochemical systems, is being studied in two dimensions by means of appropriate normal forms. Dynamical states with an unexpectedly wide variety of planar symmetries seem to be stabilized through the interplay of the nonlocal spatial coupling and the finiteness of the system.

Wolfram's cellular automata classes of increasing complexity, found through numerical simulations. The mathematical theory developed allows for an accurate identification of these dynamical behaviors in terms of symmetry breaking.

A major breakthrough came in the second half of 2011 with our finding of a general rigorous mathematical foundation for the emergence of complexity in nature. We established a theory that describes the time evolution of every dynamical system from cellular automata to continuum dynamics as described by partial differential equations. The most remarkable consequence is that analytical expressions can be systematically written down for every cellular automaton and, in most cases, they can even be analytically integrated. Universal maps have been found for all conceivable cellular automata, and they do not depend on any freely adjustable parameter. The invariances of these maps allow classification of dynamical systems into different universality classes. Complex systems belong to one of these classes and break a certain kind of symmetry that finds a precise definition in mathematical terms. This theory generalizes the traditional field of mathematical physics to the study of discrete systems and provides a unification for different kinds of calculus as they apply to physical systems: Boolean algebra, p-adic calculus, set theory, number theory, combinatorics, and differential calculus. The theory is currently being prepared for publication.

Selected Publications:

[1] V. García Morales, and K. Krischer, "Superstatistics in nanoscale electrochemical systems," *Proceedings of the National Academy of Sciences USA*, vol. 108, no. 49, pp. 19535–19539, 2011.

[2] V. García Morales, and K. Krischer, "Kinetic enhancement in nanoscale electrochemical systems caused by non-normal distributions of the electrode potential," *Journal of Chemical Physics*, vol. 134, no. 24, 244512, pp. 1–8, 2011.

Raman I. Sujith, Katharina Krischer, Vladimir García Morales

Focus Group **Advanced Computation**

Prof. Peter Schröder | Hans Fischer Senior Fellow
Jan Stühmer | Doctoral Candidate
◉ Prof. Rüdiger Westermann, Computer Graphics and Visualization, TUM

Peter Schröder

Discrete differential geometry and its applications in computer graphics

In the past year we have continued to pursue our research in discrete differential geometry and its applications. In discrete differential geometry one aims to make the tools of classical smooth differential geometry available for meshes, as they are common in computer graphics and scientific computing. One such application is geometric design, i.e., the design and editing of surfaces for purposes of geometric modeling. To this end we considered a particular class of surface deformations that are conformal; that is, locally the deformation is at most a rotation and scaling (no shearing is allowed). Such deformations maintain the mesh quality and gracefully deal with surface attributes such as texture maps. We formulated this problem in the language of quaternions, where surfaces are thought of as embedded in the imaginary quaternions rather than the standard x/y/z-space. This allows us to characterize all conformal deformations of a given surface as solutions to a first-order differential operator, the Dirac operator. Practically speaking, this amounts to setting up a linear system and then finding an eigenvector of this system. In this way we were able, for the first time, to give an algorithm for curvature-based surface deformation that does not involve nonlinear functionals, as had been the case before our algorithm. The work was published at the yearly SIGGRAPH conference, and an application that implements the algorithm is available for free download.

Selected Publication:

[1] K. Crane, U. Pinkall, and P. Schröder, "Spin Transformations of Discrete Surfaces,"
     ACM Transactions on Graphics, vol. 30, no. 4, p 104, 2011.

A giraffe model is deformed significantly in our editing system all the while maintaining conformality of the deformation. Consequently surface attributes such as texture maps gracefully deform with the surface without unsightly angle distortion.

World Development and Ecology

Global Change

Advanced Construction Chemicals and Materials

Soil Architecture

Metropolis Nonformal

Satellite Geodesy

Engineering Risk Analysis

Focus Group **Global Change**

Prof. Tim Sparks | Hans Fischer Senior Fellow
Anna Bock, Julia Laube | Doctoral Candidates
Dr. Nicole Estrella, Dr. Christian Zang | Postdoctoral Researcher
◉ Prof. Annette Menzel, Ecoclimatology, TUM

Tim Sparks

Part of a controlled day length/
temperature experiment
to assess climate change
responses of invasive, exotic,
and native tree species.

Detecting long-term climate change impacts in our environment

Global climate change has already had measurable impacts on our environment ranging from melting of glaciers to massive changes in the biosphere, including range shifts, altered phenology, and impacts on human health.

In 2011 our Focus Group concentrated on three hot topics. The first is an assessment of possible changes in yields and quality under warming conditions. Here, our doctoral candidate Anna Bock dipped deep into various archives to detect and assemble amazing long-term records that reveal a climate change response. Anna has already had her first paper published, on long-term records from the Franconian wine industry [1], and presented the essence of what will become a second paper on this topic to an international conference in New Zealand. Further data archaeology is under way.

The second important topic is invasive species, known to be highly competitive and thus able to change the composition, structure, and function of ecosystems over large areas. Doctoral candidate Julia Laube began studying climate impacts on invasive plant species that are economic and biodiversity threats in Germany and elsewhere. She is collecting a considerable quantity of data from controlled environments in the excellent TUM Dürnast experimental facilities, from field work, and from existing data resources.

Thirdly, we use historical impacts of climate on diverse systems to assess paleoclimatic information. Dr. Christian Zang uses tree rings as proxy data for the reconstruction of long-term changes in our environment. To this end, we separate endogeneous effects on tree growth, such as tree aging or effects related to stand growth and competition, from the exogenous factors of interest [2]. The recent change in the tree ring-temperature relationship (the "divergence effect") is a major concern in our reconstruction of alpine temperatures. We also succeeded in using tree-ring data as a proxy for nutrient removal from forest soils, to assess long-term change in forest productivity related to different management practices. Cooperation between our Focus Group, together with the chair of Ecoclimatology, and the TUM-IAS Focus Group on Risk Analysis and Stochastic Modeling has won an ERC Starting Grant to study extreme events in ecology.

Selected Publications:

[1] A. Bock, T. Sparks, N. Estrella, and A. Menzel, "Changes in the phenology and composition of wine from Franconia, Germany," *Climate Research*, vol. 50, no. 1, pp. 69–81, 2011.

[2] C. Zang, H. Pretzsch, and A. Rothe, "Size-dependent responses to summer drought in Scots pine, Norway spruce and common oak," *Trees - Structure and Function*, pp. 1–13, 2011. doi:10.1007/s00468-011-0617-z.

Focus Group **Advanced Construction Chemicals and Materials**

Dr. Tsuyoshi Hirata | Rudolf Diesel Industry Fellow
Alex Lange | Doctoral Candidate
◎ Prof. Johann Plank, Construction Chemicals, TUM

TUM-IAS Fellows
and their Research

## Working mechanism of polycarboxylate-based superplasticizers for concrete

Tsuyoshi Hirata

The TUM-IAS Advanced Construction Chemicals and Materials Focus Group, comprising Dr. Tsuyoshi Hirata, Prof. Johann Plank, and the doctoral candidate Alex Lange, focuses on the working mechanism of polycarboxylate-based super-plasticizers with polyethylene glycol pendants (PCEs).

PCEs have been widely used all over the world to produce highly durable concrete, such as ultrahigh-strength concrete and self-compacting concrete, because of their excellent cement-dispersing performance by steric repulsion originating from polyethylene glycol side chains grafted onto an anionic polymer backbone. The concrete industry is continuing to request superplasticizers with improved performance and usability in terms of concrete durability, strength, and fluidity as well as economy.
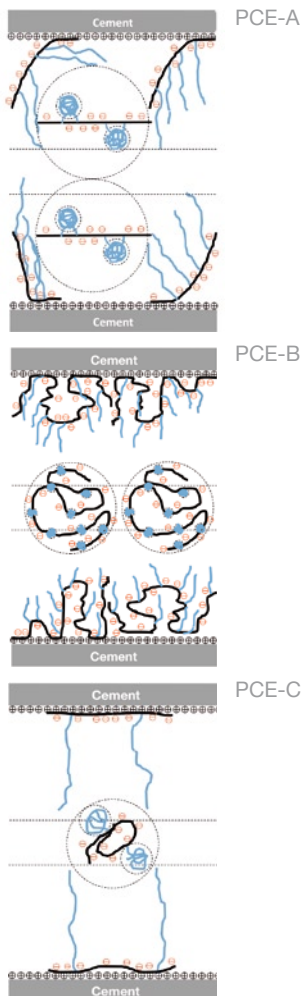
PCE-A

The composition of cement is not uniform, but rather complicated, due to variations in raw materials and production conditions. This can result in excessive and therefore less cost-efficient PCE dosage. Technical improvements leading to cost savings can have a huge impact, since cement represents the largest-volume industry-made product in the world, with a production volume of ~3 billion tons in 2010. In this respect, one of the most important features of PCEs is cement compatibility.

PCE-B

Better understanding of the working mechanism is essential for developing new PCEs that realize such quality characteristics. During the past year, we studied in detail the relationship between conformation of dissolved PCEs and their dispersing performance. Indeed, we found that in cement pore solution PCEs conform to a variety of shapes, depending on the main chain structure: rod-like (PCE-A), densely packed worm-like (PCE-B), and less densely packed worm-like or star-like (PCE-C). Furthermore, our study showed that a star-like polymer (PCE-C) requires a lower and thus more economical dosage to obtain the required initial concrete flow, because it can unfold much more easily on the cement surface.

PCE-C

Surprisingly, we found that it is likley that those PCEs disperse cement particles not only by steric interaction but also by electrostatic repulsion, and that PCE-B with short side chains is an effective ingredient in improving concrete flow.

A further goal of our project is to get a clue to an optimized polymer structure, studying the interaction between the polymer and cement hydrates. The authors wish to express their gratitude to TUM-IAS for its generous support of this fascinating research project.

Schematic diagrams of different PCE polymers adsorbed on the surface of cement.

Selected Publication:

[1] A. Lange, T. Hirata, and J. Plank, "Study on Working Mechanism of Polycarboxylate Ether (PCE) Based Superplasticizers," in *Tenth International Conference on Superplasticizers and Other Chemical Admixtures in Concrete*, Prague, 2012, accepted.

Focus Group **Soil Architecture**

Prof. Ingrid Kögel-Knabner | Carl von Linde Senior Fellow
Dr. Geertje Pronk | Postdoctoral Researcher
◉ Soil Science, TUM

Revealing the soil nano-architecture

During the biomass formation/decomposition cycle, carbon dioxide (CO_2), the most important climatic gas, is either released from soils or stabilized in soils. With the onset of soil formation, aggregation starts and soil organic carbon (SOC) is sequestered. The elucidation of the biogeochemical processes that are part of this cycle is one of the most important and most pressing scientific challenges of our time. The question that has still to be answered is: "Why, when organic matter is thermodynamically unstable, does it persist in soils, sometimes for thousands of years?"

Formation of soil interfaces in batch incubation experiments – study of reactive hot spots at the submicron scale.
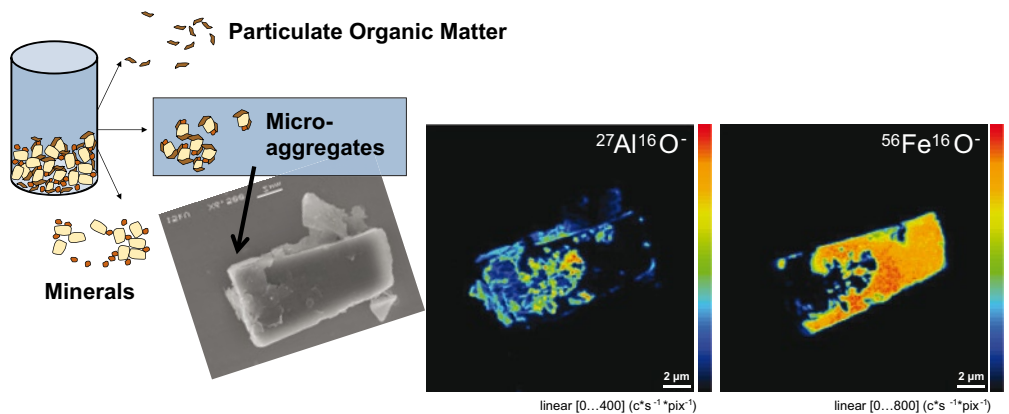
In soils a solid, liquid, and gas phase interact, producing a habitat for microbial life. The scale of spatial structures spans nearly nine orders of magnitude (from nanometer minerals to football-sized soil clods). Indeed, the spatial heterogeneity of biota, environmental conditions, and organic matter may have a dominant influence on carbon turnover and trace gas production in soils. With increasing scale and complexity in structural organization – from the primary structures of organo-mineral complexes to the architecture of the soil profile – progressively more dynamic responses to environmental perturbations and management practices occur. At present, we are far from being able to quantify the complex processes of soil structure development and fragmentation; they have different space and time scales depending on soil type, texture, and management. Thus biogeochemical and physical interactions within the aggregate system of soils have large effects on the long-term storage of SOC. The functional relation between the soil aggregate system and the organic matter stabilized in these structures is thus a key to understanding the rates and processes that control the turnover of SOC.

Obstacles to analyzing these processes are the complex architecture of soils, which is heterogeneous at different scales (aggregates, roots, and microorganisms); the broad range of temporal and spatial scales; and the opaque nature of soils, implying that no direct observation of processes and underlying mechanisms is possible.

Recent advances in physics, materials science, genomics, and computation using new techniques and experiments have enabled a new generation of research. This research has led to an emerging paradigm for soil-organic-carbon dynamics – that organic matter persists not because of its own intrinsic properties, but because of physicochemical and biological processes that reduce the probability (and therefore rate) of decomposition, allowing the organic matter to persist. In an article by Schmidt et al. (2011), we highlighted these new perspectives for soil organic matter research. Going forward, we aim to implement the simultaneous analysis of the spatial distribution of C, N, Si, Al, and Fe in organo-mineral associations and microaggregates, employing the specific features of the novel NanoSIMS (secondary ion mass spectrometry) 50L microprobe technology with the simultaneous analysis of up to seven ion species with high sensitivity and resolution. NanoSIMS technology boosts our ability to locate the association of elements/isotopes in soil structural components.

Selected Publications:

[1] M.W.I. Schmidt, M.S. Torn, S. Abiven, T. Dittmar, G. Guggen-berger, I.A. Janssens, M. Kleber, I. Kögel-Knabner, J. Lehmann, D.A.C. Manning, P. Nannipieri, D.P. Rasse, S. Weiner, and S.E. Trumbore, "Persistence of soil organic matter as an ecosystem property," *Nature*, vol. 478, no. 7367, pp. 49–56, 2011.

[2] K. Eusterhues, T. Rennert, H. Knicker, I. Kögel-Knabner, K.U. Totsche, U. Schwertmann, "Fractionation of organic matter due to reaction with ferrihydrite: coprecipitation versus adsorption," *Environmental Science & Technology*, vol. 45, no. 2, pp. 527–533, 2011.

Ingrid Kögel-Knabner
graduated in geo-ecology in 1983 and received her doctorate from the University of Bayreuth, Germany, in 1987, working on the chemical composition of organic matter in forest soils. She became a professor of soil science and soil ecology at the Ruhr-Unive-ristät Bochum in 1992. In 1995 she joined the Life Sciences Center of TUM as Professor in soil science. Ingrid Kögel-Knabner directed a German nationwide priority research program on soils as source and sink of CO_2. She is a member of both German national scientific academies, Akademie der Naturforscher Leopoldina (since 2000) and Akademie der Technik-wissenschaften acatech (since 2007).

Focus Group **Metropolis Nonformal**

Prof. Christian Werthmann | Hans Fischer Senior Fellow
◉ Prof. Regine Keller, Landscape Architecture and Public Space, TUM

Metropolis nonformal

Illegal - irregular - clandestine - uncontrolled - slum - skid row - favela - barrio - bidonville - shantytown. Our common vocabulary for nonformal urbanism emphasizes its outcast nature, but not its formidable dynamic, moral legitimacy, and ubiquity. Over the last hundred years, nonformal urban growth has greatly increased and accounts for about one third of our urban population. In the coming decades, nonformal cities will constitute not only close to half of our urban growth on this planet, but will house the majority of our young urban population. As global design practice becomes a commonplace, not many practitioners are prepared to be effective in the highly dynamic conditions of cities that grow to innate orders independent of conventional planning paradigms. As we experience the rise of the auto-constructed city in synchronicity with the ascent of global practice, a whole new generation of designers has to learn a set of new navigation modes.

What constitutes the role of professional designers in cities where everybody is a designer? The engagement of designers with nonformal urbanization is as old as the phenomenon itself, stretching from Haussmann's slum clearances in Paris to John Turner's self-help initiatives in Peru. However, attitudes, means, and operations of designers working in nonformal cities have radically changed over the centuries and are continuously evolving. Today, a new generation of designers engages highly conflicted and incredibly dense urban territories through carefully calibrated infrastructure, urban, and landscape interventions. Nonformal cities are not primarily viewed as a malfunction, but as a brave response of the urban migrant to the government's inability to provide shelter.

The Focus Group Metropolis Nonformal pursues two avenues of research: It traces the particular modes of operation of an emerging professional field, and it develops new modes of engagement based on a carbon-reduced, culturally adaptive, and economically stimulative integration of green infrastructure into nonformal cities.

Concerning the first avenue of research, I invited nine professionals and academics who have performed outstanding work in nonformal settlements to Munich, to give presentations at the symposium *Metropolis Nonformal* in the fall of 2011 (see documentation under www.tum-ias.de/metropolis-nonformal-symposium/documentation.html). A follow-up event, planned for spring 2013, will focus on the anticipation of nonformal urbanism.

Regarding the second avenue of research, I began a collaboration with Prof. Regine Keller, chair of Landscape Architecture and Public Space, and the chair of Urban Water Management, Prof. Harald Horn, and his interim successor Prof. Brigitte Helmreich to develop landscape-based water management strategies in the current reconstruction efforts of Port-au-Prince, Haiti. A group of six students (three environmental engineers and three landscape architects) has completed a studio in a flood plain of Port-au-Prince that is under heavy urbanization pressure. One landscape architecture master's student accompanied me on a visit there, and a doctoral candidate in environmental engineering began to formulate her thesis work under the supervision of Brigitte Helmreich. The goal for the coming two years of my Fellowship is to develop a solid foundation for future transdisciplinary collaboration in the emerging field of socio-ecologic infrastructure and nonformal urbanism.

Selected Publications:

[1] C. Werthmann, "Landscape and Infrastructure in Nonformal Cities" in Design with the Other 90%: Cities, Cynthis Smith, Ed. New York, NY: Cooper Hewitt Museum, 2011.

[2] C. Werthmann, "Squatting Infrastructure," in Infrastructural Urbanism, Hauck, Keller, Kleinekort, Eds. Munich, Germany: Dom Publishers, 2011.

Christian Werthmann received his Master of Landscape Architecture degree with a specialization in urban design at the University of Kassel in Germany. Before moving to the United States in 1997, he was a project designer in the landscape architecture office of Latz and Partners and taught as a research fellow at TUM. In the United States he worked as a landscape architect in several prominent offices, such as Peter Walker and Partners and Hargreaves Associates. Werthmann is currently an associate professor in the Landscape Architecture Department of the Harvard Graduate School of Design and serves as its director of the Master in Landscape Architecture Degree Programs. Christian Werthmann is also the co-director of the recently established Anticipatory Spatial Practices focus in the postgraduate Master in Design (MDes) program.

Focus Group **Satellite Geodesy**

Prof. Gerhard Beutler | Hans Fischer Senior Fellow
Prof. Adrian Jäggi | Carl von Linde Junior Fellow
Prof. Reiner Rummel | Carl von Linde Senior Fellow

Reiner Rummel

GOCE gravity and dynamic topography

GOCE, the focal point of our project, is a satellite mission of the European Space Agency (ESA) that was launched in March 2009. The Institute of Astronomical and Physical Geodesy (IAPG) has invested considerable energy in getting this mission realized and is still coordinating the science data processing on an ESA contract (see TUM-IAS Annual Report 2009, p 66–71). GOCE measures Earth's gravity field. Its core instrument is a gravitational gradiometer that delivers all components of the gravitational field tensor, and it is the first instrument of its kind. Gradiometry was chosen in order to amplify the short-scale gravity signals and to counteract the attenuation of the field at satellite altitude. From two years of mission data we know that the strength of the system is at spatial length scales between about 250 km and 80 km. Length scales longer than 250 km have to be reproduced from the orbits, while those shorter than 80 km require terrestrial measurements.

What is the scientific objective? In short one may say it is "dynamic topography." Discovering the connection between processes observed on the Earth or in space and their internal dynamics is an essential goal in solid Earth physics. Dynamic topography in geophysics means the deformation of the surface of the Earth, supported by the vertical stresses at the base of the lithosphere that are generated by flow in the mantle below. Comparison of the geoid signal as measured by GOCE with an Earth model in hydrostatic equilibrium predominantly reflects dynamic topography. It is shown in terms of gravity variations in figure 1. In oceanography, dynamic topography is the deviation of the actual mean ocean surface from the geoid. In this case the geoid serves as a reference, an idealization of the world's oceans at complete rest. The actual ocean surface is measured from space by radar altimetry, and GOCE provides the geoid. Figure 2 shows a world map of the mean dynamic ocean topography based on GOCE. This marks the first time that dynamic ocean topography was measured from space with great detail and precision and without the use of oceanographic *in situ* data.

The main goal of the TUM-IAS Focus Group is the development of optimal methods of gravity field recovery from measured GOCE orbits and gravitational gradients. Prof. Gerhard Beutler and Prof. Adrian Jäggi, our TUM-IAS Fellows from the Astronomical Institute of the University of Bern, conceived and refined a new method of orbit analysis; the method is known as the Celestial Mechanics Approach (CMA). It was very successful when applied to orbit analysis and gravity field determination of the satellite gravimetric missions GRACE and GOCE (see TUM-IAS Annual Report 2010).

