Annual Report

Technische Universität München

Institute for Advanced Study

2013

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TUM President's Foreword

More than ever since its inception in 2006, the TUM Institute for Advanced Study both reflects and helps to shape the dynamic life of the Technische Universität München. The mutual interplay between the TUM-IAS and the larger community, which was "designed in" from the start, has become more active year by year. While serving as a forerunner, not only on new frontiers of research but also in important areas such as internationalization and establishment of the new TUM Faculty Recruitment and Career System, the TUM-IAS is increasingly integrated with the university as a whole.

During the past few years, much of our collective effort has been focused on new beginnings, chiefly though by no means exclusively within the context of the Excellence Initiative. We've taken action in many different ways – including of course through the TUM-IAS – to boost top-level research and education, reinforce our entrepreneurial culture, orient the TUM community toward international competition, and promote talents in all their diversity. Between 2002 and 2013, while our total faculty grew by 38 percent, the number of women on the faculty grew by 230 percent. In 2013, TUM recruited three outstanding female scientists as Liesel Beckmann Distinguished Professors as well as 12 TUM Faculty Tenure Track Professors – including the first TUM-IAS Mößbauer Tenure Track Professor, Bjoern Menze.

Now we are placing an added emphasis on consolidating gains and following through on all those promising beginnings, while at the same time managing unprecedented growth and pushing ahead on new fronts. This new emphasis can be seen across the university but particularly in the TUM-IAS, where a critical transition in leadership took place in 2013. Winning external support from the European Union in 2012 was one sure sign that the TUM-IAS had moved decisively beyond its startup phase; another was the smooth handoff from founding director Patrick Dewilde to Gerhard Abstreiter. I want to thank them for doing such a fine job and congratulate them for making it look so easy.

Already during Patrick Dewilde's tenure as director, the TUM-IAS had outstanding results to validate its effectiveness as a catalyst for high-risk/high-gain research. It certainly played a role as well in enhancing TUM's image and international visibility. In addition to securing these achievements and keeping research on track, Gerhard Abstreiter is further strengthening ties within the university – in part by taking a TUM-IAS road show to the 13 departments on our various campuses, and in part by encouraging even more activity at the TUM-IAS building in Garching.

In this effort a more Bavarian leadership style has not hurt the cause. To the ongoing program of workshops, visiting lectures, and Fellows' Lunches, the TUM-IAS has added public talks, an art exhibit, weekly coffees featuring informal research presentations, and twice-yearly Faculty Day get-togethers where professors from every campus can network with a view of the Alps at sunset. These are incremental but effective contributions toward making the TUM-IAS more definitively "at home" within TUM and vice versa. That, in turn, helps to ensure that our Institute for Advanced Study can fulfill its intended role well into the future.

Prof. Wolfgang A. Herrmann
President

TUM-IAS Director's Message

It has been almost one year now since I took the helm from Patrick Dewilde as director of TUM-IAS. During this time, I have made an effort to continue Patrick's successful undertakings, while also soliciting and contributing new ideas to prepare the Institute for the challenges ahead.

The first major task was the appointment process for the new Rudolf Mößbauer Tenure Track Professors. The tenure track system is an innovation both to the German academic landscape and to TUM. The Rudolf Mößbauer Professorship is even more innovative, as calls are published largely without thematic restrictions; the Joint Search and Evaluation Committee therefore had to develop new procedures on judging and comparing the achievements and potential of early-career scientists of vastly different fields. Many excellent candidates have presented themselves thus far in the selection process, and the first Rudolf Mößbauer Tenure Track Professors have already been appointed. In this way we continue to broaden the research and teaching portfolio of TUM in exciting and highly relevant scientific and technological domains.

Last summer term I visited most TUM faculties to present the Fellowship program and its changes. The well-established Hans Fischer Fellowships will continue as it is to further foster top-level international research collaborations and networks. The Rudolf Diesel Industry Fellowship, however, needs new boundary conditions to enhance interaction with local and international industry. The TUM-internal Carl von Linde Fellowship program also underwent changes: In the future, one such Fellowship will be given to an outstanding TUM faculty member per year. This Fellowship grants the awardee both time for cutting-edge research, and a platform for taking a leading role in establishing and promoting new investigative fields at TUM.

To improve interaction between faculties and scientists, and to further entrench TUM-IAS as an intellectual center on the Garching campus, we organized a number of new events. Faculty Days enable TUM professors from all faculties to spend an informal evening together twice a year. At the weekly Wednesday Coffee Talks, scientists on all career levels gather at the Institute to listen to short talks on recent and relevant TUM publications, specifically designed for a non-expert audience. Finally, invitations to scientific Sunday Matinees encourage our neighbors of the surrounding towns to discover what "those researchers in Garching actually do."

In examining the past year, it could be said that TUM-IAS has undergone a reshaping, but one in which we have also taken care to maintain our unique position as a flagship for initiating and supporting top-level research at TUM. Special emphasis has been laid on the Institute's prominence inside and outside the university – not as a detached "ivory tower," but as a lively hub where scientists from the various TUM research fields interact, both with one another and with researchers of international institutions and industry, discussing and enthusiastically participating in scientific events and inquiry.

Prof. Gerhard Abstreiter
Director

People

Board of Trustees

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

Members

Chairman: Prof. Wolfgang A. Herrmann
Technische Universität München, President

Prof. Patrick Aebischer École Polytechnique Fédérale de Lausanne (EPFL), President
Dr. Enno Aufderheide Alexander von Humboldt Foundation, Secretary General
Dr. Christian Bode German Academic Exchange Service,
Secretary General (retired)
Dr. Klaus Engel Evonik Industries AG, Chairman of the Executive Board
Prof. Manfred Erhardt Association for the Promotion of Science and Humanities in Germany, Secretary General (retired)
Prof. Angelika Görg Technische Universität München, Emerita Proteomics Research Group
Prof. Burkhard Göschel MAGNA International Europe AG, Chief Technical Officer, BMW Executive Board of Management (retired)
Prof. Joachim Hagenauer Technische Universität München, Emeritus Chair for Communications Engineering
Prof. Heather Hofmeister Goethe-Universität Frankfurt, The Center for Leadership and Behavior in Organizations (CLBO), Scientific Director
Hildegund Holzheid Bavarian Constitutional Court, President (retired)
Prof. Klaus-Olaf von Klitzing Max Planck Institute for Solid State Research, Professor of Physics, Nobel Prize in Physics 1985
Prof. Jürgen Mittelstraß University of Konstanz, Emeritus Chair of Philosophy
Prof. Lars Pallesen Technical University of Denmark, President (retired)
Prof. Bert Sakmann Max-Planck-Institute of Neurobiology, Max-Planck Florida Institute, Research Group Leader, Nobel Prize for Physiology or Medicine 1991
Prof. Janis Sarra Peter Wall Institute for Advanced Studies, University of British Columbia, Director
Dr. Georg Schütte Federal Ministry of Education and Research, State Secretary
Prof. Dr. med. Markus Schwaiger Technische Universität München,
Clinic for Nuclear Medicine, Director
Prof. Frank E. Talke University of California, San Diego, Center for Magnetic Recording Research
Prof. Peter Wilderer Institute of Advanced Studies on Sustainability,
Technische Universität München, Emeritus Chair of Water Quality Control and Waste Management

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. 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

Prof. Hans-Joachim Bungartz
Chair of Scientific Computing, Graduate Dean of the TUM Graduate School
Prof. Andrzej Buras
Department of Physics
Prof. Martin Buss
Institute of Automatic Control Engineering
Prof. Sandra Hirche
Chair for Information-Oriented Control
Prof. Horst Kessler
Department of Chemistry
Prof. Claudia Klüppelberg
Chair of Mathematical Statistics
Prof. Ingrid Kögel-Knabner
Chair of Soil Science
Prof. Arthur Konnerth
Institute of Neuroscience
Prof. Gerhard Kramer
Institute for Communications Engineering
Prof. Klaus Mainzer
Chair of Philosophy and Philosophy of Science,
Director of the Munich Center for Technology in Society and the
Carl von Linde-Akademie
Prof. Ernst Rank
Chair for Computation in Engineering, Director of the IGSSE
Prof. Gerhard Rempe
Max Planck Institute of Quantum Optics, Quantum Dynamics Group
Prof. Wolfgang A. Wall
Institute for Computational Mechanics
Prof. Isabell M. Welpe
Chair for Strategy and Organization

Management Office

People

Prof. Gerhard Abstreiter
Director

Stefanie Hofmann
Managing Director

Tatjana Steinberger
Program Manager

Anna Fischer
Program Manager

Sigrid Wagner
Event Manager /
Web Coordinator (on maternity leave since Dec. 2013)

Annette Sturm
Event Manager /
Web Coordinator
(since Nov. 2013)

Nora Eichinger
Project Manager (IESP)

Nina Jelinek
Secretary (Building Coordination)

Christina Schmid
Secretary

Fellows

Carl von Linde Senior Fellows

2008 Prof. Horst Kessler
2010 Prof. Gerhard Abstreiter
2011 Prof. Ingrid Kögel-Knabner
2013 Prof. Annette Menzel

Carl von Linde Junior Fellows

2009 Dr. Julia Kunze-Liebhäuser
2010 Dr. Wilhelm Auwärter, Dr. Vladimir García Morales, Prof. Miriam Mehl, Dr. Dirk Wollherr
2011 Prof. Dongheui Lee, Dr. Angelika Peer
2013 Dr. Peer-Hendrik Kuhn

Hans Fischer Senior Fellows

2009 Prof. Matthew Campbell
2010 Prof. Robijn Bruinsma, Prof. Markus Hegland, Prof. Michael Ortiz, Prof. Tim H. Sparks, Prof. Raman I. Sujith
2011 Prof. Silvio Aime, Prof. Polly L. Arnold, Prof. Daniel Gianola, Prof. Frank Kschischang, Prof. Christian Werthmann
2012 Prof. Stephen Goodnick, Prof. Dietmar W. Hutmacher
2013 Prof. Harald Brune, Prof. Zvonimir Dogic, Prof. Josef P. Rauschecker, Prof. Jelena Vuckovic

Hans Fischer Fellows

2012 Prof. George Biros, Dr. Franz Hagn
2013 Prof. Matthias Batzill, Dr. Christian Hirt

Hans Fischer Tenure Track Professors

2010 Prof. Hendrik Dietz

Rudolf Diesel Industry Fellows

2010 Dr. Matthias Heller, Dr. Tsuyoshi Hirata, Dr. Chin Man W. Mok, Prof. Gernot Spiegelberg
2012 Dr. René-Jean Essiambre, Dr. Michael Friebe, Dr. Bruno Schuermans
2013 Dr. Thomas Koehler, Dr. Peter Lamp

Rudolf Mößbauer Tenure Track Professors

2013 Prof. Kathrin Lang, Prof. Bjoern Menze, Prof. Alessio Zaccone

Alumni Fellows

Carl von Linde Senior Fellows

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

Carl von Linde Junior Fellows

2007 Prof. Adrian Jäggi
2008 Dr. Martin Gorbahn, Dr. Ulrich Rant, Prof. Robert Stelzer
2009 Dr. Kolja Kühnlenz, Dr. Marco Punta, Dr. Ian Sharp
2010 Prof. Alexandra Kirsch, Dr. Christian Stemberger

Hans Fischer Senior Fellows

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. Richard Davis, Prof. Gino Isidori, Prof. Shuit-Tong Lee, Prof. Wolfgang Porod, Prof. Stanley Riddell, Prof. Peter Schröder, Prof. Zohar Yosibash
2010 Prof. Stefan Pokorski

Hans Fischer Tenure Track Professors

2007 Prof. Thomas Misgeld

Rudolf Diesel Industry Fellows

2009 Prof. Khaled Karrai, Dr. Dragan Obradovic, Dr. Georg von Wichert

Honorary Fellows 2013

ERC Grantees

Dr. Wilhelm Auwärter | Molecular Nanoscience and Chemical Physics of Interfaces, TUM
Dr. Olaf Groß | Clinical Chemistry and Pathobiochemistry, TUM
Prof. Sandra Hirche | Information-Oriented Control, TUM
Prof. Thomas Misgeld | Biomolecular Sensors, TUM
Dr. Zeynep Ökten | Molecular and Cellular Biophysics, TUM
Dr. Björn Schuller | Human-Machine Communication, TUM

Alexander von Humboldt Research Awardees

Honorary Hans Fischer Senior Fellows
Prof. Peter Boncz | Centrum Wiskunde & Informatica (CWI); Vrije Universiteit Amsterdam
Prof. Dieter Fox | University of Washington, Seattle
Prof. Shu Kobayashi | The University of Tokyo

Liesel Beckmann Distinguished Professors

Prof. Susanne Albers | Efficient Algorithms, TUM
Prof. Sandra Hirche | Information-Oriented Control, TUM
Prof. Sabine Maasen | Sociology of Science, TUM

Gottfried Wilhelm Leibniz Prizewinners

Prof. Vasilis Ntziachristos | Biological and Medical Imaging, TUM

TUM Distinguished Affiliated Professors

Prof. Patrick Dewilde | Delft University of Technology; TUM Institute for Advanced Study
Prof. Gerhard Ertl | Fritz Haber Institute of the Max Planck Society, Berlin
Prof. Helga Nowotny | ETH Zurich; European Research Council

Visiting Fellows 2013

Prof. Harald Brune
Institute of Condensed Matter Physics
École Polytechnique Fédérale de Lausanne
Hosts: Prof. Johannes Barth, Prof. Karsten Reuter

Prof. Imre Dékány
Department of Medical Chemistry
University of Szeged
Host: Prof. Johann Plank

Prof. Zvonimir Dogic
Department of Physics
Brandeis University
Host: Prof. Andreas Bausch

Prof. Alan Fiske
Department of Anthropology
University of California, Los Angeles
Host: Prof. Isabell M. Welpe

Prof. Alexej Jerschow
Department of Chemistry
New York University
Host: Prof. Steffen Glaser

Prof. Dianne Newell
Peter Wall Institute for Advanced Studies
University of British Columbia, Director (retired)

Prof. Dimitris Politis
Department of Mathematics
University of California, San Diego
Host: Prof. Claudia Klüppelberg

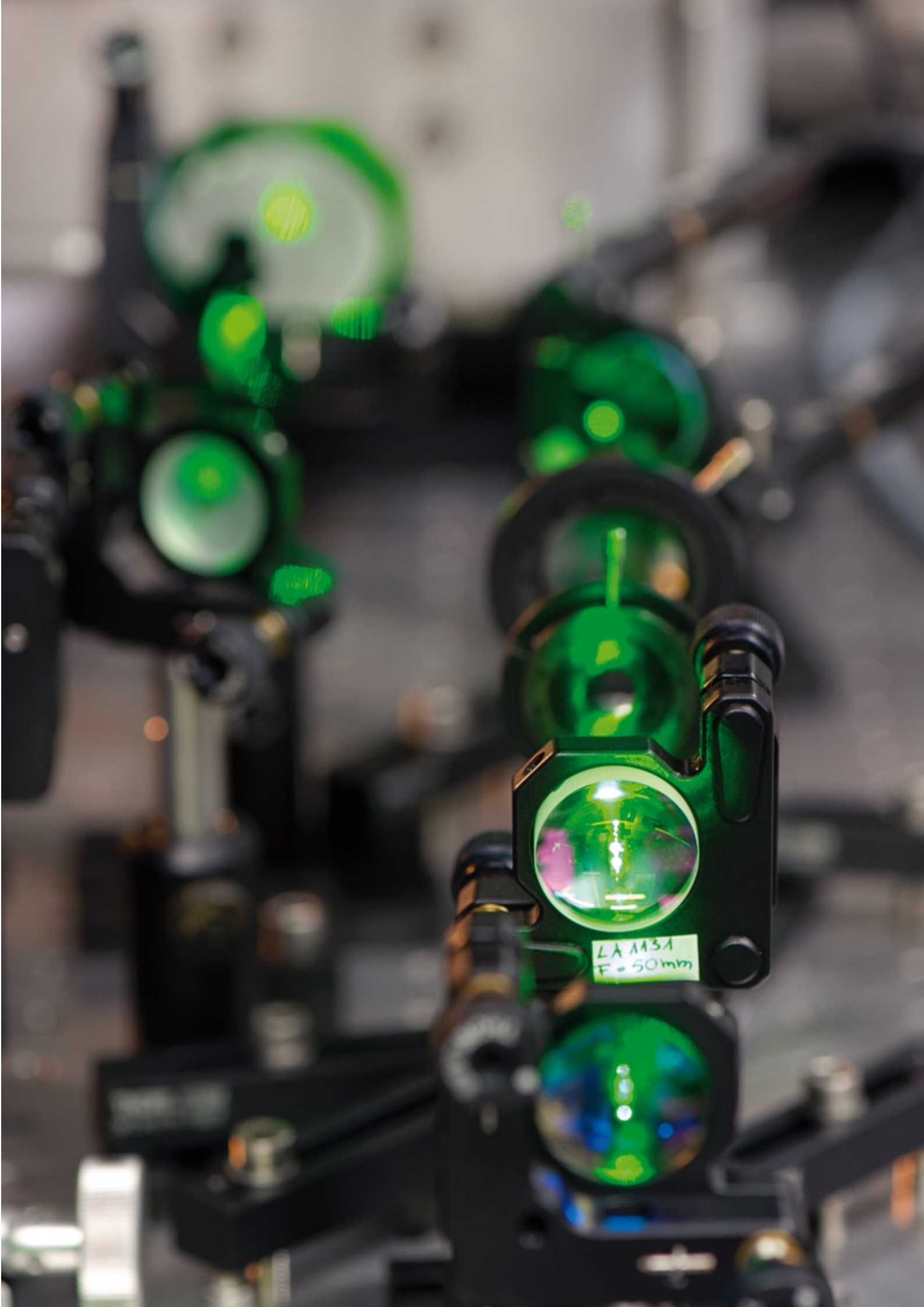
Prof. J. Edward Swan II
Department of Computer Science and Engineering
Mississippi State University
Host: Prof. Nassir Navab

Prof. Jinglin Zuo
School of Chemistry and Chemical Engineering
Nanjing University
Host: Prof. Fritz E. Kühn

TÜV Süd Stiftung Visiting Professors 2013

Prof. Shinji Hara
Department of Information Physics and Computing
The University of Tokyo
Host: Prof. Sandra Hirche

Prof. P. S. Thiagarajan
School of Computing
National University of Singapore
Hosts: Prof. Samarjit Chakraborty, Prof. Javier Esparza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Focus Groups

Focus Groups

TUM-IAS Focus Groups are the basic units of organization of the Institute. They are fully integrated into TUM and provide the social environment where Fellows, Hosts, their students, and collaborators meet to develop their project, organize activities, and be mutually supportive. Ideally, the teams' compositions reflect the Institute's interdisciplinary and diverse character. The list below shows the Focus Groups that have been active in 2013.

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

Advanced Computation
Prof. Matthew Campbell | Oregon State University, USA
Host: Prof. Udo Lindemann | Product Development, TUM

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

Advanced Stability Analysis
Dr. Bruno Schuermans | Alstom, Switzerland
Prof. Raman I. Sujith | Indian Institute of Technology Madras
Hosts: Prof. Wolfgang Polifke,
Prof. Thomas Sattelmayer | Thermodynamics, TUM

Aircraft Stability and Control
Dr. Matthias Heller | Airbus Defence & Space, Germany
Host: Prof. Florian Holzapfel | Flight System Dynamics, TUM

Biochemistry
Dr. Franz Hagn | Harvard Medical School, USA
Host: Prof. Horst Kessler | Chemistry, TUM

Biophysics
Prof. Robijn Bruinsma | University of California, Los Angeles, USA
Prof. Zvonimir Dogic | Brandeis University, USA
Prof. Hendrik Dietz | TUM
Host: Prof. Andreas Bausch | Molecular and Cellular Biophysics, TUM

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

Cognitive Technology
Prof. Dongheui Lee | TUM
Dr. Angelika Peer | TUM
Dr. Dirk Wollherr | TUM
Host: Prof. Martin Buss | Automatic Control Engineering, TUM

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

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

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

Engineering Risk Analysis
Dr. Chin Man W. Mok | GSI Environmental Inc., USA
Host: Prof. Daniel Straub | Engineering Risk Analysis, TUM

Fiber-Optic Communication and Information Theory
Dr. René-Jean Essiambre | Bell Laboratories Alcatel-Lucent, USA
Prof. Frank Kschischang | University of Toronto, Canada
Host: Prof. Gerhard Kramer | Communications Engineering, TUM

Functional Interfaces
Prof. Matthias Batzill | University of South Florida, USA
Host: Prof. Johannes Barth | Molecular Nanoscience and Chemical Physics of Interfaces, TUM

Global Change
Prof. Tim H. Sparks | Coventry University, UK
Host: Prof. Annette Menzel | Ecoclimatology, TUM

High-Resolution Gravity Modeling
Dr. Christian Hirt | Curtin University, Australia
Host: Prof. Roland Pail | Astronomical and Physical Geodesy, TUM

High-Performance Computing (HPC)
Prof. George Biros | University of Texas at Austin, USA
Prof. Markus Hegland | Australian National University
Prof. Miriam Mehl | University of Stuttgart
Host: Prof. Hans-Joachim Bungartz | Scientific Computing, TUM

Image-Based Biomedical Modeling
Prof. Bjoern Menze | Computer Aided Medical Procedures & Augmented Reality, TUM

Intra-Operative Therapy
Dr. Michael Friebe | IDTM GmbH, Bochum
Host: Prof. Nassir Navab | Computer Aided Medical Procedures & Augmented Reality, TUM

Metal Organic Superlattices of Quantum Magnets
Prof. Harald Brune | École Polytechnique Fédérale de Lausanne, Switzerland
Hosts: Prof. Johannes Barth | Molecular Nano-science and Chemical Physics of Interfaces, TUM
Prof. Karsten Reuter | Theoretical Chemistry, TUM

Metropolis Nonformal
Prof. Christian Werthmann | Leibniz Universität Hannover
Host: Prof. Regine Keller | Landscape Architecture and Public Space, TUM

Molecular Aspects in Interface Science
Dr. Julia Kunze-Liebhäuser | TUM
Host: Prof. Ulrich Stimming | Physics, TUM

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

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

Nanophotonics
Prof. Gerhard Abstreiter | Walter Schottky Institute and Physics Department, TUM

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

Nanoscience for Renewable Energy Sources
Prof. Stephen Goodnick | Arizona State University, USA
Host: Prof. Paolo Lugli | Nanoelectronics, TUM

Neuroscience
Prof. Thomas Misgeld | TUM
Host: Prof. Arthur Konnerth | Neuroscience, TUM

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

Proteomics
Dr. Peer-Hendrik Kuhn | TUM
Host: Prof. Stefan Lichtenthaler | Neuroproteomics, TUM

Regenerative Medicine
Prof. Dietmar W. Hutmacher | Queensland University of Technology, Australia
Host: Prof. Arndt F. Schilling | Plastic Surgery and Hand Surgery, TUM

Soil Architecture
Prof. Ingrid Kögel-Knabner | Soil Science, TUM

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

Activities and Events

TUM-IAS General Assembly 2013

April 25 – 26








As in past years, the TUM-IAS General Assembly took place at the beautiful castle of Hohenkammer. For two days, the TUM-IAS community came together to hear about the Focus Groups' and TUM-IAS projects' progress, to get to know new members and meet old acquaintances, to discuss, exchange ideas, and relax in the castle's beautiful premises.

As always, the talks came from scientific areas that were as interdisciplinary as the TUM-IAS itself: application-oriented topics such as robotics in human environments or the future of image-guided therapies, topics that touch today's big issues such as climate change and ecosystems or landscape and infrastructure strategies for low income populations of a rapidly urbanizing planet, but also fundamental research touching questions such as "Fundamental Physics after Higgs Discovery: What Next?".

This year's conference dinner was particularly festive, being held in honor of our parting director, Prof. Patrick Dewilde. Laudatory speeches came from the president of TUM, Prof. Wolfgang A. Herrmann, former TUM-IAS Board of Trustees member and Visiting Fellow Prof. Dianne Newell (Peter Wall Institute for Advanced Studies, UBC, retired director), Dr. Markus Zanner, once TUM-IAS Managing Director, now chancellor of the University of Bayreuth, Prof. Joachim Hagenauer, TUM-IAS Board of Trustees member, and Prof. Klaus Diepold (TUM Vice President for Diversity and Talent Management), who had been Host Professor for Patrick Dewilde when he first came to TUM as an Alexander von Humboldt Awardee.

Fellows' Lunches

In 2013, TUM-IAS continued with its popular monthly Fellows' Lunches. Invited speakers from diverse fields presenting their research projects – or a chosen topic of general interest – to a broad, scientific audience has, once again, proven to be a lively and engaging format. The multidisciplinary talks often sparked spirited and fruitful discussions among the participants: The relaxed atmosphere inspired TUM-IAS Fellows and members to exchange ideas across fields and benefit from very valuable – and, to that point, unfamiliar – points of view on their research questions. Fellows' Lunches provide a platform for scientists to meet and, in doing so, they also draw the Institute's community closer together and foster interdisciplinary exchange and approaches.

There was a wide variety of talks for this year's Lunches. With the second round of the Excellence Initiative having just begun, cluster coordinator Prof. Stephan Paul gave an overview of the Excellence Cluster Universe, its main ideas, and the interesting scientific questions it raises. This Lunch was followed by March's session, in which former TUM-IAS director Prof. Patrick Dewilde invited the TUM-IAS community to contribute to the topic of novel elementary numerical methods – and presented "Gaussian Elimination Revisited" himself, as inspiration. At the next Fellows' Lunch, Prof. Gerhard Abstreiter introduced himself as the new TUM-IAS director by giving a talk on the future of the Institute. Further highlights throughout the year included a broad glimpse into biomedical imaging with presentations on "Clinical MR/PET Imaging," "Molecular Imaging," and "Advanced X-Ray CT Imaging" by TUM-IAS members Prof. Markus Schwaiger, Prof. Silvio Aime, and Prof. Franz Pfeiffer; in September, the Focus Group High-Performance Computing – represented by Prof. Markus Hegland and doctoral candidate Christoph Kowitz – enlightened the participants with "From Sparse Grids to Tensor Trains and Fractals." TUM-IAS was also very pleased to welcome Alexander von Humboldt Professor Prof. Matthias Tschöp, who spoke on "Discovering New Diabetes Therapies." Finally, the year concluded with the introduction of the new Focus Group "High-Resolution Gravity Modeling": Dr. Christian Hirt and doctoral candidate Moritz Rexer capped 2013 – and another successful year of Fellows' Lunches – with "The Gravity Field of Planet Earth – Modeling with Ultra-High Resolution."

Scientists Meet Scientists – Wednesday Coffee Talk

When we created “Scientists Meet Scientists – Wednesday Coffee Talk” in the summer of 2013, we had several intentions: Firstly, we wanted to give scientists on all career levels from the various research fields of TUM (especially those of the Garching research campus – and those working in our building) a chance to meet and get to know each other in a relaxed, informal atmosphere. Secondly, we wanted to give outstanding TUM publications a platform – by inviting their authors to present their work in a short, simple presentation that would be understandable to non-experts, too. Then, quite simply, we hoped to encourage people from outside the TUM-IAS community to come and get to know the Institute and its building, thus adding to TUM-IAS’s standing as an intellectual center on campus. In a nutshell, our Wednesday Coffee Talk stands for chatting to colleagues over a cup of coffee, getting to know other scientists, and finding out more about exciting projects currently happening at TUM.

We are rather pleased with how our new creation has turned out. After five months of Wednesday Coffees, 10 of which featured a presentation, we seem to have gathered a substantial crowd of regulars, each week mixed with new faces. We have had very interesting talks as well as great, inspiring discussions. And the fact that many of our regulars volunteered to bring along cake from time to time certainly did not hurt either!

Scientists Meet Scientists – Wednesday Coffee Talk will continue in 2014: As last year, there will not be a presentation every Wednesday, but we will always serve coffee.

Wednesday Coffee Talks in 2013

July 10, 2013	Opening of the exhibition “Insights Into Nanoworlds”
July 17, 2013	Prof. Dirk Busch (Medical Microbiology, Immunology and Hygiene) on an assay identifying T cells as most capable of fighting infections and cancers
July 24, 2013	Prof. Thorsten Hugel (Biophysics) on frictions in the nanoworld
October 10, 2013	Dr. Stefan Huber (Organic Chemistry) on halogen bonds in catalysis
November 06, 2013	Prof. Burkhard Rost (Bioinformatics) on the functional diversity of protein and its impact on health
November 13, 2013	Josef Lichtinger (Experimental Physics) on neutrons showing the accumulation of the antidepressant lithium in the brain
November 20, 2013	Prof. Arndt F. Schilling (Plastic Surgery and Hand Surgery) on Emacure, a patient-specific wound healing therapy
November 27, 2013	Dr. Alaa Abdellah (Nanoelectronics) on carbon nanotubes as a path to flexible, low-cost sensors
December 4, 2013	Dr. David Écija (Molecular Nanoscience & Chemical Physics of Interfaces) on molecular forming 2D-patterns that had never been observed before
December 18, 2013	Julia Laube (Ecoclimatology) on climate change altering the timing of spring growth in forests

TUM-IAS Faculty Days

June 26 / December 3





While it is a university professor's daily routine to meet with scientists from his own department and collaborating institutions, there is hardly ever a chance to meet with fellow professors from all the other TUM departments. This is what brought about the idea of creating a regular semestral event to which all TUM professors as well as the Emeriti of Excellence would be invited: the TUM-IAS Faculty Days.

The first Faculty Day took place on June 26. About 110 faculty members, not only from the Garching departments, but also from Weihenstephan, the city campus, and the hospitals, met for a casual get-together and Bavarian-style snacks and drinks. Chats and discussions lasted well into the evening, at which time the faculty club, with its panorama windows, provided the opportunity to watch the sun set on campus at a summerly late hour (21:08 that day).

Sunset also played a crucial part in the next Faculty Day – taking place in winter on December 3; however, on this occasion sunset was chosen as the event's starting time (16:21). This Faculty Day the program was a little more formalized with a talk by Prof. Jürgen Ruland (Clinical Chemistry) on "Animal Modeling and Cancer Research," but the rest of the evening was again dedicated to informal scientific and social interaction.