Weiyong Yi | Doctoral Candidate

◎ Prof. Reiner Rummel, Astronomical and Physical Geodesy, TUM
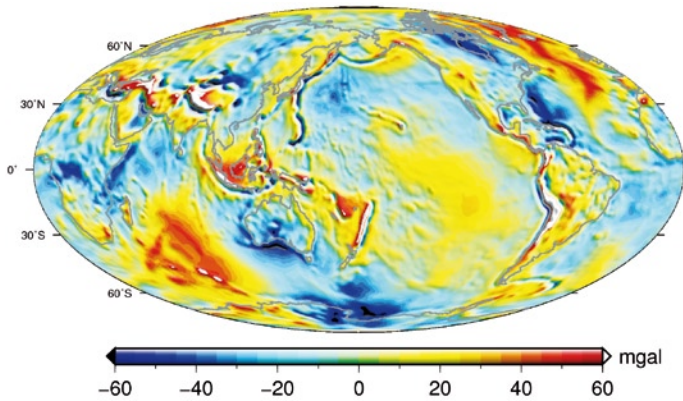
1 | Global map of variations of gravity as derived from GOCE. The units are milliGal, i.e., parts per million of "g." All geodynamic collision zones are clearly visible, such as the so-called "ring of fire" surrounding the Pacific Ocean.
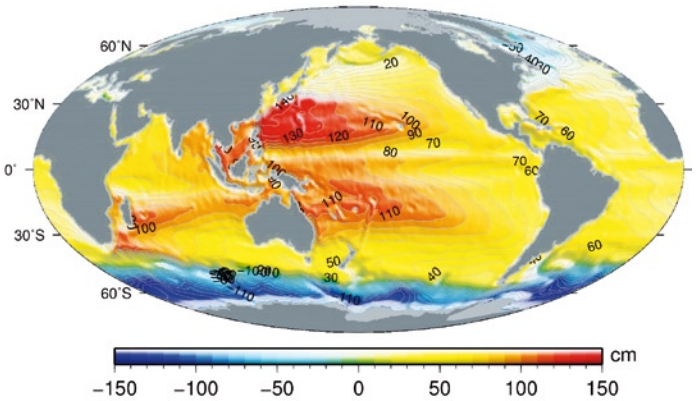
2 | Global map of the dynamic ocean topography. It shows the deviation of the actual mean ocean surface (averaged over almost twenty years of satellite radar altimetry measurement of the ocean surfaces) from the geoid as derived from GOCE. The values are given in centimeters; they range between -1.5 m and +1.5 m.

In parallel, the gravitational gradients have been studied along with their individual spectral behavior and their characteristics on the Earth's sphere [1]. The joint analysis of orbit and gradients resulted in a global field model. It is represented as a spherical harmonic series up to degree and order 215, i.e., using close to 50,000 representation coefficients. The relative contribution of each of the tensor components and of the orbits could also be quantified.

With support from TUM-IAS and IAPG, ESA jointly organized a user workshop at TUM from March 31 to April 1, 2011, where TUM-IAS Director Prof. Patrick Dewilde gave the opening address. More than 200 participants from 26 countries discussed GOCE data

analysis and first results in geophysics, oceanography, and geodesy. The workshop received great interest in the international news media.

In December 2011, Carl von Linde Junior Fellow Dr. Adrian Jäggi was appointed as a professor and the head of the Astronomical Institute of the University of Bern.

Selected Publications:

[1] R. Rummel, W. Yi and C. Stummer "GOCE Gravitational Gradiometry," *J. of Geodesy*, vol. 85, no. 11, pp. 777–790, 2011.

[2] R. Rummel, M. Horwath, W. Yi, W. Bosch and R. Haagmans "GOCE, Satellite Gravimetry and Antarctic Mass Transports," *Surveys in Geophysics*, vol. 32, no. 4–5, pp. 643–657, 2011.

Focus Group **Engineering Risk Analysis**

Dr. Chin Man W. Mok | Rudolf Diesel Industry Fellow
◎ Prof. Daniel Straub, Engineering Risk Analysis, TUM

Developing holistic and adaptive risk-based decision support for hydrologic, geologic, and environmental applications

Conventional approaches for designing engineering systems and evaluating natural systems rely on conservative assumptions to account for uncertainties associated with various non-anthropogenic and anthropogenic factors. In most cases, there is no further examination of the safety of such systems unless failure has occurred. With the advancements in measurement devices and remote sensing techniques in recent years, more systems are being monitored to provide data for evaluation of their current state and performance. However, future risk is often subjectively evaluated on the basis of professional judgment and experience. The Engineering Risk Analysis Group aims to steer research toward developing holistic and adaptive reliability-based decision support techniques that utilize monitoring data to predict future risk and incorporate decision support tools to minimize the predicted risk. Monitoring data not only provide statistical information for conditional prediction of future conditions, but also can serve as the basis for bias correction and for prediction error reduction. We consider applications to hydrologic, geologic, and environmental problems, such as water resources management, landslide warning, and health risk assessment.

Our group has been gaining momentum since its formation in May 2011. One of our current focuses is on development of a stochastic rainfall model that simulates the spatial and temporal characteristics of rainfall. We investigated the possibility of using Bayesian methods to integrate rain gauge and radar rainfall data. Rain gauge data are more accurate, but they only yield information at point locations. Radar data provide continuous spatial information but they are less accurate. As demonstrated by Marian Heimann in his master's thesis, integrating these two types of data provides more accurate and continuous rainfall interpretation [1]. We are developing this method further to a non-parametric approach allowing rainfall spatial structures to be intensity-dependent. Another student, Wolfgang Betz, began refining the temporal resolution of rainfall estimation using Bayesian networks. A journal publication is in preparation.

Through the Rudolf Diesel Industry Fellowship, the TUM-IAS has enabled Wolfgang Betz to continue with our group, as of March 2012, as a doctoral candidate; his research will focus on reliability-based decision support for flood hazard management. At the same time, another doctoral candidate, Ji Yuan, starts his doctoral research on risk assessment of landslide hazards using rainfall information in near-real time. We are currently seeking funds to support a third doctoral candidate to work on stochastic modeling of rainfall and climate. In addition, we are collaborating with Dr. George Matanga of the US Bureau of Reclamation on a similar research topic related to water resources management. Finally, we have been investigating the use of Bayesian networks in flood management with Daniel Frey, a TUM doctoral candidate working on remote sensing [2]. This collaboration was initiated at a TUM-IAS workshop.

Posterior mean estimates of rainfall intensity
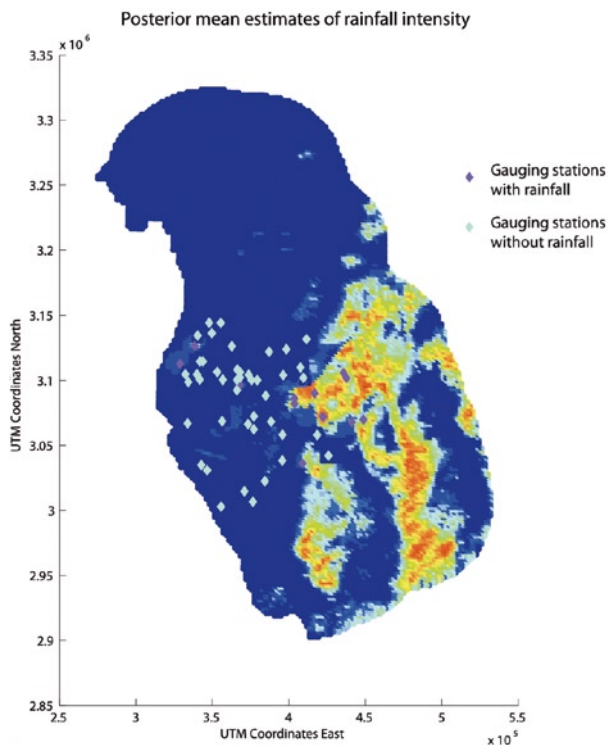
Estimation of rainfall by integrating rain gauge and radar rainfall data with Bayesian methods.

Further activities in 2011 included the organization of a professional five-day short course series on risk-based environmental management, with Dr. Ravi Arulanantham and Fulbright specialist James Jacobs; a master's thesis on probabilistic health risk assessment; and several short seminars by Dr. Chin Man W. Mok for students of environmental and civil engineering.

Selected Publications:

[1]   M. Heimann, "Bayesian Integration of Radar Rainfall into Point Measurements Developing Profile for Downscaling Climate Models," *MSc thesis*, Engineering Risk Analysis Group, TUM, Munich, Germany.

[2]   D. Frey, M. Butenuth, and D. Straub, "Probabilistic graphical models for flood state detection of roads combining imagery and DEM," *IEEE Geoscience and Remote Sensing Letters*, to be published.

Chin Man W. Mok

graduated with BSc (Eng.) in civil and structural engineering from the University of Hong Kong in 1985. After working in Hong Kong as a structural and geotechnical engineer for over a year, he moved to the University of California at Berkeley, where he obtained his MS and PhD degrees in civil and environmental engineering. He joined Geomatrix Consultants, Inc. (acquired by AMEC in 2008) in 1987 and is currently a principal engineer and hydrogeologist in AMEC's Oakland, California, office. He has 26 years of consulting experience in hydrogeology as well as in geotechnical, earthquake, environmental, hydrologic, and structural engineering worldwide. Apart from his industry practice, he is active in academia. He is currently an adjunct professor (hydrogeology) at the University of Waterloo and has been a part-time associate professor (geotechnical engineering) at the University of Hong Kong. He has taught continuing professional development short courses in many countries and has been a principal investigator in numerous research studies funded by national agencies and AMEC. His expertise is in computational modeling, reliability/risk/hazard analysis, resource and operations optimization, and field testing. He is interested in applied research and is currently supervising several graduate students.

Cells and Molecules

Biochemistry

Neuroscience

Biophysics

Clinical Cell Processing and Purification

Biomedical Engineering

Focus Group **Biochemistry**

Prof. Horst Kessler | Carl von Linde Senior Fellow
◎ Chemistry, TUM
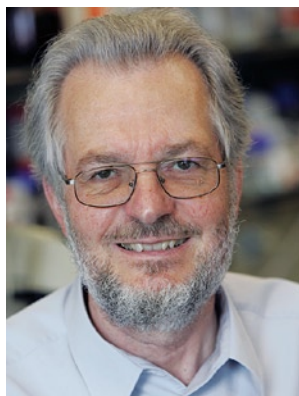
Highlights from the Kessler group

Horst Kessler

Our main topic is the improvement of activity and selectivity of integrin ligands for molecular imaging and biophysical studies in cell adhesion. In addition, we investigated other peptidic ligands for GPCR receptors and studied protein-protein interactions by NMR spectroscopy. In 2011 we published 15 manuscripts with a total impact factor of 100. Two highlights are given below.
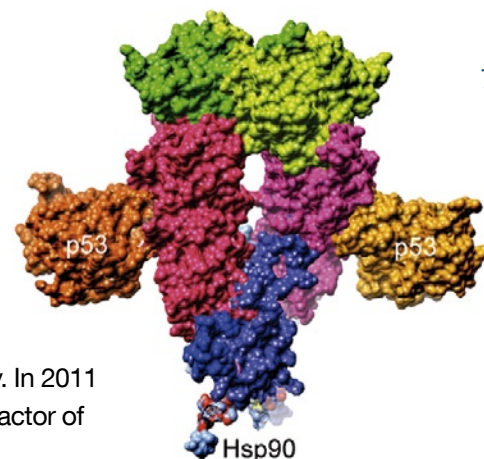
Interaction of Hsp90 with p53: The tumor suppressor protein p53 has an essential role in controlling the stability of the genome. When DNA damage is detected by p53, the cell cycle gets arrested until a repair of the DNA is achieved. If this is impossible, the cell is sent to death (apoptosis). Therefore, p53 is often called the "guardian of the genome." However, in more than 50% of all cancers this important control function is impaired. The structural integrity of p53 itself is strongly dependent on the function of the heat shock protein 90 (Hsp90). By using NMR and other biophysical methods we were able to show that p53 has multiple binding sites on Hsp90 and to obtain a structural model for the complex between the two proteins. Our data represent the first detailed analysis of the interaction of Hsp90 with a client protein and therefore contribute to the general understanding of the function of molecular chaperones. This was a collaboration with the group of Prof. Johannes Buchner (Chemistry, TUM). [1]

PET imaging of the CXCR4 receptor: This chemokine receptor subtype is a central part of signaling systems in human body. In addition to its function as regulator of stem cell trafficking, it is involved in tumor metastasis and more than 30 human tumors. We have developed a Ga68 radiolabeled cyclic peptide that addresses this receptor with high specificity. This allows for detection of cancer in mice via positron emission tomography (PET). This work is a collaboration with the group of Prof. Hans-Jürgen Wester (Pharmaceutical Radiochemistry, TUM) and Prof. Markus Schwaiger (Clinic for Nuclear Medicine, TUM). [2]

A

60 min

Selected Publications:

[1] F. Hagn, S. Lagleder, M. Retzlaff, J. Rohrberg, O. Demmer, K. Richter, J. Buchner, and H. Kessler, "Structural analysis of the interaction between Hsp90 and the tumor suppressor protein p53," *Nature Structural and Molecular Biology*, vol. 18, no. 10, pp. 1086–1093, 2011.

[2] O. Demmer, I. Dijkgraaf, U. Schumacher, L. Marinelli, S. Cosconati, E. Gourni, H.-J. Wester, H. Kessler, "Design, synthesis, and functionalization of dimeric peptides targeting chemokine receptor CXCR4," *J. Med. Chem.*, vol. 54, no. 21, pp. 7648–7662, 2011.
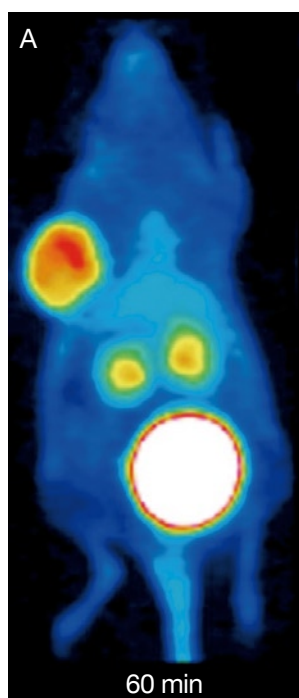
Focus Group **Neuroscience**

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   Rita Förster | Doctoral Candidate

Across scales: From organelles to circuits

The challenge of neuroscience lies in size. This challenge exists not only because the brain's decisive elements are small – as indeed, they are, with single contact sites ("synapses," the brain's transistors) approaching what a light microscope can barely resolve (<1μm). At the same time, the brain is enormous in dimensions, with a single cell's myriads of synapses spread over macroscopic distances of centimeters or even meters. Hence, technology to explore the brain's circuits needs to span such orders of magnitude. The TUM-IAS Neuroscience Focus Group is addressing this challenge by combining techniques ranging from *in vivo* electrophysiology and imaging to genetic circuit tracing and electron microscopy.
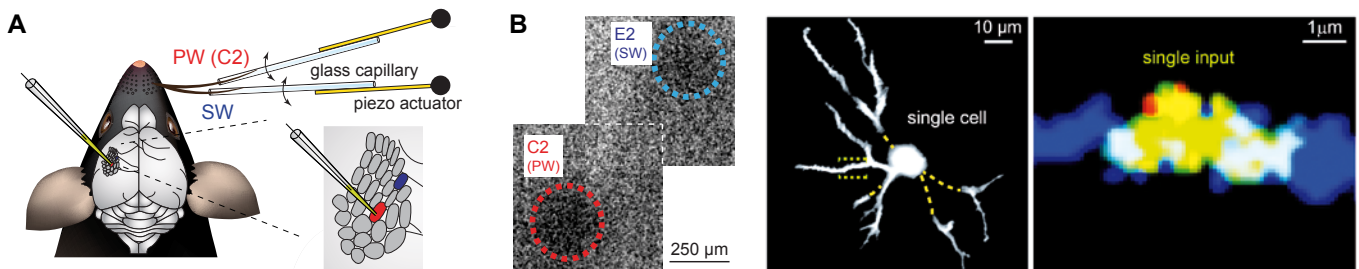
1 | Schematic workflow to use *in vivo* electrophysiology and imaging of sensory circuits to cover the range from whole circuits to single inputs, covering tissue level activity (2nd panel from left; active areas of cortex appear dark and are circled), single cells (3rd panel) and single inputs (4th panel).

One focus of our work in 2011 was to further explore the functioning of sensory networks, specifically the tactile circuits of small rodents. As nocturnal animals, mice heavily depend on their whiskers to explore their environment. One attractive feature of this system is its simple anatomy: Each facial whisker of a mouse is neatly represented in its own site in the cerebral cortex (figure 1). This allows us to identify brain areas and cells that primarily respond to sensory stimulation (i.e., deflection) of a given whisker. However, even cells in a brain area that primarily responds to one whisker receive inputs that indicate stimulation of another one. This lets us address the question of how inputs relating to these "principal" and "secondary" whiskers are organized on a target cell. Are they distributed all over? Can they come so close as to actually stimulate the very same synaptic site? The Konnerth and Sakmann groups combined forces to answer these questions (Varga et al., PNAS 2011). We found that indeed signals from different whiskers can converge on the same part of a target cell, and even onto the same synaptic site. Still, by carefully analyzing the activation patterns that arise from stimulating the principal or a secondary whisker, we could tell these distinct signal origin sites apart – and most likely, so can neurons.

A parallel focus of our work in 2011 was disease-related change to neuronal circuits. Given the size of neuronal processes, it is not surprising that these cell appendages are easily damaged in neurodegenerative or neuroinflammatory disorders. For instance, motor neurons, the cells that innervate muscle, can span up to a meter in humans. And indeed, in a group of disorders known as "motor neuron diseases," which includes amyotrophic lateral sclerosis (ALS), these cells degenerate, leading to disability and death in a few years.

Arthur Konnerth   Thomas Misgeld   Bert Sakmann

25 µm
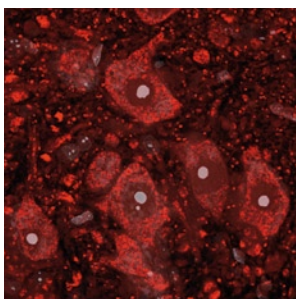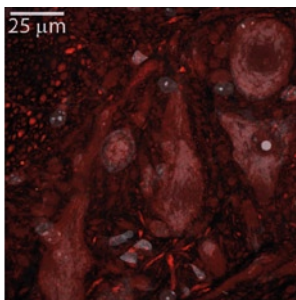
2 | Confocal microscopic images showing motor neurons in the spinal cord of transgenic mice that overexpress either wild-type (top) or ALS-mutated (bottom) forms of the human superoxide dismutase protein (red; a neuronal counterstain is shown in gray). Note the intercellular aggregation of the ALS-mutated protein.

The Misgeld group focused for a while on analyzing the mechanisms by which motor neurons maintain and remodel their long processes. One leading hypothesis is that in ALS transport of organelles inside motor neuron processes is disrupted. By developing tools that allow visualization of such organelles in living mice, we were able to refute this hypothesis for one genetic form of ALS, where the gene for superoxide dismutase is mutated (figure 2: Marinković et al., PNAS 2012). To our surprise, while disruptions of transport are present in some animal models of this form of ALS, others lack this abnormality. At the same time, some manipulations unrelated to ALS (such as overexpressing a normal form of the superoxide dismutase gene that we all carry in our genome) can cause such deficits. We are now focusing on other neurological diseases (e.g., multiple sclerosis) to understand whether transport disruptions might contribute to neurological diseases other than ALS.

Another highlight in 2011 was the "The 12th Otto Loewi and 1st ELSC Conference" that the Konnerth group organized in collaboration with TUM-IAS Visiting Fellow Prof. Yosi Yarom. Held at the Inter University Institute in Eilat, Israel, the conference featured 25 international speakers, who covered the entire range of current cellular and systems neuroscience.

Selected Publications:

[1] S. Varga, H. Jia, B. Sakmann, and A. Konnerth, "Dendritic coding of multiple sensory inputs in single cortical neurons *in vivo*," *Proc. Natl. Acad. Sci. USA*, vol. 108, no. 37, pp. 15420–15425, 2011.

[2] X. Chen, U. Leischner, N.L. Rochefort, I. Nelken, and A. Konnerth, "Functional mapping of single spines in cortical neurons *in vivo*," *Nature*, vol. 475, no. 7357, pp. 501–505, 2011.

[3] M. Oberlaender, C.P. de Kock, R.M. Bruno, A. Ramirez, H.S. Meyer, V.J. Dercksen, M. Helmstaedter, and B. Sakmann, "Cell type-specific three-dimensional structure of thalamocortical circuits in a column of rat vibrissal cortex," *Cereb. Cortex*, to be published.

[4] M.S. Brill, J.W. Lichtman, W. Thompson, Y. Zuo, and T. Misgeld, "Spatial constraints dictate glial territories at murine neuromuscular junctions," *J. Cell. Biol.*, vol. 195, no. 2, pp. 293–305, 2011.

[5] D. Bishop, I. Nikić, M. Brinkoetter, S. Knecht, S. Potz, M. Kerschensteiner, and T. Misgeld, "Near-infrared branding efficiently correlates light and electron microscopy," *Nat. Methods*, vol. 8, no. 7, pp. 568–570, 2011.

[6] P. Marinković , M.S. Reuter , M.S. Brill , L. Godinho , M. Kerschensteiner (*), T. Misgeld (*), "Axonal transport deficits and degeneration can evolve independently in mouse models of amyotrophic lateral sclerosis," *Proc. Natl. Acad. Sci. USA*, 2012 (* equal contribution).

Focus Group **Biophysics**

Prof. Robijn Bruinsma | Hans Fischer Senior Fellow
◉ Prof. Andreas Bausch, Molecular and Cellular Biophysics, TUM

Structural engineering of living cells

The biopolymer F-actin is a crucial component of the "cytoskeleton," the backbone of cells that can grow, shrink, and re-form into different morphologies, depending on the needs of the cell. In cells, F-actin filaments are arranged into multiple geometries by a variety of cross-linking proteins through a fascinating spontaneous
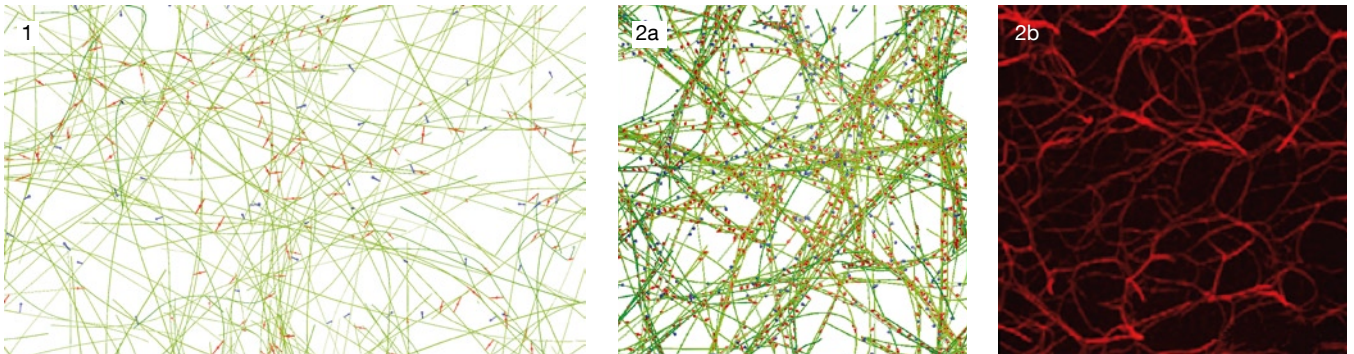
1 | Isotropic gel phase. The 208 filaments are represented by green lines. The diameter of the filaments was reduced for clarity. Doubly-bound linkers are marked as red rods, singly-bound linkers as blue rods. Free linkers are not shown. The system is homogeneous.

2a | Simulated network of bundles. The system was composed of 3,000 isotropic linkers and 208 filaments.

2b | Confocal image of an F-actin/Filamin network of bundles for an F-actin concentration of 2.4 microMolar and a Filamin/Actin molar ratio of 0.1. The scale bar is 100 microns.

process known as "self-assembly" that is not controlled by the DNA of the cell. We carried out simulations of the interaction of F-actin by linker molecules with the aim of understanding the self-assembly of F-actin aggregates. We used a novel simulation platform developed by Dr. Christian Cyron and Prof. Wolfgang A. Wall that was much more realistic in terms of the basic physics of the F-actin filaments and also increased the effective simulation times to about 1,000 seconds of real time. These represent the absolute state of the art in terms of simulations of biopolymer networks. We found that at low linker concentrations, the system formed homogeneous "universal" gels with physical properties independent of the linker molecules. An example of such a universal gel is shown in the figure 1.

These universal gels had been first described in theoretical studies, and they are well known from experimental studies. In the biophysics literature, it is believed that these universal gels are representative of the F-actin systems of living cells. Our study has now cast serious doubt on this.

When we increased the linker concentration, we discovered there is a point at which the F-actin linker system undergoes a "phase transition." Suddenly the system becomes extremely sensitive to the properties of the linker molecules. If the linker molecules are able to connect filaments at all possible angles, then this phase transition is actually a "glass transition" – the system falls out of thermodynamic equilibrium for fundamental reasons, forming networks of bundles that slowly coarsen over time. An example is shown in the figure 2, where our simulation results are compared with F-actin condensation induced by the linker molecule filamin.

Note the similarity between the simulated and observed networks. Our results strongly suggest that the observed networks must be identified with these glassy networks. We discovered that these networks "try" to evolve into a single thick bundle but are frustrated by the linkages between smaller bundles.
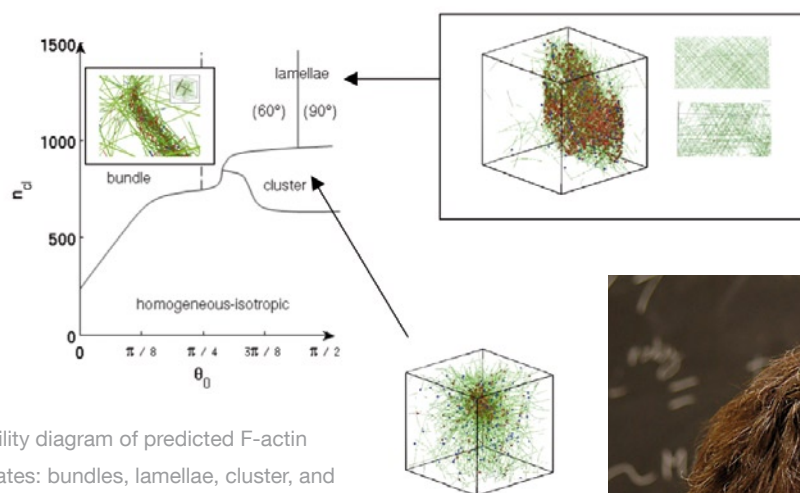
3 | Stability diagram of predicted F-actin condensates: bundles, lamellae, cluster, and homogeneous-isotropic network. Transitions that are discontinuous are shown as straight lines and continuous transitions as dashed lines. Lamellae can exhibit a hexagonal or square symmetry.

When we restricted the permitted range of binding angles between filaments, we encountered a rich "phase diagram" shown in figure 3. The vertical axis is the number of linkers and the horizontal axis the preferred binding angle of the linker molecules.

These different morphologies are not glassy but instead are in full thermodynamic equilibrium. The square and hexagonal lamellar structures had been recently predicted in an analytical study done in Göttingen but had never been seen before. The cluster phase observed experimentally in the group of Prof. Andreas Bausch at TUM was a complete surprise. The results of our simulations led us to formulate a new theory for the self-assembly of F-actin filaments, based on the concept of "dimensional reduction" driven by the entropy of the linker molecules.

We are currently extending these simulations by including the key concept of *biomolecular chirality*. This, again, is only possible because of the new code developed at TUM.

In collaboration with Dr. Christian Cyron, Kei Mueller, and Prof. Wolfgang A. Wall (TUM).

Selected Publication:

[1] K. Zhao, R. Bruinsma, T.G. Mason, "Entropic crystal-crystal transitions of Brownian squares," *Proc. Natl. Acad. Sci. USA*, vol. 108, no. 7, pp. 2684–2687, 2011.
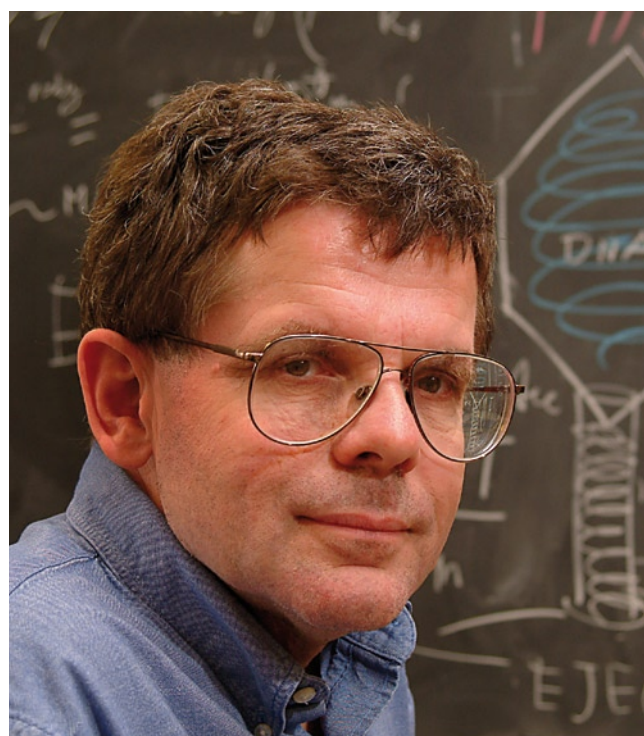
Robijn Bruinsma

received his bachelor's and master's degrees in physics from the Vrije University Amsterdam in 1974 and the Rijks University Utrecht in 1976 respectively. In 1976, he was awarded his doctoral degree from the University of Southern California. Bruinsma joined Harvard University as a postdoctoral fellow from 1979 to 1980. He subsequently became a research associate at the Brookhaven National Laboratory in 1980, where he stayed for two years, followed by a position as visiting scientist at the IBM Research Center in Yorktown. Bruinsma is a Distinguished Professor at the University of California (UCLA), where he started as an assistant professor in 1984. Since 2001, he also holds the chair of Theoretical Physics for the Life Sciences at Leiden University. Among other honors, he has been awarded the Pierre et Marie Curie Visiting Professorship (ESPCI) and the Rothschild Foundation Fellowship. He is a Fellow of the American Physical Society.

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

Stanley Riddell

Christian Stemberger

The vision of the Focus Group "Clinical Cell Processing and Purification" is to establish a fully integrated cell processing platform to facilitate clinical preparation of highly functional and minimally manipulated therapeutic cells for highly individualized medical care.

Building on our recent success in developing the tools necessary for optimal cell purification, we focused on transferring our technology to its first clinical application in cancer immunotherapy.

Our cell processing technology enables us to specifically target and isolate specialized cells of the immune system that provide unique properties for next-generation immunotherapy. Especially in the setting of cancer therapy, it is crucial that therapeutic cells are able to completely eradicate the tumor, including single disseminated malignant cells that might give rise to metastases. Furthermore, these highly effective therapeutic T cells should optimally persist long-term in the patient to prevent re-occurrence of tumor. We identified a special CD8+ T cell subset – a so-called central memory T cell – that fulfill both criteria. This cell type can only be characterized by expression of several surface markers for which we successfully developed selection reagents. These reagents not only allow for the first time enrichment of these T cells from peripheral blood to high purity, but in addition can be completely removed afterwards. By performing sequential positive selections for several different markers, we are now able to isolate specific T cell subsets defined by multiple parameters with excellent purity. Our current work involves automation of these multiple reversible selection regimens to provide an easy-to-use, highly standardizable clinical interface.

To continue the extensive exchange of knowledge between our teams in Munich and Seattle, two doctoral candidates from Munich joined Prof. Stan Riddell's laboratory at the Fred Hutchinson Cancer Research Center in Seattle for six months. During their stay in Seattle, they developed protocols to subsequently engineer highly pure T cell products by genetic modification with a molecularly designed tumor-specific receptor as well as a stably integrated novel "emergency safety" mechanism. The addition of a clinically approved reagent leads to elimination of cells that carry the safety marker on their surface. The doctoral candidates obtained the first data demonstrating the feasibility and efficiency of this safety mechanism in different animal models.

To further extend the applicability of designed tumor-reactive receptors, we have constructed a programmable tumor-specific receptor that allows post-transfer tuning of the receptor. The specificity of the engineered cells is interchangeable by choosing a different small molecule from vast libraries of tumor-specific adaptors. The strategy of using versatile cell products that can be directed against multiple tumor targets promises to become a highly innovative concept for individualized and adaptable therapy.

Selected Publications:

[1] S. Terakura, T. N. Yamamoto, R. A. Gardner, C. J. Turtle, M. C. Jensen, S. R. Riddell, "Generation of CD19-chimeric antigen receptor modified CD8+T cells derived from virus-specific central memory T cells," *Blood*, vol. 119, no. 1, pp. 72–82, 2012.

[2] C. Stemberger, S. Dreher, C. Tschulik, C. Piossek, J. Bet, T. N. Yamamoto, M. Schiemann, M. Neuenhahn, K. Martin, M. Schlapschy, A. Skerra, T. Schmidt, M. Edinger, S. T. Riddell, L. Germeroth, and D. H. Busch, "Novel serial positive enrichment technology enables clinical multiparameter cell sorting," *PloS Medicine*, submitted for publication.
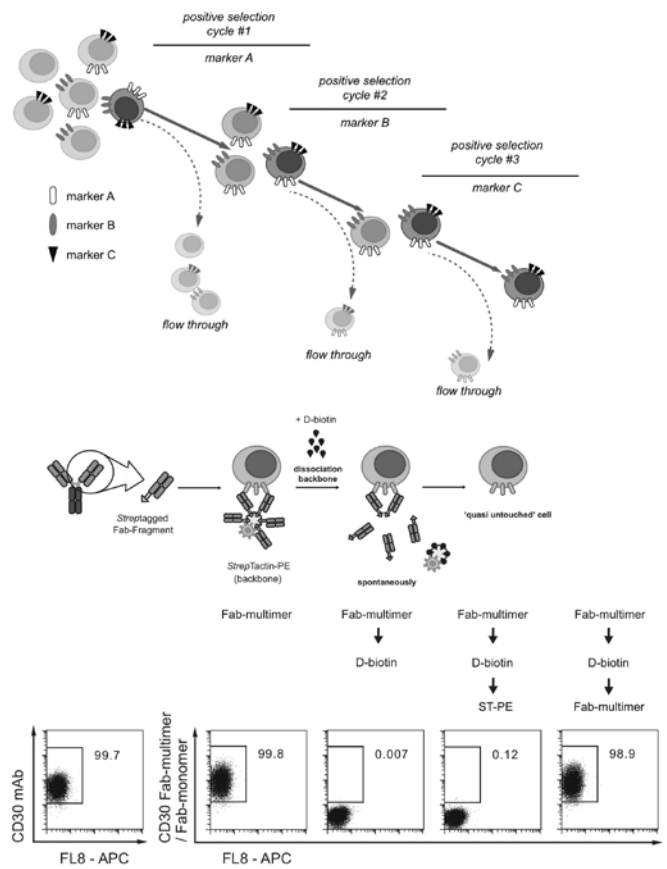
Patrick Regan, Dirk Busch, Christian Stemberger, Stanley Riddell

Focus Group **Biomedical Engineering**

Prof. Axel Haase | Carl von Linde Senior Fellow
Thomas Gaaß, Marika Kuschan | Doctoral Candidates
◎ Prof. Markus Schwaiger, Clinic for Nuclear Medicine, TUM

Axel Haase

Time course of ^{13}C NMR lactate signal in the kidney of a rat following the injection of three different concentrations (20 mM/l, 40 mM/l, 80 mM/l) of ^{13}C-hyperpolarized pyruvate (at time point 0). The normalized signal should reach the same intensity. Lower normalized signal after the injection of high concentrations of pyruvate indicates a partial saturation of the biological system. [2]

In vivo dynamic metabolic MR imaging

NMR imaging is a powerful diagnostic tool as long as ^{1}H NMR signals of water and lipids are used for image reconstruction. However, in order to detect *in vivo* metabolic information, nuclear magnetic resonances from other nuclei, such as ^{31}P, ^{13}C, etc. must be measured from substances having concentrations in the milli-molar range or less. Here, the NMR signal is more than 100,000 times smaller than the ^{1}H signal. In some cases, a method called dynamic nuclear polarization (DNP) can increase the ^{13}C signal of certain metabolites by the same factor. ^{13}C-labeled substances like pyruvate were successfully hyperpolarized in a separate machine and immediately injected into anesthetized rats. During a measuring time of about two minutes, the local concentration of pyruvate and its downstream metabolites, lactate, alanine and bicarbonate, could be measured in several metabolic maps [1].

We have investigated this experiment in more detail and applied it to implanted tumor models. We were especially interested in dose effects of the injected pyruvate. As a major result [2] we found that the dose should be of the order of 10 mmol/l or less to avoid satura-

tion effects *in vivo*. Hyperpolarized ^{13}C metabolic mapping is a promising new tool for diagnostic imaging, especially when the signal-to-noise ratio of the method is further improved by new NMR hardware and imaging techniques. Our experiments are partly funded by a BMBF grant and are performed in cooperation with Prof. Markus Schwaiger, Clinic for Nuclear Medicine, Prof. Steffen Glaser, Department of Chemistry, GE Global Research Laboratory, Garching (Dr. Menzel, Dr. Schulte), and Rapid Biomedical GmbH (Dr. Lanz).
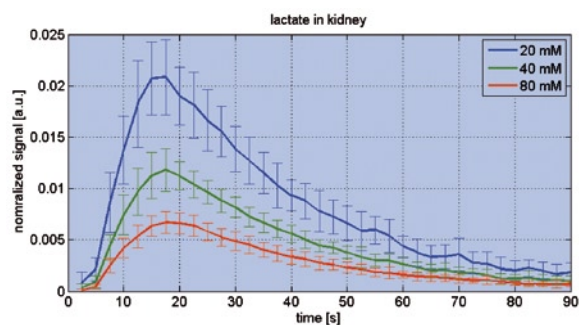
Further experiments in our group are concentrated on magnetic nanoparticles that are optimized to interact with selected proteins and pathogens. We detect the interaction of these particles by changes in NMR relaxation times, and we will use this effect in NMR imaging and diagnostic NMR in general.

Selected Publications:

[1]   F. Wiesinger, E. Weidel, M.I. Menzel, M.A. Janich, O. Khegai, S.J. Glaser, A. Haase, M. Schwaiger, R.F. Schulte, "IDEAL spiral CSI for dynamic metabolic MR imaging of hyperpolarized [1-(13)C] pyruvate," *Magn Reson Med.*, 2011. DOI: 10.1002/mrm.23212. [Epub ahead of print] – to be published.

[2]   M. A. Janich, M.I. Menzel, F. Wiesinger, E. Weidl, O. Khegai, J.A. Ardenkjaer-Larsen, S.J. Glaser, A. Haase, R.F. Schulte, M. Schwaiger, "Effects of pyruvate dose on *in vivo* metabolism and quantification of hyperpolarized ^{13}C spectra," *NMR in Biomedicine*, vol. 25, no. 1, pp. 142–151, 2012.

Focus Group **Nanophotonics**

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

Gerhard Abstreiter

Yasuhiko Arakawa

Silicon is by far the most important semiconductor for device applications in the field of micro- and nanoelectronics. However, limits of conventional downscaling are already being witnessed, and new paradigms are required for future information processing and communication. One promising concept is the development of optical interconnects that could directly link the universally electronic information-processing units with optical information distribution, but efficient silicon-based light emitters do not yet exist. Within our Nanophotonics Focus Group, we are working on two different concepts with the goal of achieving novel photonics devices on a silicon platform.

Project 1: Silicon-based nanophotonics

Silicon-based optical circuits with integrated light emitters are of great technological interest since they would allow for the development of fast optical interconnects with CMOS compatibility. However, the indirect bandgap of silicon results in an extremely low quantum efficiency.

This may be overcome by engineering the photonic environment of optical emitters in Si (Ge islands or impurities).

1 | Three-dimensional Si-based photonic crystal nanocavity with embedded Ge islands as active optical emitters.

We have studied the correlation between emission intensity of self-assembled Ge islands and the quality factor of two-dimensional photonic crystal nanocavities. We observe a clear reduction of the average mode emission intensity under conditions of strong optical pumping as the cavity mode quality factor increases. This is attributable to reabsorption of photons due to free carriers created at high excitation intensities [1]. In addition, we have started in a strong collaborative effort between TUM and the University of Tokyo to fabricate very promising silicon-based three-dimensional photonic crystal nanocavities with embedded Ge islands; these show strongly enhanced spontaneous emission and record high quality factors. An example of such a woodpile 3-D photonic crystal nanocavity is shown in figure 1.

Stefan Funk, Norman Hauke, Thomas Zabel | Doctoral Candidates
Dr. Ilaria Zardo | Postdoctoral Researcher

Project 2: Semiconductor hetero-nanowires on silicon

Another concept for combining optical functionality with Si technology is the integration of III-V semiconductors such as GaAs or InAs on Si. The large mismatch of the lattice constants, however, leads to many defects in conventional III/V hetero-epitaxy. This can be overcome by using novel semiconductor nanowires in which the lattice mismatch is relaxed elastically due to the small footprint on Si.

Our goals in this project are:
· Realization of high-quality optically active III-V nanowires on a Si platform
· Semiconductor hetero-nanowires for quantum electronics, photonics, and sensing
· New-generation photodetectors, solar cells, and thermoelectrics on Si

In the past year we have mainly concentrated on optimization of arsenide-based hetero-nanowires on Si substrates. High-purity GaAs- and InAs-based nanowires with diameters ranging from 30 to 150 nm have been achieved, without external catalyst, by molecular beam epitaxy. The nanowires nucleate in predefined holes in thin SiO_2 on Si (as an example see figure 2) [2, 3]. Also, InGaAs segments can be embedded along the growth axis by adding In in the GaAs case or Ga in the InAs case, forming potential wells or barriers, respectively. The wire growth can be terminated by increasing the arsenic pressure and thus crystalizing the Ga droplet. We can then overgrow the side facets under optimized growth conditions with AlGaAs barrier layers, resulting in coaxial hetero-nanowires with strongly enhanced optical emission efficiency.

2 | Ordered array of InAs nanowires on Silicon fabricated by selective area growth with molecular beam epitaxy.

Selected Publications:

[1] N. Hauke, S. Lichtmannecker, T. Zabel, F. P. Laussy, A. Laucht, M. Kanniber, D. Bougeard, G. Abstreiter, J. J. Finley, and Y. Arakawa, "Correlation between emission intensity of self-assembled germanium islands and quality factor of silicon photonic crystal nanocavities," *Physical Review B*, vol. 84, no. 8, 085320, 2011.

[2] S. Hertenberger, D. Rudolph, S. Bolte, M. Doblinger, M. Bichler, D. Spirkoska, J. J. Finley, G. Abstreiter, and G. Koblmüller, "Absence of vapor-liquid-solid growth during molecular beam epitaxy of self-induced InAs nanowires on Si," *Applied Phys. Letters*, vol. 98, no. 12, 123114, 2011.

[3] D. Rudolph, S. Hertenberger, S. Bolte, W. Paosangthong, D. Spirkoska, M. Döblinger, M. Bichler, J. J. Finley, G. Abstreiter, and G. Koblmüller, "Direct Observation of a Noncatalytic Growth Regime for GaAs Nanowires," *Nano Lett.*, vol. 11, no. 9, pp. 3848–3854, 2011.

Focus Group **Nanophotonics**

Dr. Ulrich Rant | Carl von Linde Junior Fellow
Matthias Firnkes, Markus Schuster, Alexander Schwemer | Doctoral Candidates
◎ Prof. Gerhard Abstreiter, Experimental Semiconductor Physics, TUM

Ulrich Rant

Getting to know proteins – one at a time

Understanding how biomolecules interact with each other is a prerequisite for comprehending the molecular biology of life. Which set of proteins is present in a cell at a given point in time? What functions do the individual proteins fulfill? Which proteins team up (associate) in order to perform different, more sophisticated functions?

In principle, answers to these questions can be found either by looking at many biomolecules simultaneously (ensemble measurements) or by interrogating the properties of one biomolecule after the other (single-molecule measurements). Statistical knowledge about ensembles may often suffice, but sometimes it is important to pay attention to the specific features of individuals. (For example: statistically speaking, humans exactly have one ovarian tube, although this is not the case for anyone I know.) From an experimental point of view, the single-molecule approach poses many challenges, since proteins are delicate objects, being only several nanometers in size. Moreover, they are easily "offended" when scrutinized insensitively, and often lose their function in the attempt to modify them with chemical reporter groups (labels) for detection.