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

An exciting new development this year for TUM-IAS was the conception of the lecture series “Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?,” a program aimed at engaging local residents – particularly high school students – in the research activities of the scientists on the Garching campus. These Sunday talks target a broad, non-scientific audience and offer discussions on such questions as “Why does one need a supercomputer?” and “What is a black hole?” The first of these fascinating topics was presented in November 2013 by Prof. Heinz-Gerd Hegering of the Leibniz-Rechenzentrum – the computing center for Munich’s universities and the Bavarian Academy of Sciences and Humanities. Prof. Hegering’s talk, “Der Supercomputer SuperMUC und seine Anwendungen,” was an excellent kick-off to TUM-IAS’s emerging program. The schedule moves ahead in March 2014 with Prof. Andreas Burkert of the Max Planck Institute for Extraterrestrial Physics addressing the second question in “Das Schwarze Loch im Zentrum unserer Milchstraße.” If one recognizes the name of Prof. Burkert, it is perhaps because he or she knows the small planet 267003 Burkert, the professor’s celestial namesake.

It is hoped that in 2014 and beyond the lecture series will continue to attract those members of the public who, although not necessarily scientists themselves, wish to expand their scientific knowledge, and who are curious about the bold enterprises of their neighbors, the researchers in Garching.

Liesel Beckmann Symposium 2013

Mein Informatik-Puzzle (Puzzling out Informatics)

In 2013, the Department of Informatics designed the Liesel Beckmann Symposium with the theme “Mein Informatik-Puzzle,” or “Puzzling out Informatics,” as part of the faculty’s activities to promote diversity and gender equality. The symposium was chaired by Prof. Anne Brüggemann-Klein (TUM), with advisors Prof. Karin Zachmann (TUM), Veronika Oechtering (Universität Bremen), and the Informatik-Forum Frauen IFF (TUM). The concept for the symposium was based on the conviction that informatics thrives in an environment that values a rich spectrum of approaches to and perspectives on the field. A multifaceted image of informatics grows best in a heterogeneous community that reflects society’s composition with respect to gender, social and cultural background, age, and life experience, the unifying forces being a common interest in computational thinking and the vision to contribute to the well-being of society with the tools of the trade (cultural perspective). The symposium provided a forum for computer science students and professionals in academia and industry to puzzle out individual perspectives on informatics and to contribute to a comprehensive, effective, and sustainable concept of the field. The symposium facilitated exchange, reflection, and validation; delegates developed a rich image of informatics and its practitioners.

The symposium was organized into two sections, offering talks in the morning and workshops in the afternoon. Two talks in the morning dealt with career paths in informatics. First, Prof. Ute Schmid, University of Bamberg, provided a bird’s-eye perspective, reporting on the European Social Funds-sponsored study “Alumnae Tracking.” The study is unique in generating insights into subjective and objective career barriers for women, specifically in informatics; it is also unique for its approach in methodically analyzing matched pairs of men and women. Second, Sara Adams (Google Munich), in her inspirational talk “Becoming a software engineer at Google,” allowed for a fascinating and very personal close-up view, spotlighting love for foundational work and applications in mathematics and informatics, dedication and hard work, self-reflection, resilience in the face of adversity, persistence, inventiveness, high professional standards, and her puzzle pieces of work-life balance.

In the afternoon, four parallel workshops provided opportunities to puzzle out one’s own image of informatics in an informal atmosphere. (1) An improvisational theater workshop, led by Dorothea Anzinger (Anzinger Team Training) under the title “Der Homo Informaticus — Wer sind wir und wenn ja, wie viele?!”, addressed stereotypes in a creative and humorous way. It also – and more importantly – provided first-hand experience with a team-building technique for heterogeneous teams.

(2) For the second workshop, Prof. Schmid returned with two colleagues, Anja Gärtig-Daugs and Silvia Förtsch, to present “Selbstwahrnehmung und Fremdwahrnehmung von Studentinnen und Studenten der Informatik.” An empirical study prompted reflection on delegates’ personal experiences. (3) “Nerds or Geeks — Public and Self-Image of Computer Scientists in Different Countries”: that was the title of an image workshop presented by Christine Müller (TUM) and Nastaran Matthes (infoAsset). The two workshop leaders work and worked, respectively, as international student advisors at TUM. They created the highly esteemed International Café and other community-building events for international students in the Department of Informatics. They were uniquely positioned to guide workshop participants in exploring the image of informatics in Germany versus the international perspective, inspiring a widening of the horizon. (4) In the World Café Computational Thinking, we discussed computational thinking as a mindset that contributes to problem solving outside informatics. The format of this workshop had been designed by Michaela Gluchow (TUM), who was ill on the day of the symposium, so Prof. Brüggemann-Klein took over.

The symposium concluded with live improvisational theater, presented by the first workshop, and a lively final discussion. There was general agreement that Sara Adams’s talk had been exceptionally inspirational and that the improvisational workshop had provided novel experiences. The symposium was generally well received, although some participants were critical of its perceived gender bias. Participants appreciated goodies that were donated by Google, and Amazon gift coupons that were donated by infoAsset.

The symposium has had lasting impact: The University of Bamberg and TUM continue to explore collaboration on statistics, the materials from the World Café Computational Thinking have been integrated into the teaching of introductory classes and outreach programs, and we hope to further explore improvisational theater as a development technique for diverse teams at TUM.

International Expert Group on Earth System Preservation (IESP)

The International Expert Group on Earth System Preservation (IESP) is a global network of scientists, engineers, and members from governmental and non-governmental organizations. Its purpose is to contribute to advances in Earth system science through thematic-based conferences, workshops, seminars, lectures, and publications. It also serves as a liaison between experts, decision makers, and the public. The IESP promotes the exchange of knowledge and provides access to current scientific results. Its activities contribute to widespread policy debates by establishing a platform for discussion on sustainable development of ecosystems, economic and societal systems, and their interrelationships. The IESP network has more than 50 international members from the fields of sustainability research, energy and environmental sciences, resource technology, environmental engineering, climate dynamics, risk assessment, industrial ecology, political sciences, economics, and more. The IESP is supported by the Bavarian State Ministry of the Environment and Consumer Protection. In addition, the IESP is hosted by TUM-IAS, where the organizational staff is located. Prof. Peter Wilderer acts as chairman of the IESP.

Earth system science

The thematic-based activities of the IESP focus mainly on the promotion of scientific knowledge in Earth system science. The Earth system is to be understood as the sum of the planet's interacting physical, chemical, biological, and anthropogenic processes. As the human population is growing rapidly, the extent of anthropogenic impact is increasing as well, leading to problematic environmental changes: for example, global warming caused by excess emission of greenhouse gases. Obviously, humankind is changing the Earth system and its function, deeply affecting its dynamic, its stability, and its resilience. Therefore one of the most important concerns of the scientists of the IESP is how to protect the functioning of the Earth system in favor of the continued existence of life on Earth and decent living conditions for future generations.

IESP Events

July – October 2013	International Online Workshop **Post-2015 Development Goals** Organizer: IESP
November 4 – 5, 2013	International Workshop **Centralized versus Decentralized Energy Systems** Organizers: IESP; TUM-IAS
November 5, 2013	International Workshop **Importance of Forest Ecosystems for Climate Regulation** Organizers: IESP; European Water Partnership (EWP), Brussels
December 3 – 5, 2013	International Workshop **Directions in Ecological Modeling: Principles and Practice** Organizers: IESP; LRZ; TUM-IAS

TUM-IAS Events

February 5

Lecture Series “Science and Society – Meet with Excellence”
Weshalb es keine wissenschaftliche Olympiade geben kann
Organizers: TUM-IAS, MCTS
Speaker: Prof. Helga Nowotny (European Research Council) | TUM Distinguished Affiliated Professor

March 11–12

Symposium **Along the Frontiers of Nanoelectronics: From Nanoimprinting to Nanoenergy**
Organizers: TUM-IAS, Nanosystems Initiative Munich (NIM), TUM Institute for Nanoelectronics
Speakers: Prof. Paolo Lugli (Institute for Nanoelectronics, TUM)
Prof. Khaled Karrai | Rudolf Diesel Industry Fellow
Prof. Wolfgang Porod | Hans Fischer Senior Fellow

March 12

Kick-Off Meeting of the Focus Group **Nanoscience for Renewable Energy Sources**
Organizers: TUM-IAS, Institute for Nanoelectronics
Speakers: Prof. Stephen Goodnick | Hans Fischer Senior Fellow
Dan Popescu (Institute of Nanoelectronics, TUM)
Prof. Aldo Di Carlo (University of Rome)
Dr. Ahmed Abdellah (Institute of Nanoelectronics, TUM)

March 14–15

Munich Battery Discussions **Lifetime and Ageing of Battery Materials and Systems**
Organizers: TUM-IAS, BMW Group, TUM,
Dr. Julia Kunze-Liebhäuser | Carl von Linde Junior Fellow
Prof. Hubert A. Gasteiger (Technical Electrochemistry, TUM)

March 18

Inaugural Lecture **MRI & Molecular Imaging: What's Good for Clinical Translation?**
Organizers: Prof. Markus Schwaiger (Clinic for Nuclear Medicine, TUM)
Prof. Axel Haase | Carl von Linde Senior Fellow
Speaker: Prof. Silvio Aime | Hans Fischer Senior Fellow

March 18–21

11th German Peptide Symposium
Organizer: Prof. Horst Kessler | Carl von Linde Senior Fellow

April 10–12

Workshop **Surface-Supported Molecular Nanostructures: Foundations and Functionality**
Organizers: Dr. Wilhelm Auwärter | Carl von Linde Junior Fellow
Prof. Johannes Bart, Dr. Florian Klappenberger
(Molecular Nanoscience & Chemical Physics of Interfaces, TUM)

April 25–26

Scientific Symposium at the **General Assembly**
Organizer: TUM-IAS

May 3

Exploratory Workshop **Bio-Inorganic Chemistry**
Organizer: Prof. Fritz E. Kühn (Molecular Catalysis, TUM)

May 4–7

International Workshop **The Future of Ptychography**
Organizers: Dr. Pierre Thibault (Biomedical Imaging, TUM)
Dr. Irene Zanette (Biomedical Physics, TUM)
Martin Dierolf (Biomedical Physics, TUM)

May 8

Talk **High-Resolution CT of the Breast at Very Low Dose**
Organizer: TUM-IAS
Speakers: Prof. Willi A. Kalender (University of Erlangen-Nuremberg)
Prof. Axel Haase | Carl von Linde Senior Fellow

May 13–15

Short Course **Model-free Versus Model-based Prediction Intervals**
Organizers: TUM-IAS; TUM Mathematics Department
Speaker: Prof. Dimitris Politis (University of California, San Diego) | Visiting Fellow

May 17

Inaugural Lecture **Intraoperative Image Guided Therapies – I2gT**
Organizer: TUM-IAS
Speakers: Dr. Michael Friebe | Rudolf Diesel Industry Fellow
Prof. Nassir Navab (Computer Aided Medical Procedures & Augmented Reality, TUM)
Dr. Helmut Schönenberger (UnternehmerTUM)
Dr. Jörg Traub (Surgiceye)

May 29

Lecture Series “Science and Society – Meet with Excellence”
Innovation-Driven Futures and Knowledge-Able Citizens
Organizers: MCTS, TUM-IAS
Speaker: Prof. Ulrike Felt (University of Vienna)

June 4

Kick-Off Workshop **Redefining Ecosystem Services in Human Habitats: Cradle to Cradle® in Building and Planning**
Organizers: TUM-IAS, Cradle to Cradle®
Speaker: Prof. Michael Braungart | Start-up Cradle to Cradle®

June 6 — Lecture Series “Science and Society – Meet with Excellence”

Emerging Science and Technology – Modes of Tentative Governance
Organizers: MCTS, TUM-IAS
Speaker: Prof. Stefan Kuhlmann (University of Twente)

June 7 — Talk **How Do We Measure Depth Perception in Near-Field Augmented Reality?**
Organizers: Chair for Computer Aided Medical Procedures & Augmented Reality, TUM-IAS
Speaker: Prof. J. Edward Swan II (Mississippi State University) | Visiting Fellow

June 14 — Talk **Multifractality in Combustion Noise: Prediction of Impending Combustion Instability**
Organizer: TUM-IAS
Speaker: Prof. Raman I. Sujith | Hans Fischer Senior Fellow

June 14 — Talk **The New Product Development Process for MEDTEC Products - A Holistic Observation**
Organizer: Dr. Michael Friebe | Rudolf Diesel Industry Fellow
Speaker: Dr. Rolf Sauter (former Director of Engineering at SIEMENS Healthcare)

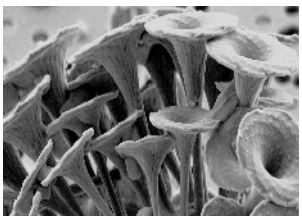
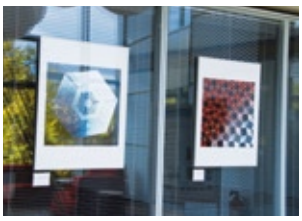
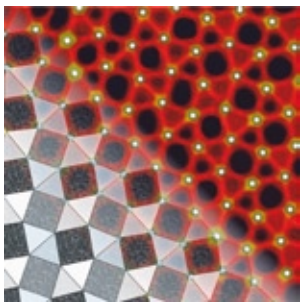
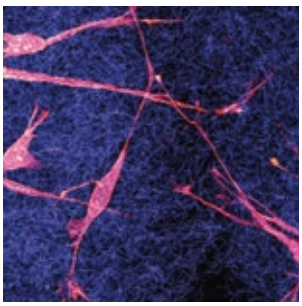
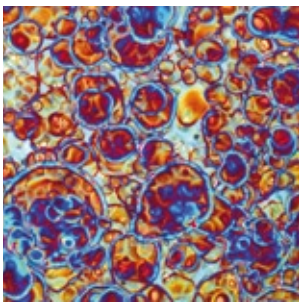
June 18 — Talk **Relational Models Theory and its Implications for Managing Organizations**
Organizers: Chair for Strategy and Organization, TUM-IAS
Speaker: Prof. Alan Fiske (University of California, Los Angeles) | Visiting Fellow

June 18–21 — Summer School and Workshop **Non-Normal and Nonlinear Effects in Aero- and Thermoacoustics**
Organizers: TUM-IAS, Ercoftac,
Prof. Raman I. Sujith | Hans Fischer Senior Fellow
Prof. Wolfgang Polifke (Thermodynamics, TUM)

June 26 — **Summer Faculty Day – Professoren treffen Professoren**
Organizer: TUM-IAS

July 1 — Talk **Oberflächen-Modifizierung von schichtartigen Nanostrukturen: Flüssigkeitsadsorption und Benetzung an fest/flüssigen Grenzflächen**
Organizer: TUM-IAS
Speaker: Prof. Imre Dékány (University of Szeged) | Visiting Fellow

July 10 Opening of the 1st Exibition “Science and Technology Meet Art”
Insights into Nanoworlds
Organizer: TUM-IAS

July 10 Talk **MRI Methods for *In Vivo* and for Battery Materials Imaging**
Organizer: IMETUM
Speaker: Prof. Alexej Jerschow (New York University) | Visiting Fellow

July 10–11 1st International Workshop **Latest Advances in Cardiac Modeling**
Organizers: Dr. Cristóbal Bertoglio, Prof. Wolfgang A. Wall
(Focus Group Advanced Cardiac Mechanics Emulator; Computional Mechanics, TUM)
Speakers: Prof. Dominique Chapelle (INRIA)
Prof. Sasha Panfilov (Gent University)

July 18–19; 22 Workshop **A Short Course on Estimation Theory**
Organizers: TUM-IAS, TUM Faculty of Mechanical Engineering
Speaker: Prof. Arun K. Tangirala (IIT Madras) | Visiting Fellow

July 24 Talk **Sodium and Chemical Exchange MRI:**
Opportunities for Clinical Studies in the Joints and Brain
Organizer: TUM Rechts der Isar University Hospital
Speaker: Prof. Alexej Jerschow (New York University) | Visiting Fellow

July 29–31 Workshop **Novel Numerical Methods**
Organizers: Prof. Patrick Dewilde | Former TUM-IAS Director
Prof. Miriam Mehl | Carl von Linde Junior Fellow
Prof. Markus Hegland | Hans Fischer Senior Fellow

August 13 — Inaugural Lecture **N-body Algorithms in Computational Physics and Statistical Inference**
Organizer: TUM-IAS
Speaker: Prof. George Biros | Hans Fischer Fellow

August 18–23 — 2013 Gordon Research Conference **Soft Condensed Matter Physics: Bio-Soft Matter: Dynamical and Structural Complexity**
Organizers: Prof. Andreas Bausch (Molecular and Cellular Biophysics, TUM)
Prof. Robijn Bruinsma | Hans Fischer Senior Fellow

September 19 — Workshop **Adaptive and Local Model Order Reduction with Machine Learning for Parametrized Systems**
Organizers: Prof. Hans-Joachim Bungartz (Scientific Computing, TUM)
Prof. Karen Willcox (Aeronautics and Astronautics, MIT)
Speaker: Prof. Markus Hegland | Hans Fischer Senior Fellow

September 24 — Workshop **Probabilistic Health Risk Assessment & Environmental Decision Making**
Organizer: TUM Faculty of Civil, Geo and Environmental Engineering
Speakers: Dr. Chin Man W. Mok | Rudolf Diesel Industry Fellow
Dr. Ravi Arulanantham (Geosyntec, USA)

October 6–8 — Kloster Seeon Meeting **BACE Proteases in Health and Disease**
Organizer: Prof. Stefan Lichtenthaler (Neuroproteomics, TUM)
Speaker: Dr. Peer-Hendrik Kuhn | Carl von Linde Junior Fellow

October 9–11 — Workshop **Targetry for laser-driven proton (ion) accelerator sources**
Organizers: Prof. Paul Bolton (Kansai Photon Science Institute)
Prof. Fridtjof Nüsslin | TUM Distinguished Affiliated Professor
Prof. Jörg Schreiber (Ludwig-Maximilians-Universität München)
Prof. Jan Wilkens (Advanced Technologies in Radiation Therapy, TUM)

The first of its kind, this international workshop brought together 34 participants (23 from Europe, four from Asia, five from the United Kingdom, and two from the USA) to focus on the current state and future of ‘targetry’ as a rapidly evolving and critically enabling component in the development of integrated laser-driven ion accelerator systems (ILDIAS). Target and laser pulse parameters constitute the source parameter space for such innovative accelerator systems. Subject matter in the workshop included basic types of targets, target conditioning, fabrication, positioning, handling, target performance, unique diagnostics, and important technical challenges.

The 26 talks presented over two days described 17 different target types. Motivated by the success of this first workshop, a similar event will be held in the future as part of an ongoing workshop series aimed at highlighting progress and challenges in promoting coordinated development of key ILDIAS components.

Workshop participants represented research laboratories from nine countries. Presented by the Munich-Centre for Advanced Photonics (MAP), the workshop was supported by the TUM Institute for Advanced Study (TUM-IAS) which provided the venue, the LEX Photonics and CALA programs, the Technische Universität München (TUM), the Ludwig-Maximilians-Universität München (LMU), and the Kansai Photon Science Institute (KPSI) in Japan.

October 16

Lecture Series “TUM Frontiers in Science and Technology”
Globally Networked Risks and How to Respond
Organizers: TUM-IAS, MCTS
Speaker: Prof. Dirk Helbing (ETH Zurich)

October 19

Tag der offenen Tür
Talk **IESP – Die Funktion des Erdsystems retten – wie soll das gehen?**
Speaker: Prof. Peter Wilderer (Emeritus Waste and Water Management, TUM)
Talk **DNA – Die Sprache der Pflanzen**
Speaker: Prof. Chris-Carolin Schön (Plant Breeding, TUM)
Exhibition **DNA-Nanotechnologie aus dem 3D-Drucker**
Organizer: Prof. Hendrik Dietz | Hans Fischer Tenure Track Professor

October 22, 29 & November 5
Lecture Series **Glocal Control for Hierarchical Dynamical Systems**
Organizer: Chair for Information-Oriented Control
Speaker: Prof. Shinji Hara (University of Tokyo) | TÜV Süd Stiftung Visiting Professor

October 28–29
Focus Workshop **Advances in Semiconductor Nanowire-based Photonics**
Organizers: TUM-IAS, Nanosystems Initiative Munich (NIM),
Prof. Gerhard Abstreiter | TUM-IAS Director
Prof. Jonathan Finley, Dr. Gregor Koblmüller
(Nanotechnology and Nanomaterials, TUM)

November 7
Kick-off Minisymposium **Magnetism and Chemistry of Metal-Organic Networks at Surfaces**
Organizers: Prof. Harald Brune | Hans Fischer Senior Fellow
Prof. Johannes Barth (Molecular Nanoscience & Chemical Physics of Interfaces, TUM)
Prof. Karsten Reuter (Theoretical Chemistry, TUM)

November 17


Lecture Series „Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?“ **Der Supercomputer SuperMuc und seine Anwendungen**
Organizer: TUM-IAS
Speaker: Prof. Heinz-Gerd Hegering (Leibniz-Rechenzentrum)

November 20–23


Symposium **Metropolis Nonformal – Anticipation**
Organizers: UN-Habitat, TUM-IAS,
Prof. Regine Keller (Chair of Landscape Architecture and Public Space, TUM)
Prof. Christian Werthmann | Hans Fischer Senior Fellow

November 22
Liesel-Beckmann-Symposium **Mein Informatik Puzzle (Puzzling Out Informatics)**
Organizers: TUM-IAS, TUM Faculty for Informatics

December 2
Research Alumni Forum **Everything You Always Wanted to Know about Working as a Researcher Internationally – But Never Dared to Ask** and **Science Fiction: TUM Ambassadors Talk about their Visions for the Future**
Organizer: TUM Alumni & Career
Speakers: Prof. Gerhard Abstreiter | TUM-IAS Director
Prof. Patrick Dewilde | Former TUM-IAS Director

December 3
Winter Faculty Day – Professoren treffen Professoren
Talk **Animal Modeling and Cancer Research**
Organizer: TUM-IAS
Speaker: Prof. Jürgen Ruland (Clinical Chemistry, TUM)

December 9–10
Lecture Series **Approximate Verification of Probabilistic Dynamical Systems**
Organizer: TUM Faculty for Informatics
Speaker: Prof. P.S. Thiagarajan | TÜV Süd Stiftung Visiting Professor

In Focus:
Metropolis Nonformal – Anticipation

Metropolis Nonformal – Anticipation

A global gathering where voices for the poor echoed through a royal ballroom

Medellin, Colombia

“Wherever a city's planned infrastructure and officially sanctioned housing stock are inadequate for waves of new residents, or simply out of reach for the poor, people do what they can to create their own.”

One of the most striking differences between the symposium “Metropolis Nonformal – Anticipation” and other meetings hosted by the TUM Institute for Advanced Study was in the language participants used to present their work and argue with each other. It tended to be poetic, political, and rich in invented terms – often contested – designed to capture the essence of complex social and economic phenomena, to convey the nuances of problems and ways they might be approached, and to draw distinctions between seemingly similar points of view. “This is so new,” said Hans Fischer Senior Fellow Christian Werthmann, “that we're still struggling to find the right terminology.”

At the same time, this symposium exemplified a core characteristic of the Institute: the ability to couple a starkly realistic view of 21st-century society's great challenges with irrepressible optimism, engagement, and creativity.

In this case, the focus was on how urban planning, design, and architecture might ease the distress of people leading a marginal existence in and around the world's megacities. Wherever a city's planned infrastructure and officially sanctioned housing stock are inadequate for waves of new residents, or simply out of reach for the poor, people do what they can to create their own. The results – ranging from huts on hillsides to improvised low-rise row homes and gangster-dominated camps under bridges in flood zones – are the slums of our time. “People are forced into living conditions that increase their health, environmental, economic, and social vulnerability, and there's nothing nice about that,” said Claudio Acioly of UN Habitat, the United Nations agency for human settlements.

Over a period of decades, authorities and to some extent academics have responded to these self-made slums – “informal” or “nonformal,” “self-constructed” or “self-produced” – in a series of stages: denial, eradication, tolerance, and improvement. The next stage, according to Werthmann, must be anticipation. The global population of such communities is expected to swell by an additional two billion children, women, and men between now and 2050.

Claudio Acioly and Christian Werthmann

The starting assumption for the Metropolis Nonformal Focus Group of the TUM-IAS is that most of these migrants will have a hand in building and shaping their own urban environments.

The total number of academics and professionals devoted to accommodating this looming human tsunami is relatively small, of course. Thus the 50 speakers and 250 other participants in the November 20–23 “Anticipation” symposium constituted a significant fraction of that community. Their meeting also served as the official launch of the new UN Habitat University Initiative Hub on Informal Urbanism. This “UNI” Hub, Acioly explained, is expected to develop new kinds of research and knowledge that can support needed changes in policy and practice globally. He said the Hub would provide more relevant training for future leaders, build trust among stakeholders, and facilitate match-making across a global network.

Nearly every continent was represented at the Munich meeting. The opening lecture by Mumbai-based Rahul Mehrotra focused on stories from his experience in India while, conceptually, ranging far and wide. Speakers shared their research and experience in critical areas of the Asia-Pacific region, Central and South America, and Africa. From every region, descriptions of the demographic trends, living conditions, and political obstacles often made the situation sound hopeless. Yet somehow hope nearly always was part of the message,

Ninik Suhartini

together with confidence and commitment – for example in the assertion by Harvard's Anna Heringer that “architecture is a tool to improve lives.” She talked about “handmade architecture” as a catalyst for developing shelter, communities, skills, and work opportunities. “And it's also,” Heringer added, “strongly linked with the longing for beauty and dignity.”

A common theme was the claim that meaningful advances could in fact be achieved by simultaneously harnessing “global creativity” and local knowledge. Cynthia Smith of Cooper-Hewitt argued that solutions could be transferable: “Innovative strategies developed for locations with limited resources and challenging environments can be adapted for use in cities around the globe, including in the US and Europe, where resource consumption needs to be reduced.”

The optimistic strain was tempered, however, by skeptical comments and accounts of well-intended interventions that failed. Edgar Pieterse, from the University of Cape Town, took a deliberately provocative stance: “We should get more real here. I think that there's been a kind of naivete about politics and about power and about popular culture, and in some ways a kind of silence about these things, which are absolutely fundamental to structuring the condition of informality.”

While explaining how his group, based at the National University of Singapore, accomplishes precision mapping and modeling of river settlements over time, Jörg Rekittke asserted that it was “not helpful” to differentiate between formal and nonformal. “That's why I call it ‘permanent residence on board a sinking ship,’” Rekittke said, adding that in the Jakarta settlements he is engaged with, “the people on board are celebrating life.”

More than one speaker commented on the incongruity between the event’s topic and its location in the Sophiensaal, a royal ballroom designed and named for a 19th-century princess. If anything, though, that may have sharpened attention to present-day conditions underlying urban poverty, such as the grotesque inequality between the world's richest families and nearly everyone else.

Words of the writer Samuel Beckett, equally brilliant and bleak, were invoked to express the paradox of persistently striving toward a probably impossible goal: “Ever tried. Ever failed. No matter. Try again. Fail again. Fail better.”

Patrick S. Regan

Rahul Mehrotra and Hubert Klumpner

Martim O. Smolka and Maria Teresa Diniz

Edgar Pieterse

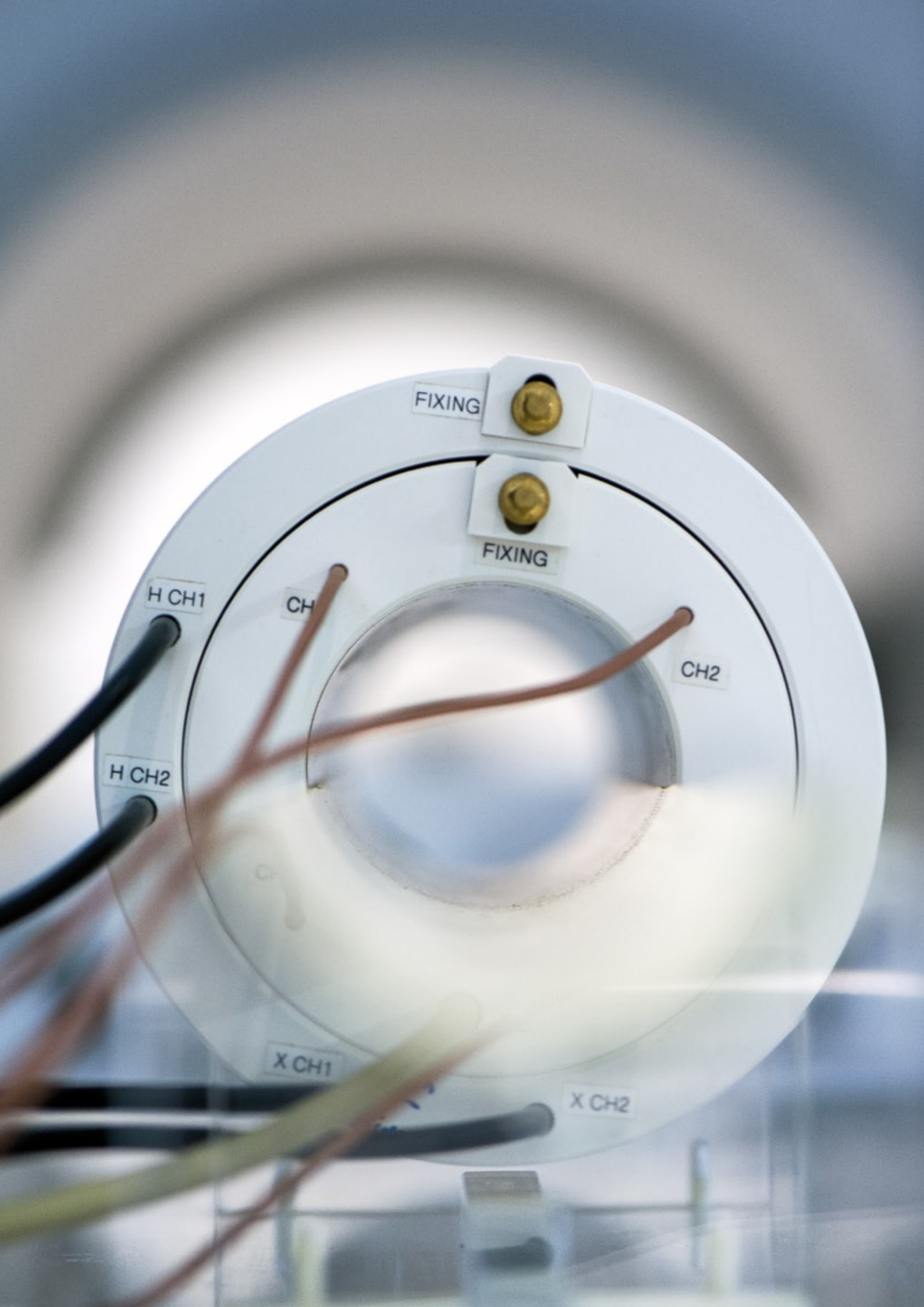
Scientific Reports

Engineering Sciences

Life Sciences

Medicine

Natural Sciences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Scientific reports of the Focus Groups

In this section, the TUM-IAS Focus Groups highlight their major achievements of 2013 or briefly describe their goals in the case of newly started activities. The more interested reader is referred to the original publications and reviews which are listed in total in the publications section. The scientific reports are grouped according to the main research areas, namely engineering sciences, life sciences, medicine, and natural sciences. The color codes for the four different areas are kept consistent throughout the report, also for the facts and figures as well as for the finances sections.