Nanopores are electrical devices capable of the label-free detection of single molecules. A single nanoscale hole is fabricated in a membrane separating two fluidic compartments, which contain the molecules of interest. A voltage is applied between the compartments, electrically driving the molecules through the nanopore. As they pass, molecules briefly disturb (block) the ionic current flowing through the pore and leave a characteristic pico-Ampere footprint in the measured current trace. This scheme has been realized with biological (bacterial protein) channels and artificial (solid-state) pores. Solid-state pores offer technical advantages, since they are robust and can be engineered with state-of-the-art nanotechnology. However, because they are made of inorganic materials such as silicon, they do not exhibit biological function and thus were mainly used as passive orifices and molecular counters up to now.

During the last three years, much of our research focused on "breathing life" into "inanimate" solid-state pores. Recently, our attempts were successful, as we achieved the anchoring of a single protein in a nanopore. This primary protein probes and specifically retards other secondary proteins as they travel through the pore. In so doing, it lends its own chemical properties and biological function to the pore. Because the coupling chemistry used to anchor the primary protein relies on a generic scheme (tris-NTA and His-tags), the primary protein may be selected from a vast number of available proteins, and the pore's biochemical nature can thus be adapted easily.

We demonstrated that such a pore can be employed to discriminate subclasses of IgG antibodies. Differentiating subtle, yet biologically crucial features in molecules proves that chemically modified solid-state nanopores are well suited as stochastic sensors for the analysis of protein-protein interactions on a single-molecule level.

Selected Publications:

[1] R. Wei, V. Gatterdam, R. Wieneke, R. Tampé, and U. Rant, "Stochastic Sensing of Proteins with Receptor-Modified Solid-State Nanopores," *Nature Nanotechnology*, 2012. DOI: 10.1038/NNANO.2012.24

[2] D. Pedone, M. Langecker, G. Abstreiter, and U. Rant, "A Pore-Cavity-Pore Device to Trap and Investigate Single Nanoparticles and DNA Molecules in a Femto-Liter Compartment: Confined Diffusion and Narrow Escape," *Nano Letters*, vol. 11, no. 4, pp. 1561–1567, 2011.
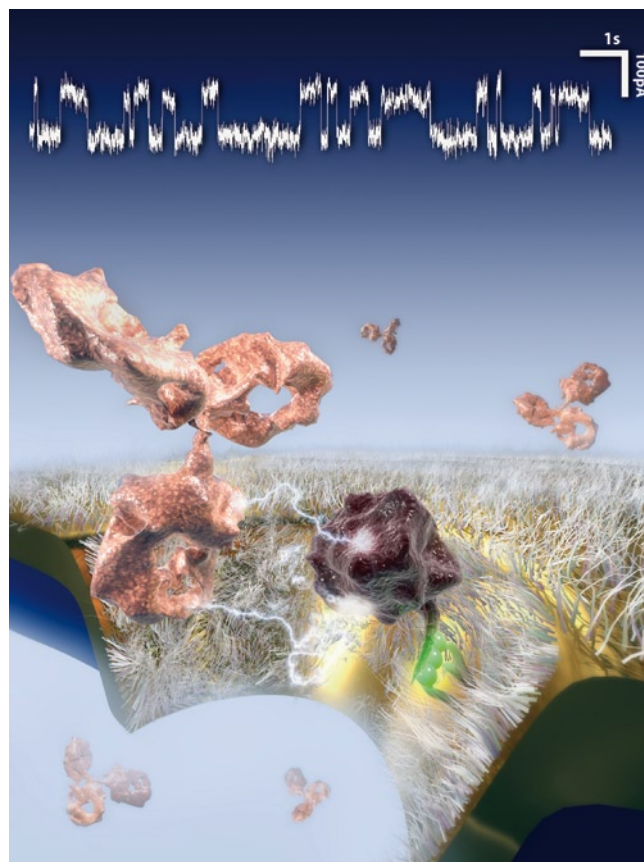
Single proteins are probed with artificially engineered nanopores in solid-state membranes. A primary protein (dark red) anchored within the pore transiently binds an IgG antibody (light red) passing through the pore. Because the pore's ionic conductance is lowered while the antibody resides in the pore, the interaction time can be measured electrically. It reveals the antibody's biological function. A carpet of self-assembled molecules (white hairs) is used to coat the gold pore walls, rendering the surface biologically inert. (Image by Christoph Hohmann, NIM)

Focus Group **Nanoscale Control of Quantum Materials**

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

Probing functionality on the single-molecule level

During the past year, we broadened and deepened our understanding of molecular interaction processes on surfaces. In general, we aim at the controlled assembly and comprehensive characterization of molecular nanostructures on metallic surfaces.

Here, we focus on two highlights. First, we introduced a new approach to extend supramolecular assembly protocols on surfaces to the third dimension [1]. To this end, we developed a bottom-up synthesis procedure that resulted in molecular double- and triple-decker complexes assembled directly on a smooth Ag(111) surface under clean and controlled ultrahigh-vacuum conditions. Specifically, we fabricated cerium bis- and trisporphyrinato species, which are of considerable interest given their electronic properties and potential for molecular rotation. Indeed, rotational motion of the upper porphyrin of these complexes was demonstrated by manipulation with the atomically sharp tip of a scanning tunneling microscope.

As a second example, we explored the binding of carbon monoxide molecules to surface-anchored porphyrin units [2]. The interaction of diatomic molecules with Fe or Co centers embedded in a molecular framework is significant for many biological processes. Notably, metallotetrapyrrole units carry respiratory gases or provide catalytic and sensing functions. We used saddle-shaped Fe- and Co-porphyrins arranged in two-dimensional arrays as templates to study the carbon monoxide adsorption. Complementary molecular-level scanning tunneling microscopy observations and density functional theory calculations revealed a novel binding scheme expressed in a cis-dicarbonyl configuration.

Our future efforts will concentrate on more complex surfaces as templates for molecular adsorption and self-assembly. Specifically, ultrathin textured boron-nitride layers epitaxially grown on metallic substrates bear great promise for an electronic decoupling of molecular nanosystems.

Willi Auwärter

STM image displaying both rod-shaped bare porphyrins and cross-like carbonyl species where CO selectively bridges specific metal-center-nitrogen bonds. Reprinted by permission from Macmillan Publishers Ltd: [Nature Chemistry] [2], copyright (2011).

Selected Publications:

[1] D. Ecija, W. Auwärter, S. Vijayaraghavan, K. Seufert, F. Bischoff, K. Tashiro, and J.V. Barth, "Assembly and Manipulation of Rotatable Cerium Porphyrinato Sandwich Complexes on a Surface," *Angew. Chem. Int. Ed.*, vol. 50, no. 17, pp. 3872–3877, 2011.

[2] K. Seufert, M-L. Bocquet, W. Auwärter, A. Weber-Bargioni, J. Reichert, N. Lorente and J.V. Barth, "Cis-dicarbonyl binding at cobalt and iron porphyrins with saddle-shape conformation," *Nature Chem.*, vol. 3, no. 2, pp. 114–119, 2011.

Focus Group **Functional Nanosystems**

Dr. Ian Sharp | Carl von Linde Junior Fellow
Matthias Sachsenhauser, Sebastian Schöll | Doctoral Candidates
◎ Prof. Martin Stutzmann, Experimental Semiconductor Physics, TUM

Functional nanomaterials for biosensing, dosimetry, and everything in between

Ian Sharp
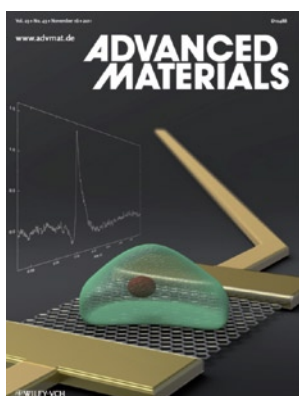
A living cell is cultured on top of a graphene solution-gated field effect transistor (FET) and the cell action potential is detected with the transistor. Arrays of graphene solution-gated FETs can be successfully used to record the electrical activity of living cells, demonstrating superior performance for bioelectronic applications.

At the nanoscale, the properties of materials are primarily governed by their surfaces, where defects and chemical instabilities can be deleterious to function. Fortunately, surfaces also provide powerful opportunities for precisely controlling the properties of nanomaterials for emerging applications, such as artificial photosynthesis, biological sensing, and molecular electronics. Within the Functional Nanosystems Focus Group, we seek to develop new methods of altering surfaces in order to tune the structural, chemical, and electronic properties of advanced materials such as silicon carbide, gallium nitride, and graphene. Through close collaborations, we have applied these fundamental advancements to the formation of active devices for ionizing radiation detection, photocatalysis, and biosensing.

During the past year, we significantly advanced the range of methods available for covalent chemical functionalization of graphene, an ideal two-dimensional material that has a tremendous technological potential due to its unique electronic and structural properties. We demonstrated a process by which covalent grafting occurs at defined chemical sites on the material, thus allowing for precise control over the grafting density. In parallel work, we demonstrated the detection of action potentials from live electrogenic cells grown on graphene transistor arrays.

In collaboration with the Helmholtz Zentrum München, we continued to investigate the sensitivity of AlGaN/GaN heterostructure devices. Working at the BESSY II synchrotron in Berlin, we performed a series of X-ray measurements that proved these devices to be exceptionally sensitive to ionizing radiation, with response times that are unprecedented for wide-bandgap semiconductors. Thus, these devices enable real-time dosimetry, along with the capability for simultaneous biosensing. In addition, we participated in a study to develop gallium nitride for photocatalysis. This included a fundamental study of the properties of this material in electrochemical environments, the coupling of platinum nanoparticles to the surfaces, and analysis of light-induced chemical reactivities. Finally, great progress has been made in functionalization of silicon carbide. In particular, we showed that surface states can be nearly completely passivated by a physical halogenation procedure. Historically, large defect concentrations at silicon carbide surfaces and interfaces have greatly hindered the use of this material for device applications; our findings have the potential to eliminate this obstacle to more widespread commercial use of silicon carbide.

Selected Publications:

[1] M. Steenackers, A.M. Gigler, N. Zhang, F. Deubel, C.H.Y. Xuan Lim, K.P. Loh, J.A. Garrido, R. Jordan, M. Stutzmann, and I.D. Sharp, "Polymer brushes on graphene," *J. Am. Chem. Soc.*, vol. 133, 10490, 2011.

[2] S.J. Schoell, J. Howgate, M. Hoeb, M. Stutzmann, M.S. Brandt, and I.D. Sharp, "Electrical and chemical passivation of SiC surfaces by halogen termination," *Appl. Phys. Lett.*, vol. 98, 182106, 2011.

Focus Group **Functional Nanosystems**

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

Shuit-Tong Lee

The core of our research is devoted to addressing major scientific challenges in areas of long-term and real-time bioimaging by using fluorescent nanoscale materials. To ensure scalability, and thus maximize the impact of new technologies in these fields, we focus on utilizing silicon, which is the leading semiconductor material for technological applications and a naturally abundant material that can be processed at the nanoscale. Our approach includes the design of new nanoscale silicon materials, the creation and study of silicon-based hybrids, and the fabrication of high-performance silicon-based fluorescent biological probes. Two exemplary studies are described here to highlight our approach to integrated nanoscale materials design and implementation.

Fluorescent silicon quantum dots (SiQDs) are highly promising for biological and biomedical applications, due to favorable biocompatibility and low toxicity. However, SiQDs studied to date are hydrophobic and require additional surface modification to render them hydrophilic. In addition to being relatively complicated procedures, such post-treatments often produce adverse effects on the physical/chemical properties of SiQDs. Recently, we have made significant advancements in achieving high-quality SiQDs featuring excellent aqueous dispersibility, strong fluorescence, and robust stability. In particular, we have developed a simple microwave-assisted method for one-pot synthesis of water-dispersible SiQDs. Remarkably, the SiQDs prepared in this way feature excellent aqueous dispersibility, robust stability, strong fluorescence (~ 15%), and favorable sizes (~ 4 nm). They can be easily and rapidly prepared in large quantities in short reaction times (e.g., 15 min). We further demonstrate that the resultant SiQDs are promising biological probes for long-term and real-time immunofluorescent cellular imaging.

Silicon-based nanohybrids made of silicon nanowires (SiNWs) decorated with fluorescent nanoparticles have been developed and utilized for biological sensor applications. Last year, we reported a novel kind of SiNWs decorated with multicolor CdTe quantum dots (QDs), which were directly prepared in aqueous phase via a straightforward one-pot microwave synthesis. Significantly, the QD-decorated SiNWs possess excellent aqueous dispersibility, strong photoluminescence, and ultrahigh photostability, rendering them a promising candidate for various biological applications.

Selected Publications:

[1] Y. He, Y.-L. Zhong, F. Peng, X.-P. Wei, Y.-Y. Su, Y.-M. Lu, S. Su, W. Gu, L.-S. Liao, and S.-T. Lee, "Microwave Synthesis of Water-Dispersible, Ultraphoto and pH Stable, and Highly Fluorescent Silicon Quantum Dots," *J. Am. Chem. Soc.*, vol. 133, no. 36, pp. 14192–14195, 2011.

[2] Y. He, Y.-L. Zhong, Y.-Y. Su, Y.-M. Lu, Z.-Y. Jiang, F. Peng, T.-T. Xu, S. Su, Q. Huang, C.-H. Fan, and S.-T. Lee, "Water-Dispersed Near-Infrared-Emitting Quantum Dots of Ultrasmall Sizes for in Vitro and in Vivo Imaging," *Angew. Chem. Int. Ed.*, vol. 123, no. 25, pp. 5813–5816, 2011.
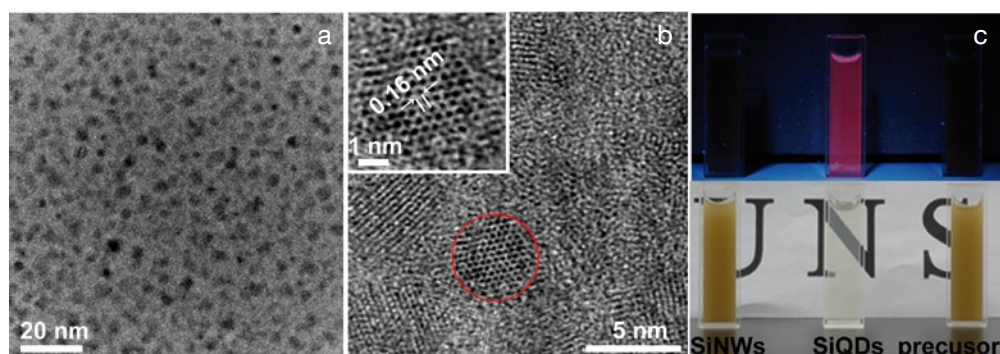
1 | TEM and HRTEM images (a, b) of as-prepared SiQDs. Inset in (b) is HRTEM image of a single SiQD. (c) Photographs of aqueous solutions of dispersed SiNWs (left), as-prepared SiQDs (middle), and reaction precursors (right) under 365 nm irradiation (up) or ambient light (bottom). SiQDs featuring excellent aqueous dispersibility, ultrahigh photo and pH stability, strong photoluminescence, and favorable biocompatibility are facilely and rapidly prepared via a one-pot microwave-assisted method. Such SiQDs are promising biological fluorescent probes particularly suitable for long-term and real-time immunofluorescent cellular imaging.
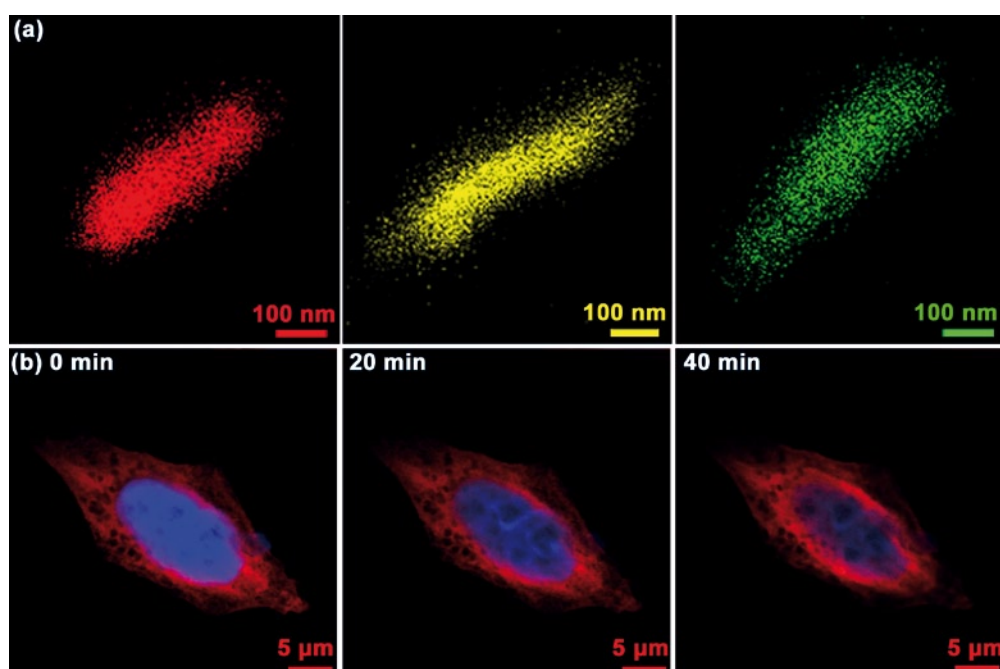
2 | (a) Fluorescence photos of the "green," "yellow," and "red" SiNWs imaged by laser-scanning confocal microscope, and (b) long-term immunofluorescent cellular imaging using the "red" SiNWs hold great promise for multicolor long-term and real-time immunofluorescent cellular imaging.

Focus Group **Nanoimprint and Nanotransfer**

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

Toward cost-effective nanofabrication techniques

Wolfgang Porod

Khaled Karrai

Nanoimprint techniques have been developed in recent years with the motivation of providing an alternative to optical lithography for the realization of silicon integrated circuits. It has in the meantime become clear that the demands and constraints posed by IC fabrication (alignment in the nanometer domain over several layers) can only be met by nanoimprinting if novel alignment methodologies are developed. Nevertheless, a variety of new applications have emerged in the field, including bioelectronics, sensors, and nanofabrication. The aim of the Focus Group is to demonstrate that nanoimprint lithography and nanotransfer are indeed valuable techniques for nanofabrication, in particular when low-cost (and possibly large-area) processes are required.

In recent work, we have shown that metallic nanostructures in the form of lines or dots can be transferred from a patterned mold onto a substrate of choice without any need for post-processing. This is of great interest, for instance, with respect to realization of semitransparent electrodes for electronic and optoelectronic devices exploiting plasmonic effects associated with nanometer dimensions. Alternatively, metallic transferred nanostructures can possibly be used as efficient catalyzers for hydrogen or oxygen production in electrochemical cells.

Not only did we succeed in transferring individual metallic nanostructures, but we also demonstrated that entire functional nanometer-scale devices can be produced with such nanoimprint and nanotransfer techniques. As an example, figure 1 shows an array of metal-oxide-metal diodes that have been transferred from a stamp onto a silicon substrate. The diameter of each diode is around 60 nm, and the thickness of the oxide layers is just 4 nm. The utility of this method is validated by the fact that the transfer process has a yield of more than 90%, with virtually all diodes working properly. Part of this work was performed while TUM-IAS-supported student Mario Bareiss visited the group of Prof. Wolfgang Porod at the University of Notre Dame.

In a related effort, patterning via nanoimprinting allowed us to fabricate nanomagnets, which in turn are the building block of a new class of circuits based on magnetic field coupling. This activity on nanomagnet logic (NML) is part of a DARPA-sponsored research collaboration that includes, among others, the University of Notre Dame, the University of California at Berkeley, and IBM.

We have also developed a novel compact nanoimprinter based on Attocube positioners. It operates with flexible PDMS molds and can transfer micro- and nanostructures onto a variety of substrates. Compact in size, it could be used inside a vacuum or inert-gas chamber. The need for multichannel, compact, non-invasive and accurate displacement sensing solutions has increased dramatically in just the past couple of years. Ultrahigh-precision systems such as metrological atomic force microscopes, deep-UV mask aligners and nanoimprinters, and ultralarge telescopes require extremely ambitious specifications for nm accuracy and sub-nm sensitivity.

Edgar-Otto Albert, Mario Bareiß, Armin Exner, Qingqing Gong, Muhammad Imtaar,
Klaus Thurner, Anandi Yadav | Doctoral Candidates

The challenging constraints include immunity against drift on the subnanometer scale over hours and even days, compactness, low energy budget, and affordable cost. During the last year we tested the limits of novel original technological solutions invented a few years earlier at Attocube Systems AG. The multiple-channel sensor system is entirely based on optical fiber technology operating at telecom wavelength, and its sensing heads are small enough (typically sub-cm) to conveniently fit in tight or constrained spaces. A quadrature signal of the interferometric beats is generated using a novel patented technique that can account for both the amount and direction of displacement. The initial subsystem consists of a multitude of very compact and passive interferometer displacement sensing heads. The second consists of a central laser and electronic control unit capable of simultaneously analyzing the displacement for each interferometer head channel with a 1-MHz bandwidth. The sensing heads are passive, consisting of a single-mode fiber and a collimating lens tube. The sensing head is non-invasive as it produces neither heat nor electromagnetic disturbances. We have verified the functionality of our displacement sensing system (shown in figure 2) with up to 1 km of fiber length connecting the sensor head to the control unit. To ensure a wavelength accuracy of better than 0.5 ppm, we actively locked the telecom laser to a NIST traceable molecular absorption gas cell. The accuracy could be significantly improved if required, with the tradeoff being higher cost.

1 | Micrograph of large-scale array of metal-oxide-metal diodes fabricated by the nanotransfer process. The inset shows a conductive bridge used to make contacts for electrical characterization.
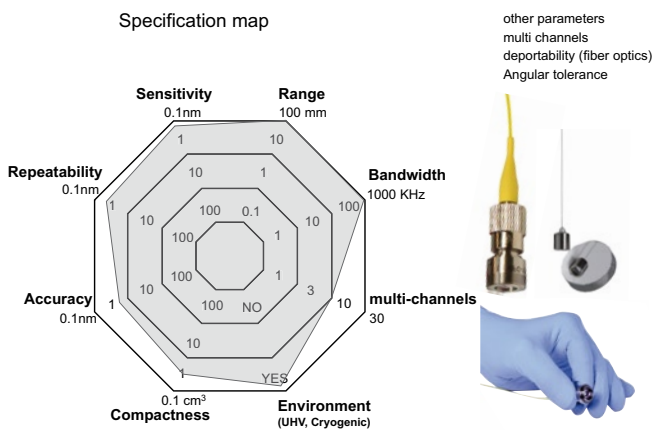
2 | Left, specification chart for the multichannel interferometer. The shaded area corresponds to the specifications reached up to now. The hand is shown holding the larger of the two sensor heads.

Selected Publications:

[1] O. Fakhr, P. Altpeter, K. Karrai and P. Lugli, "Easy Fabrication of Electrically Insulating Nanogaps by Transfer Printing," *Small*, vol. 7, no. 17, pp. 2533–2538, 2011.

[2] M. Bareiss, B.N. Tiwari, A. Hochmeister, G. Jegert, U. Zschieschang, H. Klauk, B. Fabel, G. Scarpa, G. Koblmuller, G.H. Bernstein, W. Porod, and P.Lugli, "Nano Antenna Array for Terahertz Detection," *IEEE Transactions on Microwave Theory and Techniques*, vol. 59, no. 10, pp. 2751–2757, 2011.

[3] M. Bareiss, A. Hochmeister, G. Jegert, U. Zschieschang, H. Klauk, R. Huber, D. Grundler, W. Porod, B. Fabel, G. Scarpa, and P. Lugli, "Printed array of thin-dielectric metal-oxide-metal (MOM) tunneling diodes," *J. of Applied Physics*, vol. 110, no. 4, 044316, 2011.

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
Prof. Stefan Pokorski | Hans Fischer Senior Fellow

Fundamental physics at the dawn of big discoveries
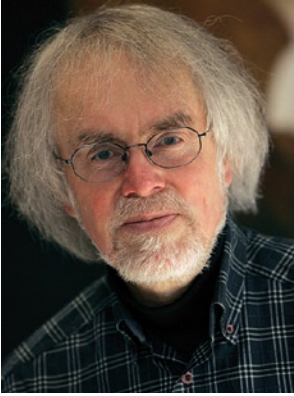
The first important data from the Large Hadron Collider (LHC) at CERN, presented at the summer conferences in 2011, opened an exciting era for fundamental physics or more specifically elementary particle physics. In addition to the direct search for the famous Higgs particle and new particles present in various extensions of the Standard Model of particle physics enabled by the ATLAS and CMS experiments, the LHCb experiment provides the first more precise information on very rare decays of the so-called B-mesons, which are governed by quantum fluctuations. While ATLAS and CMS experiments will provide new insight into the origin of mass, the LHCb experiment will bring new understanding of the origin of the matter-antimatter asymmetry of the universe that is essential for our existence. All three experiments already probe distance scales of order 10^{-19} m, and this resolution will be reached by complementary high-precision experiments in Europe, Japan, and the USA later in this decade.

Extensive research studies of the last 30 years demonstrate that at such short distance scales new phenomena, new heavy particles, and new forces should be discovered, enhancing our understanding of the hierarchical structure of quark and lepton masses and of their interactions. Moreover, a number of deviations from the Standard Model predictions have been identified in high-precision measurements in the last few years. While no definitive signal of Higgs particle or new phenomena could be identified at the LHC in 2011, many particle physicists expect that this will be the case in 2012 when the experimental data from the three LHC experiments in question will improve.

The research in the Focus Group Fundamental Physics related to the exploration of shortest distance scales is primarily dealing with the flavor physics - that is, the physics describing different kinds (flavors) of leptons and quarks, their flavor violating interactions, and their masses. While some of our research is related to the phenomena explored by ATLAS and CMS, in particular those related to Higgs particles, our studies are more closely related to the LHCb experiment, which opens up new era of precision experiments addressing flavor violating interactions. In this context our group has been performing, for several years already, detailed analyses of various extensions of the Standard Model of particle physics, identifying patterns of flavor violation and correlations between various observables that would allow us with the help of future precise experiments to uncover what kinds of dynamics, new interactions, and new particles exist at the scales of order 10^{-20} m and even shorter distance scales. These activities were intensified in 2011 through the ERC Advanced Grant awarded to Prof. Andrzej Buras. This project has as the main goal the construction of the fundamental theory of flavor and had its start in May 2011. It will continue until April 2016 and will be predominantly performed in the TUM-IAS building. In addition to project leader Prof. Andrzej Buras and his group, the groups of Prof. Gino Isidori and three professors in Munich, Prof. Gerhard Buchalla (LMU) and Prof. Alejandro Ibarra and Prof. Michael Ratz (both TUM) will be involved in this expedition to shortest distance scales.

Andrzej Buras

Martin Gorbahn

Emmanuel Stamou | Doctoral Candidate
Dr. Luca Merlo, Dr. Robert Ziegler | Postdoctoral Researchers
◉ Prof. Andrzej Buras, Theoretical Elementary Particle Physics, TUM

A very important role in these activities is played by the postdoctoral researchers contributing to the life of our group in the TUM-IAS building: Dr. Jennifer Girrbach, Dr. Luca Merlo, Dr. Minoru Nagai, and Dr. Robert Ziegler. The ERC grant awarded in 2011 will enable three new postdoctoral researchers to join our efforts in the fall of 2012.

The highlights of our research in 2011 can be summarized as follows:

One of the important results of our efforts toward flavor theory was the construction of a minimal theory for quark masses [1]. This theory attributes the observed hierarchy in the quark masses to the hierarchy of interactions of SM quarks with new very heavy fermions with masses of order of a few TeV and in the reach of the LHC. While the Higgs particle is present in this framework, it is only responsible for the generation of the masses of SM gauge bosons W and Z and the spontaneous breakdown of the SM gauge symmetry. The observed masses of quarks and their flavor-violating interactions are generated through the dynamics of new heavy quarks. We made significant progress toward a detailed analysis of phenomenological implications for flavor physics with participation of Jennifer Girrbach.

One of the main properties of the Standard Model 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, in a more fundamental theory at much shorter distance scales, parity could be a good symmetry implying the existence of right-handed (RH) charged weak currents. In 2010 Prof. Andrzej Buras, Katrin Gemmler, and Prof. Gino Isidori formulated an effective theory with the goal to study these phenomena in a bottom-up approch. In 2011 a different team [2] in a top-down approach investigated properties of right-handed (RH) currents in a specific model with increased gauge symmetries and new heavy gauge bosons and Higgs scalars. In particular it has been pointed out that the heavy Higgs particles in this model, having masses well beyond the reach of the LHC high-energy experiments, could leave footprints in precision flavor observables. This analysis demonstrates clearly that flavor physics can probe distance scales as short as 10^{-20} m. On the other hand, the corresponding new gauge bosons having masses of order of a few TeV could be discovered at the LHC.

Recently models with large-gauged flavor symmetries have been proposed in the literature. The goal of these constructions is again the explanation of the quark mass spectra and their observed flavor interactions. This time, in addition to new heavy fermions, heavy neutral gauge bosons are also invoked for this purpose. The question then arises whether such models for fermion masses are consistent with rare flavor-violating transitions. While such claims have been made in the literature, our group has demonstrated [3] that the models of this type appear to have problems in satisfying all existing data on the rare transitions in question.
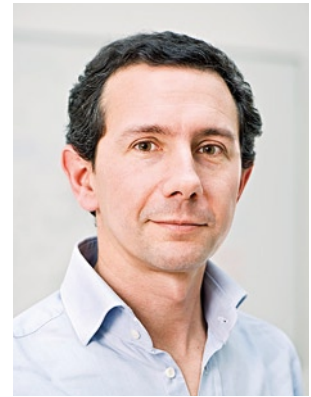
Gino Isidori
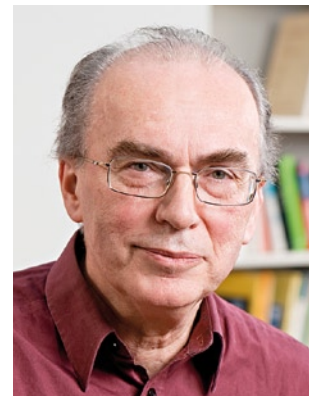
Stefan Pokorski

Supersymmetric Grand Unified Theories (SUSY GUTs) are very popular and well motivated extensions of the Standard Model (SM). In GUTs all three forces of the SM merge to a single force at a very high energy scale, 10^{-16} GeV, which corresponds to times shortly after the big bang. Furthermore quarks and leptons are related to each other, which is not the case in the SM, and these correlations can be tested in experiment. Such correlations between quark and lepton physics can be investigated in a controlled manner in an SO(10) SUSY GUT model studied in [4], where the atmospheric neutrino mixing angle induces large new effects in B physics and charged lepton transitions. The current data is still compatible with this model. However, with the help of this analysis and further data from the LHC this model can be probed more precisely in the coming years and depending on the measurements could even be ruled out.

In the context of supersymmetric extensions of the SM, we have analyzed a possible flavor symmetry able to accommodate current data from the LHC (in particular the absence of direct signals of supersymmetry) and, at the same time, solve some of the existing tensions in low-energy data (in particular the tiny discrepancy between the predicted and the observed amount of CP violation in B meson mixing). We found that the minimal supersymmetric extension of the SM with a flavor symmetry is a particularly interesting candidate in this respect, and we have further investigated its signatures at the LHC [5]. On the other hand, more exotic supersymmetric models are needed to explain the anomalous forward-backward asymmetry in top-quark production observed at the Tevatron [6].

A significant deviation of the measured size of CP violation in K meson decays from SM prediction has attracted significant attention in the past years. Improved theory predictions are needed to truly falsify the Standard Model, in this case with the currently observed deviations of high-precision measurements. Through a demanding calculation Dr. Martin Gorbahn and Dr. Joachim Brod [7] were able to show that hitherto unknown quantum corrections in the SM lead to a significant shift away from the experimental value, and that previous analyses underestimated the theoretical uncertainty. A calculation analogous in spirit has been done for theoretically clean rare K decay [8].

Selected Publications:

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[2] M. Blanke, A. J. Buras, K. Gemmler and T. Heidsieck, "$\Delta F=2$ Observables and $B \to Xq\gamma$ Decays in the Left-Right Model: Higgs Particles Striking Back," *Journal of High Energy Phys.*, vol. 2012, no. 3, 024, 2012.

[3] A. J. Buras, M. V. Carlucci, L. Merlo and E. Stamou, "Phenomenology of a Gauged Flavour Model," arXiv:1112.4477 [hep-ph].

[4] J. Girrbach, S. Jäger, M. Knopf, W. Martens, U. Nierste, C. Scherrer and S. Wiesenfeldt, "Flavor Physics in an SO(10) Grand Unified Model," *Journal of High Energy Phys.*, 2011, no. 6, 044, 2011.

[5] R. Barbieri, G. Isidori, J. Jones-Perez, P. Lodone, and D. M. Straub, "U(2) and Minimal Flavour Violation in Supersymmetry," *Eur. Phys. J. C*, vol. 71, 1725, 2011.

[6] G. Isidori and J. F. Kamenik, "Forward-Backward $t\bar{t}$ Asymmetry from Anomalous Stop Pair Production," *Phys. Lett. B*, vol. 700, pp. 145–149, 2011.

[7] Joachim Brod and Martin Gorbahn, "The NNLO Charm-Quark Contribution to CP-violation and Delta M(K)," *Phys. Rev. Lett.*, to be published.

[8] Joachim Brod, Martin Gorbahn, and Emmanuel Stamou, "Two-Loop Electroweak Corrections for Rare K-Decays," *Phys.Rev. D*, vol. 83, no. 3, 034030, 2011.

From TUM-IAS to the World: Carl von Linde Junior Fellows

After just a few short years in operation, the TUM Institute for Advanced Study has the evidence to back up a fairly bold claim: that it is not only a good place for a researcher to be, but also a good place to be *from*. This shows most clearly in the trajectories of promising young scientists whose careers the Institute has helped to launch, particularly through the Carl von Linde Junior Fellowship. The first "alumni" of this program for advanced postdoctoral researchers have already achieved prominent positions and impressive results.

At the age of 30, Robert Stelzer left the TUM-IAS for a full professorship at Ulm University. For Adrian Jäggi, the Carl von Linde Junior Fellowship was a step toward a full professorship at the University of Bern. Marco Punta, Ian Sharp, and Ulrich Rant are principal investigators and project leaders at prominent research institutes in England, the United States, and Germany, respectively. In addition, intellectual property generated by Uli Rant's research is on a path toward commercialization in a novel type of scientific instrumentation.

Adrian Jäggi

On January 1, 2012, Adrian Jäggi became director of the Astronomical Institute of the University of Bern (AIUB) and a professor in the university's Faculty of Natural Sciences. The research focus at the AIUB is on fundamental astronomy: About 25 co-workers cope with a wide variety of problems in celestial mechanics, astrometry, satellite geodesy, and the history of astronomy. The AIUB operates the CODE (Center for Orbit Determination in Europe) Analysis Center of the International GNSS Service (IGS) in a consortium with the Swiss Federal Office of Topography (swisstopo, Wabern), the German Federal Agency for Cartography and Geodesy (BKG, Frankfurt), and the TUM Institute for Astronomical and Physical Geodesy. Every day precise GPS and GLONASS satellite orbits, coordinates of GPS/GLONASS tracking stations, Earth rotation parameters, satellite and receiver clock corrections, global ionosphere maps, and station troposphere parameters are computed and made available to the scientific community for geodetic research. A prime example of such research is the GOCE project for the determination of Earth's gravity field, where the AIUB, within the framework of the European GOCE Gravity Consortium, is in charge of computing the precise science orbits of the GOCE satellite. The AIUB also operates the Zimmerwald observatory near Bern, which is equipped with a 1-m multipurpose astronomical telescope used for satellite laser ranging and for astrometric and photometric observations of natural and artificial celestial bodies. The combination of observational skills and development of algorithms for data analysis and interpretation has a long tradition at the AIUB, which will be continued in the future.

"Thanks to the Carl von Linde Junior Fellowship," Jäggi says, "I was able to establish my academic profile in a very short time span. The TUM-IAS was the perfect stage for establishing a long-lasting cooperation between Bern and TUM, and it helped to establish gravity field research performed in our TUM-IAS Focus Group, Satellite Geodesy, as a new branch at the AIUB. I would like to express my sincere thanks to the entire TUM-IAS team and to Reiner Rummel, my host at TUM, for the unique time I spent in Munich."

Marco Punta

As a project leader at the Wellcome Trust Sanger Institute near Cambridge, UK, Marco Punta is in charge of developing and maintaining the Pfam protein sequence database; he and his co-workers also use the database to produce original research. The Sanger Institute is a world-renowned center for genome sequencing and analysis, primarily funded by the Wellcome Trust, an independent charity. A leader in the Human Genome Project, it is now focused on understanding the role of genetics in health and disease. For example, the Institute has an important role in the 1000 Genomes and UK10K projects, which seek to shed further light on human genetic variation and on its links to human disease.

Pfam is a database that clusters conserved protein regions into families based on sequence similarity. A large number of scientists around the world use Pfam for manual or automatic functional annotation of protein sequences. "I am enjoying my new job greatly," Punta reports, "along with new challenges in terms of project, people and time management. The Sanger, sharing the Genome Campus with the European Bioinformatics Institute, is a great place to work and do research."

"I am very thankful to the TUM-IAS," he adds, "for having given me the opportunity to further develop my skills and improve my publication record over the course of my year and a half in Munich. After spending a number of years as a postdoctoral researcher at Columbia University in the city of New York, it was especially important to me to have a chance to return to Europe in a top institution. The associated funding, which I used mainly for traveling and for inviting other researchers to Munich, was a great added value. I have very fond memories of the time I spent at TUM as a Carl von Linde Junior Fellow in Burkhard Rost's group. In fact, since I left in March 2011, I've already been back to visit my old group and the TUM-IAS twice, keeping up with my scientific collaborations at TUM. I wish also to thank all of the TUM-IAS staff, as everybody has always been extremely helpful and kind to me. I think the people working at the TUM-IAS create a most graceful atmosphere for the Fellows, and I am always happy to go back to Munich and visit the beautiful new Institute building on the Garching campus."

Ulrich Rant

Uli Rant continues to advance his research and his career here at TUM, within the framework of the Walter Schottky Institute and the Chemistry Department. He leads the 20-person Bio-Nanostructures research group, which currently has projects focusing on the interaction of biomolecules down to the single-molecule level and the optical properties of nanostructures. The group has pioneered the switchsense technology, a novel method for analyzing proteins and DNA with a biochip. It will be commercialized by the Munich-based startup company Dynamic Biosensors, which was recently founded by Rant and colleagues from TUM and Fujitsu Ltd.

Reflecting on his Carl von Linde Junior Fellowship, Rant says: "Getting started as an independent scientist is hard. You've got many ideas, but only a limited track record to prove that you will actually make them work. It may sound cheesy, but what you need is someone who believes in you, even if you are pursuing ideas off the beaten track. The TUM-IAS gave me the means and the time to follow my interests and simply work. The results obtained during my TUM-IAS Fellowship were not only of scientific merit, but they also were important for building my personal track record. Eventually, this enabled me to raise funding to continue my work in the future.

"Administrative issues usually are the researcher's nightmare. While knowing that it is necessary to track how public funds are spent, at the same time you despise every minute wasted on working through regulations and filling in forms. It simply keeps you from focusing on what you are actually paid for: figuring out why your experiments didn't work! The TUM-IAS lets you do exactly that. You talk about ideas, and they help you put them into practice. Lean, efficient, constructive.

"The TUM-IAS not only facilitates science through direct support but also through the environment and social network it generates. I remember a dinner after a TUM-IAS annual meeting where I complained to Bert Sakmann (a Hans Fischer Senior Fellow) about lacking a special current amplifier that I needed for single-molecule experiments with nanopores. Two days later, I was standing in Bert Sakmann's lab. He handed me one of his instruments and said, 'Do something useful with it.' In the two years that followed we published six papers on the topic."

Ian Sharp

Ian Sharp's research propelled him from the TUM-IAS to the Joint Center for Artificial Photosynthesis (JCAP), a United States Department of Energy Innovation Hub with sites at Caltech and Lawrence Berkeley National Laboratory. JCAP's stated mission is to develop and demonstrate a manufacturable "solar-fuels generator," made of Earth-abundant elements, that will take sunlight, water, and carbon dioxide as inputs and produce fuel from the sun.

Critical requirements for achieving highly efficient solar-fuel generation devices include detailed understanding and control over interfacial charge-transfer pathways, along with reduction of charge-trapping centers. Ian Sharp is responsible for overseeing the design, construction, and operation of a comprehensive measurement facility being developed at Lawrence Berkeley National Laboratory to address these scientific challenges. In addition, his core research program will include both collaborative and independent investigations of complex interfacial phenomena that are inherent to artificial photosynthesis devices.

"As a staff scientist and principal investigator at JCAP," Sharp says, "I not only have the privilege of interacting with the world's leading scientists in the renewable energy field, but I also have the honor to assist in finding a solution to the foremost challenge facing humankind: the search for a clean and renewable source of energy to drive the modern world forward.

"The TUM-IAS played a critical role in preparing me for this. I was given both the freedom and the resources necessary to establish an independent research group. The opportunity to manage students and scientists, develop new research programs, and closely interact with leading researchers provided the experience required for success in my current position. As I build up my research group at the Lawrence Berkeley National Laboratory, I will constantly draw on the invaluable experiences and connections that I gained as a Carl von Linde Junior Fellow. I am extremely appreciative of the unique opportunities afforded me by the TUM-IAS."

Robert Stelzer

Currently a full professor at the Faculty of Mathematics and Economics of Ulm University, Robert Stelzer also heads the university's Institute of Mathematical Finance. Among other responsibilities, he teaches financial mathematics and stochastics for programs including "Mathematics and Management" – the first of its type in Germany and a success story taken over by TUM and many other universities – as well as an international English-language master's program in finance. Stelzer is an active member of the faculty's focus research area "Financial services and their mathematical foundations" and a principal investigator and deputy speaker of the DFG-funded research training group 1100, "Modeling, analysis, and simulation in economy mathematics." Currently he supervises, in Ulm and at TUM, four doctoral candidates and two postdocs.

"The TUM-IAS Fellowship enabled me to set up my own research group starting with two doctoral candidates," Stelzer recalls, "and thus I could learn how to be a good advisor and how to devise and lead a research group. I was also able to teach master's courses of my own, which led to advising several students on their master's theses. Moreover, I had the opportunity to deepen and broaden my knowledge and research, and to extend my scientific network, thanks to the international composition of our TUM-IAS Focus Group – Risk Analysis and Stochastic Modeling, chaired by Carl von Linde Senior Fellow Claudia Klüppelberg – and its international workshops on current research topics. I worked on many interesting research projects related to risk analysis and stochastic modeling, and I continue to be very active in a number of special topics that I first explored through the TUM-IAS.