Several Focus Groups were terminated in 2013 after three years of funding. Among these are *Advanced Computation* (Campbell, Lindemann), *Advanced Cardiac Mechanics Emulator* (Ortiz, Wall), *Aircraft Stability and Control* (Heller, Holzapfel), *Diesel Reloaded* (Spiegelberg, Knoll), *Engineering Risk Analysis* (Mok, Straub), *Nanoimprint and Nanotransfer* (Karrai, Porod, Lugli), *Clinical Cell Processing and Purification* (Riddell, Stemberger, Busch), *Neuroscience* (Konnerth, Misgeld), *Advanced Construction Chemicals and Materials* (Hirata, Plank), *Nanophotonics* (Abstreiter), *Nanoscale Control of Quantum Materials* (Auwärter, Barth), and *Non-equilibrium Statistical Mechanics at the Nanoscale* (García Morales, Krischer). Fortunately several of these very successful collaborative projects continue and have expanded through different support, such as ERC grants or joint DFG, NSF or EU-funded initiatives.

Some longer-existing Focus Groups continued and strengthened their successful work within TUM-IAS by integrating newly appointed Fellows. These are *Advanced Stability Analysis* (Schuermans, Sujith, Polifke, Sattelmayer), *High Performance Computing* (Biros, Hegland, Mehl, Bungartz), *Global Change* (Menzel, Sparks), and *Biochemistry* (Hagn, Kessler).

A few new Focus Groups started their work in 2012/2013 and have their first reports already included in this section. The subjects are *Intra-Operative Therapy* (Friebe, Navab), *Nanoscience for Renewable Energy Sources* (Goodnick, Lugli), *Proteomics* (Kuhn, Lichtenthaler), *Regenerative Medicine* (Hutmacher, Schilling), and *Cradle to Cradle* (Braungart, Lang).

In 2013 we granted several new Fellowships, and those groups started their activities in fall 2013 or will do so in the beginning of 2014; therefore, they have not yet contributed a scientific report. The newly established Focus Groups cover the areas *Nanophotonics and Quantum Optics* (Vuckovic, Finley) as a continuation of the former *Nanophotonics* project, *Metal-Organic Superlattices of Quantum Magnets* (Brune, Barth, Reuter), *Functional Interfaces* (Batzill, Barth), *Neuroimaging* (Rauschecker, Hemmer), *High Resolution Gravity Modeling* (Hirt, Pail), *Phase Contrast Computing Tomography* (Koehler, Pfeiffer), and *Electrochemical Interfaces in Batteries* (Lamp, Gasteiger), as well as a continuation of the *Biophysics* project (Dogic, Dietz, Bausch). In addition, the first Rudolf Mößbauer Tenure Track Professors have been appointed and have recently started their work on *Synthetic Biochemistry* (Lang), *Image-Based Biomedical Modeling* (Menze) or *Theory of Soft Matter* (Zaccone) at TUM.

However, the total number of new Fellows and starting Focus Groups was kept smaller in 2012 and 2013 due to uncertainties in the long-term funding situation of TUM-IAS. After the success of TUM in the second round of the Excellence Initiative we are now planning an increase of new Hans Fischer and Hans Fischer Senior Fellowships – up to nine in total – and Rudolf Diesel Fellowships – up to four – in the year 2014. Additionally we started, as a new initiative, the Rudolf Mößbauer Tenure Track Professorships, with the goal of giving highly talented young researchers an optimum start to their independent research careers with great perspectives for the future. We hope to establish a substantial number of such research groups by the end of 2014, covering a broad spectrum of interdisciplinary research areas. We expect and hope for exciting research and groundbreaking results in the coming years.

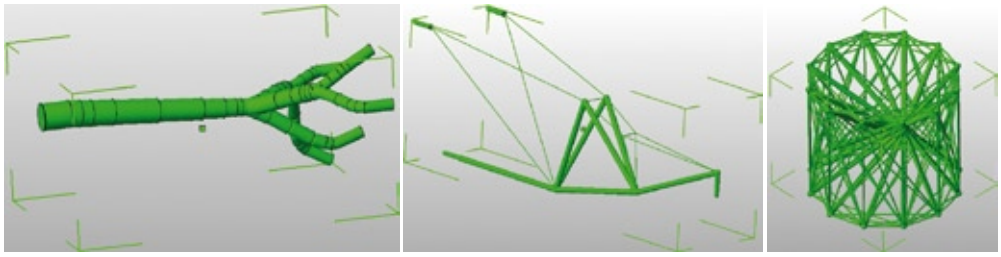
Engineering Sciences

Prof. Matthew Campbell | Hans Fischer Senior Fellow
Amir Hooshmand | Doctoral Candidate
Prof. Udo Lindemann, Product Development, TUM

Matthew Campbell

Solving engineering design problems through a combination of generative grammars and simulations

The significant amount of computing power and memory of today's computers has enabled the development of new methods and algorithms for diverse areas of application. However, the amount of design automation in different fields varies drastically. In mechanical engineering, computer-aided design (CAD) technologies are used mainly for analysis and representational purposes. These tools concentrate mainly on analysis and optimization of very specific details in a proposed solution. They leave the most critical part of finding a conceptual design solution to human designers. Design synthesis is an area of research which is focused on developing methods and tools to support the generation of solutions at the early phases of the design. One of the main problems of automated design synthesis is that solutions are too often simple and fail to capture the real complexities of the problem since they are traditionally based on theoretical principles instead of common sense heuristics. This work seeks to overcome the simplicity and time-consuming computation by utilizing design knowledge and information during the synthesis process. During the last 36 months, Prof. Matthew Campbell's research group has developed a framework for capturing and using design knowledge in



1 | The automated synthesis of fluid channels is created for a complex test problem consisting of one input and five outputs. The result shows a solution with smooth curvature and smooth changes in diameter to minimize loss. In the second problem, a cantilever truss is created by applying rules that include heuristics to minimize beam bending. This approach to shape synthesis is unlike many current approaches which take hours to complete. The third problem is a tensegrity structure where static equilibrium is achieved despite the fact that beams are connected only by cables. Constraints such as these as well as other meaningful manufacturing constraints can be incorporated to achieve near-optimal solutions within reasonable time limits through Prof. Campbell's approach.

the synthesis processes using generative graph grammars. On top of this framework, the group has been solving three engineering design problems to validate the framework. The design decision-making process is made more efficient by an appropriate leveraging of design information and knowledge. The results show that utilizing design information and knowledge not only produces many alternative valid and optimum solutions, but also that it reduces computation by avoiding the generation of invalid design candidates, which normally constitutes a significant portion of research performed by other approaches.

Selected Publications

[1] A. Hooshmand and M. I. Campbell, "Topology optimization of fluid channels using generative graph grammars," in *39th Design Automation Conf. (ASME2013),* 2013. doi:10.1115/DETC2013-13058

[2] A. Hooshmand, M. Schlaich, L. Belaus, and M. I. Campbell, "CDS platform - a platform for multi-physics computational design synthesis," in *Proc. of the 19th Int. Conf. on Engineering Design (ICED13), Design for Harmonies,* vol.9: Design Methods and Tools, Seoul, 2013, pp. 099–108.

Focus Group **Aircraft Stability and Control**

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

Flying into a *novel* future

1 | SAGITTA multidisciplinary advanced research Demonstrator – Flying Wing UAS.

Matthias Heller

The main objective of the Focus Group Aircraft Stability and Control is to investigate new techniques in the field of dynamics, performance, stability, and control of innovative unmanned aircraft systems (UAS) in order to bridge the currently existing gap between theory and real flight. Hence it is our vision and mission statement to maturate novel (adaptive) control techniques towards their valuable application within real flying systems by overcoming the so-called “certification collapse”: i.e. to develop certifiable flight control systems (FCS) featuring guaranteed stability, robustness, and performance properties which satisfy the rigid requirements on safety, accuracy, availability, and survivability which are common in aviation.

In the year 2013, the development and build-up of the SAGITTA Demonstrator, an unstable Flying Wing UAS (see figure 1), moved into focus in order to bundle the outcomes and synergies of the fruitful collaboration between a broad range of outstanding partners towards the maiden test flight in 2015 (figure 2). Within the dedicated “lighthouse project SAGITTA” and in embodiment of our vision, the progressive construction of this multidisciplinary advanced research flying test bed represents a joint effort to provide the evidence of validity and feasibility of the novel approaches and theoretical research results via in-flight demonstration. One major achievement was passing the Flight Management System (FMS) Preliminary Design Review (PDR) in summer 2013 – for this safety critical core system the TUM-IAS Focus Group holds the overall design responsibility – after proofing the configuration's controllability and stabilization capability (figure 3) and the definition of the entire flight control system hardware design.

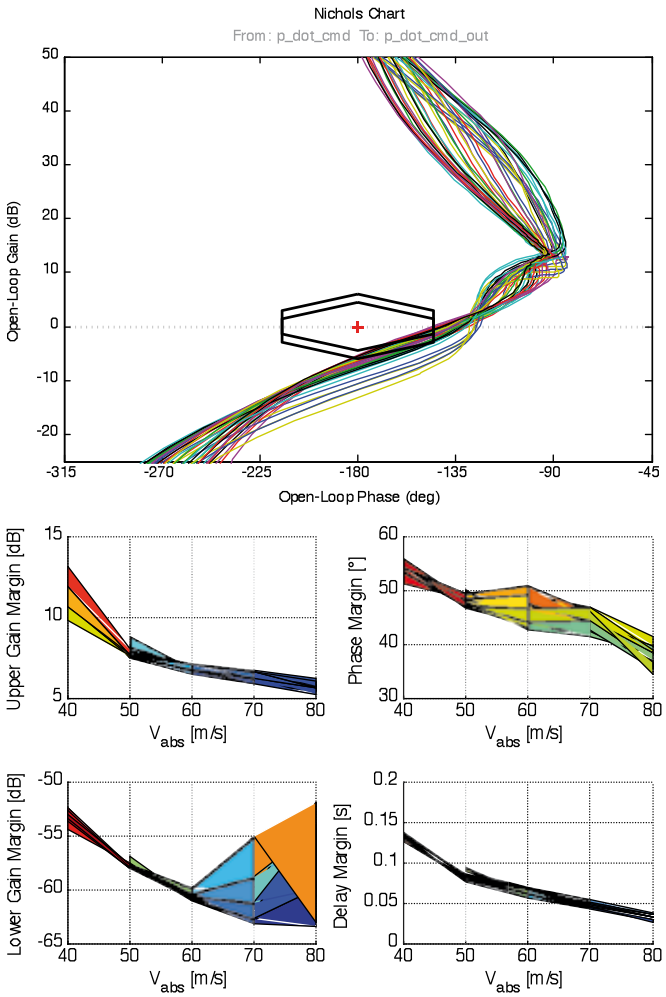
2 | The research program partners directly after commitment to integration and first flight schedule within the SAGITTA Program Review in November 2013.

Additionally, as a fundamental component of the entire safety concept, two UAV test pilots verified the manual landing capability (via remote control) of the SAGITTA Demonstrator. This manual landing study was conducted in the hardware and integration laboratory at the Institute of Flight System Dynamics of TUM, running the (stabilizing) reversionary control laws in real-time on the original backup flight control computer (BFCC) and thus, effectively performing the first hardware-in-the-loop simulation (HILS) validation tests of the system (figure 4).

Subsequently, the systems architecture was frozen and the overall demonstrator PDR could be accomplished successfully, as the mandatory prerequisite for the further development, manufacturing, and integration steps. Currently, following development and testing of core elements, the Focus Group is entering the definition and layout process of the crucial flight controller, followed by an integration and testing phase, in order to prepare and support the first flight tests. In addition, the automatic landing functionality is going to be integrated adequately together with the general auto-flight algorithm structure.

Complementary, ongoing research of an adaptive control scheme providing a pre-normalized ideal plant serving as robust basis for the actual flight control laws to be developed is advanced. Here, the adaptation focuses on output-feedback methodologies, enhancing flexibility in the sensors to be utilized. Moreover, the theoretical foundation for incorporation of thrust vector control into the feedback loops, which - in contrast to aerodynamic control surfaces - enters the dynamics nonlinearly, has been prepared and the resulting algorithm is integrated into a dynamic inversion control system structure.

A novel formulation of a Lyapunov-based stability theorem, which is tailored to the proposed flight control system structure, provides a tool for guaranteed stability characteristics of the adaptive closed loop system in the presence of unmatched uncertainties.



3 | Controllability and Stabilization Capability Assessment study as fundamental prerequisite for the demonstrator Preliminary Design Review (PDR).

In parallel to the demonstrator development activities, noteworthy research is being conducted within the frame of the TUM-IAS Focus Group Aircraft Stability and Control in two associated areas: “Excellent Handling Qualities Design of General Aviation Aircraft” [1] and “Active Control Systems dedicated to Future Small Aircraft” [2], each represented by a doctoral candidate.

The SAGITTA research program attracted plenty of attention as it was presented to a wide public at the Dubai and International Paris (Le Bourget) Air Show and the DWT (Deutsche Gesellschaft für Wehrtechnik e.V.) Symposium in Bonn.

4 | Manual Landing Study conducted in the hardware and integration laboratory at Flight System Dynamics of TUM in July 2013.

The project has repeatedly been the subject of reports and discussions in various aviation specialist journals (e.g. Flight International, UAS Vision) and the corresponding SAGITTA UAS configuration has been recently included in professional reference books (e.g. Janes) highlighting the great interest in this exceptional venture. In 2014, the research group will expedite the respective investigations and development work towards the Critical Design Review (CDR) in order to realize our vision and let the SAGITTA Demonstrator fly (unmanned) into a novel future.

In collaboration with Stanislav Braun, Simona Wulf, Falko Schuck, and Thaddäus Baier.

Selected Publications

[1] F. Schuck, M. Heller, T. Baier, and F. Holzapfel, “Longitudinal robust controller for excellent handling qualities design of a general aviation aircraft using QFT,” in *AIAA Guidance, Navigation & Control Conf.*, Boston, MA, 2013. doi:10.2514/6.2013-5180

[2] M. Heller, T. Baier, and F. Schuck, “Lateral fly by wire control system dedicated to future small aircraft,” in *Advances in Aerospace Guidance, Navigation and Control. Selected Papers of the Second CEAS Specialist Conference on Guidance, Navigation & Control,* Q. Chu et al., Eds. Berlin: Springer-Verlag, 2013, pp. 353–372.

More publications by this Focus Group can be found on page 120.

Focus Group **Advanced Cardiac Mechanics Emulator**

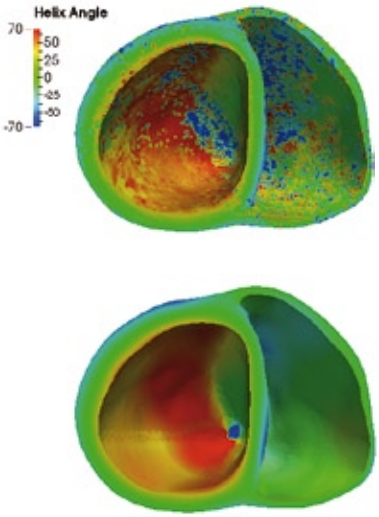
Prof. Michael Ortiz | Hans Fischer Senior Fellow
Dr. Cristóbal Bertoglio | Postdoctoral Researcher
Andreas Nagler | Doctoral Candidate
Prof. Wolfgang A. Wall, Computational Mechanics, TUM

Multiscale and multiphysics modelling of the heart

Michael Ortiz

The Advanced Cardiac Mechanics Emulator (ACME) is a collaborative effort between 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 aims to combine state-of-the-art biophysical models of myocardial tissue, hemodynamics, and the electrophysiological response of the heart within a high-performance computing framework.

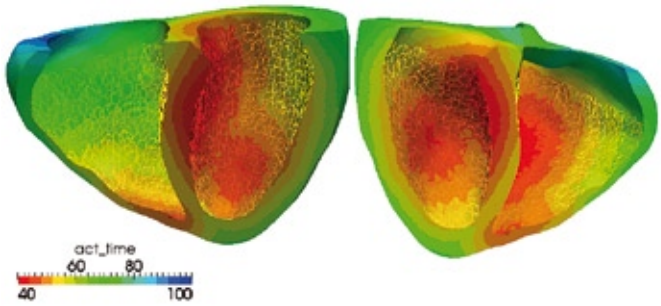
The first challenge was to model the geometry of the human heart, which we have addressed by using *in vivo* ECG-gated computer tomography (CT) in order to construct a finite element (FE) discretization. After that, in order to simulate the physiology of the heart, a model of the myocardium histology – 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 geometry. In particular, we have developed a methodology for synergistically combining mathematical models and fibers measured through diffusion tensor magnetic resonance imaging (DT-MRI). Specifically, we estimate – through the solution of an inverse problem – the degrees of freedom of the model, namely, the parameters of the angle distribution on the epi- and endocardial surfaces. Future work may consist of acquiring fiber data and dynamic geometrical sequences in the same patient in order to study the influence of the fibers in the contraction dynamics and stress distribution.



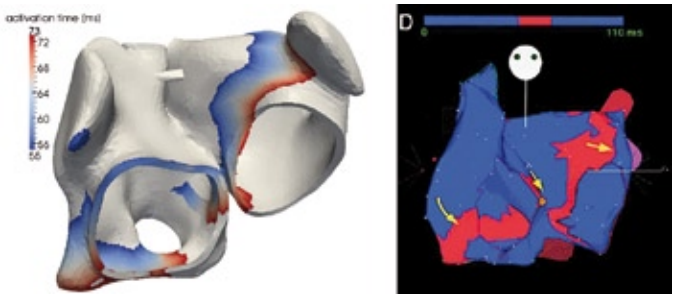
1 | Comparison of the fiber angle (with respect to the short axis plane) between 3D DT-MRI (top) and estimated (bottom).

The cardiac contraction is triggered by an electrical impulse, which is transmitted in the first instance by the so-called fast cardiac conduction system (FCCS), a set of specialized cells isolated from the rest of the myocardium which allow the rapid conduction of the electrical impulse for homogeneously activating the working heart muscle. Hence, including it in the computations remains a necessity in every detailed cardiac model. We achieved a first version of the FCCS based on 1D elements interacting with 3D elements, but with a higher electrical conductivity. Figure 2 shows the achieved times of electrical activation with the combined 1D-3D elements.

During this year, we made our first steps in modeling the electromechanical physiology and pathophysiology of the atria, taking advantage of the previously segmented 4-chamber geometry. After a devoted literature research, we constructed the fiber model of the atria, which is generally much more intricate than that of the ventricles. This allowed us to run coupled electromechanical simulations, which have the potential to quantify the atrial contractile performance far beyond the current clinical imaging capabilities. Concretely, a precise electromechanical model of the atria would allow clinicians to predict the impact of their electrophysiological surgical procedures on the mechanics. Figure 3 presents an example of an electrophysiology simulation. Even though they are from different individuals, the agreement is satisfactory.

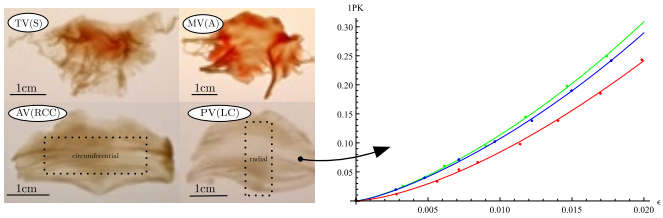


2 | Activation times (in ms) computed using a combined myocardial-FCSS electrophysiological model. Note that in the left ventricle, the muscle is activated from endocardium to epicardium as it does in reality.



3 | Comparison of the activation times (in ms) between an electrophysiology simulation (left) and data from a real patient (right).

Maybe the most challenging component of the heart from the mechanical point of view is the valves separating the cardiac chambers. An obstacle to the predictive modeling of human heart valves is the current paucity of data regarding their mechanical properties. In order to fill this gap, we have conducted uniaxial and biaxial tensile tests on porcine heart valve leaflets in order to characterize the mechanical properties of the entire complement of valves and leaflets under tensile loading. Sample specimens and the resulting stress-strain data for the posterior tricuspid valve are shown in figure 4. The data exhibit a high degree of reproducibility across different specimens and provide a wealth of quantitative information and insight into the structure and mechanical properties of heart valves.



4 | Left: leaflet samples for the four porcine cardiac valves. Right: fitting of experimentally measured strains and stress (dots) by an analytical biomechanical valve model including fiber reinforcing (lines) for three different leaflets of the same pulmonary valve.

Finally, we would like to remark that during 2013 the Focus Group achieved two international successes. At the end of June, the 7th International Conference on Functional Imaging and Modeling of the Heart took place in London, UK, where Andreas Nagler obtained the Best Poster Award.

The second achievement was the organization of the very successful 1st International Workshop on Latest Advances in Cardiac Modeling, held at the TUM-IAS facilities from July 10 to 11 (www.tum-ias.de/lacm2013). During two intense and exciting days, around 35 leading researchers from Europe and North America presented and discussed the latest results in cardiac modeling.

Selected Publications

[1] A. Nagler, C. Bertoglio, M. Gee, and W. Wall, “Personalization of cardiac fiber orientations from image data using the unscented Kalman filter,” in *Lecture Notes in Computational Sciences 7945: Functional Imaging and Modeling of the Heart,* S. Ourselin, D. Rueckert, N. Smith, Eds. Berlin: Springer, 2013, pp. 132–140.

[2] A. Nagler, C. Bertoglio, and W. Wall, “Complex modeling and estimation of the cardiac tissue anisotropy,” in *Proc. of the 3rd Int. Conf. on Mathematical and Computational Biomedical Engineering,* Hong Kong, 2013, pp. 57–60.

Focus Group **Advanced Stability Analysis**

Prof. Raman I. Sujith | Hans Fischer Senior Fellow
Dr. Bruno Schuermans | Rudolf Diesel Industry Fellow
Ralf Blumenthal, Sebastian Bomberg, Tobias Hummel | Doctoral Candidates
Prof. Wolfgang Polifke, Prof. Thomas Sattelmayer, Thermodynamics, TUM

Raman I. Sujith

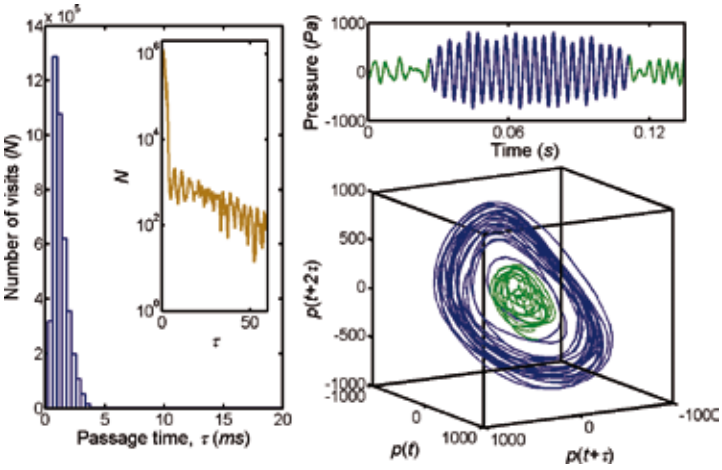
Bruno Schuermans

The occurrence of thermoacoustic instability – also known as combustion instability – has been a problem plaguing the development of combustors for rockets, jet engines, and power generating gas turbines. Our ultimate goal of predicting and controlling instability in industrial combustors requires an understanding of the interactions between the combustion process and the acoustic waves. Our cause was strengthened by Dr. Bruno Schuermans (Alstom, Switzerland), who joined the group as a Rudolf Diesel Industry Fellow. He will contribute his rich experience and a unique control- and systems-theory-based perspective on thermoacoustics to our studies. The Diesel Fellowship will also strengthen the industrial perspective and bridge the gap between the academic and the industrial worlds.

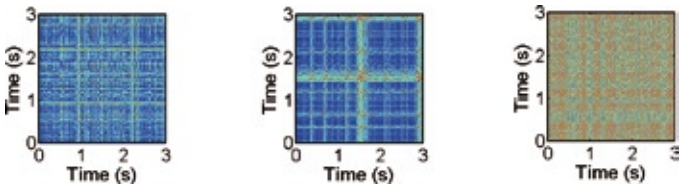
In the summer, Prof. Raman I Sujith, along with his doctoral candidates Vineeth Nair, Ennappadam Gopalakrishnan, Meenatchi Devi, and Vishnu Unni, visited Munich. Prof. Arun Tangirala (IIT Madras), with whom we collaborated on system identification as applied to flame dynamics, also visited TUM. During the summer, we made significant progress in our DFG project titled “Non-normality in flow – premixed – flame – acoustic interactions and its consequences for combustion instability.” There were intensive discussions on the question of the most appropriate energy norm for thermoacoustic processes. This question is crucial for the proper description of non-normal effects. A joint publication is in preparation. We also organized a short course on estimation theory, in which Prof. Tangirala delivered lectures that attracted audiences from many TUM departments. Further, Prof. Sujith had extensive interactions with Dr. Schuermans that are now leading to collaborative work.

Ralf Blumenthal visited IIT Madras in the last quarter of 2013. We worked on completing the formulation of models of thermoacoustic systems in the time domain, where the dynamics of the heat source are incorporated in terms of a distributed time lag response function. We showed that the linear response of the heat source in a thermoacoustic system should be represented in terms of a distributed time lag response function rather than a single time lag model, with a view to retain the rich complexity that is present even in such a low-order model for the heat source. A joint paper has been submitted. Our experimental studies involved performing experiments on industrial combustors that have swirling turbulent flow. We are also examining the onset of thermoacoustic instabilities in greater detail. This involves studying the mechanisms underlying the transition from broadband combustion noise to narrowband thermoacoustic oscillations. Combustion noise was identified to be the result of chaotic dynamics of the global system comprising turbulence, combustion, and the chamber acoustics. Further, we showed that these chaotic fluctuations display scale invariance and multifractality, which provides evidence for the multiple scales involved in the energy transfer.

An international summer school and workshop on Non-normal and Nonlinear Effects in Aero- and Thermoacoustics (N3L) was held during June 18–21, 2013 at TU Munich. The conference was funded by TUM-IAS and the Marie Curie Initial Training Network TANGO (Thermo-acoustic and Aero-acoustic Nonlinearities in Green combustors with Orifice structures). We had about sixty participants: Half of them were experienced researchers and half of them were doctoral candidates and postdoctoral researchers.



1 | The distribution of the time spent by the dynamics in the low-amplitude aperiodic segments is seen to have an exponential tail indicative of the formation of homoclinic orbits in the phase space. Shown next to it is a single burst of oscillations in the pressure signal and its corresponding evolution in an embedded phase space showing the formation of a homoclinic orbit.



2 | The recurrences or repeating patterns in the dynamics of pressure signals during the various states – chaotic, intermittent, and periodic – are shown in terms of a pairwise distance matrix in phase space called a recurrence plot. The recurrence plot, which is grainy during chaotic dynamics, develops perforated enlarged rectangular structures during intermittency. The recurrence plots during periodic oscillations are composed of parallel diagonal lines indicative of a bifurcation in the underlying system.

Selected Publications

[1] R. S. Blumenthal, P. Subramanian, R. I. Sujith, and W. Polifke, "Novel perspectives on the dynamics of premixed flames," *Combust. Flame*, vol. 160, no. 7, pp. 1215–1224, 2013.

[2] V. Nair and R. I. Sujith, "Identifying homoclinic orbits in the dynamics of intermittent signals through recurrence quantification," *Chaos*, vol. 23, no.3, pp. 033136-033136-6, 2013.

More publications by this Focus Group can be found on page 120.

During the summer school (June 18 and 19), a series of invited lectures by leaders in the subject reviewed the state of the art on topics of current interest. Speakers included Prof. Tim Lieuwen (Georgia Tech), Prof. Oliver Paschereit (Berlin), Prof. Ganesh Raman (Illinois Institute of Technology), Prof. Guillaume Penelet (Université du Maine), Nicolas Noiray (Alstom Power), Dr. Matthew Juniper (Cambridge), and Prof. Sujith (IIT Madras, TUM-IAS). The speakers provided an overview of the rapid developments in the field, and offered a glimpse of things to come. The video recordings of these lectures are an excellent resource for researchers in this topic. The summer school was followed by the workshop (June 20 and 21), which brought together researchers active in aero- and thermoacoustics to present and discuss original, recent research results on non-normal and nonlinear effects in these disciplines. The papers from this meeting are presently undergoing peer review; the accepted papers will be published in a special issue of the International Journal of Spray and Combustion Dynamics. Until recently most research in thermoacoustic instability was performed in the framework of linear stability analysis. N3L highlighted, in a stimulating atmosphere, the rapid developments that are taking place in the nonlinear analysis of aero- and thermoacoustic instabilities. Both the summer school and the workshop were grand successes.