"The great amount of time and freedom for research at TUM-IAS allowed me to publish many papers in leading journals and to finish my habilitation in February 2011. All these possibilities and the excellent research conditions were essential in preparing me to leave TUM, after 2½ years as Carl von Linde Junior Fellow, to assume the position of a full professor."
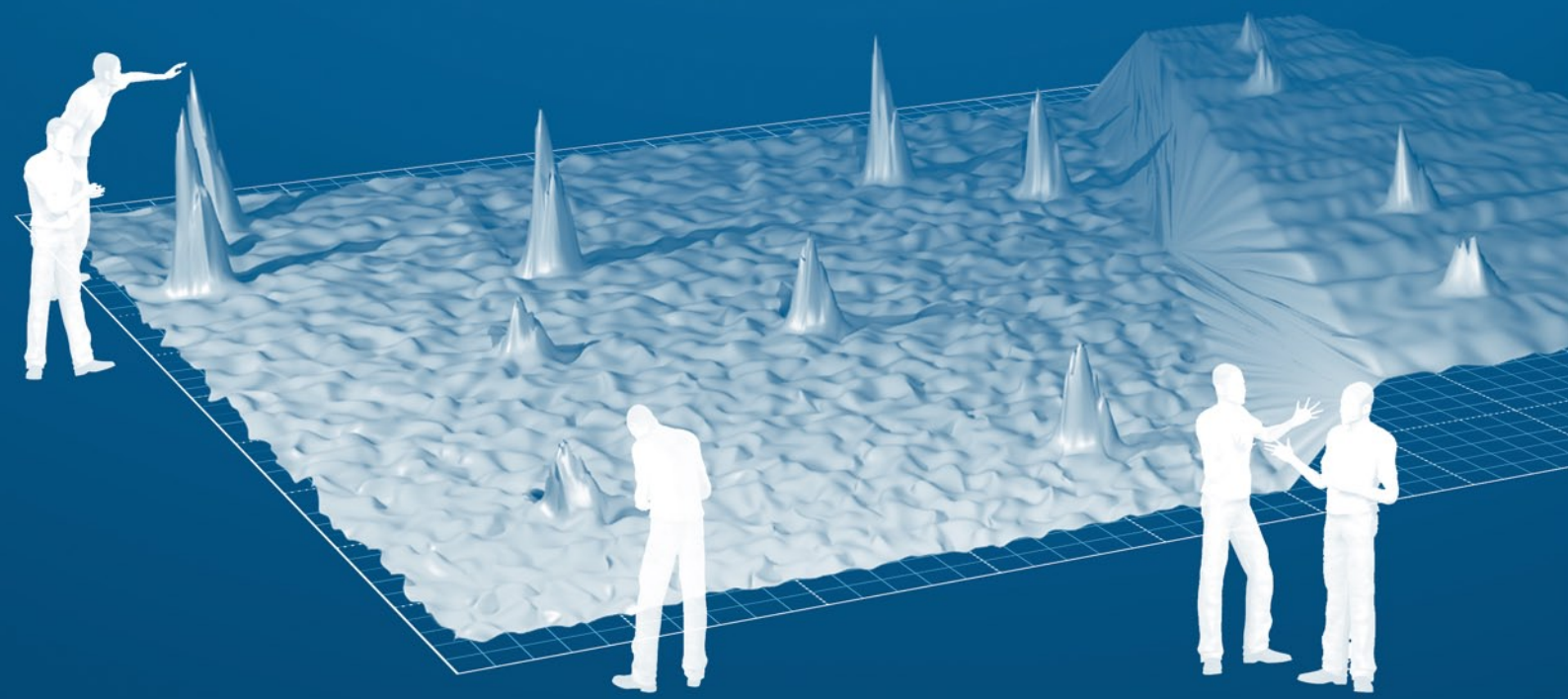
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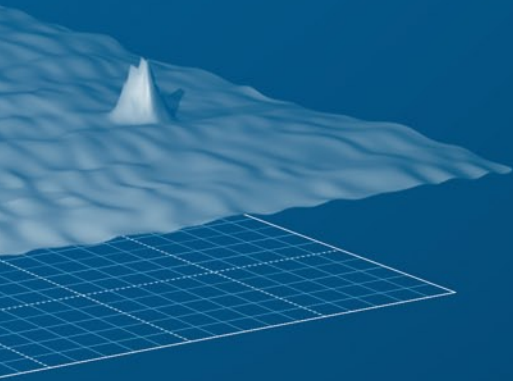
In Focus **High-Performance Computing**
Excerpts from an interview on January 30, 2012

Patrick Regan

At one end of the Internet-video call, Hans Fischer Senior Fellow Markus Hegland (MH) and TUM doctoral candidate Christoph Kowitz (CK) were easing into a warm summer evening. Still shaking off the chill of a winter morning were Carl von Linde Junior Fellow Miriam Mehl (MM), postdoctoral researcher Dirk Pflüger (DP), doctoral candidate Valeriy Khakhutskyy (VK), and TUM Professor Hans-Joachim Bungartz (HB), host of the High-Performance Computing Focus Group (and co-coordinator of a new DFG Priority Program on "Software for Exascale Computing").

Meetings like this, linking TUM's Garching campus with Hegland's home institution, the Australian National University in Canberra, are nothing unusual for this tightly knit group of researchers. The only thing out of the ordinary was devoting a whole meeting to answering a reporter's questions, all the while doing a remarkable job of seeming unaware of the circling, snapping photographer. The aim of the meeting was – and the aim of this article is – to offer a special kind of insight into how the TUM-IAS functions by looking inside its basic working unit, the Focus Group.

As in most of the TUM-IAS Focus Groups, basic scientific questions and application-oriented issues intertwine with and enhance each other throughout a program that is, by necessity and design, multidisciplinary. In this case, the research focuses on problems in computer science, mathematics, engineering, and physics that have been brought to the fore by advances in supercomputing technology; at the same time, applications ranging from aerospace engineering to plasma physics stand to benefit from the results. (PR)

PR: The concept of high performance gets redefined a lot more frequently for computers than, say, for automobiles. What does "high-performance computing" mean today, and looking ahead over the next decade or so? And why do the performance trends raise new research problems?

HB: It has always meant the top level of computing power that is available. Today a typical benchmark would be several petaFLOPS, meaning 10^{15} floating-point operations per second, and within ten years we definitely will have entered into the "exa" era, 10^{18} FLOPS. For decades, beginning in the 1960s, it was the machines themselves that dominated the field of high-performance computing. But over the past ten years, algorithms and software have been getting more of the focus.

People see that if you have a fast car, a Ferrari, you need someone who is really able to drive it. That's basically where we are today: People see that if the hardware moves on at such a speed, then there won't be that many groups that are really able to manage all the software issues.

There's another reason this is a turning point. For a long time, people in application areas could avoid the difficult transition to parallel computing – which requires parallel programming – by buying a bigger machine with a small number of faster processors. But today, at around 3 GHz, the processors are coming to a physical boundary, and going into the parallel is your only chance.

MM: That's something we all have to face, the problem of getting a complex algorithm, either composed of different models or involving multiple dimensions, to a multicore computer.

HB: I always give this analogy: If a field needs to be ploughed, typically a farmer would prefer four big oxen to one billion ants. But what we will have in the future is one billion ants, and the farmer has to think about how he can do his classical jobs, no longer with four strong oxen but with the ants. And that's the technological challenge we have now.

PR: Coming from a farming family, I can say that sounds like a discouraging prospect. But I get the point: A change as radical as that is unavoidable for high-performance computing. What are the implications?

MM: In the past if you did parallelization, 64 processors was already a lot. That's what you still hear in some fields. But now we have to face a hundred thousand processors, and we have to do completely different things. For example, you have to handle faults. You have hardware that doesn't work as you would expect it to. Think about having a hundred thousand cores, and you can calculate the probability that something doesn't work.

HB: It will get even harder to get pieces of software that run decently, to get data into and out of the computer, to get the data processed, and also to extract the knowledge out of the numbers. Imagine that you have just one set of data with 10^{18} bytes – someone has to tell us what this means, whether it is a weather forecast or some technical project. Parallelization, and in particular in a massively parallel way – not tens or hundreds, but hundreds of thousands of processors – is the biggest issue. However, this goes beyond a mere parallelization in the sense

Hans-Joachim Bungartz, Miriam Mehl

of taking existing codes and algorithms and turning them into something parallel by force. Many current algorithms have intrinsically sequential parts. Think of a coffee machine – the standard joke that coffee comes first and the cup drops out at the end is an example of a sequential part of an algorithm. One interpretation of that, called Amdahl's law, led to a very critical perspective on parallelism for decades. However, not all that is sequential in an algorithm is enforced by the underlying problem. Sometimes, we just have to think about a completely new algorithm design. To "think parallel" – designing algorithms and programs that are inherently parallel, and which could only be sequentialized by force – that's what is needed.

PR: This transition to larger-scale multicore processing is just part of a whole constellation of "multi" issues that come up in your group's research plans and publications: multiphysics – meaning the coupling of multiple physical models – multidimensional, multiscale, multilevel. What's the best way to sort them out for people, like me and most of our readers, who are outside this field?

HB: There is a way of classifying all these multis. Maybe this reduces the jungle a bit. There are multis that come from the problem, which is typically multiscale. A phenomenon like turbulence, for example, is multiscale. You have very tiny vortices, but these tiny vortices define the macroscopic picture. Multidimensional is also coming from the problem, because you have the dimensionality in the problem. Then you have a second group of multis that deal with the algorithms, how you want to work on these problems. Multilevel for example is a classical approach to tackling multiscale; it's the algorithmic weapon that lets you represent a multiscale phenomenon in a very efficient way.

And then you have a third group, not the algorithmic but the technological weapons, such as multicore. Multicore has nothing to do with the problem, has not that much to do with the algorithms; that's just the machine part. If you think in terms of the three boxes associated with problems, algorithms, and hardware, then maybe there's less chance for confusion about all these multis and the interplay between them.

MM: They are all related with each other, and that means you cannot just focus on one topic. You need them all to be high-performing in the end. Why do we do multiphysics? Because one model is not accurate enough. Typically you neglect something. If you simulate an airplane only simulating the flow, you don't include the flexing, up-and-down movements of the wings and their interaction with the flow again. So to be more accurate you need multiphysics, and then you have to be accurate on each field. And for that you need the multicore. And if you want to optimize in addition you have multiple parameters, and then you are in the multidimensional field.

DP: To tackle today's challenges, you can't as a scientist just choose a problem, go back to your room, and come back a few years later with a solution. That just doesn't work any more. The problems are too complex. So you need to bring different ideas together, and you need a group that tackles a variety of sub-problems. That's one of the big advantages of the TUM-IAS Focus Group.

Patrick Regan

Valeriy Khakhutskyy and Dirk Pflüger

PR: That puts the spotlight on the other big "multi" in the picture, multidisciplinary. I'm interested in understanding how the group divides the problems and melds the diverse activities into an integrated program bigger than the sum of the parts.

HB: There's a strong bias toward the multidimensional right now, with Markus, Christoph, Dirk, and Valeriy working mainly on that. Miriam is concentrating on multiphysics. We're hoping to be joined in 2012 by someone who will focus more on multicore; for now I'm wearing the multicore hat, which is natural since I serve on the directorate and steering committe of the Leibniz Supercomputing Center. I'm eager to spend more time thinking about parallel concepts, working on parallel solutions for important problems where the current state of algorithmics faces huge roadblocks. But to be honest, finding time for that will not be easy for me, since I'm also serving as the "glue" for our Focus Group, helping to keep the three threads together.

As Miriam said, these things are interwoven, much more than you'd suspect from the way they have been addressed in the past. Typically the groups are quite separated, especially the multidimensional, which lies more in classical computer science or applied mathematics and not that much in physical modeling. But here we are bringing in a classical multiphysics problem from plasma physics and trying to combine it with a multidimensional approach and then to bring it into a multicore machine.

That's a unique chance we have here with this group, but it calls for an orchestrator, so that's my main role.

PR: Sometimes it helps to have a musician in the group, any kind of group.

HB: It's true, over the weekend I was playing Beethoven and Bruckner. Yes, I like the orchestrator metaphor better than glue.

PR: One common theme seems to be that models and predictive analyses are inherently limited for the same reason that they work, because you've abstracted something out of reality. Could you tell me more about the various ways you're working to close the distance between simulation and the real world, or between prediction and the way things happen?

MH: Let's consider the multidimensional aspects. In the early days of computation, the first flow simulations for example were in two dimensions. That's as you say an abstraction from the real world, and the real world is three-dimensional. So it was a big

improvement of course when we got simulations that could really deal with three-dimensional effects; that's especially important in fluid flow. But now we're looking at breaking the barrier and adding even extra dimensions. Why do we need extra dimensions? Well, let's say with fluid flow, in addition to our three-dimensional spatial variables, we can have different velocities, for example in gases, in the same places. So we have an additional three dimensions, and that gives us six. Now why don't we have that in traditional fluid dynamics? That's because a distribution is assumed at every point. We assume a so-called Boltzmann law or a Gaussian law of the velocities. But for realistic simulations, in many areas we need at least six dimensions.

VK: My research will be on data mining in high dimensions, where we have problems with ten, twenty, or a hundred dimensions. We're looking at actual data, any measured data, either from simulations or from real measurements, and here "dimensions" means the number of parameters that we can simultaneously deal with. For data mining this means

Christoph Kowitz and Markus Hegland

having lots of data, looking at the relationships be-tween the data, and trying to induce the rules and make predictions. The challenge is how to master these problems using methods from computational science. And there are a lot of applications.

For example, one of the next projects we'll be working on has to do with time series predictions in all kinds of applications, like financial series or physics. Every-where we have data depending on time, measures are taken every moment of time, and in order to get the prediction correct, you have to consider everything that happened in the past. That's where high dimen-sions can appear.

MH: Talking about predictions, that is a very impor-tant problem too. Starting in the 1990s, for example, we worked together with insurance companies and predicted risk. Insurance companies need to be able to predict the risk of having an accident, and banks need to predict the risk of default. These predictions are based on features, lots of different features that will al-low you to predict the risk that some event will happen. Similarly, companies like Google and Amazon try to predict what an individual might be interested in, and agencies involved with security or immigration control have questions that are basically not so different.

The main tools used for prediction are mathematical functions. You can have functions of many variables, and of course each variable can take on many differ-ent values. If you have a new customer, typically this new customer will have features that are different from the ones you've seen in other customers. How do you interpolate between all these other customers? So you have a function with 20 varia-bles, and you need to interpolate what you've seen before. Or you need to do a regression. That's a classic problem, which Valeriy and Dirk have also worked on. And of course my main interest is in computation.

How can we do this fast? And there's this curse of dimensionality. So one way is to calculate the values of your functions for all possible customers. And again you have this curse of dimensionality. So if you have your first feature, and you can take ten different values, and the second one can take ten different values, you have a hundred combina-tions. It's a combinatorial problem really. And if you have a third feature, you know, you have already a list with a thousand values. If you have ten features, you have ten to the ten different values. That's a lot of values. And it's infeasible to even store these things. That's one reason we use so-called sparse grids. But another interesting aspect is that a col-league of mine, Jochen Garcke, found that some of the traditional combinatorial techniques we used were unstable.

PR: Meaning what?

MH: Unstable means basically that small perturbations or small errors can have a big effect. That's something that you know from extrapolation. These techniques are related to extrapolation. Weather forecasting, for example, is extrapolation. It's very difficult. You can get it wrong. The further you want to extrapolate, the worse it is. So you tabulate on a regular grid, and you want to extrapolate what is in between the values on the grid. And you have exactly the same effects as if you would like to predict what happens to the stock market in the future. It can go wrong. Extrapolation is, we call it, inherently unstable. But we have an answer. We have a cure for this instability. We have a stable approach based on relatively classical numerical techniques, an idea in numerical analysis; you can show that you can solve these problems, partial differential equations, by relating them to minimization problems. Minimization problems are inherently stable, whereas extrapolation problems are inherently unstable, and we found a way to cure this instability by reframing it as an optimization problem. I'm working also with Christoph on applying this concept, which originally came from our work in data mining, in more general contexts in physics.

PR: I'd like to hear more about this "curse" of dimensionality, which comes up regularly in group members' papers. What exactly does it mean?

CK: It may be easiest to explain in connection with an application. I'm collaborating with scientists at the Max Planck Institute for Plasma Physics in Garching. The larger context is research toward a future energy source from nuclear fusion rather than fission. The basic idea is to magnetically confine isotopes of hydrogen in a really hot vessel so that nuclei fuse together and produce energy.

The problem there is they want to simulate the behavior of a hot fusion plasma in this vessel, a so-called tokamak. The simulations are done to be able to confine the plasma effectively, to prevent the particles from going out of the interesting zone, the hot zone in the plasma, so that they are fusing. You have a spectrum of applicable models. You can have a single-particle description, where you just take every plasma particle

for itself, to look how it's moving through the magnetic field. At the other end of the spectrum you can have a fluid-like description of the plasma, where you say, this is a continuum, or more or less a gas, which is acting a bit stranger than a regular gas. And somewhere in between these extremes are the gyrokinetic simulations that the IPP physicists are doing. They don't have single particles – the particles are not resolved themselves – what you have is more like a statistical description of these particles; but it's still more complicated and more detailed than a gas-like description or a fluid description. So, somewhat "in between."

What the physicists are especially interested in is simulating the turbulence, with high resolution in space and time, to be able to understand how it works in detail. And there we're not just using a three-dimensional fluid simulation, but a five-dimensional simulation, a so-called gyrokinetic simulation. The problem is now if you want to simulate something in five dimensions, you have to resolve it in this space. And just to get a moderately high resolution in this space, you already need vast amounts of data points. So there are huge amounts of data you have to handle and you have to do computations with. Here we've really come to the curse of dimensionality.

Just imagine a really small one-dimensional space. If you want to have a cube in one-dimensional space, it's basically just two points, left and right. If you extend that cube to two dimensions you get a square, and that's already four points. If you extend it to three dimensions, you already get eight points, which is a three-dimensional cube. Now imagine just adding two more dimensions. You're suddenly at 32 points for that cube, and this is just the smallest cell that you can resolve – but for this plasma physics code you need vast amounts of these unit-squares or unit-cubes. For current simulations, which run on supercomputers for days or even weeks, they have up to one billion data points, which is 200 gigabytes of data they do computations with.

For each of them you have to do some computations, and then you move on to the next time step. Then you do all the calculations again, and then again you move a tiny bit forward in time. But only that way are you able

to resolve the turbulence, to understand what's really going on in that tokamak. If you don't understand that, then it will be harder to confine that 200 million degree plasma.

PR: And this is without even considering any multiphysics aspects of the fusion plasma simulation.

CK: That's right. I'm focusing at this point on ways to handle the multidimensionality of the gyrokinetic turbulence simulation using the IPP code called GENE.

PR: Meanwhile, Miriam, you are leading the multiphysics effort. I guess the most familiar example of multiphysics would be the coupling of atmosphere and ocean models to produce more reliable weather reports or climate simulations. Here you're focusing mainly on coupling flow models for fluids such as air, water, or circulating blood with models of flexible solid structures. What are the difficulties, and how are you addressing them?

MM: Imagine two people meet at a conference and decide to couple one code that solves for fluid flows with another that does structural mechanics computations. You first have to tackle this technically, how to make these two codes talk to each other, and then you probably notice that you get something that is not reasonable at all. You may get for example large oscillations, wings breaking away from the plane, and that's just the numerical instability. So then you have to add something there, and once you have done all this, you probably want to concentrate on efficiency, how to make the solving fast, not only stable, and of course also accurate. And the next step will be to bring this onto a large machine, so there of course you have additional difficulties. We have several codes, they should run in parallel, preferably in a load-balanced way, so you should prevent a situation where one part is ready very fast and the other one runs over a long time and you have idle processors. It's a challenge to run just one code efficiently on a multicore machine.

One of the things we use to address multiphysics problems is a coupling environment called preCICE, which was originally developed in our group under a grant from the German Research Foundation. That was originally developed for fluid-structure interactions. The idea was to have something that works in a way that computer scientists always like things to work, in a very modular way. The idea is you have two solvers, fluid solver and structure solver, and you just plug them together with this glue software, and then everything works. And once you decide you want to exchange your flow solver – because you want to simulate a different application with different needs, and you've found a specific solver that works for that – you exchange it and all the other parts remain unchanged.

That's something you don't find in currently available commercial tools. There is commercial multiphysics software, but it's not modular in this sense. There also is coupling software, but it doesn't have the full functionality. You don't just need a tool that performs data communication between two codes. There's also numerics in it: So, how do you iterate, how many

times do you call the flow solver, the structure solver, in one time step, and in which order, and what data do they exchange? There is a lot that should be in that central coupling unit, because if it's in one of the solvers, you have to redo everything every time you exchange one of the parts. That was the original idea, and it has more and more become a generic tool for coupling different physics. That's the direction we are going, to make it more generic, not only for fluid and structure, but also to make it work for other kinds of multiphysics applications. And on the solver side, we've found we can greatly enhance performance by implementing certain kinds of data structures, particularly tree-structured adaptive computational grids. We have a home-grown flow solver called Peano that brings both hardware efficiency and numerical efficiency to simulations of fluid-structure interactions.

PR: A concept that comes up a lot in your papers, in all kinds of different contexts, is "sparse grids." What does it mean, and how does it help?

DP: If you are dealing with high-dimensional problems, you can't just use your brute force approaches, the classical ones. You have to try to represent the important structures with as little effort as possible, and you have to try to adapt to certain properties of the problem at hand. With sparse grid techniques you focus on the most important things first, and then try to express the less important parts, and if you can start to neglect some of those parts, you can tackle really high-dimensional problems. And that's where my focus is, trying to express, with as little work as possible algorithmically, computationally, the high-dimensional problems.

We're also building a software toolbox called SG++, for dealing with these high-dimensional problems using spatially adaptive sparse grids. We're trying to include the basic ingredients for different types of high-dimensional problems, from plasma physics to data mining to other problems, option pricing in finance for instance, bringing those things together to provide the means of tackling that whole range of problems.

HB: If you have one dimension, you have n points. If you have d dimensions, then you have n to the d points. So n square, n cube. So to achieve a specific accuracy for your problem, you have to invest n to the d points. If d increases, this is the curse of dimensionality. So the question now is: Is there any strategy you could develop where you can do only with n – that is, where you always invest, say, 117 grid points, and it doesn't matter if you are in a one-dimensional or a 15-dimensional domain. And the answer is funnily yes, and this is Monte Carlo; there you don't work with grid points, but you work with degrees of freedom. So you need 117 shots, and you can get similar quality, and the problem is not interested in the dimension of your domain. But the drawback is that you get a very lousy approximation quality.

So that's the reason why so many people work with Monte Carlo. It works, it is easy. But as soon as they have something else, they turn to something else, because something else is basically always better. And now the question was, is there anything else? This was the idea of sparse grids, and the result is now – I simplify strongly but – the result is that you get an algorithm that lets you work with a number of grid points that only moderately depends on the dimensionality and still obtain the same quality that you get with the n to the d approach. So that means you get a product of the same quality but for a much smaller price. It is attractive for three dimensions – you can just increase your resolution and make things finer – but it is essential for the higher-dimensional case, because now you can do something numerically in situations where you could not do anything numerically apart from Monte Carlo before. That's a very rough idea of it.

PR: Research involving sparse grids has a history in Munich, doesn't it – including your own contributions?