Bruno Schuermans received his M. Sc. degree in mechanical engineering from Delft University of Technology in the Netherlands in 1998. He joined the ABB Corporate Research Center in Switzerland to conduct research in the field of thermoacoustic combustion instabilities. In 2003, he obtained a Ph.D. in mechanical engineering from the Swiss Institute of Technology in Lausanne (EPFL). His Ph.D. thesis was on the subject of modeling and active control of thermoacoustic instabilities. He is currently a principal engineer at Alstom in Switzerland where he leads a team that is responsible for the development of numerical and experimental methods for analysis of combustion dynamics of gas turbine combustion systems. Dr. Schuermans is the holder of more than 30 patents in the field of combustion control, diagnostics, and optimization.

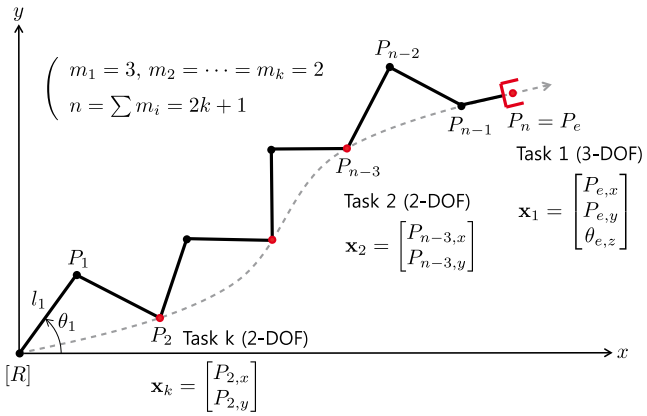
Prof. Dongheui Lee | Carl von Linde Junior Fellow
Sang-Ik An | Doctoral Candidate
Prof. Martin Buss, Automatic Control Engineering, TUM

Control strategies for multiple tasks with priority

Dongheui Lee

Performing multiple tasks at the same time is an important human skill because it allows us to be more efficient and reliable in unstructured and unpredictable environments. For the same reason, in the history of robotics there have been intensive studies to develop control strategies for multiple tasks with priority. Technically, this is a problem of finding forward and inverse mappings between the joint space and the task space of a robot such that the joint motions corresponding to the task motions are determined to minimize the task execution errors while preserving the task priority. A widely-used mathematical tool for this problem is projection theory. The lower-priority tasks are projected to the null-space of the higher-priority tasks while the inverse solutions are calculated. The variants of conventional methods can be divided into two groups, based on the projection between tasks: iterative and non-iterative methods. The non-iterative method directly calculates the inverse solutions with null-space projectors, while the iterative method constructs a series of optimization problems and searches for the inverse solution iteratively.

We have proposed new non-iterative methods using QR and Cholesky decompositions for the purpose of separation of orthogonalization and inversion processes, as the conventional methods perform both simultaneously. The strength of our proposal is the elimination of the interference between two processes. Our basic idea is to perform the QR decomposition of the Jacobian transpose without pivoting, allowing the original Jacobian to be decomposed into two parts, the lower triangular square matrix multiplied by the row-orthonormal matrix. In this frame, the prioritized inverse solutions can be derived in the recursive or closed forms. When a manipulator operates near the singularity, the Jacobian loses its full rank and the inverse or pseudo-inverse of the Jacobian diverges. Therefore, the damped-least squares pseudo-inverse must replace the original inverse or pseudo-inverse. In the conventional method, this replacement can affect both orthogonalization and inversion processes, and this unnecessary interference between two processes can produce inaccuracy or instability in the prioritized inverse solutions. However, our method does not suffer from this interference because the inversion process is totally decoupled from the orthogonalization process thanks to the QR and Cholesky decompositions.



1 | Geometry of the n-link manipulator

To show the effect of the proposed methods, we have performed simulations using the two-dimensional n-link manipulator shown in figure 1 with various numbers of tasks. The tasks are designed for each control point to reach to the outside of its workspace in order to introduce singularities. If the inverse solution preserves the priorities accurately, the task errors of the higher-priority tasks should be close to zero, while the lower-priority tasks cannot be performed perfectly and result in task errors. To verify the proposed methods, four different prioritized inverse solutions are tested, two conventional methods and two proposed methods. In the simulation, the proposed method using both QR and Cholesky decompositions gives the best results.

In the case of the iterative method, the multiple task problem can be formulated as a cascade of quadratic programming (QP) problems. At each level of priority, a separate QP is constructed and the search space of lower priority QP is restricted to be the optimal solution set of higher priority QP. The advantage compared with non-iterative methods is that unilateral constraints can be added explicitly. Based on the QP formulation, we proposed a framework to imitate the human walking motion online both in task and joint spaces, targeting more human-like behaviors. Two aspects are essential for a successful walking imitation: stable footprints represented in task space; and motion similarity represented in joint space. The human footprints are recognized through the captured motion data and imitated by the robot through a conventional zero-moment point control scheme. Additionally we focus on similar knee joint trajectories for the motion similarity, which are related to knee stretching and swing leg motion. Conventional walking controllers usually produce knee-bended walking because of the joint singularity and this can be solved by adding an inequality constraint to the knee joint position.

The inverse kinematics suffers strongly conflicting tasks and underactuation because of the knee joint tracking task. We solve this problem by formulating conflicting tasks as dynamic constraints, and a continuous task switching is realized by introducing an activation buffer, resulting in a cascaded QP form.

We evaluate the effectiveness of the proposed approach on the DLR humanoid robot TORO as shown in figure 2. Captured human walking motion is imitated by the TORO with additional knee joint tracking. The cascade of two QPs with 12 variables considering more than 20 constraints can be solved in 1000 Hz frequency on the robot's onboard computer. The proposed framework results in a more natural-looking and energy-efficient walking style.

2 | Human walking imitation based on quadratic programming.

Selected Publications

[1] S. An and D. Lee, "Prioritized Inverse Kinematics using QR and Cholesky Decompositions," *IEEE Int. Conf. on Robotics and Automation (ICRA),* 2014, accepted.

[2] K. Hu, C. Ott, D. Lee, "Online Human Walking Imitation in Task and Joint Space based on Quadratic Programming," *IEEE Int. Conf. on Robotics and Automation (ICRA),* 2014, accepted.

More publications by this Focus Group can be found on page 121.

Dr.-Ing. Angelika Peer | Carl von Linde Junior Fellow
Milad Geravand | Doctoral Candidate
Prof. Martin Buss, Automatic Control Engineering, TUM

Haptic interaction and collaboration in human-human and human-robot dyads

Angelika Peer

Touch is an indispensable component of interaction in real and virtual collaborative environments. Compared to other fields of interaction research like communication via speech and gestures, haptic interaction is still largely underrepresented. Doubtlessly, however, haptic interaction is an essential component for future robotic systems that are supposed to collaborate closely with humans in performing physical tasks, as required when assisting elderly persons in standing up, walking, and sitting down, or when enhancing motor training and rehabilitation.

In such situations, people are not only expected to interact, but to collaborate, which means that both partners try to accomplish a common goal and therefore share intentions and action plans. Thus, haptic collaboration not only implies the physical coupling of two bodies either directly or via an intermediate object, but also involves higher-level cognitive processes. The underlying principles of involved coordination and decision-making processes, however, are largely unknown, which makes their implementation on a robotic platform challenging.

1 | Recording of motion capture data of a caregiver assisting an elderly person while walking. Recording performed at Agaplesion Bethanien Geriatric Clinics in Heidelberg.

Thus, our approach is to first analyze haptic coordination and decision making in human-human dyads and then to transfer gained knowledge to human-robot dyads. In doing so, special attention is paid to the investigation of typical role and strategy distributions adopted by partners and their evolution over time, as well as the investigation of intention estimation and negotiation processes. To gain better insight into processes involved in haptic coordination and decision making, a series of recordings of human-human dyads were made over the last year. This involved the recording of pairs of healthy subjects in typical decision-making situations as well as the recording of more complicated situations capturing the interaction of a caregiver and an elderly person in the situations of standing up, walking, and sitting down.

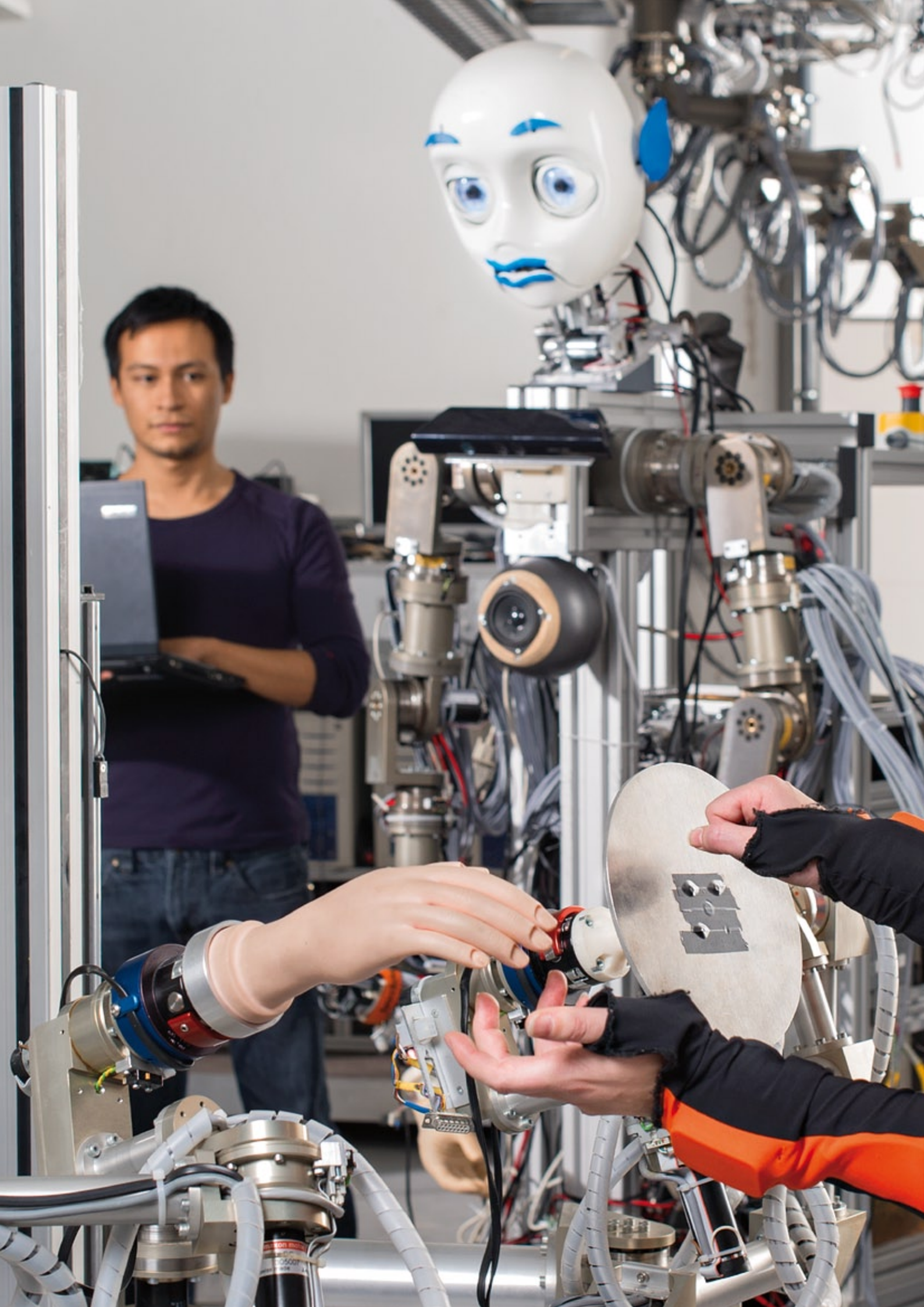
As a first attempt to model decision-making processes we further investigated the win-stay, lose-switch rule and the drift-diffusion model first introduced in cognitive science. Both models were analyzed for their capability to model haptic interaction in human-human dyads and were finally also implemented on a robotic platform to mimic human-like haptic assistance behavior. While these first models can capture basic human decision-making rules, our future work will focus on extending these models and gaining even further insight into the underlying processes of haptic coordination and decision making and the joining of these efforts with attempts to model human movements based on theories of human motor control.

Selected Publications

[1] C. Passenberg and A. Peer, “Exploring the design space of haptic assistants: the assistance policy module,” *IEEE Trans. Haptics*, vol. 6, no. 4, pp. 440–452, 2013.

[2] N. Stefanov, C. Passenberg, A. Peer, and M. Buss, “Design and evaluation of a haptic computer assistant for telemanipulation tasks,” *IEEE T. Syst. Man Cyb.*, vol. 43, no. 4, pp. 385–397, 2013.

More publications by this Focus Group can be found on page 121.



Focus Group **Cradle to Cradle**

Prof. Michael Braungart | EPEA Internationale Umweltforschung GmbH
Martin Korndoerfer, Michiel Kulik | Research Members
Prof. Werner Lang, Energy Efficient and Sustainable Design and Building, TUM

Hakuna Matata – Cradle to Cradle inspired building in east Africa

Michael Braungart

The UNO predicts that, given current conditions, in the 21st century the majority of population increase will occur in developing countries. The population in these parts of the world will increase from 5.4 to 7.9 billion people. In order to prevent and preempt rural depopulation and the explosion of urban centers, it has to be a primary goal of this century to make rural spaces more attractive, primarily but not exclusively through raising rural standards of living and creating attractive, fulfilling job prospects.

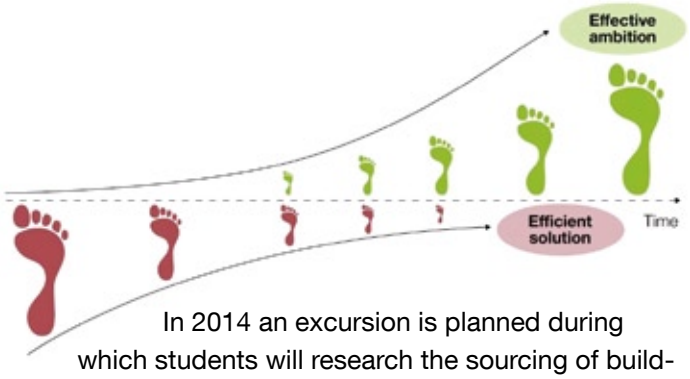
A growing population as well as new infrastructure and production facilities necessary for positive rural development demands the construction of new, and the refurbishment of existing, buildings. These developments have already become apparent through the immense growth rates in the building sector of developing countries around the world. The biggest challenge for these countries to tackle now is to shape the expansion of the built environment in such a way that its construction is socially and environmentally acceptable, and, further, to choose materials that do not get lost as 'waste' after their use phase in the building has ended, nor that endanger functioning ecosystems through unsound sourcing.

The innovative design concept Cradle to Cradle® applied to architecture has the potential to result in buildings that – their primary function of providing a living space for humans aside – are able to provide a net-positive impact on the realms of society, ecology, and economy. This design concept retains the natural capital assets utilized for construction as recyclable building materials, instead of producing a liability at the point of their disposal.

This positive ambition is highly compatible with the aims of the Hakuna Matata Project, which seeks to provide orphans and elderly women in the region around Meru/Isiolo, Kenya with a long-term perspective for the future.

During the winter semester 2013/2014 tutors of the Institute of Energy Efficient and Sustainable Design and Building (ENPB) and the Cradle to Cradle work group have been working with this year's ENPB architecture design master class towards designing a cradle to cradle inspired school and clinic for the Hakuna Matata Project.

The buildings in the complex have been designed as plus-energy buildings with additional ecosystem services, such as the provision of clean drinking water for the occupants throughout the year, including the long dry season, and the continuous cycling of nutrients through the system. The only building materials chosen were those with little impact on the surrounding ecosystems, were locally available, and which can go back into the biological cycle after their use phase without negatively impacting biological systems. The buildings were designed to have the biggest positive environmental footprint as possible, functioning themselves like ecological systems where synergies and added-value for the surrounding environment (human and ecological) were optimized.



1 | EPEA 2012

In 2014 an excursion is planned during which students will research the sourcing of building materials and get to know the building site and the local culture, partake in a stakeholder dialogue to identify the best design, and initiate an exchange on cradle to cradle inspired building with their counterparts at the University of Nairobi. During the summer semester of 2014, the chosen design will be finished to the stage of execution. In parallel, efforts will be undertaken to raise the necessary funds by the end of the year to have the project realized in March 2015.

Building Integrated Greenhouses (BIG)

Air quality in public buildings has often been a topic in the news. High occupation of small rooms combined with bad ventilation creates a bad work and learning environment: Research has shown that focus and performance of occupants can be reduced by as much as 20%. For comparison, on pig farms more budget is available per pig for ventilation than per person in schools.

In cities the indoor air quality is often negatively influenced by the surroundings. Busy roads are a main cause of high concentrations of, among other things, NO_x, CO_2, and fine dust. Additionally, in school classrooms and office meeting rooms relatively high occupation levels lead to high concentrations of CO_2, resulting in the previously mentioned drops in performance. Computers and other equipment and furniture can also contribute to the pollution of indoor air.

The Building Integrated Greenhouse (BIG) concept is a greenhouse on top of a school in China that – combined with a green double facade and interior solutions – acts as a lung in heavily polluted cities. In nature many plants have specialized in metabolizing unwanted polluting substances; most plants even grow faster in higher concentrations of CO_2. Besides the filtration of air, research is done on how specific plant species or other organisms can improve the work or learning environment. The BIG research focuses on how this can all be implemented in buildings as effectively as possible.

2 | happyhealthyschool.com

The research has shown there is great potential for symbiosis between greenhouses and buildings in general, not just in the field of climate control, but also in household energy: for example in heat exchange and storage, and nutrient cycles ('waste is food'). As an illustration, the greenhouse has an abundance of heat in spring and autumn, which can be used to preheat the building. The project won a prestigious award at the 2010 World Expo in Shanghai.

The project is a multidisciplinary cooperative effort between TUM, TU Delft, Utrecht University, Wageningen University, and Priva – a Dutch company specialized in climate and process control of greenhouses. The project is now in the process of acquiring a substantial subsidy for further tests and prototyping.

Focus Group **Diesel Reloaded**

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

Pulling into the final station – summary and final report

Gernot Spiegelberg

1 | Innotruck at the VDI Congress Elektronik in Fahrzeug in Baden-Baden in 2013.

The TUM-IAS Focus Group Diesel Reloaded has ended its activities in 2013, after three challenging and inspiring years on the border between research and engineering. In this report, we present our results and key contributions. Our activities were divided into three distinct automotive areas: energy management, information and communication technology architecture, and human-machine interaction.

Energy management

The main challenge in devising an energy management system that can be used for various commercial vehicles is the smart definition of the interfaces between a central unit for controlling the power conversion and distribution, and the energy components in the vehicle (sources and sinks). The approach consists of several stages:

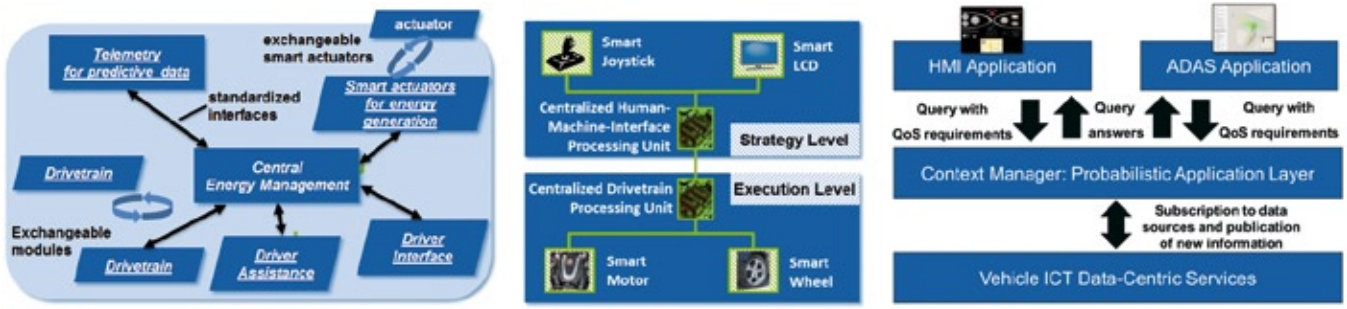
- design of a vehicle model with different power sources and sinks
- validation of the vehicle model based on measurements with a real hybrid-electric commercial vehicle
- development and implementation of flexible energy management
- generalization of the approach for other vehicle types

Information and communication technology architecture

The effort to integrate new functionalities in today's vehicles is increasing as the interconnection and verification of the growing amount of heterogeneous and distributed electric control units, sensors, and actors become more difficult. The demand for a new architectural approach that can cope with the increasing complexity and that

offers possibilities for smooth integration of future technologies is urgent. Such technologies are, for example, drive-by-wire systems and advanced driver assistance systems that make use of multiple sensors and coordinate several actors. With our work, we introduced a centralized ICT architecture for future cooperating intelligent vehicles by a close look into

The project focus was initially placed on the common demonstrator platform InnoTruck. Several integration stages of the InnoTruck were presented at various public and industry events. Throughout the project's course we extended the scope of the individual research topics and added new integration and demonstration platforms, such as the Siemens eHighway



2 | Flexible energy management on the left, centralized ICT architecture in the middle, context-centric HMI design on the right.

possible software, hardware, and system architecture and their properties. In addition, a migration path from the current vehicle architecture was suggested and economic impacts of suggested improvements were shown. Adaptability, safety, and self-reliance will be the key enablers in this future world of intelligent vehicles.

Human-machine interaction

A context-centric design of the human-machine interface has been developed, placing the emphasis on knowledge modeling and knowledge usage by the vehicle applications. The goal was to improve interaction context processing and situation awareness mechanisms on a common automotive computing platform. The context is defined by driver, vehicle, and environment descriptions. The concept of inference quality-of-service and the resulting requirements are introduced, in order to handle the processing of the driver-vehicle-environment context by both driver assistance and human-machine interface applications. The main contribution is given in the area of exact inference on a commonly used probabilistic structure called dynamic Bayesian networks and its optimized derived model, called junction tree. The contribution, under the name of probabilistic application layer (PAL), provides inference as a service to the HMI application space and performs all the housekeeping tasks, such as network reconfiguration and inference scheduling. The approach is validated by experiments in a driving simulator and by synthetic benchmarks of the knowledge network.

truck and a personal vehicle driving simulator.

We would like to thank the Institute for Advanced Study of the Technische Universität München for all the help and the practical support, especially with the organization of various media events. This work would not have been possible without the excellent industry cooperation framework provided by TUM-IAS. Many thanks to our key industry partner Siemens Corporate Technology for sponsoring the doctoral candidates through the International Graduate School for Science and Engineering (IGSSE).

Selected Publications

[1] C. Buitkamp, G. Spiegelberg, and M. Lienkamp, "Reducing costs during development and operation of hybrid commercial vehicles through a market-based electric energy management," *Elektrik/ Elektronik in Hybrid- und Elektrofahrzeugen und elektrisches Energiemanagement IV*, U. Brill, Ed. Essen: expert verlag, 2013, pp. 347–362.

[2] H. Stähle, L. Mercep, G. Spiegelberg, and A. Knoll, "Towards the deployment of a centralized ICT architecture in the automotive domain," *2013 2nd Mediterranean Conf. on Embedded Computing (MECO),* Budva, 2013, pp. 66–69.

[3] L. Mercep, G. Spiegelberg, and A. Knoll, "Context processing for automotive human-machine interfaces," *IEEE Science and Information Conf. (SAI)*, London, 2013, pp. 979–984.

More publications by this Focus Group can be found on page 122.

Focus Group **Engineering Risk Analysis**

Dr. Chin Man W. Mok | Rudolf Diesel Industry Fellow
Wolfgang Betz | Doctoral Candidate
Prof. Daniel Straub, Engineering Risk Analysis, TUM

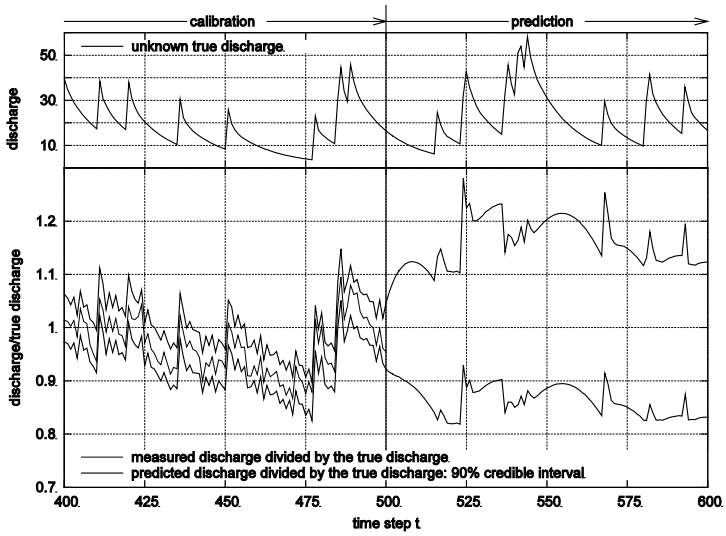
Probabilities, risk, and decision making in environmental systems

Chin Man W. Mok

A more optimal and scientific approach to managing uncertainty in the environment, particularly with regard to hydrologic and geologic risks, is our aim. In this context, a major challenge is bridging the gap between the fundamental (scientific) understanding and the practical (engineering) implementation. Besides our research, we also invested time in 2013 in a number of activities to educate the engineering and scientific communities and to enhance their understanding of the challenges underlying the risk questions. In this third year of the Fellowship, we have also set the basis for future research in the direction of smarter systems and adaptation to climate change.

Smarter use of data in near-real-time risk assessments through the use of Bayesian analysis in combination with numerical (engineering) models is a central theme: Our goal is to be able to continuously update probabilistic process models and corresponding risk estimates as data becomes available from monitoring, sensors, and other sources. We are active in developing efficient numerical methods for the representation of uncertainty in realistic systems through random fields models [4] and for Bayesian updating of these models [5]. In this context, the representation of the modeling error and its effect on the prediction in dynamical systems remains an open question that we are investigating [2].

On the application side, we worked on reliability analysis of dam erosion assessment with monitoring data (Terrestial LiDAR and 3-dimensional photogrammetry) in collaboration with Drs. Robert Wright and Engsew Aw of AMEC Environment and Infrastructure [3]. A number of existing tall dams worldwide have experienced scour and erosion of foundation, abutment, plunge pool, and unlined spillway materials due to flood flows larger than those designed for, and unrecognized adverse geologic conditions. Global climate change and the associated potential increase in future flood events further enhance the dam erodibility risks. Related to this, we also continued our work on the risk assessment of landslide hazard using rainfall information in near real-time [1]. Using instrumented site data provided by the Hong Kong government, we are currently working with Dr. Albert T.-C. Yeung and doctoral candidate Javy Guan to develop an integrated analysis framework for predicting surface runoff, infiltration, and landslide risk. Finally, we also continued our research in hydraulic tomography, which delineates subsurface condition in high resolution to improve environmental risk assessment. With the support of the United States Department of Defense, we have been collaborating with Prof. Walter Illman at the University of Waterloo, Prof. J. T. C. Yeh at the University of Arizona, and Yemia Hashimoto of Amec Environment and Infrastructure. Aquifer tests have been conducted at the North Campus Research Site at the University of Waterloo and additional test data will be collected at the Air Force Plant 44 site in Tucson, Arizona, USA.



1 | Learning of a hydrological model with rainfall and discharge measurements through Bayesian analysis: learning and prediction phase. The upper figure shows absolute values, the lower figure shows the 90% credible interval of the model estimate relative to the true value. In this application, the challenge is finding a realistic description of the model error.

2 | Google Earth view of Spaulding Lake Dam where dam erodiblity research was conducted.

Within the Focus Group, a new project was developed on “adaptive risk-informed decision making for flood management and water resource planning under climate change uncertainty (AdaptRisk),” together with Prof. Markus Disse and Prof. Claudia Klüppelberg. The project starts in January 2014 within the IGSSE Focus Area Water, with additional funding from DNV-GL. In this project, we investigate methods for identification of optimal watershed management strategies, in which we explicitly account for the uncertainties in extreme events under climate change.

Our work also included multiple student projects and M.Sc. theses. Two of these students will continue their research in 2014 during a 6-month stay hosted by Prof. Nicholas Sitar at the University of California at Berkeley. In September 2013, we organized a short course on probabilistic environmental risk assessment in Munich with Dr. Ravi Arulanantham, as an extension of an earlier short course. Finally, in December we presented several of our ongoing works at a symposium that was held at the IAS of the Hong Kong University of Science and Technology.

References

[1] J. Yuan, I. Papaioannou, C. M. Mok, and D. Straub, “Effect of rainfall on reliability of infinite slope,” in *4th Int. Symp. on Geotechnical Safety and Risk*, Hong Kong, 2013.

[2] W. Betz, C. M. Mok, I. Papaioannou, and D. Straub, “Bayesian model calibration using structural reliability methods: Application to the simple hydrological abc model,” in *Proc. 2nd Int. Conf. on Vulnerability and Risk Analysis and Management*, Liverpool, 2014, to be published.

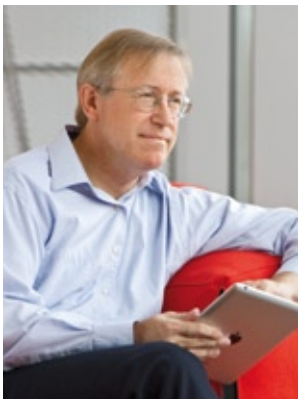
[3] C. M. Mok, E. S. Aw, R. Wright, and J. Cooley, "Probabilistic Dam Erosion Risk Evaluation," in *Proc. 2nd Int. Conf. on Vulnerability and Risk Analysis and Management,* Liverpool, 2014, to be published.