HB: It has a history in Munich, and it has a history beyond Munich. The new era of sparse grids started in Munich around 1990 with the work of Christoph Zenger and his PhD students at that time. The older part of the story is like always. I always say you have to do this "cherchez le Russe" – you have to find

the Russian or the Chinese guy who did it before. In the case of sparse grids, we haven't discovered the Chinese guy yet, but there are definitely Russian guys in the 1950s, in approximation theory. But no one did anything practical with it, or even thought of solving partial differential equations. The equations are something that definitely came with this reinvention, but the mathematics behind it goes way back, to Archimedes. So now I have to draw a picture. The task of Archimedes was to get the area of the parabola, but he didn't have calculus, he didn't know about an integral. But he could make points here, and then trapezoids, and calculate the area of each trapezoid and sum them up. As the story goes, Archimedes' wife came along and said that's not accurate enough, so you have to introduce additional ones. And the problematic thing is then you have to forget everything you've calculated so far; you have to do it completely from scratch for every change in the grid points, which is extremely expensive if you don't have a pocket calculator.

Good mathematicians are always lazy. So he thought about something to improve that, and this is where this picture comes in, where he invented this so-called hierarchical basis. He said let's start with a big triangle, and let's add smaller and smaller triangles. And you see with this first big triangle, it already is quite a decent approximation. And if you add the next two, then you've already improved the precision. This is how Archimedes in the third century before Christ was basically defining all the ingredients you need for the sparse grids. Not in higher dimensionality in this case – that came later – but the main idea.

So I would therefore say that the first hour as far as we know so far is actually Archimedes sitting on the beach and thinking about integrals.

At this point, laughter was heard from the Australian end of the videoconference.

MM: And now they're sitting on the beach.

HB: They are trying to mimic this, sitting on the beach and thinking and getting great ideas like Archimedes.

PR: That brings me to a simple, practical question. You've explained a lot about what makes the group a group, such as the interconnectedness of the problems and the active role of Hans as orchestrator. But I'm also interested in how the advantages of this geographically challenging collaboration outweigh the potential disadvantages.

HB: We met Markus before, at conferences, but thanks to the TUM-IAS we have now a framework to collaborate in a deeper way – together with time and free space to think about things – and I think that's a very important contribution you cannot overestimate in that context.

DP: We are spending a great effort to bridge the gap between Australia and Germany. Currently Christoph is over there, and I was in Australia the last three months of 2011. At the beginning of June, Markus will be here. We have video group meetings on a regular basis.

MH: We talk to each other of course when there are pressing scientific questions that we need to discuss. But in addition to that, our colleagues from Munich join by video in an extended research group meeting I have every Wednesday, typically a group of ten or so including five or six doctoral candidates.

CK: When I'm here at ANU, I can work intensively with Markus, and that's definitely one advantage. But it's not only Markus. We are now working together with Mike Osborne and other scientists here. I'm not a mathematician, so for me it's always

interesting to hear what the mathematical PhD candidates or professors are thinking. It's interesting to get in this different environment where people see my problem in a completely different way, or bring up problems where I don't see any problems at all.

DP: When I was there, we even started new projects. We were able to look at new scientific problems, which is not that easy to do via electronic communications alone.

PR: Can you give an example?

DP: There is one subtask I ran into using sparse grids for classification. We found a solution that works, but we didn't understand how it works or why it works from a theoretical point of view. Now, bringing together our hands-on approach from computer science and Markus's knowledge from mathematics, we've been able to study that and gain a deeper understanding. This is something that needs plenty

of discussions, that needs intensive cooperation, and that just doesn't work electronically, in my experience.

MH: And of course this close connection to Munich, to Garching in particular, has advantages for me and my research group at ANU.

HB: I think if you look on a European scale, from a computational point of view, there is no better place to do this. Facing each other across Boltzmannstrasse in Garching are, on one side, our computer science and mathematics departments and the Leibniz Supercomputing Center, and on the other side, the Max Planck Institute for Plasma Physics (among others!) and their computing center. Complementary expertise in theory, practice, and applications situated right here, and now we have crossed the street. But beyond that, there's another special advantage over other places that have big machines, challenging applications, and active research – that is the ease with which we can bring in the young scientists, for example through TUM's International Graduate School of Science and Engineering and our computational methods study programs.

Going back to the "multi" of multidisciplinarity: It is invoked today actually in an inflationary way, but I think it's really true for this group, and it can be an especially mind-opening experience for young scientists. In your everyday work you can be trapped in your discipline. That starts with teaching, with the colleagues you typically meet, and with your way of thinking. But here we can really bring together mathematics with computer science and with the applications in physics and engineering, with a great scope for different ideas and perspectives. It can be difficult to get your mind open in this way if you are 50 or above – I can say this because I am 49 – and I think it's important that we really put this into researchers' lives very early. Then you see the mixture as a natural thing, and monodisciplinary research as more or less the exception. That's where we should be heading, and I think this is a splendid opportunity where we can actually live it. ∎

Institute Activities
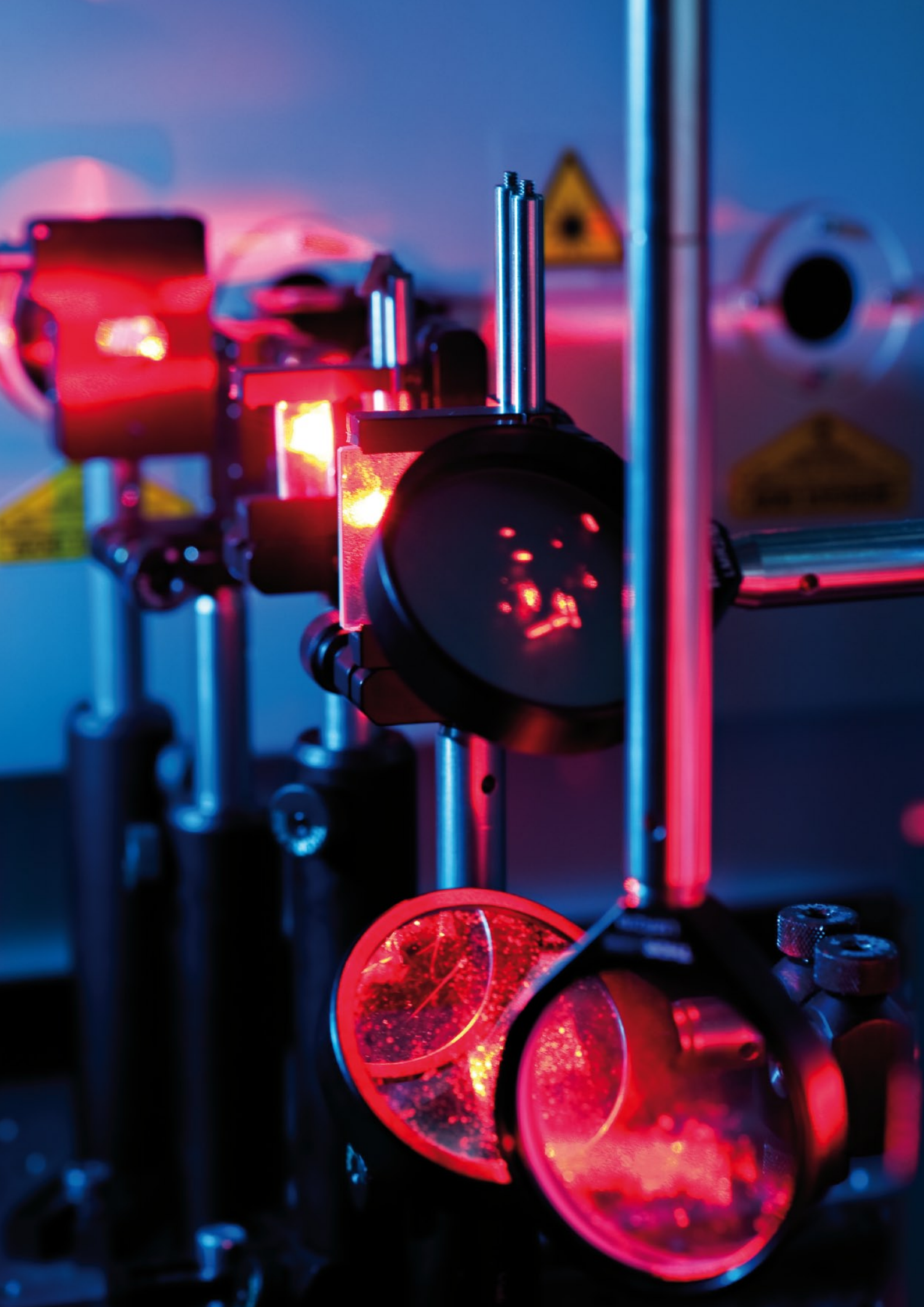
Fellows' Lunches

To cultivate the spirit of multidisciplinary exchange among its scientific community, TUM-IAS made it a tradition to host a monthly Fellows' Lunch during the academic year. Every Fellows' Lunch is dedicated to a topic of general interest to the members of the Institute, which is presented and subsequently discussed among the participants. The aim of these lunches is not only to strengthen the network within the Institute's community but first and foremost to advocate a multidisciplinary approach among the TUM-IAS Fellows.

The following topics have been launched into in 2011: "Information" (Prof. Gerhard Kramer), "Carbon" (Prof. Gerhard Abstreiter, Dr. Jose Antonio Garrido), "Rebuilding the Energy Infrastructure" (Dr. Philipp Gerbert), "Extreme Event Ecology" (Prof. Annette Menzel), "Climate from Tree Rings" (Dr. Christian Zang), "Soil Architecture" (Prof. Ingrid Kögel-Knabner), "Probing Molecular Interactions with Highly Amplified Magnetic Resonance Spectroscopy" (Prof. Song-I Han), "Biophysics" (Prof. Robijn Bruinsma), "Engineering Risk Analysis" (Dr. Chin Man W. Mok), and "Technology and Society" (Prof. Isabell Welpe), as well as a general discussion on "Systems and Biology."

Several lunches have also been dedicated to summaries of the latest workshops and the input they brought to the different areas of expertise the TUM-IAS is covering. Last but not least, the lunches are also a means to identify promising topics and research fields for the future of the Institute.

Inaugural Lectures

January 27

Exploring Functional Molecules on Surfaces

Speaker:
Dr. Willi Auwärter
Carl von Linde Junior
Fellow
Molecular Nanoscience
and Chemical Physics of
Interfaces, TUM

Abstract: The comprehensive characterization and engineering of low-dimensional nanostructures on surfaces is of great current interest, both from scientific and technological points of view. Specifically, the growth of molecular architectures on well defined surfaces, applying self-assembly protocols inspired from supramolecular chemistry, is a maturing and rapidly advancing field of research.

Dr. Willi Auwärter's group puts particular emphasis on systems based on porphyrin molecules. 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. Scanning tunneling microscopy (STM) and spectroscopy (STS) allow the researchers to look at the interior of these molecules and to address key questions related to their functionality: How do the molecules adapt to a surface? What stabilizes highly regular self-assembled structures? How do the porphyrins respond to small gas molecules, and can they act as conductance switches or molecular rotors?

February 9

Entropy of Systems with Nonlocal Interactions

Speaker:
Dr. Vladimir García
Morales
Carl von Linde Junior
Fellow
Nonequilibrium Chemical
Physics, TUM

Abstract: Statistical mechanics of complex systems with memory, dynamical correlations, and nonlocal and nonlinear interactions are the subject of current intense study. The complex dynamics of these systems render standard Boltzmann-Gibbs thermostatistics unapplicable in many situations. Boltzmann entropy is a well established concept close to equilibrium if correlations and nonlocality are negligible and the available phase space is densely filled by the trajectory of the system.

In his talk Dr. Vladimir García Morales considered situations where Boltzmann entropy cannot be used. He demonstrated that a new formalism, generalized statistical mechanics, leads to the appropriate entropic form for fractal phase spaces in the microcanonical ensemble. Several applications to physico-chemical and electrochemical systems were described and elucidated through this theory including: correlations in highly charged electrolyte solutions, capacitance of monolayer protected nanoclusters, and enhanced electrochemical kinetics at the nanoscale. Possible applications to spatially extended electrochemical oscillators and electrochemical turbulence were also discussed.

February 23

Farewell Lecture: Sequence, Structure, Function: An Insider's View on Protein Structural Genomics

Speaker:
Dr. Marco Punta
Carl von Linde Junior
Fellow
Bioinformatics, TUM

Abstract: Structural knowledge is critical for understanding and for being able to manipulate protein function at the molecular level. From its inception ten years ago, structural genomics (SG) has greatly contributed to the increase of structural

coverage of the protein sequence space and to the development of new methods that accelerate structure determination. In the first part of this talk, Dr. Marco Punta discussed his experience of several years in SG with a particular focus on recent advances in the study of challenging targets such as membrane proteins. Overall, as of January 2011, SG has deposited close to 10,000 structures into the public domain, with one particular twist regarding their annotation: A significant fraction of these structures are for proteins of unknown function. In the talk's second part, he argued that these proteins represent an important, yet still largely untapped, resource. Protein discoveries might be just a click (or two) away.

February 24

Speaker:
Dr. Ian Sharp
Carl von Linde Junior Fellow
Experimental Semiconductor Physics, TUM

Physics and Chemistry at Hybrid Semiconductor Interfaces

Abstract: Hybrid materials offer significant potential for applications ranging from renewable energy generation to biological and chemical sensing. However, the inherent complexity of multiphase systems composed of inorganic semiconductors, (bio)organic molecules, and electrolytes remains a critical hurdle to fully exploiting their properties.

Dr. Ian Sharp explained that the aim of his group's work is to develop a more complete understanding of charge transfer processes occurring at the bio-inorganic interface and to exploit such findings for formation of functional structures at the nanoscale. They utilize a variety of physical and chemical processes to create electrically passivated surfaces with tailored chemical reactivities onto which functional molecules and proteins may be bound. The alignment of energy levels within the various components of these bio-inorganic systems is investigated at all stages of assembly.

In this talk, the general approaches to functionalization of various semiconductors were addressed. Furthermore, recent results on photo-induced charge transfer between wide bandgap semiconductors and short chain molecules, as well as photosynthetic reaction centers, were presented. Dr. Ian Sharp concluded with a discussion of the group's efforts to extend these methods to graphene, an ideally two dimensional material that presents both great opportunities and new challenges.

May 26

Speaker:
Prof. Raman I. Sujith
Hans Fischer Senior Fellow
Aerospace Engineering, Indian Institute of Technology, Madras

Non-normal & Nonlinear Dynamics of Thermoacoustic Instabilities

Abstract: Thermoacoustic instability is a serious problem encountered during the development of practical combustion systems such as gas turbine combustors, ramjet engines, rocket motors, burners, and furnaces. It is manifested in the form of large amplitude pressure oscillations. These oscillations induce structural vibrations that are highly detrimental to the system. This instability occurs due to the feedback between the unsteady heat release and the acoustic oscillations in a system.

In this talk, Prof. Raman I. Sujith presented theoretical and experimental investigations of the non-normal and nonlinear nature of thermoacoustic interactions. The role of non-normality in subcritical transition to instability (known in the thermoacoustics community as triggering instability) was examined. The multiscale and multiphysics aspects of thermoacoustic instabilities were also discussed.

1/3 – Toward a Global Design Exchange

Speaker:
Prof. Christian Werthmann
Hans Fischer Senior
Fellow
Graduate School of
Design, Harvard
University

Abstract: 1/3 of our urban population lives in cities that were built without the help of planners, architects, or engineers. While Europe keeps shrinking, the nations of the Global South will expand, and with it nonformal urbanism. The matter of fact is that the nonformal condition will account for almost half of our future urban growth; the sheer magnitude of the phenomenon will force us to speak of future nonformal metropolises. The problematic nature of uncontrolled urbanization has been emphasized in the past, as described by Mike Davis in his influential book *Planet of Slums.* But, there is also a growing understanding of the virtues, inevitableness, and moral legitimacy of self-built cities.

Despite all well known shortcomings these cities provide a place for the urban poor to live. Today, a new generation of designers in the Global South has found strategies of useful and very pragmatic engagement. They tactically insert into the conflicted and large territory of self-made cities carefully calibrated infrastructures and landscape interventions. At the same time, European and North American trained designers and engineers increasingly pursue work outside of their countries. Whether willingly or not, they will encounter conditions in the nonformal cities that they are insufficiently prepared for. Can the designers of the Northwestern hemisphere learn from the designers of the Global South? What are key strategies and tactics? What can the designers of the Northwestern hemisphere add to the growing knowledge of urban poverty and nonformal city improvement in the Global South?

Calender of Events 2011

February 10 **Japanese-German Energy Symposium**
             Organizer: Prof. Ulrich Stimming | Carl von Linde Senior Fellow
             Including a panel discussion "Why do we need electromobility?"

February 10 Workshop **Statistical Methods and Models**
             Organizers: Prof. Claudia Klüppelberg | Carl von Linde Senior Fellow
             Prof. Daniel Straub (Engineering Risk Analysis)

February 28 Symposium **Frontiers in Medicinal Chemistry**
             Organizer: Prof. Horst Kessler | Carl von Linde Senior Fellow

March 22   Talk **Innovationen als Schlüssel für die Zukunft der Mobilität**
             Organizers: Prof. Markus Lienkamp (Automotive Technology) and TUM-IAS
             Speaker: Dr. Thomas Weber, Daimler

March 23   Workshop **Grid and Cloud Computing for Computational (Bio-) Statistics**
             Organizers: Prof. Burkhard Rost (Bioinformatics) and TUM-IAS

March 29   Fireside Chat **Batteries and Storage of Electrical Energy**
             Organizers: BMW and TUM-IAS

March 31– April 1 **4th International GOCE User Workshop**
             Organizer: Prof. Reiner Rummel | Carl von Linde Senior Fellow

April 6   Talk **Rebuilding the Energy Infrastructure**
             Organizers: Dr. Dragan Obradovic | Rudolf Diesel Industry Fellow
             Prof. Sandra Hirche (Automatic Control Engineering)
             Speaker: Dr. Philipp Gerbert (Boston Consulting Group)

May 4 – 6   TUM-IAS General Assembly

After two years at the same location (Hotel Schloss Berg at Lake Starnberg), we decided to move our General Assembly to a real castle. For 2.5 days TUM-IAS community members gathered at Schloss Hohenkammer, an old castle lying off the beaten track outside of Munich. The grand hall offered the perfect atmosphere to

explore new avenues for the Institute and to enhance communication between our scientists. Special emphasis was put on the introduction of research projects by our Fellows nominated the previous year, ranging from talks on "Recent Advances in Cellular Therapies" to "Diesel Reloaded" and "Magnetic Resonance in Medicine." Among others the Focus Groups Global Change and High-Performance Computing, the Research Area Nanoscience, and groups in the fields of Construction

Chemicals and Materials and Stability Analysis outlined their main research issues. The beautiful courtyard and historic arch room were ideal places to have intermissions during which our researchers engaged in vivid scientific discussions across fields. Groups that presented either new ideas or recent results during an animated communication session at the end of each day included the Neuroscience and Satellite Geodesy Focus Groups and the Research Area Risk Analysis. In the afternoon of the last day, the members of our international Board of Trustees came together to discuss the future strategy of the Institute.

May 10	Talk **CH Activation Versus O Insertion in Selective Oxidation of Ethylene and Benzene** ERIC Catalysis Colloquium Speaker: Prof. Rutger A. van Santen (Eindhoven University of Technology, Netherlands)	TUM-IAS Visiting Fellow
May 12	Talk **A Variational Approach to Nonlinear Estimation** Speaker: Prof. Sanjoy K. Mitter (Massachusetts Institute of Technology, Cambridge, USA)	TUM-IAS Visiting Fellow
May 13	Talk **Hydrodynamic Instabilities in Aircraft Gas Turbine Engines** Speaker: Dr. Matthew Juniper (University of Cambridge, England)	TUM-IAS Visiting Fellow
May 17	Panel discussion **Integrative Organization of Complex Dynamical Systems** Moderator: Prof. Klaus Mainzer (Carl von Linde-Akademie) Speakers: Prof. Sanjoy K. Mitter (Control Theory), Prof. Jürgen Scheurle (Dynamical Systems), Prof. J. Leo van Hemmen (Theoretical Biophysics), Prof. Gerhard Kramer (Communications Engineering)
May 24	Talk **When Do We Want it? Now! A Query Theory and Neuroscience Account of Intertemporal Preference Construction** Speaker: Prof. Elke Weber (Columbia University, New York)	TUM-IAS Visiting Fellow

May 27	Talk **A Broader Look at the Magnitude-9 Tohoku Earthquake** Organizer: Institute for Astronomical and Physical Geodesy, TUM Speaker: Prof. Fumiko Tajima (Guest Professor, Dept. of Earth and Environmental Sciences, LMU Munich)
May 27	Talk **Flow Control Design by Galrkin Projection and System Identification** Speaker: Prof. Peter Schmid (LadHyX, École Polytechnique, Paris) ǀ TUM-IAS Visiting Fellow
May 31	Talk **Nanotechnology and Design Problems in Present and Future Hard Disk Drives** Speaker: Prof. Frank E. Talke (University of California, San Diego, USA) ǀ TUM-IAS Board of Trustees Member
June 1	**4th Joint Nanoworkshop of TU/e, DTU, and TUM** Organizers: nanoTUM, TUM-IAS
June 6, 20, 27, July 11, 25	Lecture Series **Schaltstelle Gehirn. Von der Evolution des Geistes zur Neurotechnologie und Robotik** Organizers: Carl von Linde-Akademie, TUM-IAS
June 7	**Diesel Reloaded - Efficiency and Simplicity Through Innovative Technology** Focus Group Kick-off Meeting Organizer: Prof. Gernot Spiegelberg ǀ Rudolf Diesel Industry Fellow Keynote speaker: Prof. Luigi Colani
June 14	**Statistical Space-Time Modeling for Wind Power Forecasts** IGSSE/TUM-IAS Doctoral Symposium
June 15	Talk **Bio-Electrochemical Processes – A New Platform Technology with Broad Applications** Speaker: Prof. Jurg Keller (The University of Queensland, Australia) ǀ TUM-IAS Visiting Fellow
June 19–22	**International Scanning Probe Microscopy Conference, ISPM 2011** Organizers: Dr. Willi Auwärter ǀ Carl von Linde Junior Fellow Prof. Johannes Barth (Molecular Nanoscience and Chemical Physics of Interfaces)
June 24	**Munich Bioinformatics Retreat 2011** Organizer: Rostlab (TUM)
June 30	Talk **An Adaptive Reliability-Based Decision Framework For Water And Hazard Management** Speaker: Dr. Chin Man W. Mok ǀ Rudolf Diesel Industry Fellow
July 5	Talk **Handling Qualities Research in Russia** Organizers: Dr. Matthias Heller ǀ Rudolf Diesel Industry Fellow Prof. Florian Holzapfel (Flight System Dynamics) Speaker: Prof. Alexander V. Efremov (Moscow Aviation Institute)
July 6	Talk **Environmental, Hydrologic, and Geotechnical Applications of Reliability Analyses** Speaker: Dr. Chin Man W. Mok ǀ Rudolf Diesel Industry Fellow

July 11	**The Expanding World of Engineering: A Glimpse from My Path** Lecture Series "World of Engineering" Organizer: Munich School of Engineering (MSE) Speaker: Dr. Chin Man W. Mok	Rudolf Diesel Industry Fellow
July 13	**MAC Summer Workshop 2011** In combination with the Munich Multiphysics Meeting Organizer: Munich Centre of Advanced Computing
July 14	Talk **Lithium Batteries – A Look into the Future** Speaker: Prof. Bruno Scrosati (University "La Sapienza," Rome)	TUM-IAS Visiting Fellow
July 14	Talk **Probing Molecular Interactions with Highly Amplified Magnetic Resonance Spectroscopy** Speaker: Prof. Song-I Han (UC, Santa Barbara)	TUM-IAS Visiting Fellow
July 14	Talk **On the Rank of Cutting-Plane Proof Systems** Speaker: Prof. Andreas S. Schulz (Massachusetts Institute of Technology) Honorary Hans Fischer Senior Fellow
July 15	Talk **Fukushima – Nuclear Safety Being Put to the Acid Test** Speaker: Prof. Wolfgang Kröger (ETH Zurich)	TUM-IAS Visiting Fellow
July 19	Fireside Chat **The City of the Future** Organizers: BMW and TUM-IAS
July 20	Workshop **Adaptive Control and Its Transition to Practice** Organizers: Dr. Matthias Heller	TUM-IAS Rudolf Diesel Industry Fellow Prof. Florian Holzapfel (Flight System Dynamics) Speaker: Dr. Naira Hovakimyan (University of Illinois at Urbana-Champaign, USA)

Abstract: While the benefits of adaptation in the presence of failures and uncertainties could be shown in various flight tests over the last decades, the major challenge related to stability/robustness assessment of adaptive systems is still being resolved on the basis of testing the closed-loop system for all possible variations of uncertainties in Monte Carlo simulations. This talk gave an overview of the limitations inherent to the conventional adaptive controllers and introduced the audience to the L1 adaptive control theory, the architectures of which had guaranteed robustness in the presence of fast adaptation. Various applications, including flight tests of a subscale commercial jet were discussed during the presentation to demonstrate the tools and the concepts. With its key feature of decoupling adaptation from robustness, L1 adaptive control theory has facilitated new developments in the areas of event-driven adaptation and networked control systems. A brief overview of initial results and potential directions concluded the presentation.