[4] W. Betz, I. Papaioannou, and D. Straub, “Numerical methods for the discretization of random fields by means of the Karhunen-Loève expansion,” *Comput. Method. Appl. M.*, vol. 271, pp. 109-129, 2014.

[5] D. Straub and I. Papaioannou, “Bayesian updating with structural reliability methods,” submitted for publication.

Focus Group **Fiber-Optic Communication and Information Theory**

Prof. Frank Kschischang | Hans Fischer Senior Fellow
Dr. René-Jean Essiambre | Rudolf Diesel Industry Fellow
Dr. Luca Barletta, Dr. Mansoor Yousefi | Postdoctoral Researchers
Prof. Gerhard Kramer, Communications Engineering, TUM



Frank Kschischang

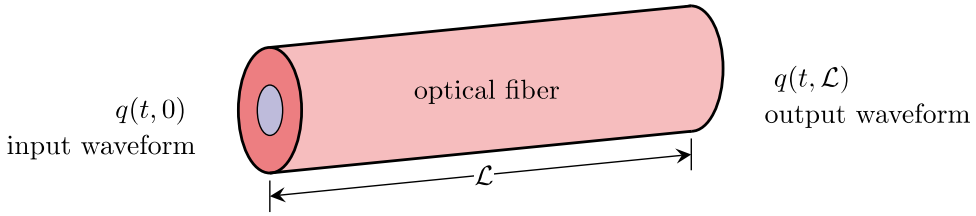
Communication over optical fiber channels

Optical fiber forms the backbone of the world's communication networks, carrying much of the Internet traffic. A huge bandwidth, on the order of THz, is available in silica fiber, allowing transmission of information over distances as long as 6000 km with only 0.2 dB/km loss and very low probability of error. Pulse propagation is well modeled by the stochastic nonlinear Schrödinger (NLS) equation. Three factors interact in this equation: chromatic dispersion, Kerr nonlinearity, and additive white Gaussian noise. Recent studies suggest that global fiber-optic networks face a looming "capacity crunch" due to the impact of the Kerr nonlinearity. This alarming observation has called for research into understanding the challenges presented by the fiber nonlinearity.

The central objective of the Focus Group in the past year was to study the nonlinear fiber channel from the point of view of information theory, establishing fundamental limits on communication rate. We have made progress in two main directions.

1. A well-established method for communication over linear channels is orthogonal frequency-division multiplexing (OFDM). The method is based on the Fourier transform and encodes information into orthogonal modes. Channel users are assigned the modes that do not interact with one another. Remarkably, the NLS equation has an integrable structure, meaning that it also supports signals without interaction. Exploiting this structure, we effectively "diagonalize" the channel with the help of the nonlinear Fourier transform (NFT), a powerful tool for solving integrable nonlinear dispersive partial differential equations. Using the NFT, a signal is represented by discrete and continuous nonlinear spectra. While the signal propagates along the fiber, the action of the channel on its spectral components is given by simple independent linear equations. Thus, just as the (ordinary) Fourier transform converts a linear channel with memory into a number of parallel scalar channels, the nonlinear Fourier transform converts a nonlinear dispersive channel described by a Lax convolution into a number of parallel scalar channels. A new transmission method, termed nonlinear frequency-division multiplexing, arises that – in analogy with OFDM – encodes information in the nonlinear spectra [1]–[2],[7]–[9].

2. The lasers used for up-conversion and down-conversion of signals in optical communications introduce phase noise. We studied the impact of this noise on the achievable rates of discrete-time and continuous-time channels, through sophisticated numerical and analytical upper and lower bounds on the mutual information rate between the input and output of the phase noise channel [3]–[6].



$$\frac{\partial q(t,z)}{\partial z} = \underbrace{-\frac{j\beta_2}{2}\frac{\partial^2 q(t,z)}{\partial t^2}}_{\text{dispersion}} + \underbrace{j\gamma|q|^2 q}_{\text{nonlinearity}} + \underbrace{n(t,z)}_{\text{noise}}$$

1 | Optical fiber channel described by the nonlinear Schrödinger equation. Here q (t,z) is the signal as a function of time t and distance z.

Selected Publications

[1] M. I. Yousefi and F. R. Kschischang, “Integrable communication channels and the nonlinear Fourier transform,” in *2013 IEEE Int. Symp. on Information Theory*, Istanbul, 2013, pp. 1705–1709.

[2] M. I. Yousefi and F. R. Kschischang, “Communication over fiber-optic channels using the nonlinear Fourier transform,” in *2013 IEEE Int. Symp. on Information Theory*, Istanbul, 2013, pp. 1710–1714.

[3] H. Ghozlan and G. Kramer, “Multi-sample receivers increase information rates for Wiener phase noise channels,” in *IEEE GLOBECOM 2013*, Atlanta, GA, 2013.

[4] H. Ghozlan and G. Kramer, “On Wiener phase noise channels at high signal-to-noise ratio,” in *2013 IEEE Int. Symp. on Information Theory*, Istanbul, 2013, pp. 2279–2283.

[5] L. Barletta, M. Magarini, and A. Spalvieri, “Tight upper and lower bounds to the information rate of the phase noise channel,” in *2013 IEEE Int. Symp. on Information Theory*, Istanbul, 2013, pp. 2284–2288.

[6] L. Barletta, M. Magarini, S. Pecorino, and A. Spalvieri, “Bayesian tracking as extraction of information,” submitted for publication.

[7] M. I. Yousefi and F. R. Kschischang, “Information transmission using the nonlinear Fourier transform, Part I: Mathematical tools,” submitted for publication. arXiv:1202.3653v2 [cs.IT]

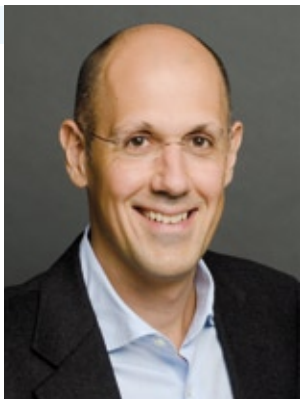
[8] M. I. Yousefi and F. R. Kschischang, “Information transmission using the nonlinear Fourier transform, Part II: Numerical methods,” submitted for publication. arXiv:1204.0830v1 [cs.IT]

[9] M. I. Yousefi and F. R. Kschischang, “Information transmission using the nonlinear Fourier transform, Part III: Spectrum modulation,” submitted for publication. arXiv:1302.2875v1 [cs.IT]

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

Prof. George Biros | Hans Fischer Fellow
Prof. Markus Hegland | Hans Fischer Senior Fellow
Prof. Miriam Mehl | Carl von Linde Junior Fellow

Tackling the multi-challenge



George Biros

Markus Hegland

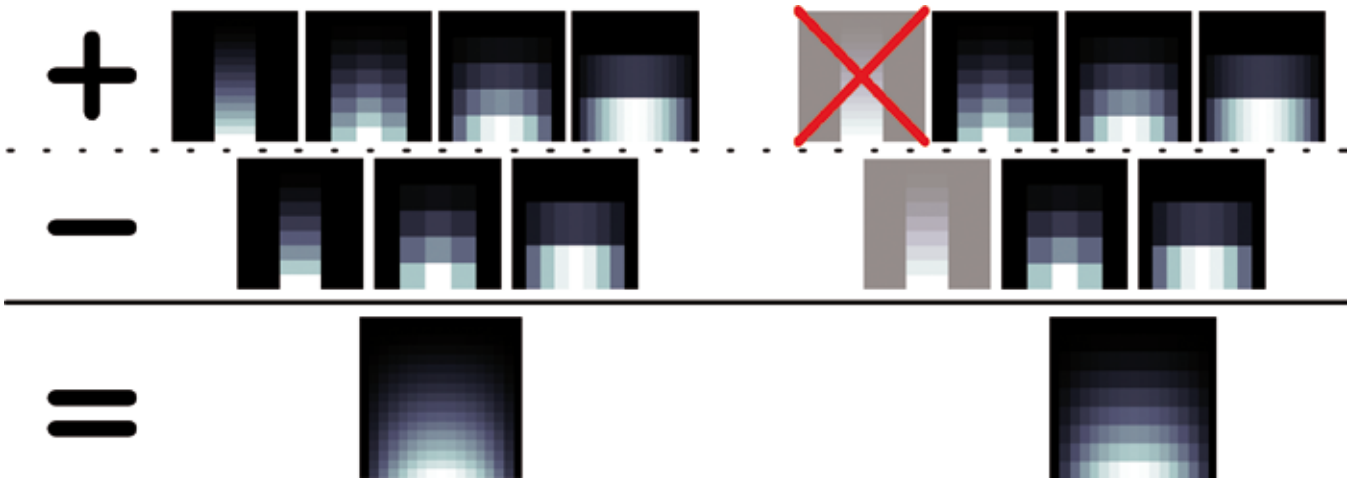
Miriam Mehl

In the past year, the composition of our Focus Group changed. Prof. Mehl received offers for full professorships from the University of Stuttgart and from the Technische Universität Kaiserslautern, and has chosen the former. Prof. Hegland's term as Hans Fischer Senior Fellow came to an end, but he will still be associated with the group as advisor for his doctoral candidates. Furthermore, new members joined the group: Hans Fischer Fellow Prof. George Biros from the University of Texas at Austin and, since December 2013, Arash Bakhtiari as his doctoral candidate. Prof. Biros stayed in Munich in the summer and started his Fellowship by giving an inaugural lecture. During his Fellowship, he and Arash Bakhtiari will refine the simulation of blood flows to replicate and refine ongoing *in vitro* experiments [1]. In particular, they will focus on improving the numerical algorithms used and on increasing the scalability of the simulations. Their research will include extensive simulations on the SuperMUC, the world's tenth fastest supercomputer, at Leibniz Rechenzentrum in Garching. They thus focus on the multi-core challenge of high-performance computing (HPC).

For tackling the multi-dimensional challenge we, along with our collaborators from Stuttgart and Zurich, recently focused on the effective parallelization of the sparse grid combination technique, which is a tool to reduce the computational effort of solving multi-dimensional problems. We tailored this approach to the plasma turbulence code GENE, which is a widely used simulation tool for research on nuclear fusion. Together with Prof. Hegland and his doctoral candidates from the Australian National University, who stayed in Munich this summer, we worked on using the combination technique for dealing with hardware faults (see figure 1), which will be likely to occur more often in the coming era of exascale computing [2]. Without fault tolerance, even simulations using tens of thousands of processors would be completely stopped when a single processor has a fault.

Furthermore, the doctoral candidate Benjamin Uekermann and Prof. Mehl worked on solving multi-physics problems. One aspect examined was the development of parallel coupling schemes for the partitioned simulation of the interaction between an incompressible fluid and an elastic structure. These methods can overcome the scalability limits to which the classical coupling schemes adhere, when the simulation is carried out on massively parallel systems. We discussed first ideas and approaches at conferences and a recently submitted paper to the *SIAM Journal on Scientific Computing (SISC)* explains and validates the developed algorithm [3]. Together with TUM-IAS, the workshop on "Novel Numerical Methods" was held in the Institute. It was organized as a tribute to the former head of the Institute, Prof. Patrick Dewilde, and our two leaving Fellows, Prof. Mehl and Prof. Hegland. The excellent line-up of speakers included Prof. Gilbert Strang (MIT), Prof. Irad Yavneh (Israel Institute of Technology), Prof. Eugene Tyrtyshnikov (Russian Academy of Sciences), Prof. Paul Van Dooren (Université catholique de Louvain), Prof. Uwe Helmke (University of Würzburg), and Prof. Joos Vandewalle (KU Leuven). It also included scientists from TUM, such as Prof. Klaus Diepold and Prof. Samarjit Chakraborty. The line-up was completed by high-quality presentations by TUM doctoral candidates.

Arash Bakhtiari, Benjamin Uekermann, Christoph Kowitz, Valeriy Khakhutskyy | Doctoral Candidates
Prof. Hans-Joachim Bungartz, Scientific Computing, TUM



1 | The sparse grid combination technique represents each solution as a sum of approximations of the solutions on coarser grids (left). If the computation of a single coarse grid approximation fails, the combination can still recover and retrieve an only slightly deteriorated approximation of the solution (right).

Other workshops and conferences co-organized by the Focus Group included the workshop on Adaptive and Local Model Order Reduction with Machine Learning for Parametrized Systems at TUM-IAS, the 5th Workshop on High-Dimensional Approximation in Canberra, and the International Conference on Parallel Computing - ParCo2013.

As another highlight of the year, a team of researchers, including the Focus Group Host Prof. Hans-Joachim Bungartz, received the PRACE award for running a multi-trillion particle simulation on the SuperMUC using 140.000 cores and achieving 591 trillion floating point operations per second (TFLOPS).

George Biros received his B.Sc. at the Aristotle University of Thessaloniki, Greece, in 1995. He received his M.Sc. at Carnegie Mellon University, Pittsburgh, USA, in 1996, and was awarded his doctoral degree at the same university in 2000. After a postdoctorate at the Courant Institute in New York City and assistant and associate professorships at the University of Pennsylvania, George became associate professor and assistant dean for Technology Infrastructure at the Georgia Institute of Technology. In 2011 he became a full professor of the University of Texas at Austin, where he is currently holding the chair in Simulation-Based Engineering Sciences. In 2010 Prof. Biros received the Gordon Bell Prize for the petascale simulation of blood flow.

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[2] J. W. Larson, M. Hegland, B. Harding, S. Roberts, L. Stals, A. P. Rendell, P. Strazdins, M. M. Ali, C. Kowitz, R. Nobes, J. Southern, N. Wilson, M. Li, and Y. Oishi, “Fault-tolerant grid-based solvers: combining concepts from sparse grids and MapReduce,” *Procedia Comput. Sci.*, vol. 18, pp. 130–139, 2013.

[3] M. Mehl, B. Uekermann, H. Bijl, D. Blom, B. Gatzhammer, and A. van Zuijlen, “Parallel coupling numerics for partitioned fluid-structure interaction simulations,” submitted for publication.

More publications by this Focus Group can be found on page 122.

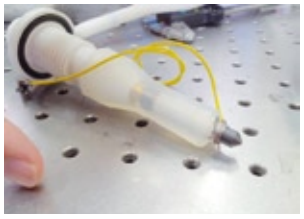
Focus Group **Intra-Operative Therapy**

Dr. Michael Friebe | Rudolf Diesel Industry Fellow
Philipp Matthies | Doctoral Candidate
Prof. Nassir Navab, Computer Aided Medical Procedures & Augmented Reality, TUM

Intra-operative therapy

Michael Friebe

Medical treatments and therapies should be as least invasive as possible, combined with the highest possible accuracy and subsequent confirmation of treatment success. Minimal-invasive therapies need to be accompanied by advanced medical imaging, otherwise these objectives are not achievable: Minimal invasive means also minimal view and minimal access. Endoscopic procedures allow a direct view only of the tissue in front of the camera system and do not provide depth, 3D images, or functional information about the tissues – but these are of particular importance for all oncological applications/surgeries. Tomographic imaging (CT, MRI, ultrasound) that could provide the needed information are diagnostic systems that are generally not used and are not optimized for therapy applications. One of the reasons is the fact that the procedures that would benefit from advanced imaging control are made to fit the imaging system, rather than the imaging system being optimized for the procedure's needs.



1 | Miniature x-ray tube connected to a high voltage power supply.

The research of our Focus Group is in the identification of translational needs for intra-operative image-guided tumor therapies. Extra-corporal radiation therapy is one of the established tumor therapies. The high megavolt linear accelerators used for these procedures are image guided and capable of radiating very small volumes, but are not ideal for very small tumors/limited local therapies/intra-operative applications, and are not an option for patients that have reached their lifetime radiation dose.

2 | Plastic guiding trokar for the miniature x-ray tube connected to tracking hardware for imaging application with a 3T MRI system.

Intra-operative radiation therapy – which means radiation delivered through a small incision – could be a possible treatment option for some types of cancer and a select patient population. You would for example identify a small tumor growth (female breast, abdominal, colon) and, after proper identification, bring a radiation source – with the help of an imaging system – directly to that tumor. Another application is radiation after surgical removal of a small tumor, to ensure that any remaining cancer cells in the surgical boundaries – plus a little beyond – are killed. The imaging could be used for target definition and potentially also as a biomarker. The intra-operative radiation treatment would be completely different to a conventional extra-corporal application in which the radiation dose is delivered in fractions. Intra-operative radiation treatments would allow the delivery of the total radiation as a boost in one session.

This possible new approach requires an innovative and very small radiation source that can be placed via a trokar/endoscopy system, and that is able to produce sufficient radiation – without generating too much heat – to allow the application of at least 1 Gy per minute.

Our Focus Group began late 2012 with some initial work, and in April 2013, after Philipp Matthies joined as a doctoral candidate, we officially started with the project definition and research setup. We started to cooperate very closely with the quantum beam engineering lab of KAIST in Daejeong (Prof. Sung Oh Cho), a leading

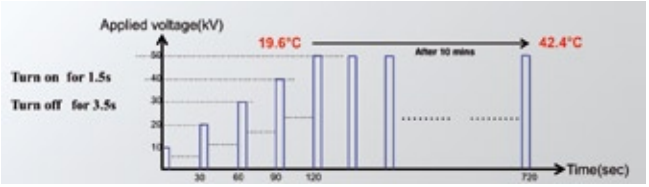
research facility for low energy x-ray tubes based on a carbon nanotube design that allows so-called cold radiation emission. We were also successful in applying for a TUM guest professorship for Prof. Cho. Through our input and collaboration activities we were able to prove and measure that the x-ray tubes can be used for radiation therapy applications in humans. With duty cycles of 30% we were able to produce close to 0.8 Gy/min radiation (1 cm in water) without raising the temperature at the surface of the radiation source to significantly over 40°C.

MRI tests at the TUM rechts der Isar University Hospital in München (3T, Prof. Ernst Rummeny, Dr. Peter Noël) showed that the setup that we envisioned – placing a trokar as a placeholder for the radiation source under MRI guidance and MRI control – was feasible and could be further pursued.

We also identified a German partner from industry who is willing to financially support our activities in the future. For that we are in the process of formulating a comprehensive research plan and have already successfully applied for some public research funding. Several talks and congress papers on the subject were submitted and accepted (IEEE EMBS, MICCAI, SMIT) and four patents filed.

The goals for the coming months will be to minimize the radiation source – together with our Korean and industrial partners – and to further define the clinical needs for intra-operative radiation therapy using small low-energy radiation sources in combination with advanced diagnostic imaging for visualization and as biomarkers.

Temperature of Miniature X-ray Tube Surface



3 | Miniature x-ray tube temperature development over time with 30% duty cycle.

Selected Publications

[1] P. Matthies, S. O. Cho, and M. Friebe, “Integration of a low energy radiation source in MRI environment for intraoperative applications - a feasibility evaluation,” in *25th Int. Conf. of the Int. Society for Medical Innovation and Technology*, Baden-Baden, 2013.

[2] P. Matthies, A. Okur, T. Wendler, N. Navab, and M. Friebe, “Combination of intraoperative freehand SPECT imaging with MR images for guidance and navigation,” in *35th Annu. Int. Conf. of the IEEE Engineering in Medicine and Biology Society*, Osaka, 2013, pp. 3383-3386.

[3] S. Bock, S. Dahl, M. Schneider, A. Hartmann, M. Kramer, H.-W. Henke, M. Friebe, and G. Krombach, “Entwicklung eines MR-kompatiblen Kathetersystems zur bildgesteuerten intramyokardialen Injektion,” presented at the *94. Deutscher Röntgenkongress*, Hamburg, 2013. (winner of poster award)

Michael Friebe was educated as an electrical engineer with a scholarship from IBM Germany. After graduation he left Germany for a 5-year work (MRI engineer and project manager at TOSHIBA MRI and University of California, San Francisco, RIL research laboratory) and study (graduate degree in technology management) period in San Francisco. He returned to the fascinating Ruhr valley in 1993 – with an American wife – to pursue and finish his doctoral studies (1995, interventional MRI, University Witten) and start his first company (Neuromed). In the next 15 years he invested a lot of time and effort in creating new ventures, all related to diagnostic and interventional imaging. Dr. Friebe has filed more than 20 patent families, is on the advisory board of several start-up companies, is a non-executive director of a publicly traded MEDTEC company, and currently runs a MEDTEC advisory boutique. Since 2010 he has been a very enthusiastic lecturer of “Medical Technology Entrepreneurship” and “Innovation in Image-Guided Surgeries” at Prof. Navab’s department. In 2011 he was named Germany’s Business Angel of the Year.

Focus Group **Metropolis Nonformal**

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

Christian Werthmann

1 | Johann-Christian Hannemann is a TUM urbanism master's student, who volunteered for an eight-week stay with the NGO "Techo" to conduct workshops regarding the further urbanization of Onaville.

The year 2013 was characterized by the ongoing research activities of our Focus Group Metropolis Nonformal in the earthquake refugee settlement Onaville in Port-au-Prince, Haiti, and by a symposium titled "Metropolis Nonformal – Anticipation," during which a worldwide "Hub for Informal Urbanism" was launched under the auspices of UN-Habitat.

Focus Group Onaville, Haiti

In 2011 I began a collaboration with the chair of Landscape Architecture and Public Space, Prof. Regine Keller, the lecturer Thomas Hauck, 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 still-ongoing reconstruction efforts of Port-au-Prince, Haiti. The idea was to develop – through a string of master theses – tactical, small-scale, and small-step enviro-urbanistic strategies to improve living conditions in the poorest neighborhoods of Port-au-Prince.

The research design of this Focus Group's activities is a reaction to past experiences in the difficult terrain of Haiti. Previous research has shown that large scale master planning has not been successful in an environment of weak governance and a powerful but complex set of international NGOs and governments (the "international community") with diverse and often conflicting goals and uncoordinated actions. Three years after the devastating earthquake that flattened Port-au-Prince, it became obvious that the Haitian government and the people it represents are not, despite their best efforts, in control of reconstructing their own country. In a situation determined by outsiders, our Focus Group decided in 2012 to collaborate with a small Chilean NGO, "UN Techo Para Mi Pais," because of its small financial footprint and its full integration of ordinary Haitians in all their efforts. "UN Techo Para Mi Pais" has been working with a small budget and a highly participatory process since 2010 in the earthquake refugee settlement "Onaville" with approximately 3,000 souls in the northeast of Port-au-Prince. Two environmental engineering students, Valentin Heimhuber and Maria Alejandra Casanova, and two urbanism master students of TUM, Johann-Christian Hannemann and Raphaela Guin, began to assist the NGO by mapping the settlement, developing improvement scenarios focusing on storm water and flood modeling, and advancing sanitation and urbanization scenarios for the tremendously fast growing settlement.

In 2013 the two urbanism students volunteered to stay for extended periods with "Techo" (on their own budget!) and conducted workshops with the community. In turn, they provided valuable field data for their colleagues in Munich to run flood calculations and sanitation scenarios. In the meantime, two master's theses on flooding and sanitation have been completed which will give the urbanism students valuable data on which to build their development proposals. Their proposals can then in turn be tested through our partner on the ground, "Techo."

The Focus Group for Onaville interweaves education, research, and practice. Once a critical point of data and proposal collection has been reached, the publishing of results is planned. This small group functions like a living laboratory with an indeterminate outcome. It is completely based on the interest, passion, and volunteerism of the students and the faculty. All of them should be thanked for their engagement in this endeavor.

2 | Onaville is an emerging city informally founded by families who lost their homes during the 2010 earthquake in Port-au-Prince.

3 | Raphaela Guin is a TUM urbanism master's student, who volunteered for a six-week stay with the NGO "Techo" to conduct workshops regarding the further urbanization of Onaville.

Symposium Metropolis Nonformal – Anticipation

I also continued with my efforts to convene outstanding scholars on the topic of nonformal urbanism in Munich. Back in fall 2011 I invited nine professionals and academics to TUM. They gave a presentation at the symposium "Metropolis Nonformal" (see documentation under www.tum-ias.de/news-and-events/documentation/2011/metropolisnonformal.html). In the end of November 2013 a total of 50 speakers gathered at the symposium "Metropolis Nonformal – Anticipation" in Munich. The main question was what alternative strategies could be developed to provide assistance to a projected additional two billion slum dwellers by 2050.

The symposium operated under the understanding that self-produced cities are the only viable urbanization model for low-income migrants when formal planning models continue to fail (as they have in the past). Over the course of two days, 22 renowned international experts gave short talks and engaged in discussion with an audience of over 250 participants. On the third day, 28 doctoral students presented their ongoing research on nonformal (self-built) settlements. All talks were documented on video and are published with an executive summary on the TUM-IAS website: www.tum-ias.de/news-and-events/documentation/2013/metropolis-nonformal-symposium.html (see also page 42 ff).

The symposium also served as the launching event of two new initiatives. First a new "Hub on Informal Urbanism" as part of the UN-Habitat University Initiative (UNI) was officially launched in Munich. UNI seeks to strengthen ties between academic institutions of higher education and UN-Habitat, creating a mutually beneficial relationship between urban research, education, knowledge production, and global normative works. Everybody who is interested in the activities of the hub can find more information under: www.unhabitat.org.

Secondly, the "Laufen Manifesto for a Humane Design Culture" was made public for the first time. The two page manifesto was developed by a group of 20 design and planning professionals and is an urgent call to fundamentally change our design culture and education towards more effectively addressing the growing inequality on our planet: www.laufenmanifest.org.

For the organization of this large gathering I want to thank the TUM-IAS team led by Prof. Gerhard Abstreiter, my TUM Host Prof. Keller, and my chief coordinator, Juliane Schneegans, and her whole team. All of them have proven to be excellent partners in this enterprise.

Focus Group **Nanoimprint and Nanotransfer**

Prof. Khaled Karrai | Rudolf Diesel Industry Fellow
Prof. Wolfgang Porod | Hans Fischer Senior Fellow
Armin Exner, Muhammad A. Imtaar, Klaus Thurner, Anandi Yadav | Doctoral Candidates
Prof. Paolo Lugli, Nanoelectronics, TUM

Towards cost-effective nanofabrication techniques

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-based integrated circuits. An important challenge posed by compatibility with IC fabrication technology is the need for alignment on the nanometer scale over several layers, which can only be met if novel alignment methodologies are developed for nanoimprinting. Our work, in collaboration with attocube systems AG, has addressed this critical issue. In addition, our work has contributed to a variety of new applications, such novel nanoantenna-based infrared detectors [1] and nanomagnetic logic structures [2]. 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 large-scale processes are required.

Wolfgang Porod

We have recently demonstrated that nanoimprinting is a valuable alternative to electron-beam lithography for patterning silicon substrates and can thus provide templates for the growth of InAs nanowires via molecular beam epitaxy [3]. In addition, we have shown that conductive films made either with metals or conductive polymers can be patterned in order to alter the film optical properties. Over this past year we have also developed novel position readout of the wafer or stamp location by long range Fabry-Pérot interferometry [4]. This novel technology will assist multistep nanoimprinting at later stages of development and has been now implemented in fixed beam scanning optical lithography. We were fortunate to establish a breakthrough in terms of laser position sensing in that we overcame the limitation typical to interferometry, that of being able to read only a displacement [5]: We are now able to read a distance and not only a displacement, and with nanometer sensitivity and over distances in the submeter range. Such a feature should allow more complex multistep imprinting procedures without loss of position information.

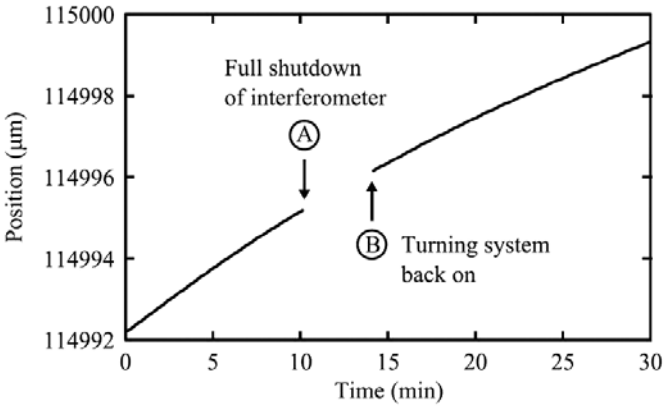
In previous work, we demonstrated that entire functional nanometer scale devices can be produced with such nanoimprint and nanotransfer techniques. More specifically, we demonstrated the transfer of arrays of metal-oxide-metal and metal-metal structures as rectifying elements in large-scale nanoantenna arrays for infrared detection and/or energy harvesting. This so-called “rectenna” – a device concept first proposed in the late 1960s – combines an antenna, which collects electromagnetic radiation, and a nanoscale metal-insulator-metal (MIM) diode, which acts as a rectifier in the terahertz region. Previous theories hold that the MIM tunnel diode rectifies the induced terahertz currents using the nonlinearity of the tunnel diode characteristic.

Over this past year, we were able to revisit these long-held assumptions and to elucidate the physical mechanism at work for IR detection, and we were able to show that it is the heating caused by the radiation-induced antenna currents that gives rise to a thermoelectric response, which provides the detector signal.

Our results unambiguously demonstrate that the thermoelectric Seebeck effect is the actual dominant rectifying mechanism. This new realization that the underlying mechanism is thermal based, rather than tunneling based, can open the way to important new developments in the field, since the fabrication process of rectennas based on the Seebeck effect is far simpler than existing processes that require delicate tunnel junctions. We demonstrated for the first time the fabrication of a rectenna array using an efficient parallel transfer printing process featuring nearly one million elements.

It should also be mentioned that the participants of this Focus Group were successful in being awarded a new NSF International Collaborative Program, and several of the workshop participants are partners in this new project. As such, this Focus Group will continue on in a modified form, taking advantage of the collaborative ties developed over these past years. Moreover, Prof. Stephen Goodnick will participate in this new project, which thus also acts as a link between this outgoing Focus Group and the new Focus Group on "Nanoscience for Renewable Energy Sources." This new international collaborative program also features a component on societal impact, and involves Prof. Klaus Mainzer with the Munich Center for Technology in Society. Last but not least, Klaus Thurner, a doctoral candidate of our Focus Group, is now fully employed in attocube systems AG as a development engineer in the sensing department and will work on a commercial version of the interferometric techniques discovered in this collaborative work.

More publications by this Focus Group can be found on page 123.



1 | The displacement of a sample holder (such as in a nanoimprinting machine or other forms of multistep lithography) is accurately tracked by laser interferometry. When the measurement is interrupted, for instance by a shutdown or by dismounting the sample holder, the position measured by standard single wavelength interferometry readout is irreversibly lost. This is not the case with our newly developed dual wavelength laser interferometer which allows one to measure a distance very accurately, and not just a displacement. Here, in (A) the dual laser interferometer was turned off for five minutes. In (B) the interferometer is turned on again without loss of memory of the position. See reference [5] for more details.

Selected Publications

[1] M. Bareiß, P. M. Krenz, G. P. Szakmany, B. N. Tiwari, D. Kälblein, A. O. Orlov, G. H. Bernstein, G. Scarpa, B. Fabel, U. Zschieschang, H. Klauk, W. Porod, and P. Lugli, "Rectennas revisited," *IEEE T. Nanotechnol.*, vol. 12, no. 6, pp. 1144–1150, 2013.

[2] M. A. Imtaar, A. Yadav, A. Epping, M. Becherer, B. Fabel, J. Rezgani, G. Csaba, G. H. Bernstein, G. Scarpa, W. Porod, and P. Lugli, "Nanomagnet fabrication using nanoimprint lithography and lectrodeposition," *IEEE T. Nanotechnol.*, vol. 12, no. 4, pp. 547–552, 2013.

[3] S. Morkötter, S. Funk, M. Liang, D. Markus, S. Hertenberger, J. Treu, D. Rudolph, A. Yadav, J. Becker, M. Bichler, G. Scarpa, P. Lugli, I. Zardo, J. J. Finley, G. Abstreiter, and G. Koblmüller, "Role of microstructure on optical properties in high-uniformity $In_{1-x}Ga_xAs$ as nanowire arrays: Evidence of a wider wurtzite band gap," *Phys. Rev. B*, vol. 87, no. 20, 205303, 2013.

[4] K. Thurner, P. F. Braun, and K. Karrai, "Fabry-Pérot interferometry for long range displacement sensing," *Rev. Sci. Instrum.*, vol. 84, 095005, 2013.

[5] K. Thurner, P. F. Braun, and K. Karrai, "Absolute distance sensing by two lasers optical interferometry," *Rev. Sci. Instrum.*, vol. 84, 115002, 2013.

Focus Group **Nanoscience for Renewable Energy Sources**

Prof. Stephen Goodnick | Hans Fischer Senior Fellow
Pietro Luppina | Doctoral Candidate
Prof. Paolo Lugli, Nanoelectronics, TUM

New focus on solar energy

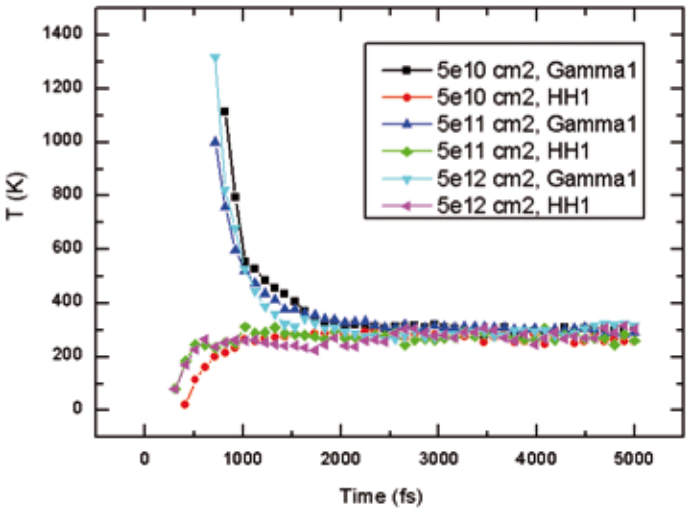
Stephen Goodnick

During 2013, Prof. Stephen Goodnick started his research program in collaboration with Prof. Paolo Lugli as part of the TUM-IAS Focus Group Nanoscience for Renewable Energy Sources. This program of research was initiated by the inaugural lecture given by Prof. Goodnick on March 12, 2013, entitled “Next Generation Photovoltaics,” as part of a half-day workshop to kick off the Nanoscience for Renewable Energy Sources Focus Group. Other presenters for the Focus Group kick-off included Prof. Aldo di Carlo from the University of Rome II, and talks were given by Dan Popescu and Dr. Alaa Abdellah (Institute for Nanoelectronics).

During several short term visits the specifics of the research project were discussed, and a new TUM-IAS-funded doctoral candidate, Pietro Luppina, joined the team. A kick-off meeting was held during a visit on October 17, 2013 at TUM concerning a newly funded international project led by the University of Notre Dame (Prof. Wolfgang Porod, Dr. Kathy Eggleson, Prof. Scott Howard) and including Arizona State University (Prof. Goodnick, Prof. David Guston), TUM (Prof. Lugli, Prof. Klaus Mainzer), the Pázmány P. Catholic University, Budapest (Dr. Tamas Roska), and the University of Seville (Prof. Ángel Vazquez). The project, funded under the Early Concept Grants for Exploratory Research (EAGER) program from the National Science Foundation in the US, is entitled “Computer Architectures for 2020 and Beyond.”

The Focus Group research project Nanoscience for Renewable Energy Sources utilizes advances made by Prof. Lugli’s efforts on modeling and fabrication of nanostructures and nanodevices, and builds on the expertise of Prof. Goodnick in two distinct application areas: (1) hybrid solar cells, and (2) light and energy harvesting. The development of sustainable and efficient energy conversion processes and systems is of central importance for our future. The limited availability of fossil fuels as primary energy sources and the concomitant emission of pollutants leading to negative local and global effects on the environment pose an enormous challenge for our future energy supply. Solar energy is by far the most abundant clean energy source available today.

However, the efficiency of present day solar cells is well below the maximum conversion efficiency dictated by thermodynamics. The motivation for the project comes from the necessity to develop tools which can help improve the efficiency of existing solar energy conversion systems, or to design novel advanced concept devices. Current commercial modeling tools lack the sophistication and necessary physics to accurately model novel energy conversion concepts which may significantly improve photovoltaic efficiencies.



1 | Electron and hole energy relaxation in InAs quantum wells under femtosecond excitation for different injected densities simulated using ensemble Monte Carlo simulation.

The project aims at setting up a simulation framework based on a series of physical models and Monte Carlo tools able to describe the fundamental processes determining the operation of PC devices and ultimately to provide accurate design tools for their optimization. While the use of such tools is widely established for the design of electronic devices, this is not the case for solar cells and other energy conversion devices. The theoretical effort will be supported by experimental investigations carried out in the Host Institute and in cooperation with other groups at TUM and Arizona State University.

Selected Publication

[1] S. M. Goodnick, N. Faleev, and C. Honsberg, "Nanoscale photovoltaics and the terawatt challenge," *Nanoscale Applications for Information and Energy Systems*, A. Korkin and D. J. Lockwood, Eds. New York: Springer Science, 2013, pp. 77–117.

Stephen Goodnick received a B.S. degree in engineering science from Trinity University, USA, in 1977, and M.S. and Ph.D. degrees in electrical engineering from Colorado State University in 1979 and 1983. He was an Alexander von Humboldt Fellow with TUM (1985) and the University of Modena (1986); he was an engineering faculty member at Oregon State University for more than a decade. His subsequent academic career has comprised leading positions at Arizona State University, the Ira A. Fulton School of Engineering, the Arizona Institute for Nanoelectronics, and the Arizona Initiative for Renewable Energy. He is presently deputy director of ASU Lightworks, an initiative focused on use-inspired applications of light, including solar energy. Some of his main research contributions include analysis of surface roughness at the Si/SiO_2 interface, Monte Carlo simulation of ultrafast carrier relaxation in quantum confined systems, global modeling of high frequency devices, full-band simulation of semiconductor devices, transport in nanostructures, and fabrication and characterization of nanoscale semiconductor devices.

Life Sciences

Focus Group **Global Change**

Prof. Annette Menzel | Carl von Linde Senior Fellow
Prof. Tim H. Sparks | Hans Fischer Senior Fellow
Ecoclimatology, TUM

Unravelling the impacts of climate change

Annette Menzel

Tim H. Sparks

The study of climate change and its impacts on nature is in constant danger of stereotypically trusting supposedly well-established findings without any further scrutiny of their long-term validity under globally changing conditions. For instance, the assessment of observed increases in the intensity or duration of droughts since 1950 was revised from the IPCC AR4 report in 2007 (likely in many regions since the 1970s) and the IPCC SREX report (medium confidence in some regions), to the IPCC AR5 report in 2013 (low confidence on a global scale). In this sense, the members of the Focus Group Global Change questioned the well-known and documented fact that the observed lengthening of the growing season in temperate regions such as Central Europe is exclusively triggered by spring warming.

In a climate chamber experiment in TUM Dürnast glasshouse facilities, Julia Laube (TUM-IAS doctoral candidate) tested the response of twigs of 36 different species to (1) winter chilling needed to break dormancy; (2) photoperiod, which is seen as a factor restricting premature spring development; and (3) spring warming. Contrary to previous assumptions, the increasing length of the day in spring plays no big role in the timing of budding. Instead, her research has brought a new correlation to light: The colder the winter, the earlier native plants begin to grow again. Since warmer winters can be expected as the climate changes, spring development of typical forest trees might start later and later – giving an advantage to shrubs and invasive trees that do not depend on a chilling period. A subsequent TUM press notice and an TUM-IAS Wednesday Coffee Talk were titled “Warm winters let trees sleep longer.” The related publication in *Global Change Biology* [1] – with an IF of 6.9 – even used photographs from Julia Laube’s experiment for the cover of that issue.

The existing literature suggests that besides spring warming there are no other factors explaining much of the observed variability in spring onset dates. Dr. Susanne Jochner and Julia Laube could demonstrate in two papers [4]–[5] that factors reinforcing turgor pressure and thus cell extension may significantly accelerate leaf development in spring. The experimental evidence demonstrated that air humidity is an important – so far overlooked – factor influencing budburst, likely via simple water uptake by aboveground tissue. More surprisingly, a new concept of chilling and forcing based on drying out in winter and subsequent humidity uptake was presented in a paper just accepted by *New Phytologist*. An urban gradient study in Munich revealed that increased foliar concentration of potassium, boron, zinc, and calcium of birch trees was significantly related to earlier onset dates of leaf unfolding.

An integral signal of the growing season, as seen for example by satellite remote sensing or in CO_2 atmospheric concentrations, also involves the activity of agricultural crops. Due to decisions of farmers and long-term adaptation of crop growing and management, phenological dates and their responses to climatic factors may differ from those of wild plants and may vary in time. A unique dataset on six decades of hay cutting in Germany was used by our other TUM-IAS doctoral candidate, Anna Bock, to show that during the last two decades, despite continuous warming, hay cutting dates were rather constant and the response

Dr. Susanne Jochner | Postdoctoral Researcher
Anna Bock, Julia Laube | Doctoral Candidates

1 | Cover of the Global Change Biology January 2014 issue.

of these dates to temperature decreased and was no longer significant. Differences in agricultural land use as well as agri-environment schemes were most likely to have confounded the overall trends in hay cutting, especially since flowering dates of commonly observed grass species did advance in the manner expected from past sensitivity to temperature [2]. Another example for diverging response could be shown in the analysis of long-term data on grape harvest yields and quality (i.e., must sugar content [°Oe]). Both viticultural variables were related to temperature, however potential increases in yields are limited by current legislation, and thus may not reach full potential in the future.

In 2014, we will focus on the study of extremes at the atmosphere-biosphere interface in order to adapt to key stressors in sustainable resource management. Major problems in the sustainability of environmental resources are interrelated through biogeochemical cycles and are equally affected by global/climate change. Whereas the main drivers (population growth, lifestyle changes) lead to subtle but gradual deterioration of the status of climate, water, and biosphere, extreme events catch public attention, as do major disturbances in ecosystems and feedbacks on atmosphere. Many of these extremes are related to water (heavy precipitation, drought). Thus, we will link our activities in the Carl von Linde Senior Fellowship to current research in E3 and the IGSSE Water Focus Area with a special emphasis on this new field of ecohydrology.

Selected Publications

[1] J. Laube, T. H. Sparks, N. Estrella, J. Höfler, D. Ankerst, and A. Menzel, “Chilling outweighs photoperiod in preventing precocious spring development,” *Glob. Change Biol.*, vol. 20, no. 1, pp. 170–182, 2014.

[2] A. Bock, T. H. Sparks, A. Menzel, and N. Estrella, “Changes in the timing of hay cutting in Germany,” *Glob. Change Biol.*, vol. 19, no. 10, pp. 3123–3132, 2013. doi:10.1111/gcb.12280

[3] A. Bock, T. H. Sparks, N. Estrella, and A. Menzel, “Climate-induced changes in grapevine yield and must sugar content in Franconia (Germany) between 1805 and 2010,” *PLoS ONE*, vol. 8, no. 7, e69015, 2013. doi:10.1371/journal.pone.0069015

[4] S. Jochner, D. Ankerst, I. Beck, A. Gottlein, J. Hoefler, C. Traidl-Hofmann, and A. Menzel, “Nutrient status - the missing factor in phenological research,” *J. Exp. Bot.*, vol. 64, no. 7, pp. 2081–2092, 2013.

[5] J. Laube, T. H. Sparks, N. Estrella, and A. Menzel, "Does humidity trigger tree phenology? Proposal for an air humitity based frame work of bud development in spring", *New Phytologist*, doi:10.1111/nph12680 (2014).

More publications by this Focus Group can be found on page 124.

Annette Menzel received her Diploma in Forestry Sciences in 1989 (LMU München), afterwards worked in the Bavarian State Forestry Commission and successfully passed the State Examination for the Higher Grade in Civil Service (Forestry) in 1992. In 1997 she was awarded her PhD in Forestry Sciences at TUM. In 2002, she received her Post doctoral lecture qualification (‘Habilitation’) and Teaching Certificate for the field of Bioclimatology (topic "Phenology as tool in global change research"). In 2007, she was appointed full professor for Ecoclimatology at TUM. Prof. Menzel was visiting scientist at the Universidade Estadual Paulista, Brazil. As expert in bio climatology and forest meteorology, she has been involved in several national and international projects and was one of the lead authors of the fourth IPCC Assessment Report (AR4), which was honoured by the Nobel Peace Prize in 2007.

Focus Group **Soil Architecture**

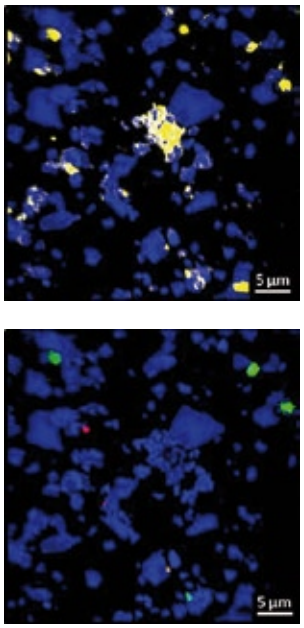
Prof. Ingrid Kögel-Knabner | Carl von Linde Senior Fellow
Dr. Geertje Pronk | Postdoctoral Researcher
Soil Science, TUM

Ingrid Kögel-Knabner

Submicron structures responsible for carbon and nitrogen sequestration in soils identified

Soils and marine sediments represent one of the largest reservoirs of organic carbon (OC) on Earth and play a crucial role in global trace gas cycles and associated climate change. In addition to occluding organic matter (OM) in aggregated mineral particles, soils and sediments sequester OC and organic nitrogen (ON) through the formation of strong bonds between OM and mineral surfaces in organo-mineral associations. The OC sequestration capacity of a soil is estimated from correlations between OC concentration and the soil's clay content or specific surface area. Understanding the dynamics of OM binding within the mineral matrix is essential for understanding the processes controlling the quantity, quality, and turnover of OM attached to mineral particles. Earlier research on marine sediments proposed a monolayer coverage of OM on clay mineral surfaces, as indicated by an indirect method (surface area calculations derived from N_2 adsorption measurements). The key technique for tracking the biogeochemical cycles of C and N is stable isotope labeling (^{13}C, ^{15}N). Nanoscale secondary ion mass spectrometry (NanoSIMS) enables the direct visualization of ^{13}C and ^{15}N down to a lateral resolution of 150 nm and can be used to identify organo-mineral associations by the simultaneous detection of ion species derived from the organic (C, N) and inorganic (Al, Si, Fe) components of the associations.

In a study incubating a sieved (<2 mm) topsoil with labeled litter, we found that only some of the clay-sized surfaces bind organic matter. Using this approach, we quantified the associations of OC and ON with mineral surfaces and identified hot spots of OM binding and label accumulation. Surprisingly, less than 19% of the visible mineral areas showed an organic matter attachment. Our data show that only some of the clay-sized mineral surfaces, namely those with rough surfaces, react with OM and thus contribute to OC and ON sequestration. Organic matter identified by NanoSIMS was preferentially associated with organo-mineral clusters with rough surfaces. We demonstrated here for the first time that small mineral particles with rough surfaces in organo-mineral clusters provide the essential reactive interfaces for OM sequestration. Our results clearly indicate that mineral particles with a smooth surface are not suited for substantial OM sequestration, presumably because they do not have etch pits, micropores, or cracks. Preferential OM sequestration on mineral clusters with rough surfaces also might be due to better hydration and nutrient conditions on rough surfaces, conditions that offer an advantageous microhabitat for microorganisms.



1 | Organic matter on mineral surfaces.
Top: Total organic matter indicated by ^{12}C- and $^{12}C^{14}N$- (yellow) secondary ion images, on mineral surfaces as revealed by ^{16}O- (blue).
Bottom: New, litter-derived, organic matter indicated by ^{13}C-/^{12}C- (green) and $^{12}C^{15}N$-/$^{12}C^{14}N$- (magenta) on mineral surfaces revealed by ^{16}O- (blue).

By combining nanoscale secondary ion mass spectrometry and isotopic tracing, we were able to distinguish between newly labeled and pre-existing organic matter. We could show that new organic matter is preferentially attached to already present organo-mineral clusters. These rough surfaces were found to be the nuclei for additional OM accumulation and therefore to control the C and N sequestration potential of soils and sediments.

Our results imply that only a limited proportion of the total clay-sized mineral particles were involved in OM sequestration. This finding was unexpected because the clay-sized mineral particles in this soil (illite, mixed layer clay minerals, and pedogenic iron oxides, such as goethite) are all considered to be reactive on all surfaces, owing to their permanent and variable charges. These findings have major implications for our understanding of fundamental soil properties that are controlled by the surface reactivity of the fine soil fraction, such as cation exchange capacity, pollutant binding capacity, and physical properties. Our data also point to the necessity for careful identification and quantification of the reactive mineral complexes that are responsible for OM sequestration and that control the OM saturation capacity of soils and sediments. Such data could be incorporated into current models for estimating the carbon sequestration capacity of soils and could be expected to considerably improve the predictive power of such models.

In collaboration with Cordula Vogel.

Selected Publications

[1] G. J. Pronk, K. Heister, and I. Kögel-Knabner, “Is turnover and development of organic matter controlled by mineral composition?“ *Soil Biol. Biochem.*, vol. 67, pp. 235–244, 2013.

[2] C. Vogel, C. W. Mueller, C. Höschen, F. Buegger, K. Heister, S. Schulz, M. Schloter, and I. Kögel-Knabner, “Submicron structures provide preferential spots for carbon and nitrogen sequestration in soils,” *Nat. Commun.*, vol. 5, 2014. doi:10.1038/ncomms3947 (2013).

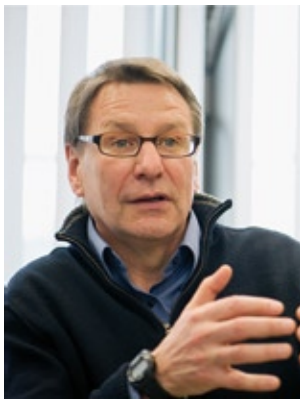
More publications by this Focus Group can be found on page 125.


BIO-RAD

Medicine

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



Stanley Riddell

Christian Stemberger

The vision of the Focus Group Clinical Cell Processing and Purification is to establish a fully integrated cell-processing platform for the clinical preparation of highly effective and minimally manipulated therapeutic cells for individualized medical care. Our recent success in developing the critical tools for optimal cell purification and their clinical transfer led to the initiation of our first clinical trials.

Our cell processing technology enables us to specifically target and isolate specialized cells of the immune system which 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 cancer cells that might give rise to metastases. Furthermore, highly effective therapeutic cells should optimally persist long term in the patient to constitutively prevent tumor reoccurrence. We have identified a special $CD8^+$ T cell subset – the so-called central memory T cell (Tcm) – that fulfills these criteria. We demonstrated that Tcm cells comprise stem-cell properties of self-renewal and differentiation, which enables full restoration of protective immunity upon adoptive T cell transfer. In the most extreme experimental murine setting, this was accomplished by transferring a single Tcm cell. Most importantly, this basic concept of “quality over quantity” was confirmed in the first patients treated with an exceedingly low number of virus-specific T cells to provide antiviral immunity after allogeneic stem cell transplantation. Besides revealing the importance of intrinsic cellular properties in adoptive therapy, we could also show, using a novel assay for measuring the affinity of T cell receptors with the streptamer technology, that high-affine T cell receptor recognition is another crucial parameter for effective immune protection.

Tcm can only be identified by the expression of several surface markers for which we have successfully developed selection reagents. These allow – for the first time – a highly specific multi-parameter isolation of the cells. Recent work by the Focus Group, including postdoctoral fellow Stefan Dreher and graduate student Jeannette Bet, involved the establishment of isolation protocols that can be used in a GMP lab environment, which enables us to obtain these cells in clinical grade for subsequent patient treatment. The Focus Group is currently working on automating these multiple reversible selection regimens to provide an easy-to-use, standardizable clinical interface.

Dr. Stefan Dreher | Postdoctoral Researcher
Jeannette Bet, Paulina Paszkiewicz | Doctoral Candidates

Based on this new selection technology we developed protocols to subsequently engineer the obtained pure T cell products by genetic modification with a designed tumor-specific receptor that recognizes a molecule on B cell lymphomas and leukemia. This also included the introduction of a genetically stable, integrated novel "emergency stop" mechanism implemented into the cell product that has been tested in animal models by doctoral candidate Paulina Paskiewicz. Hans Fischer Senior Fellow Prof. Stanley Riddell (Seattle, USA) has launched the first clinical trial to test adoptive T cell therapy with defined composition genetically modified T cell products in patients with advanced stage B cell lymphoma that have failed conventional chemotherapy and hematopoietic stem cell transplant. Three of the first four patients treated on the trial have had complete regression of all tumor sites, suggesting that this approach has the potential be a truly transformative new cancer therapy. Plans are already being implemented to develop this approach at multiple centers in Germany, leveraging the cell manipulation and production expertise at TUMCells.

Selected Publications

[1] M. Nauerth, B. Weißbrich, R. Knall, T. Franz, G. Dössinger, J. Bet, P. J. Paszkiewicz, L. Pfeifer, M. Bunse, W. Uckert, R. Holtappels, D. Gillert-Marien, M. Neuenhahn, A. Krackhardt, M. J. Reddehase, S. R. Riddell, and D. H. Busch, "TCR-ligand koff rate correlates with the protective capacity of antigen-specific CD8+ T cells for adoptive transfer," *Sci. Transl. Med.*, vol. 5, no. 192, pp. 192ra87, 2013.

[2] V. R. Buchholz, M. Flossdorf, I. Hensel, L. Kretschmer, B. Weissbrich, P. Gräf, A. Verschoor, M. Schiemann, T. Höfer, and D. H. Busch, "Disparate individual fates compose robust CD8+ T cell immunity," *Science*, vol. 340, no. 6132, pp. 630–635, 2013.

More publications by this Focus Group can be found on page 126.

Focus Group **Molecular Imaging**

Prof. Silvio Aime | Hans Fischer Senior Fellow
Giaime Rancan | Doctoral Candidate
Prof. Markus Schwaiger, Clinic for Nuclear Medicine, TUM

Molecular imaging

Silvio Aime

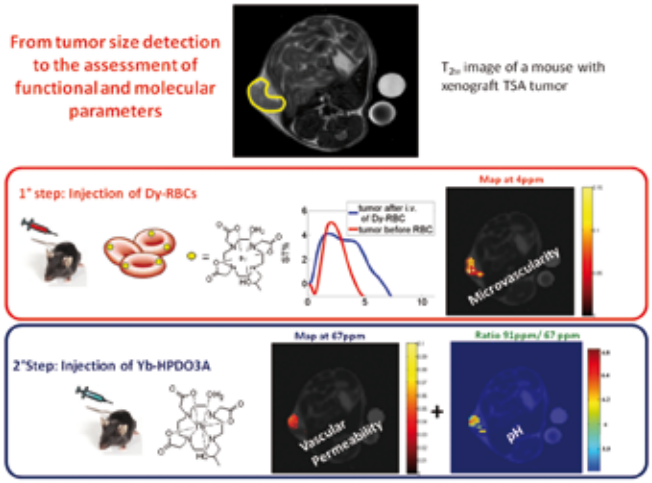
Molecular imaging procedures are undergoing intense investigation to continue the development of innovative diagnostic protocols based on the visualization of molecules and molecular events that are characteristic of the investigated pathologies. Molecular imaging relies on the use of tailored probes designed for the intended application. Our team is addressing the task of the simultaneous visualization of pH and FluoroDeoxyGlucose (FDG) by PET-MRI in tumors. Whereas FDG uptake is a well-defined PET methodology (largely used in clinical settings), procedures for pH mapping by MRI are still under investigation.

pH is an important biomarker - especially in cancer - since it has often been reported that the extracellular pH of a tumor is acidic, and the acidity plays a fundamental role in the tumor development. Among imaging modalities, MRI stands out for its superb spatial resolution, the absence of invasiveness, and its in-depth penetration capability. Different methods to measure pH by using MRI and MR spectroscopy have been developed in recent years. Our work has focused on two methods:

a) the relaxometric method [1] based on the use of paramagnetic agents whose relaxivity is predicated on the solution pH (CA-1). The method relies on the transformation of the observed ^{1}H-relaxation (R_1) data into relaxivity (r_{1p}) data. For this operation, knowledge of the concentration of the agent in each voxel is necessary. This task is accomplished by using a second complex (CA-2) analogue to the CA-1, but whose relaxivity is constant over the extended pH range;

b) the CEST (Chemical Exchange Saturation Transfer) method based on the use of diamagnetic or paramagnetic molecules whose ^{1}H-NMR spectra show two sets of mobile protons. By comparing the amount of saturation transfer (ST) on the “bulk” water resonance upon the selective irradiation of each absorption of exchangeable protons, it is possible to set-up a ratiometric method – independent from the concentration of the agent – for assessing pH.

Method b) has been tested both on a diamagnetic molecule (iopamidol) and on a paramagnetic one (YbHPDO3A) [2]. Iopamidol (Isovue®-Bracco Diagnostic Inc.) is a clinically approved x-ray contrast agent. It contains two types of amide functionalities whose exchange rates are markedly pH-dependent, thus allowing the generation of a ratiometric method for pH assessment independent from the actual concentration of the probe. The potential *in vivo* application has been tested by acquiring pH maps of kidney regions. Concerning the use of paramagnetic agents, YbHPDO3A is a chemical analogue of the clinically approved ProHance® (Gadoteridol, Bracco Diagnostic Inc.), in which the Gd^{3+} ion is replaced by Yb^{3+}. For this reason it is expected that Yb-HPDO3A will show the same good toxicological properties reported for ProHance®. This molecule is present in solution as two main isomers whose exchangeable –OH proton resonances display different ST profiles vs. pH that allow for the set-up of a ratiometric method for pH-assessment.



1 | Generation of multiparametric maps in tumor region by CEST-based probes.

The extracellular pH murine melanoma region at different development stages has been mapped using this probe. The voxels in the MR images report on the distribution of pH values with an outstanding spatial resolution (voxel 0.22 mm³).

The shifting properties of ParaCEST compounds allow the exploitation of fast exchange rates to produce considerable ST effects even at low concentrations, the limiting factor being the large irradiation energies employed. Optimizing [3] the saturation profile is thus a key element in the ongoing clinical translation of this technique. Much work has therefore been done to analytically model the CEST system through the Bloch-McConnell equations modified for three pool exchange, which represent a good approximation of the real spin exchange.

The proposed method proves, within the limitations of the employed mathematical model, that optimality has to be reached through a continuous saturation profile with rising amplitude. Access to pH-MRI maps will open new routes for novel *in vivo* diagnostic assays based on the simultaneous assessment of tissue pH and other molecular and functional parameters.

References

[1] E. Terreno, D. D. Castelli, and S. Aime, "Encoding the frequency dependence in MRI contrast media: the emerging class of CEST agents," *Contrast Media Mol. Imaging*, vol. 5, no. 2, pp. 78–98, 2010.

[2] D. D. Castelli, G. Ferrauto, J. C. Cutrin, E. Terreno, and S. Aime, "*In vivo* maps of extracellular pH in murine melanoma by CEST-MRI," *Magn. Reson. Med.*, vol. 71, no. 1, pp. 326–332, 2014. doi:10.1002/mrm.24664

[3] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, "Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms," *J. Magn. Reson.*, vol. 172, no. 2, pp. 296–305, 2005.

Selected Publications

[1] D. L. Longo, A. Busato, S. Lanzardo, F. Antico, and S. Aime, "Imaging the pH evolution of an acute kidney injury model by means of iopamidol, a MRI-CEST pH-responsive contrast agent," *Magn. Reson. Med.*, vol. 70, no. 3, pp. 859–864, 2013.

[2] D. D. Castelli, E. Terreno, D. Longo, and S. Aime, "Nanoparticle-based chemical exchange saturation transfer (CEST) agents," *NMR Biomed.*, vol. 26, no. 7, pp. 839–849, 2013.