July 21–22	International Workshop **Advances in Photovoltaics and Photocatalysis** Organizer: Prof. Paolo Lugli (Nanoelectronics)

Considerable interest is attributed these days to renewable sources, which are seen as the best way to provide the energy needed in the future while at the same time reducing the amount of CO_2 generated and diffused in the environment. Among all alternative sources, sunlight is the most abundant and cleanest one. Unfortunately, the exploitation of solar energy is limited by the reduced efficiency and high cost of solar energy conversion systems.

The workshop dealt with two approaches to energy conversion, namely photovoltaics (PV) and photocatalysis (PC). In particular, new-generation solar cells were discussed as PV applications, water splitting and CO_2 reduction for solar fuel production for PC applications. Experts in the two fields came together, mainly from Germany and Italy, but some top-level researchers from other countries were also invited. One of the main topics was the influence of nanotechnology on PV and PC energy conversion systems.

The goal of the workshop was to create a link between the two communities, which had been ignoring one another, and to open the way for a common approach that can combine effectively the know-how of physicists and engineers on PV and of chemists on PC. In order to present a coherent overview and to maximize interaction and discussion, the workshop only invited a contribution of 20 talks. The workshop was followed by a poster session for young researchers who wanted to present their results.

July 25 – 28   Multimodal and Sensorimotor Bionics

Joint international TUM-IAS and Peter Wall Institute for Advanced Studies (UBC) workshop
Organizers:
Prof. J. Leo van Hemmen (Theoretical Biophysics)
Prof. Harald Luksch (Zoology)
Prof. Dinesh K. Pai (Tier 1 Canada Research Chair in Sensorimotor Computation, UBC)
Dr. Patrick van der Smagt (Bionics Group, German Aerospace Center)

Animals are quite efficient in discerning "objects" that appear in their surroundings. Evolution has equipped them with modalities such as hearing, vision, and haptics to perceive their multiple-faceted outside world, and we can safely say that these are well adapted to the specific nature of the sensory world around them. This specific sensory triad has been studied extensively, and other, completely different, diffusely operating modalities such as the lateral line of fish and infrared vision of snakes have also attracted a lot of attention.

Each of the sensory modalities uses a specific physical means of conveying information: Vision takes advantage of a certain part of the electromagnetic spectrum, audition uses sound waves, haptics exploits pressure differences that have to get measured, the lateral line system determines the velocity field around fish (or aquatic frogs such as Xenopus), and infrared vision takes a part of the spectrum

that was left unused by normal vision (in this case, since nature cannot produce a lens that is transparent to infrared, the animal uses a big hole instead).

How do all these modalities with their specific, physically different transmission techniques function? How does the brain generate "objects" as neuronal representations of a single object in the outside world that can still be distinguished from each other? How are these different neuronal representations integrated into a single "object" in the brain, with a specific location in space-time, and how does such a "unified" object generate action of the motor system and hence sensorimotor action? The workshop Multimodal and Sensorimotor Bionics focused on precisely this circle of problems associated with integrating different modalities and transforming object formation into action, while presenting both joint biological-mathematical solutions and biomimetic implementations. Robotics hardly uses multimodal integration yet, whereas animals and humans cannot function properly without such integration. That is, the present workshop was more than timely.

The workshop was set up as a forum for communication and exchange of ideas among experimental biologists and motor experts, theorists devising mathematical models as prerequisites for technical implementation of biological algorithms, and electrical and mechanical engineers who are building robots. The program was tripartite in that the meeting started with neurobiology and modeling of multisensory integration, then turned to sensorimotor transformations, and finished with robotic implementation. The challenge of mutual internal communication was met splendidly, so it is fair to say that the TUM-IAS hosted a groundbreaking workshop. *Prof. J. Leo van Hemmen*

August 1–5   Summer Camp **Computational Design Synthesis**
Organizers: Prof. Matthew Campbell | Hans Fischer Senior Fellow
Prof. Kristina Shea (Product Development)

The week provided a deep-dive into various methods and algorithms used across the domain. Participants were divided into teams to address challenge-problems, and their results were presented at the International Conference on Engineering Design. The researchers had the opportunity to join in a week-long educational and research-intensive workshop on the foundations and practical challenges of Computational Design Synthesis.

September 3–10   **EMBO Practical Course**
Organizer: Prof. Arthur Konnerth | Carl von Linde Senior Fellow

September 6–9   Coherence and Decoherence at Ultracold Temperatures
Joint international TUM-IAS and Peter Wall Institute for Advanced Studies (UBC) workshop
Organizers:
Prof. Moshe Shapiro (The University of British Columbia, UBC)
Prof. Roman Krems (UBC)
Prof. Kirk Madison (UBC)
Prof. Valery Milner (UBC)
Prof. Gerhard Rempe (Max Planck Institute of Quantum Optics)
Dr. Francesca Ferlaino (University of Innsbruck)
Dr. Guido Pupillo (University of Innsbruck)

Ultracold temperatures characterize the state of matter in one of the most exciting research fields of modern physics. Ultracold refers to temperatures below a millikelvin, less than a thousandth of a degree above absolute zero at -273 degrees centigrade. And matter refers to atomic and molecular gases that are deliberately prevented from condensing into a solid even at such low temperatures, achieved by keeping the gas so dilute that a nucleus for the creation of a solid cannot form.

These extreme conditions create a unique testbed for fundamental studies and for exploration of new applications. Many spectacular achievements have been made throughout the last two decades with cold atoms, most notably the creation of a Bose-Einstein condensate in the mid 1990s. In fact, cold-atom research has created the coldest matter in the known universe, has revolutionized atomic physics, and was awarded six Nobel Prizes so far.

It is the aim of a still small but growing scientific community to explore ultracold matter with molecules instead of atoms. The advantage over atoms is that molecules offer a multitude of novel possibilities due to their rich internal structure. The prospects range from many-body physics to quantum information science, and from cold chemistry to tests of physics beyond the Standard Model. Developing methods to prepare the required ultracold molecular ensembles is nowadays a key area of scientific research, in particular because the most successful cooling technique for atoms, laser cooling, is not generally applicable to molecules.
It is against this backdrop that more than 100 researchers from all over the world, from countries ranging from Canada and the USA in the west to Japan in the east, came to the TUM Institute for Advanced Study to summarize the status of the field and identify open problems. They met for a four-day workshop in the wonderful environment of the Institute's new home at the center of the Garching research campus. The workshop, scientifically organized by Austrian, Canadian, and German researchers, addressed issues of coherence and how to control and minimize the deleterious effects of decoherence processes that arise due to the inability to completely isolate the experimental system from the environment. Participants discussed theoretical proposals as well as experimental methods for utilizing coherence – to control chemical reactions between and within ultracold molecules – and for controlling decoherence.

All 26 talks were 45 minutes long to allow speakers to present in-depth views of their research. Lively and well attended poster sessions took place every day during extended lunch breaks. A highly acclaimed laboratory tour was organized at the Max Planck Institute of Quantum Optics, where cold-molecule research is conducted. The success of the workshop is best documented by the fact that the next workshop on the topic is already planned for 2012, at a site in the Austrian Alps.
Prof. Gerhard Rempe, Dr. Guido Pupillo

September 7	Talk **Control and Information Architectures for Formations** Speaker: Prof. Brian D. O. Anderson (Australian National University)	TUM-IAS Visiting Fellow
September 12 – 13	International Workshop **Frontiers on Functional Interfaces** Organizers: Dr. Ian Sharp	Carl von Linde Junior Fellow Prof. Gerhard Abstreiter	Carl von Linde Senior Fellow Prof. Martin Stutzmann (Experimental Semiconductor Physics) In cooperation with WSI, ZNN, NIM

Abstract: Research into understanding and controlling interfaces lies at the confluence of nanoscience, biochemistry, microelectronics, and medicine. In recent years, significant progress in each of these fields has not only increased the importance of hybrid materials systems for applications ranging from renewable energy generation to biomedical implant technology, but also has created new challenges in synthesis, measurement, and theory. The focus of this workshop was on the advances in functional interfaces, with a particular emphasis on multi-component and multi-phase materials systems for bioelectronic, biosensing, and biomedical applications. Furthermore the workshop highlighted the roles and prospects for emerging materials such as graphene, diamond, and compound semiconductors. Addressed were the challenges in determining the complex mechanisms of interaction at interfaces between biological and inorganic systems, precisely tailoring the chemical, structural, and electronic properties, and designing and synthesizing molecular linkers and precursors to provide the desired functionality.

September 12	Workshop **The Numerical Solution of the Chemical Master Equation in Molecular Biology** Organizer: Prof. Markus Hegland	Hans Fischer Senior Fellow
September 13 – 14	Symposium **From Risk Perception to Safety Management – Today and Tomorrow** Organizer: Prof. Erik Hollnagel (University of Southern Denmark)	TÜV Süd Stiftung Visiting Professor
September 28 – 29	International Symposium **Cardiovascular Prevention in Childhood** Organizers: Prof. Renate Oberhoffer (Preventive Pediatrics, TUM) Prof. John Hess (German Heart Centre, Munich)

Abstract: In most cases, older people are those generally afflicted by strokes and heart attacks. The foundations for these diseases, however, are already laid in infancy: Abnormalities in blood vessels can already be detected between the ages of 5 and 8. Malnutrition, overweight, lack of exercise, and also lipometabolism disorders and high blood pressure are risk factors that not only can influence the severity and course of arteriosclerosis, but are also emerging at an increasing rate in children and adolescents.

If prevention – the "anticipation" of cardiovascular diseases – is to be taken seriously, it must begin in childhood. This was the topic addressed within the two-day Symposium on "Cardiovascular Prevention in Childhood," organized by the TUM Chair of Preventive Pediatrics. It took place in the German Heart Centre Munich on the occasion of the World Heart Day. Internationally renowned experts, such as Prof. Gerald Berenson (Tulane University) and Prof. James R. Morrow (University of North Texas), clarified the current state of research.

September 29–30	**Risk-Based Subsurface Environmental Management**

Professional Short Course Series
Instructors: Dr. Chin Man W. Mok | Rudolf Diesel Industry Fellow
Dr. Ravi Arulanntham (Principal Toxicologist at Geosyntec, USA)
James A. Jacobs (Fulbright Specialist and Chief Hydrogeologist at EBS, USA)

September 30, October 11,14	Seminar **Random Matrices and Free Probability**

Speaker: Prof. Víctor Pérez Abreu
(Centro de Investigación en Matemáticas, Mexico) | TUM-IAS Visiting Fellow

September 30	Talk **Market-Based Power Systems. A Control Perspective**

Organizer: TUM-IAS Focus Group Networked Dynamical Systems
Speaker: Dr. Andrej Jokic (TU Eindhoven)

October 13–14	Symposium **Metropolis Nonformal - Landscape, Infrastructure and Urbanism in the Global South**

Organizers: Prof. Christian Werthmann | Hans Fischer Senior Fellow
Prof. Regine Keller (Landscape Architecture and Public Space)

Outline: Illegal – irregular – clandestine – uncontrolled – slum – skid row – favela – barrio – bidonville – shantytown. Our common vocabulary for nonformal urbanism emphasizes its outcast nature, but not its magnitude, dynamism, and legitimacy. Today a new generation of designers engages the conflicted and large territory of self-made cities through carefully calibrated infrastructure and landscape interventions. Metropolis Nonformal traced their particular modes of operation in an emerging field that is crucial for the future of global design practice.

October 13–15	International symposium **Exercise and Cancer - Impact on Prevention and Prognosis**

Speaker: Prof. Steven N. Blair (University of South Carolina) | TUM-IAS Visiting Fellow
The goal of this international symposium was to discuss the most current knowledge and perspectives about physical activity and cancer, among a diverse group of medical experts from both large institutions and private practice.

October 15	Talks **Tag der offenen Tür Garching**

Speakers: Prof. Gernot Spiegelberg | Rudolf Diesel Industry Fellow
"Innotruck 'Diesel Reloaded' – neue Ideen zur Elektromobilität"

Prof. Annette Menzel (Ecoclimatology)
"Demnächst blaues Gold ? – Wasserressourcen im Klimawandel"

October 25	Workshop **Frontiers in DNA Nanoscience: Designed Nucleic Acid Structures in Physics, Chemistry, and Biology**

Organizer: Prof. Hendrik Dietz | Hans Fischer Tenure Track Fellow

October 27–29   Colloquium **Continuity in Energy Regimes**

Organizers: TUM-IAS, Peter Wall Institute for Advanced Studies (UBC)

The colloquium "Continuity in Energy Regimes" met at the TUM Institute for Advanced Study and at the Deutsches Museum from October 27 to 29, 2011. Financial support for speakers' travel, accommodation, and meals while in Munich came from the Peter Wall Institute for Advanced Studies of the University of British Columbia. The Deutsches Museum offered a venue for the opening session as well as extensive assistance with organization and preparation of conference materials. The TUM-IAS supplied the site for the sessions as well as organizational support before, after, and especially during the colloquium.

The meeting brought together 15 scholars from Germany, Austria, Denmark, Great Britain, Italy, the Netherlands, and Canada. They came to Munich to discuss transitions from the use of one dominant source of energy to another. While the energy history of the last 200 years is often understood as an era of coal followed by one of electricity and then oil and recently natural gas, the changes have not been sudden, nor have they been complete. Transitions in consumption have been mixed. The process of change has often proven to be a slow one, with old methods and traditional fuels continuing to contribute to energy consumption, in some places and in some instances making a considerable contribution. Papers and discussion ranged from the 18th century through the 20th, and from food to peat to coal to electricity and natural gas as sources of energy. Speakers talked about the specifics of the economics and technologies employed in the use of certain types of energy. The extensive discussion addressed incentives to shift from one type of energy to another and the barriers to implementation of new and seemingly more progressive or efficient energy carriers. Influencing the changes were factors as different as the general state of the economy, the relative costs of energy sources and other factors of production, prevailing knowledge about the sources and their effectiveness, government policies generated for various reasons, and personal tastes of consumers. The opening address, given by Prof. Robert Allen of Oxford University, explored the role of energy availability and economic transformations, and more specifically the roots of the Industrial Revolution in the 18th century. The closing roundtable, followed by an open discussion among all participants, laid out the general conclusions to be drawn from the different studies discussed by speakers.

After the last session, participants enjoyed a tour of the Deutsches Museum led by Director of Research, Prof. Helmuth Trischler. Summaries of the papers and of the conference will be published in the series Perspectives of the Rachel Carson Center, Munich.

The organizers and co-sponsors of the colloquium were very grateful to the Institute for Advanced Study and its staff for their assistance and support.
Prof. Richard W. Unger

November 10	**Engineering for a Sustainable Society – 2030, Technology that will Change the World**
	Lecture Series on Science and Society – Meet with Excellence
	Speaker: Prof. Rutger A. van Santen (Eindhoven University of Technology, Netherlands)	TUM-IAS Visiting Fellow
November 27–30	**Otto Loewi's Dream (or Nightmare) on Neurons and Synaptic Complexity**
	The 12th Otto Loewi Symposium
	Organizers: Prof. Yosi Yarom (The Hebrew University of Jerusalem)	TUM-IAS Visiting Fellow
	Prof. Arthur Konnerth	Carl von Linde Senior Fellow
	Location: Inter University Institute in Eilat, Israel
November 29–30, December 2, 5–6	Lecture Series **Risk-Based Subsurface Environmental Management**
	Instructor: Dr. Chin Man W. Mok	Rudolf Diesel Industry Fellow
December 15	**Städte im Dunkeln – Sozio-ökologische Infrastruktur für die explodierenden Megaslums der Welt**
	Lecture Series on Science and Society – Meet with Excellence
	Speaker: Prof. Christian Werthmann	Hans Fischer Senior Fellow

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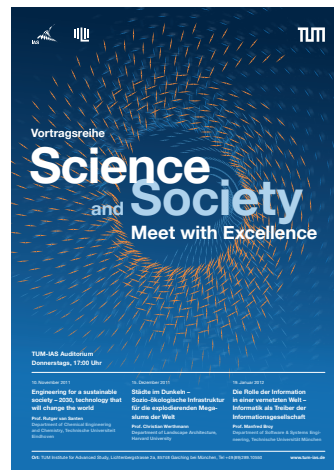
People

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
2011   Prof. Ingrid Kögel-Knabner

Carl von Linde Junior

2007   Prof. Adrian Jäggi
2008   Dr. Martin Gorbahn, Dr. Ulrich Rant, Prof. Robert Stelzer
2009   Dr. Kolja Kühnlenz, Dr. Julia Kunze-Liebhäuser, Dr. Marco Punta,
        Dr. Ian Sharp
2010   Dr. Willi Auwärter, Dr. Vladimir García Morales, Dr. Alexandra Kirsch,
        Dr. Miriam Mehl, Dr. Christian Stemberger, Dr. Dirk Wollherr
2011   Prof. Dongheui Lee, Dr. Angelika Peer

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. Robijn Bruinsma, Prof. Markus Hegland, Prof. Stefan Pokorski,
        Prof. Michael Ortiz, Prof. Tim Sparks, Prof. Raman I. Sujith,
2011   Prof. Silvio Aime, Prof. Polly Arnold, Prof. Daniel Gianola,
        Prof. Frank Kschischang, Prof. Christian Werthmann

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. Matthias Heller, Dr. Tsuyoshi Hirata, Dr. Chin Man W. Mok,
        Prof. Gernot Spiegelberg

Visiting Fellows 2011

Dr. Matthew P. Juniper
Department of Engineering
University of Cambridge, UK
Host: Prof. Wolfgang Polifke

Prof. Jurg Keller
Advanced Water Management Centre
University of Queensland, Australia
Host: Prof. Peter Wilderer

Prof. Peter Schmid
Laboratoire d'Hydrodynamique (LadHyX)
École Polytechnique, France
Host: Prof. Wolfgang Polifke

Prof. Rutger A. van Santen
Department of Chemical Engineering and Chemistry
Eindhoven University of Technology, Netherlands
Host: Prof. Johannes A. Lercher

Prof. Masahiro Watanabe
Fuel Cell Nanomaterials Center
University of Yamanashi, Japan
Host: Prof. Ulrich Stimming

Prof. Zongbin Zhao
School of Chemical Engineering,
Department of Materials Science
Dalian University of Technology, China
Host: Prof. Johann Plank

Advisory Council

TUM-IAS established its Advisory Council at the end of 2008, consisting of the main 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 (15 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. 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.

Members

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Prof. Hans-Joachim Bungartz Chair of Scientific Computing
Prof. Andrzej Buras Institute for Theoretical Elementary Particle Physics
Prof. Martin Buss Institute of Automatic Control Engineering
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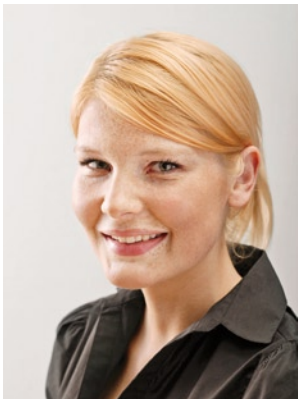
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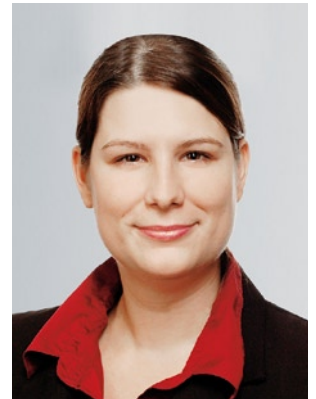
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Melanie Hüttinger
Accounting Assistant
Excellence Initiative

Patrick Regan
Science Writer and Editor

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Technische Universität München
Institute for Advanced Study
Lichtenbergstraße 2 a · 85748 Garching
Germany
Phone: + 49.89.289.10550
E-mail: info@tum-ias.de
Web: www.tum-ias.de