[3] D. D. Castelli, M. C. Caligara, M. Botta, E. Terreno, and S. Aime, "Combined high resolution NMR and H-1 and O-17 relaxometric study sheds light on the solution structure and dynamics of the Lanthanide(III) complexes of HPDO3A," *Inorg. Chem.*, vol. 52, no. 12, pp. 7130–7138, 2013.

[4] G. Ferrauto, D. D. Castelli, E. Terreno, and S. Aime, "*In vivo* MRI visualization of different cell populations labeled with PARACEST agents," *Magn. Reson. Med.*, vol. 69, no. 6, pp. 1703–1711, 2013.

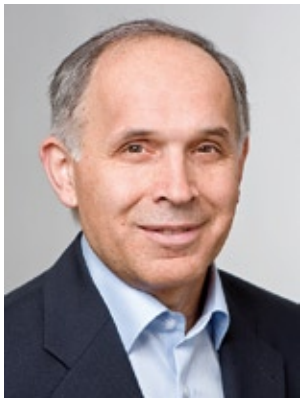
[5] V. Catanzaro, C. V. Gringeri, V. Menchise, S. Padovan, C. Boffa, W. Dastrù, L. Chaabane, G. Digilio, and S. Aime, "A R2p/R1p ratiometric procedure to assess matrix metalloproteinase-2 activity by magnetic resonance imaging," *Angew. Chem. Int. Edit.*, vol. 52, no. 14, pp. 3926 –3930, 2013.

More publications by this Focus Group can be found on page 127.

Focus Group **Neuroscience**

Prof. Arthur Konnerth | Carl von Linde Senior Fellow
Prof. Thomas Misgeld | Hans Fischer Tenure Track Professor
Institute of Neuroscience, TUM

Neuroscience



Arthur Konnerth

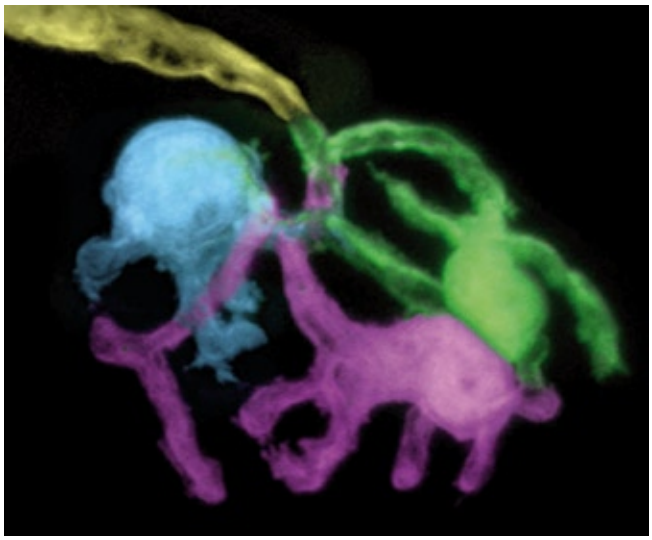
Thomas Misgeld

In 2013, the Focus Group Neuroscience – Prof. Arthur Konnerth, Prof. Thomas Misgeld, Prof. Bert Sakmann, and Prof. Yosi Yarom – continued its quest in using optical methods to explore the functions of subcellular neuronal compartments, such as interneuronal connections (synapses) or projecting processes (axons).

One important open question in neuroscience is how "spontaneous" activity found in many parts of the nervous system relates to extrinsically "evoked" activity patterns. For example, cells in the cerebral cortex spontaneously fluctuate between different functional states – known as "up" and "down" states – which are characterized by differing levels of activity. How do the subsets of synapses that are activated during such spontaneous events relate to the subset of synapses that can be activated by sensory input? The Konnerth and Sakmann groups used their unique *in vivo* approach to optically characterize calcium influx into post-synaptic structures (spines) to explore this question [1]. By comparing which synapses in a neuron are activated during "up" states in the auditory cortex with those that are activated by sound stimulation, Prof. Konnerth and colleagues could show that indeed the same subset of spines that could be activated by sensory stimulation was active during "up" states. As the "replay" of externally driven activity patterns is considered an important mechanism of neuronal plasticity and learning, these results provide an important insight into how such plasticity could play out *in vivo* at the subcellular level.

The Misgeld group similarly focused on using optical techniques to reveal the functional state of subcellular compartments in axons. They focused on energy-producing organelles (mitochondria) and could show that "opto-bioenergetic" characterization can reveal the mechanisms underlying "spontaneous" and injury-induced functional states of mitochondria. While under normal conditions, single mitochondria undergo sudden "contractions" that are accompanied by the transient dissipation of some of the ion gradients that drive energy production; after injury, permanent damage with breakdown of mitochondrial membrane integrity is induced. As mitochondrial alterations are a shared hallmark of many neurological conditions, this optical approach to mitochondrial function *in vivo* is potentially useful in deciphering the causative mechanisms that damage this important organelle [3].

Beyond these results, the Focus Group has obtained vital support to secure its existence beyond the immediate period of TUM-IAS funding, which ended in 2012. In January 2013, the DFG-funded Excellence-Cluster "SyNergy" ("Munich Cluster for Systems Neurology," coordinated by Prof. Christian Haass, LMU, as speaker, and Prof. Misgeld as co-speaker) started its funding. Prof. Konnerth and Prof. Misgeld are engaged in a number of so-called "tandem projects" with partners from LMU and the German Center for Neurodegenerative Diseases (e.g., to characterize the alterations in cortical activity induced by neuroinflammation). In parallel, Prof. Konnerth and Prof. Misgeld received support from the European Research Council (Prof. Konnerth, an Advanced ERC Grant in 2012, and Prof. Misgeld a Consolidator ERC Grant in 2013).



1 | The picture shows the glial cells of a neuromuscular synapse pseudocolored differentially based on a technique described in [2].

Selected Publications

[1] X. Chen, N. L. Rochefort, B. Sakmann, and A. Konnerth, “Reactivation of the same synapses during spontaneous up states and sensory stimuli,” *Cell Rep.*, vol. 4, pp. 31-39, 2013.

[2] M. S. Brill, P. Marinković, and T. Misgeld, “Sequential photo-bleaching to delineate single Schwann cells at the neuromuscular junction,” *J. Vis. Exp.*, vol. 71, e4460, 2013. doi:10.3791/4460

[3] M. O. Breckwoldt, F. Pfister, P. M. Bradley, P. Marinkovic, P. W. Williams, M. S. Brill, B. Plomer, A. Schmalz, D. K. St Clair, R. Naumann, O. Griesbeck, M. Schwarzländer, L. Godinho, F. M. Bareyre, T. P. Dick, M. Kerschensteiner, and T. Misgeld, “Multi-parametric optical analysis of mitochondrial redox signals during neuronal physiology and pathology *in vivo*,” *Nature Medicine, 2014*, in press.

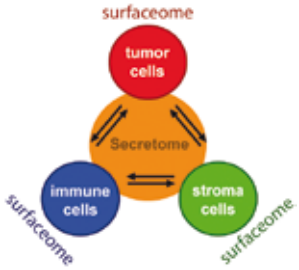
More publications by this Focus Group can be found on page 127.

Focus Group **Proteomics**

Dr. Peer-Hendrik Kuhn | Carl von Linde Junior Fellow
Alperen Serdaroğlu | Doctoral Candidate
Prof. Stefan Lichtenthaler, Neuroproteomics, TUM

Proteomic analysis of cancer secretomes upon ligands

Peer-Hendrik Kuhn



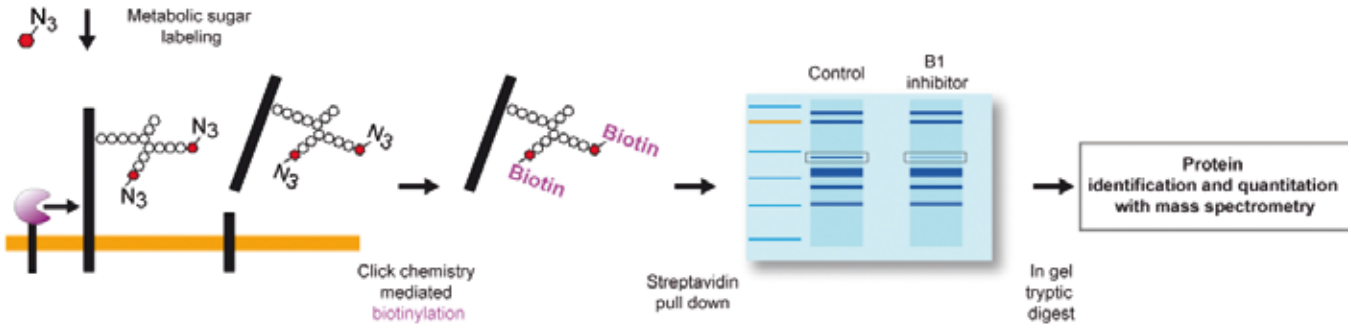
1 | Communication of tumor, immune and storm cells via the secretome.

Cancer is a major problem in our society despite recent advances in therapy for certain types of cancer. Our Focus Group is interested in understanding the biology of hematopoetic cancers with special emphasis on the secretome, the entirety of all secreted and proteolytically liberated proteins from cells, and the surfaceome, which is the entirety of all proteins on the membrane surface of cells.

Both the secretome and the surfaceome are important for the communication between tumor cells, the tumor environment, which is the surrounding stroma the tumor is embedded in, and the immune system (figure 1). In the future, we aim to investigate the impact of receptor tyrosine kinase mutations on the secretome of myeloid leukemia cells, and how this affects the stroma and tumor-invading immune cells. We plan to use mass spectrometry to identify soluble factors which are instructive in terms of understanding stroma proliferation and the generation of supportive milieus for tumor cells. However identification of these factors by analyzing the secretome of cells via mass spectrometry is almost impossible due to the predominance of exogenously introduced fetal calf serum proteins over cell-derived secretome proteins in cell culture media, a problem difficult to overcome because of insufficient analysis sensitivity of current mass spectrometers. We solved this technical problem with our recently developed technology *secretome protein enrichment with click sugars* (SPECS), which enables mass spectrometry-aided analysis of the cellular secretome out of serum containing conditioned cell culture media. SPECS comprises the successive use of metabolic labeling of glycoprotein glycan moieties during their synthesis, and click chemistry to label these metabolically labeled glycoprotein moieties with biotin for glycoprotein isolation out of a complex protein mixture (figure 2).

SPECS has already been successfully applied to the identification of substrates of the protease BACE1. BACE1 initiates the generation of Aβ, the precursor of amyloid plaques in the brain of patients suffering from Alzheimer's disease. Hence BACE1 is considered a major drug target, but mechanism-based side effects of its inhibition for therapy are far from being understood. Using the SPECS technology we identified BACE1 substrates in the central nervous system and thereby contributed to a better understanding of BACE1 physiological function in the CNS and its potential as a drug target for Alzheimer's disease. These data, along with other BACE1-related research topics, were presented at the "Kloster Seeon Conference on BACE Proteases in Health and Disease," which we organized with the support of TUM-IAS.

We are also currently developing a platform for fast and quantitative generation of highly pure recombinant proteins out of mammalian cells, to guarantee the proper folding and posttranslational modification of these proteins. This will aid in the generation of superior monoclonal antibodies against these target proteins, like ligands for receptor tyrosine kinases or rescue experiments. Both technologies will be used to understand more about tumor biology, with special emphasis on how tumors communicate with and influence their environments to improve their chances for survival.



2 | Workflow of the SPECS method: Secretome protein enrichment with click sugars.

In addition to our efforts in cancer research, we interact with other research groups within and outside the TUM-IAS community where proteomics come into play to solve biological questions.

Our Focus Group began in the middle of the year and was reinforced by the doctoral candidate Alperen Serdaroğlu at the end of the year.

Selected Publications

[1] S. Hogl, F. van Bebber, B. Dislich, P. H. Kuhn, C. Haass, B. Schmid, and S. F. Lichtenthaler, "Label-free quantitative analysis of the membrane proteome of Bace1 protease knock-out zebrafish brains," *Proteomics*, vol. 13, no. 9, pp. 1519–1527, 2013.

[2] D. N. Ivankov, N. S. Bogatyreva, P. Honigschmid, B. Dislich, S. Hogl, P. H. Kuhn, D. Frishman, and S. F. Lichtenthaler, "QARIP: a web server for quantitative proteomic analysis of regulated intramembrane proteolysis," *Nucl. Acids Res.*, vol. 41, pp. W459–464, 2013.

[3] A. K. Müller-Rischart, A. Pilsl, P. Baudette, M. Patra, K. Hadian, M. Funke, R. Peis, A. Deinlein, C. Schweimer, P.H. Kuhn, S. F. Lichtenthaler, E. Motori, S. Hrelia, W. Wurst, D. Trümbach, T. Langer, D. Krappmann, G. Dittmar, J. Tatzelt, and K. F. Winkelhofer, "The E3 ligase parkin maintains mitochondrial integrity by increasing linear ubiquitination of NEMO," *Mol. Cell*, vol. 49, no. 5, pp. 908–921, 2013.

[4] B. Schmid, A. Hruscha, S. Hogl, J. Banzhaf-Strathmann, K. Strecker, J. van der Zee, M. Teucke, S. Eimer, J. Hegermann, M. Kittelmann, E. Kremmer, M. Cruts, B. Solchenberger, L. Hasenkamp, F. van Bebber, C. van Broeckhoven, D. Edbauer, S. F. Lichtenthaler, and C. Haass, "Loss of ALS-associated TDP-43 in zebrafish causes muscle degeneration, vascular dysfunction, and reduced motor neuron axon outgrowth," *P. Natl. Acad. Sci.* USA, vol. 110, no. 13, pp. 4986–4991, 2013.

Peer-Hendrik Kuhn studied medicine from 2001 to 2008 at Ludwig-Maximilians-Universität (LMU) in Munich. During his medical studies he was a scholarship holder of the Molecular Medicine program of LMU. He joined the laboratory of Prof. Christian Haass at the Adolf Butenandt Institute to study the role of proteases in Alzheimer's disease. His state examination in medicine in 2008 was followed by the granting of a medical doctorate in 2009. After his medical studies, he joined the Medical Life Science and Technology program of the TUM and the German Center of Neurodegenerative Diseases within the Helmholtz Association (DZNE) in Munich. In 2012 he received his doctorate.

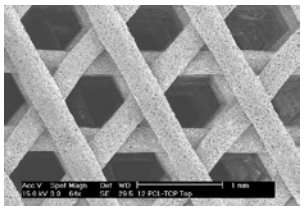
Focus Group **Regenerative Medicine**

Prof. Dietmar W. Hutmacher | Hans Fischer Senior Fellow
Dr. Elizabeth Rosado Balmayor | Postdoctoral researcher
Prof. Arndt F. Schilling, Clinic for Plastic Surgery and Hand Surgery, TUM

Tissue Engineering

Dietmar W. Hutmacher

The lack of functional integration between tissue-engineered constructs (TECs) and surrounding host tissues is a critical barrier, limiting the effectiveness and clinical translation of current soft tissue interface graft technologies. The overarching goal of this Hans Fischer Senior Fellowship is to address this challenge through the development of highly adaptable platform technologies that enable the engineering of stronger interfaces between TECs and the extracellular matrices that are distinct to particular clinical conditions. Through this project, an international network spanning scientists, engineers, clinicians, industry, and government will be established to accelerate the pace of regenerative medicine research targeting reconstruction of complex soft tissue interface defects and abnormalities.
Key outcomes of the Hans Fischer Senior Fellowship will deliver innovative strategies for additive tissue manufacturing for soft tissue interfaces whilst contributing to the education at TUM of a new generation of bioengineers, clinician scientists, and tissue engineers with a strong international profile.



1 | Scanning electron microscopy image which features the macro, micro, and nano porosity of a fully interconnected scaffold architecture.

The overall objectives of the Focus Group Regenerative Medicine:

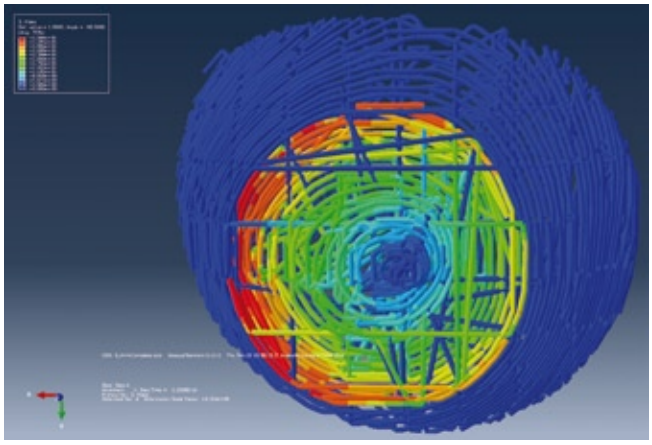
- To develop a world class tissue engineering/regenerative medicine (TE/RM) program focused on additive tissue manufacturing for the regeneration of soft tissue interfaces, specifically for breast reconstruction.
- To facilitate efforts to bridge the gap between basic research, bioengineering, and clinical positioning of regenerative therapies at TUM through strong activities supporting research translation and business development in collaboration with regional, national, and international industry partners.
- To share newly generated scientific knowledge in regenerative medicine with researchers, engineers, clinicians, and the public through educational activities, training, publications, and communication forums at national and international levels, as well as being an active advocate and discussant of ethical aspects of TE/regenerative medicine in general, and of stem cells in particular, to improve public awareness and acceptance.

In collaboration with PD Dr. Jan-Thorsten Schantz, Prof. Adorjan Kovacs, and Dr. Max Eder.

Selected Publication

[1] J. Malda, J. Visser, F. P. Melchels, T. Jüngst, W. E. Hennink, W. J. Dhert, J. Groll, and D. W. Hutmacher, “25th anniversary article: Engineering hydrogels for biofabrication,” *Adv. Mater.*, vol. 25, no. 36, pp. 5011–5028, 2013. doi:10.1002/adma.201302042

More publications by this Focus Group can be found on page 127.



2 | Finite Element Model of a patient-specific scaffold designed for breast tissue engineering.

Dietmar W. Hutmacher is a multidisciplinary biomedical engineer. Having received degrees from the University for Applied Science in Aachen and the Royal Henley Management College in the United Kingdom, he completed his Ph.D. at the National University of Singapore, in the Department of Orthopaedic Surgery, in 2001; his academic career has included positions in Germany, Singapore, and Australia. As a reflection of a pioneering ethos, his efforts have resulted in traditional scientific/academic outputs and pivotal commercialization outcomes, taking projects from holistic concept through to clinical application. His research interests and collaborations center on engineering (tissue engineering, biomaterials science, computational modeling, chemistry, nanotechnology), the life science disciplines (molecular cell and developmental biology, medicine, stem cell research, genomics, proteomics, bioinformatics), and applied clinical research (orthopaedics, plastic surgery, radiology).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Natural Sciences

Focus Group **Advanced Construction Chemicals and Materials**

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

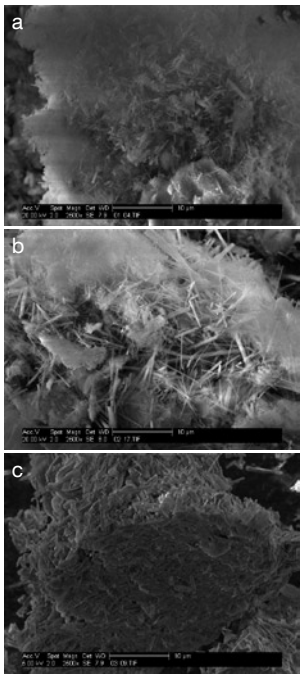
Tsuyoshi Hirata

Polycarboxylate-based superplasticizers with polyethylene glycol pendants (PCEs) have grown to be an indispensable admixture for highly durable concrete, such as (ultra) high-strength concrete and self-compacting concrete, because of their superior water-reducing capability. Furthermore, PCEs are polymers that allow easy adaption to specific needs by modification of the polymer structure: Changing the monomer ratio, the length of ethylene glycol (PEG) side chains or the molecular weight of the PCE polymer, or the introduction of other monomers, all result in quite different performance effects. Hence it is a major area of interest to understand the relationship between polymer structure and performance.

We found in the last report in 2012 that:

- There are three types of conformation in typical PCE molecules: rod-like, worm-like, and star-like.
- The star-like PCE with long PEG side chains was most effective in water-reducing performance at low dosage because of the larger adsorbed layer thickness on the cement surface.
- There is the possibility to disperse cement particles by another working mechanism originating from non-adsorbed PCE, in addition to the steric repulsion by PEG side chains originating from adsorbed PCE.

In 2013, we focused on the study of working mechanisms concerning required performance in the industry – other than water-reducing effect – such as the improvement of concrete viscosity or flow characteristics and cement compatibility.



1 | ESEM images of initial hydrate phase with and without PCE
(a) without PCE
(b) with newly developed PCE
(c) with conventional PCE.

Our conclusion is:

- Good workability such as water-like flow can be obtained from very hydrophilic PCE molecules, found especially in APEG and some IPEG PCEs. The hydrophilic and lipophilic balance in the molecule (HLB value) can be used to predict water-like flow characteristics of specific PCEs.
- Some cement constituents (C_3A, CaO) increase the PCE dosage, but two types of PCE – one a rigid polymer, the other a slightly cross-linked polymer – were found to show enhanced cement compatibility.

Our target now is to identify the working mechanism of cement compatibility. Currently it appears that conventional PCEs have a great influence on the initial hydrate crystallization when the cement includes a large amount of C_3A and CaO. The effect cannot be observed if both C_3A and CaO content are low, or if only one of the components is particularly high. Conventional PCEs require extremely high dosages to disperse these kinds of cements, whereas optimized PCEs require only a slightly higher dosage compared to easily dispersing cements.

Current research is focusing on which initial hydrate phases consume large amounts of PCE. Analytic methods include elemental analysis, SEM imaging, and thermogravimetry. The authors wish to express their gratitude to TUM-IAS for its generous support of this fascinating research project.

Publications by this Focus Group can be found on page 127.

Focus Group **C-H Activation Chemistry**

Prof. Polly L. Arnold | Hans Fischer Senior Fellow
Max McMullon, Julia Rieb | Doctoral Candidates
Prof. Fritz E. Kühn, Molecular Catalysis, TUM

Polly L. Arnold

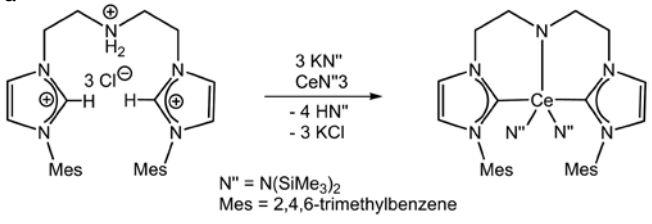
The vision of this Focus Group is to develop world-leading research in the form of the first useful catalytic conversion of the C-H bonds in hydrocarbons such as petrol or biomass, to more interesting functional groups, by the application of our molecular systems. Most homogeneous catalysis relies on the design of metal complexes to trap and convert substrates or small molecules to value-added products. Organometallic lanthanide compounds first gave a tantalizing glimpse of their potential for catalytic C-H bond transformations with the selective cleavage of one C-H bond in methane some 25 years ago. Since then, the selective activation of hydrocarbon C-H bonds by metal complexes from across the periodic table has taken off, but the challenge of making a catalytic cycle still remains; many f-block complexes show great potential in this fascinating area of chemistry. A doctoral candidate in his second year, Max McMullon, has made further new ligand frameworks to bind complementary metals, combining the C-H bond activation with cerium cations, figure 1(a), and selective oxidation steps. He has been joined by Julia Rieb, working on related systems. One heterobimetallic complex formed from the result of C-H bond scission and the bridging of the f-block and d-block element is shown in figure 1(b). Current work is now in progress to study the insertion of other hydrocarbons into the M-CH_2 bridging groups in the molecule depicted in figure 1(b), and to identify which M-C bond is more labile. The addition of hydrogen and its surrogates, such as silanes, is also in progress.

The second set of reactivity studies will focus on selective oxidation of one or both metals in the framework. The main target is a complex with one terminal metal oxo group that can participate in redox reactivity, in the anticipation that weak coordination by the other metal will enhance the oxidative capacity. Further oxidation to double oxo complexes containing the two complementary metal cations will give unusual new structures and possibilities for double C-H bond H-atom abstractions; a non-oxygen transferring route to hydrocarbon functionalization. In addition, the other principal investigator in our lab, Dr. Jason Love, is also now collaborating with Prof. Fritz E. Kühn and Dr. M. Cokoja on the development of new methods for encapsulating the industrially important metal oxo catalyst, MTO, used for hydrocarbon oxidation. This work is being patented.

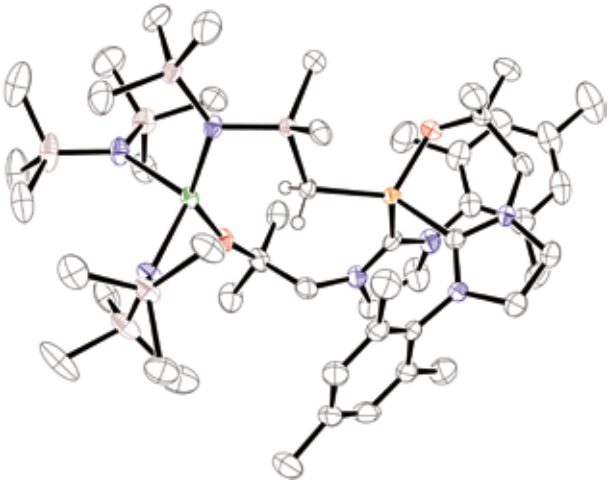
Selected Publication

[1] P. L. Arnold, M. McMullon, J. Rieb, and F. E. Kuehn, “Carbon-hydrogen bond activation by f-block complexes,” submitted for publication.

a



b



1 | (a) Cerium complexation in a tridentate carbene ligand framework (b) bridging methylidene CH_2 group in a heterobimetallic 3d-5f complex.

Focus Group **Biochemistry**

Dr. Franz Hagn | Hans Fischer Fellow
Joka Pipercevic | Doctoral Candidate
Prof. Horst Kessler, Chemistry, TUM

Structural biology of disease-linked membrane proteins

Franz Hagn

Our research is focused on the structure determination and dynamics of membrane proteins in a realistic phospholipid bilayer membrane environment, using high-resolution nuclear magnetic resonance (NMR) spectroscopy as the primary tool. NMR is a perfect tool for extracting dynamical parameters in solution that correlate with functional features of proteins during partner protein binding and enzyme catalysis.

Most membrane protein structures were solved in a detergent-solubilized form. However, for studying membrane protein complexes, detergents are less suitable as they often inhibit biological interactions and lead to chemical denaturation of soluble partner proteins. We are therefore focusing on the use of so-called phospholipid nanodiscs, a detergent-free membrane mimic that consists of a patch of phospholipid bilayer contained by two copies of a lipid-binding protein, or MSP (membrane scaffold protein). The length of the particular MSP determines the diameter of these monodisperse particles. The smallest nanodiscs reported until recently had a diameter of around 10 nm, which is still too large for high-resolution NMR spectroscopy in solution. Therefore, we constructed a series of truncated MSP variants that formed markedly smaller nanodiscs down to a diameter of 6 nm. This optimized system finally enabled the NMR structure determination of the bacterial outer membrane protein X (OmpX), which represented the first and so far only reported structure of a membrane protein in nanodiscs [1].

In another study [2], we performed a systematic comparison between various membrane-mimicking media (detergents, phospholipid nanodiscs, and amphipoles, a polymer-based membrane system). Therein, we could show that only nanodiscs confer the superior membrane protein stability required for structure determination, as probed with the seven-transmembrane–helix protein bacteriorhodopsin, a structural homologue of G-protein coupled receptors (GPCRs).

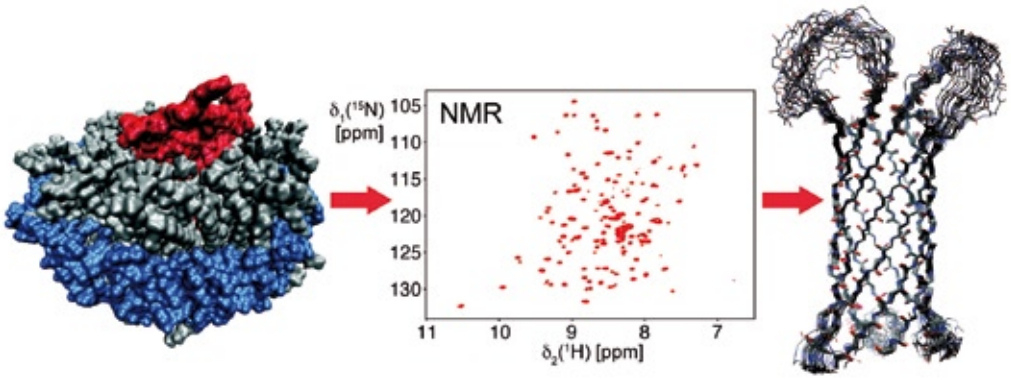
These new membrane systems are now being applied to study the pharmaceutically important interaction between GPCRs and their associated G-proteins, as well as mitochondrial membrane proteins involved in metabolic diseases and cancer.

Selected Publications

[1] F. Hagn, M. Etzkorn, T. Raschle, and G. Wagner, “Optimized phospholipid bilayer nanodiscs facilitate high-resolution structure determination of membrane proteins,” *J. Am. Chem. Soc.*, vol. 135, no. 5, pp. 1919–1925, 2013.

[2] M. Etzkorn, T. Raschle, F. Hagn, V. Gelev, A. Rice, T. Waltz, and G. Wagner, “Structural insights into cell-free expressed bacteriorhodopsin in different soluble membrane mimetics,” *Structure*, vol. 21, no. 3, pp. 394–401, 2013.

More publications by this Focus Group can be found on page 127.



Phospholipid Nanodisc

Membrane Protein Structure

1 | We are interested in the NMR structure determination of membrane proteins (red) in a novel membrane mimic, called phospholipid nanodiscs, where a patch of lipid bilayer (grey) is contained by a lipid-binding protein (blue). This system offers the unique advantage of providing a detergent free environment, which is particularly important for studying interactions between membrane proteins and soluble proteins.

Franz Hagn studied biochemistry at the University of Bayreuth and came to the lab of Prof. Horst Kessler at TUM to pursue his doctorate in the field of NMR-based structural biology of spider silk proteins, molecular chaperones, and tumor suppressor proteins. After a short postdoctoral stay at TUM, he moved to his current position as an EMBO and Human Frontier Science Program-funded research Fellow at Harvard Medical School in the lab of Prof. Gerhard Wagner. His research interests are the structure determination of membrane proteins and the development of advanced biochemical and NMR spectroscopic tools. For his work on spider silk proteins and molecular chaperones, he received the 2012 Arnold Sommerfeld Award of the Bavarian Academy of Sciences, the 2011 Hans Fischer Award of TUM Chemistry, and the 2011 Friedrich Weygand Award of the Max Bergmann Society.

Focus Group **Biochemistry**

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

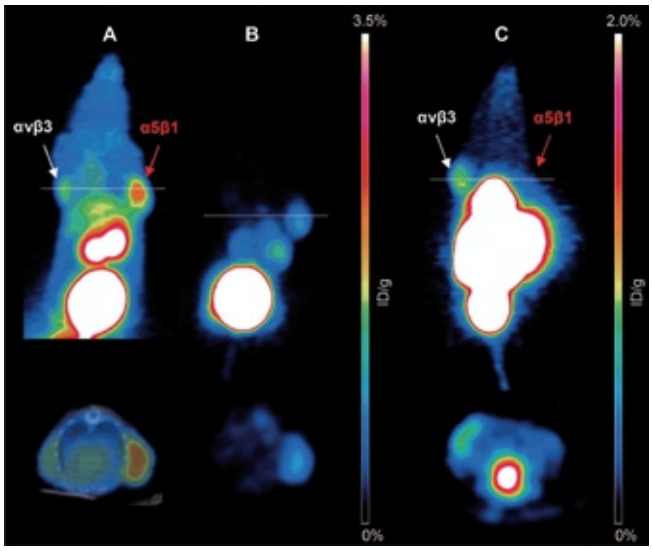
Horst Kessler

In 2013 we published 14 manuscripts with a total impact factor of 101,4. Two highlights are outlined briefly below.

Selective imaging of the angiogenic relevant integrins α5β1 and αvβ3

The binding of αvβ3 and α5β1 integrins to their corresponding extracellular matrix (ECM) proteins is essential for many biological processes, including tumor angiogenesis, development, migration, and proliferation. Currently, there is significant disagreement in the literature as to how and to what extent these RGD-binding integrins exert their functions in regular and pathological angiogenesis. Furthermore, it is unclear how the inhibition of distinct integrins is influencing the tumor growth. To answer these intriguing questions, we have developed selective RGD-based peptidomimetics for specific *in vivo* targeting and blocking of αvβ3 or α5β1 integrins. These small molecules were functionalized for molecular imaging by positron emission tomography (PET) to specifically target integrins *in vivo* (figure 1). Our studies demonstrate the first successful α5β1-based PET imaging using these different peptidomimetics and gave a striking demonstration of their integrin subtype selectivity by showing that they can differentiate between two tumor types with different patterns of integrin αvβ3 and α5β1 expression.

The development of these integrin-selective compounds will be of high medical relevance for diagnostic imaging and disease monitoring purposes (e.g., in patients afflicted with cancer). Furthermore, selective targeting of specific integrin species will be of great importance for personalized medicine, which requires the determination of distinct overexpressed receptors on the surface of the cancer cells and thus provides a good characterization of the disease on a molecular basis.

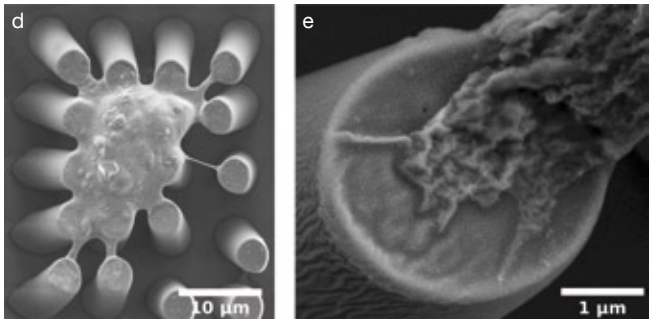


1 | Images of microPET scans. Upper row: mice bearing α5β1-expressing (RKO) and αvβ3-expressing (M21) tumor xenografts on right and left shoulder, respectively. Selective tumor uptake of the developed compounds is shown (A and C); B: Blocking experiment with α5β1-selective compound. White arrow: M21; red arrow: RKO. Lower row: axial slices corresponding to the white line in upper row.

Hydrogel micropillars with integrin selective peptidomimetic functionalized nanopatterned tops: a new tool for the measurement of cell traction forces transmitted through αvβ3- or α5β1-integrins

Additionally, integrins play a key role in cell adhesion during mechanotransduction to the cytoskeleton by regulating signaling pathways that convey physical forces into chemical signals. Several studies have focused on investigating how the activation of specific integrin types and integrin receptor clustering may contribute to adhesion strength. In particular, it has been reported that upon binding to fibronectin, αvβ3 and α5β1 integrins have a distinct role in establishing adhesion. For this reason, we functionalized the αvβ3- and α5β1-selective integrin ligands with a thiol for the coating of gold nanopatterned surfaces to investigate the cell adhesion process in biophysical experiments. In collaboration with Dr. Joachim Spatz (Max Planck Institute Stuttgart), we used hydrogel micropillars with gold nanopatterned tops (figure 2). These gold nanoparticles were functionalized with the αvβ3- or α5β1-selective molecule, respectively, and αvβ3- or α5β1-induced cell traction forces were investigated. This enabled the separate measurement of individual cellular traction forces, thus allowing us to determine the contribution of different integrin types to the total traction force. We demonstrate that cells binding to α5β1 integrin antagonists have a tendency to exert higher maximum forces on the pillars than cells binding to αvβ3 integrin antagonists.

In collaboration with T. Kapp, Dr. U. K. Marelli, Dr. S. Neubauer, and Dr. F. Rechenmacher.



2 | SEM micrographs of a fixed REF-YFP-PAX cell on gold nanoparticle PEG pillars (d) and close-up of a single pillar with an attached cell protrusion (e).

Selected Publications

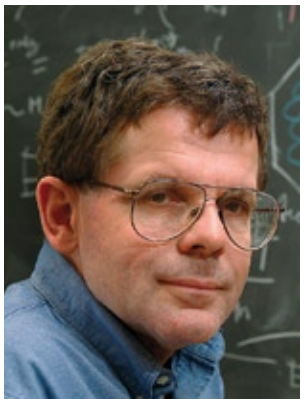
[1] S. Neubauer, F. Rechenmacher, A. J. Beer, F. Curnis, K. Pohle, C. D'Alessandria, H.-J. Wester, U. Reuning, A. Corti, M. Schwaiger, and H. Kessler, "Selective imaging of the angiogenic relevant integrins α5β1 and αvβ3," *Angew. Chem. Int. Ed.*, vol. 52, no. 44, pp. 11656–11659, 2013.

[2] S. Rahmouni, A. Lindner, F. Rechenmacher, S. Neubauer, T. R. A. Sobahi, H. Kessler, E. A. Cavalcanti-Adam, and J. P. Spatz, "Hydrogel micropillars with integrin selective peptidomimetic functionalized nanopatterned tops: a new tool for the measurement of cell traction forces transmitted through αvβ3- or α5β1-integrins," *Adv. Mater.*, vol. 25, no. 41, pp. 5869–5874, 2013.

More publications by this Focus Group can be found on page 127.

Focus Group **Biophysics**

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

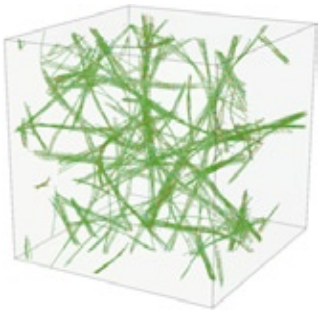


Robijn Bruinsma

The mechanical properties of cells are largely determined by the *cytoskeleton*, a dynamic network of biopolymers, and its bundles, held together by labile linker proteins. The principal constituent of the cytoskeleton is the biopolymer F-actin. In F-actin networks the *thermal persistence length* of the constituent filaments is much longer than the typical distance between consecutive cross linkers along a given filament, leading to the formation of a semi-flexible network, with surprising mechanical properties quite distinct from that of gels of synthetic, highly flexible polymers familiar to polymer science. The fundamental understanding of the elastic properties of these networks under conditions of thermal equilibrium is quite advanced. Key insights were that – despite the stiffness – small transverse thermal fluctuations dominate the single filament compliance and the high frequency rheology of these networks. This produces a *universal power-law rheology*, which was confirmed experimentally. Another consequence is that the networks' elastic moduli depend *nonlinearly* on the filament concentration. As part of our previous work at TUM, we explored the equilibrium phase diagram of these networks using Brownian dynamics simulations. In agreement with results of the Bausch Lab, we found that homogeneous networks only formed at very low linker concentrations. If the linker concentration increases, bundles or highly organized clusters and layers form.

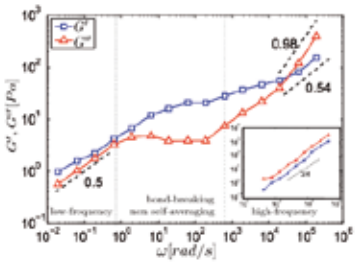
There is increasing evidence that the universal power-law rheology theory does not account adequately for the rheology of networks composed of bundles of semi-flexible filaments. Bundle formation is encountered in synthetic preparations at high linker concentrations in the form of networks of bundles. They are also ubiquitous in the cytoskeleton of eukaryotic cells. Importantly, bundle networks with labile cross linkers *are generally in a nonequilibrium state*: the network's geometry slowly evolves towards, but is never observed to reach, the final free energy minimum corresponding to just a single bundle. One would not expect to encounter any universal features.

We carried out finite-temperature Brownian Dynamics simulations of semi-flexible transient bundle networks formed from semi-flexible filaments linked by isotropic, labile cross linkers. The figure shows a typical realization.



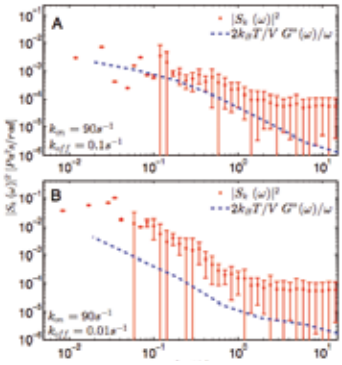
1 | Example of a bundle network produced by the Brownian Dynamics simulation. The simulation box measured 6 microns per side and has 360 filaments at a concentration of 4 micro-Molar. The filaments are in constrained thermal equilibrium with a 3 microMolar concentration of cross linkers.

The surprisingly rich rheological properties of such an evolving network are shown in figure 2.



2 | Rheology of network bundles similar to the one shown in figure 1. The vertical axis shows the real and imaginary parts of the complex modulus for linear response. The horizontal axis is the applied frequency. Dashed lines: high-frequency exponents predicted by Frey theory. Inset: rheology of free filaments. Power-law rheology is observed at high and low frequency. For intermediate frequencies, the rheology is preparation dependent.

The horizontal axis is the frequency of the applied AC shear. The vertical axis shows the real (G') and imaginary (G") parts of the response moduli – comparable to the spring and friction constants of a damped harmonic oscillator. Three regimes are visible. At high frequencies, one observes power-law scaling relations. This would seem similar to the equilibrium single-filament case, shown in the inset. However the exponents are different! In fact, the exponents agree with a recent theoretical study on bundle rheology by Prof. Erwin Frey of Ludwig-Maximilians-Universität München. At intermediate frequencies we observe a non-universal (i.e., preparation-dependent) phenomenology – as could be expected for a non-equilibrium network. The great surprise was that at low frequencies, there is a *second* universal, power-law rheology. Both moduli are proportional to the square root of the applied frequency. In this low frequency regime, large-scale rearrangements of the network were observed. We discovered that in this regime the system violates the *fluctuation-dissipation theorem* (FDT), which is the fundamental relationship that forms the basis of the linear-response theory that so far has been the basis of our understanding of the physics of semi-flexible networks. The FDT relates the power spectrum of spontaneous fluctuations, S(ω), to the imaginary part, G"(ω). The FDT predicted power spectrum is shown in blue in figure 3, the measured power spectrum in red.



3 | Test of the fluctuation dissipation theorem. Blue: predicted fluctuation power spectrum. Red: measured power spectrum. A: off rate equals 0.1 Hz. B: off rate equals 0.01 Hz.

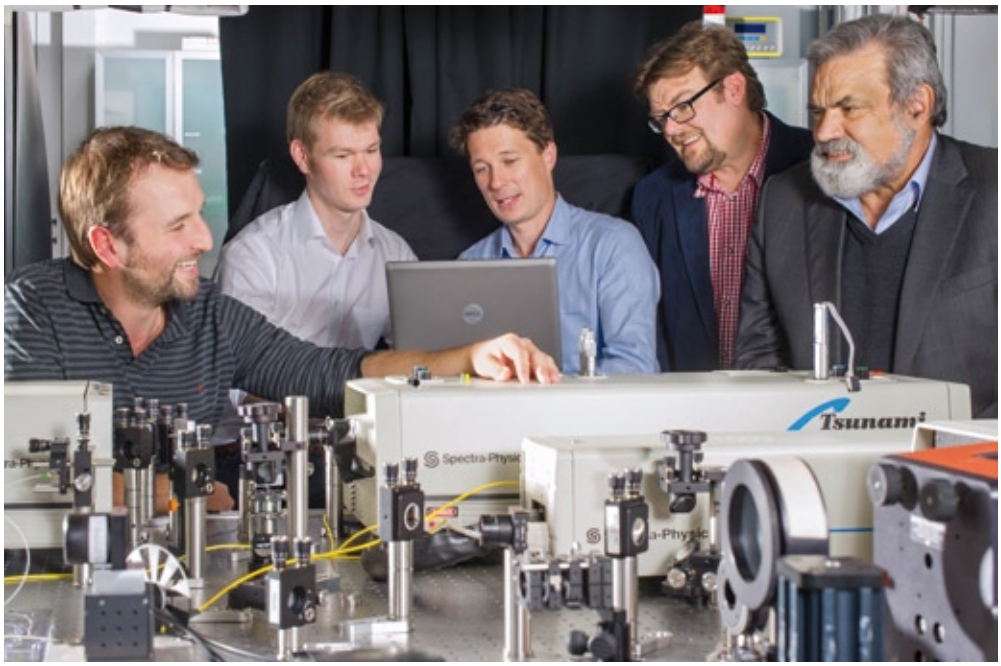
For case A, the off-rate of the labile linkers was 0.1 Hz. The FDT-predicted spectrum is within the error bars of the measured spectrum. If the off-rate is reduced by a factor of 10, as shown in B, then the measured fluctuations are an order of magnitude more intense than expected based on the FDT. The failure of the FDT demonstrates unambiguously the fundamental non-equilibrium nature of network formation of semi-flexible polymers with labile linkers.

In collaboration with Kei Mueller.

Publications by this Focus Group can be found on page 128.

Focus Group **Nanophotonics**

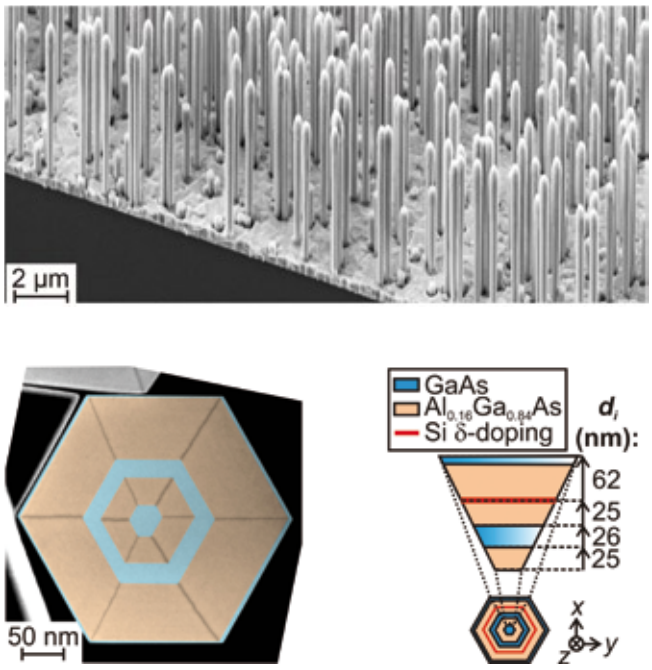
Prof. Gerhard Abstreiter | Carl von Linde Senior Fellow
Dr. Eric Hoffmann | Postdoctoral Researcher
Walter Schottky Institute and Physics Department, TUM



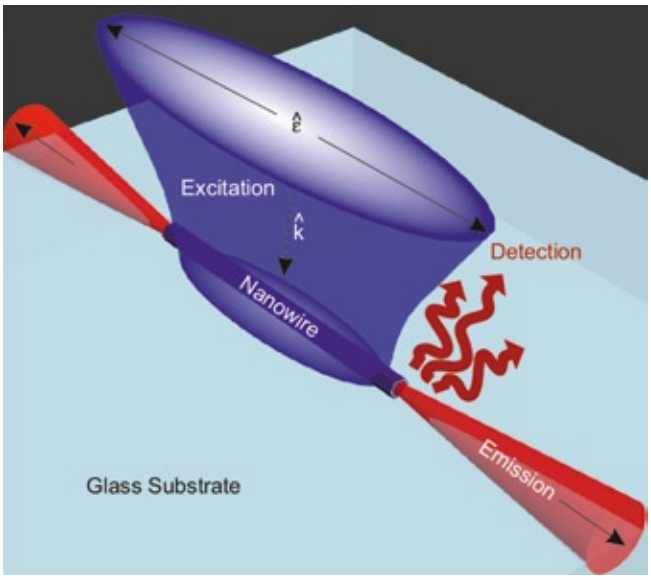
The nanowire laser is finally working. From left to right: Benedikt Mayer, Daniel Rudolph, Gregor Koblmüller, Jonathan J. Finley, and Gerhard Abstreiter.

Semiconductor hetero-nanowires on Si for nanoelectronics, nanophotonics, and photovoltaics

Major breakthroughs were achieved in the year 2013 within our hetero-nanowire research group with respect to electrical and optical properties as well as photonic applications on a Si platform. These activities resulted in several publications in *Nano Letters, Phys. Rev. B., New Journal of Physics*, and *Nature Communications*, listed in the publication section of this report. The successful work is based on the realization of high quality core-shell hetero-nanowires within the Ga(Al)As and Ga(In)As(P) materials system, synthesized directly on Si substrates. This includes the demonstration of high mobility two- and one-dimensional electron channels in remotely doped hetero-nanowires [1] as bases for future transistor integration in nanoelectronic circuits, as well as the achievement of strongly enhanced optical properties and light emission in the mid-infrared regime [2] with possible applications as broadband absorbers, photo-detectors, and next generation solar cells. The research highlight, however, is definitely the realization of GaAs-based nanowire lasers grown on Si [3]. Those lasers have potential applications for Si-based photonics, for communication, computing, and probably also for sensing.



1 | Core-shell nanowires [1].



2 | Schematics of the excitation of a nanowire laser [3].

Infrared lasing from individual core shell GaAs-AlGaAs nanowires has been achieved up to room temperature. When subject to increased optical excitation density, the nanowires show an unambiguous transition from spontaneous emission modulated by the Fabry-Perot modes of the nanowire-resonator to the lasing regime, characterized by a spectrally narrow single mode emission at low temperatures. Non-radiative surface recombination is suppressed by the AlGaAs shell. Remarkably low threshold pump power densities are observed and lasing operation persists up to room temperature. Our results show that, by carefully designing the axial and radial materials composition profile, high performance infrared nanowire lasers can be realized with III-V materials on Si.

In collaboration with Prof. Jonathan J. Finley, Dr. Gregor Koblmüller, Dr. Ilaria Zardo, and various doctoral candidates and master's students.

Selected Publications

[1] S. Funk, M. Royo, I. Zardo, D. Rudolph, S. Morkötter, B. Mayer, J. Becker, A. Bechtold, S. Matich, M. Döblinger, M. Bichler, G. Koblmüller, J. J. Finley, A. Bertoni, G. Goldoni, and G. Abstreiter, "High mobility one- and two- dimensional electron systems in nanowire-based quantum heterostructures," *Nano Lett.*, vol. 13, no. 12, pp. 6189–6196, 2013.

[2] J. Treu, M. Bormann, H. Schmeiduch, M. Döblinger, S. Morkötter, S. Matich, P. Wiecha, K. Saller, B. Mayer, M. Bichler, M. C. Amann, J. J. Finley, G. Abstreiter, and G. Koblmüller, "Enhanced luminescence properties of InAs-InAsP core-shell nanowires," *Nano Lett.*, vol. 13, no. 12, pp. 6070–6077, 2013.

[3] B. Mayer, D. Rudolph, J. Schnell, S. Morkötter, J. Winnerl, J. Treu, K. Müller, G. Bracher, G. Abstreiter, G. Koblmüller, and J. J. Finley, "Lasing from individual GaAs-AlGaAs core-shell nanowires up to room temperature," *Nat. Commun.*, vol. 4, 2931, 2013.

More publications by this Focus Group can be found on page 129.

Focus Group **Nanoscale Control of Quantum Materials**

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

Wilhelm Auwärter

Advanced molecular nanostructures on two-dimensional supports

During the last year, we broadened and deepened our understanding of molecular organization and interaction processes on surfaces. In general, we aim for the controlled assembly and comprehensive characterization of molecular nanostructures both on metallic surfaces and on advanced substrates like atomically thin boron nitride layers.

Here, we focus on two highlights. We introduced the first molecular-level realization of a two-dimensional interfacial tessellation based on five-vertex motifs. Specifically, the lanthanide-directed assembly of linear polyphenyl molecular linkers equipped with terminal carbonitrile groups yields fivefold lanthanide-ligand coordination motifs on a smooth silver substrate [1]. The resulting periodic pattern, identified as the semiregular Archimedean snub square tiling, was comprehensively characterized by scanning tunneling microscopy and spectroscopy (see figure 1).

Secondly, we have shown that an ultrathin boron nitride layer grown on copper introduces manifold new prospects for molecular adsorption compared to conventional metal supports [2]. As evidenced by scanning tunneling microscopy and spectroscopy experiments, the boron nitride electronically decouples functional porphine units from the metallic substrate, thus allowing us to image molecular frontier orbitals in real space. Furthermore, the lateral modulation of the surface potential at the boron nitride/copper interface induces a periodic, spatial modulation of the energy of the frontier orbitals and induces the unprecedented organized growth of ordered arrays of molecular assemblies, for porphines and other adsorbates (see figure 2).

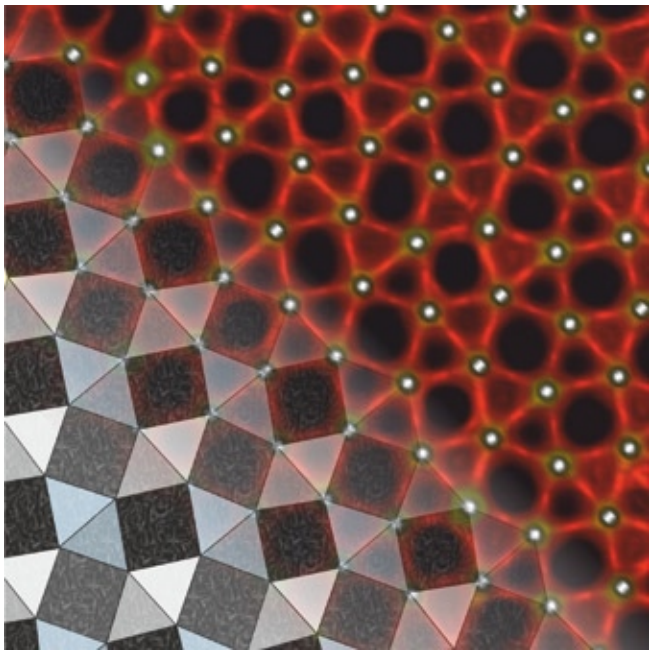
Our future efforts will concentrate on the deliberate tuning of functionalities of single molecules and supramolecular architectures on ultra-thin sp^2 layers (boron nitride or graphene). Specifically, a control on electronic and structural properties in molecule/sp^2 hybrid systems is of great interest.

Selected Publications

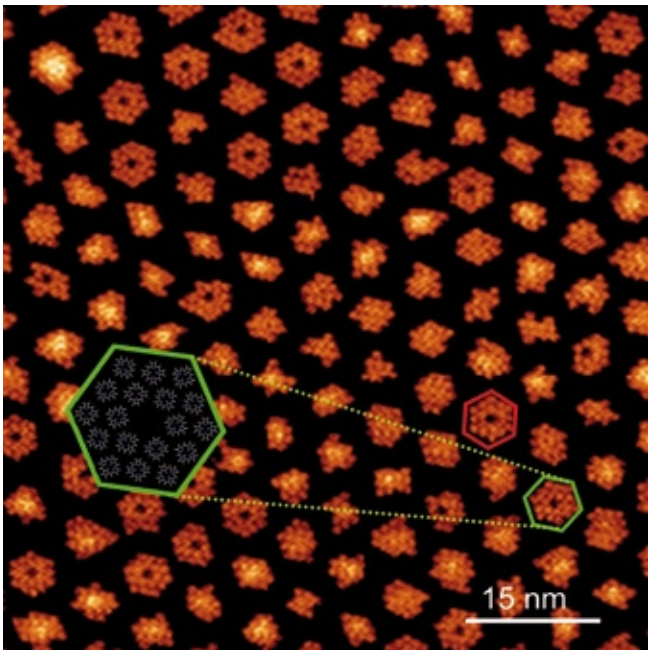
[1] D. Ecija, J. I. Urgel, A. C. Papageorgiou, S. Joshi, W. Auwärter, S. Klyatskaya, M. Ruben, S. Fischer, S. Vijayaraghavan, J. Reichert, and J. V. Barth, “Five-vertex Archimedean surface tessalation by lanthanide directed molecular self-assembly,” *P. Natl. Acad. Sci. USA*, vol. 110, no. 17, pp. 6678–6681, 2013.

[2] S. Joshi, F. Bischoff, R. Koitz, D. Ecija, K. Seufert, A. P. Seitsonen, J. Hutter, K. Diller, J. I. Urgel, H. Sachdev, J. V. Barth, and W. Auwärter, “Control of molecular organization and energy level alignment by an electronically nanopatterned boron nitride template,” *ACS Nano*, vol. 8, no. 1, pp. 430–442, 2014.

More publications by this Focus Group can be found on page 129.



1 | Nanoscale Kepler tessellation of a silver surface by a metal-organic network. The white protrusions represent lanthanide centers, linked by linear oligophenyl molecules (red rod-like features). The distance between the centers is about 2 nanometers. The STM image (top right) is overlaid with the corresponding tessellation scheme (bottom left).



2 | Scanning tunneling microscopy image revealing the formation of extended porphine assemblies (e.g., green hexagon), organized in a periodic array by the templating functionality of the supporting boron nitride/copper interface (adapted from [2]).

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

In the past year, our group has been devoted to the study of complexity in spatially extended oscillatory media, arrays of nonlinear oscillators, and discrete dynamical systems. A number of new results have been derived and confirmed by experiments and are being prepared for publication. These include the discovery of chimera states under purely global coupling in arrays of nonlinear oscillators, and a theory that allows to directly relate local and global scales for the spatiotemporal evolution of discrete systems. This latter theory has opened some possibilities that were unexpected to us and that have led us to find a systematic method of coarse-graining the microscopic dynamics of systems with many degrees of freedom, in order to accurately approximate their statistical behavior also in situations far from equilibrium.

The complex Ginzburg-Landau equation with nonlinear global coupling has been shown to lead to the spontaneous formation of chimera states, where synchrony and incoherence spatially coexist in a stable way in arrays of identical nonlinear oscillators and/or homogeneous oscillatory media [2]. These novel results show that, contrary to what has been thought until now, chimera states can form spontaneously under a pure global coupling and arbitrary initial conditions. It was previously believed that a nonlocal (but not global) coupling was strictly necessary to observe this fascinating dynamical behavior and that the initial conditions had to be carefully selected in order to keep the basin of attraction where chimera states are stable. Our work has shown that, far from being an exotic dynamical behavior, chimera states mediate – in a very general and ubiquitous way – the transition from order and synchrony to disorder and incoherence in ensembles of nonlinear oscillators.

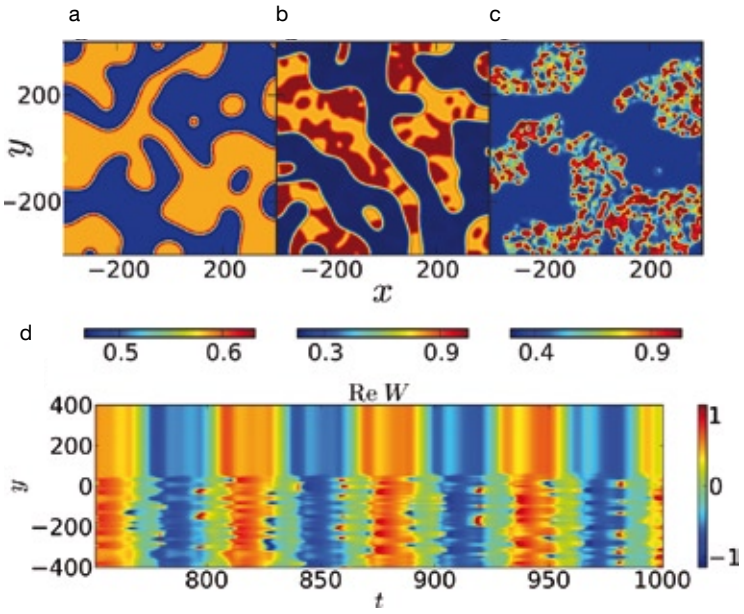
We have also shown that the origin of complexity in dynamical systems has its foundations on a symmetry breaking process that occurs already at the level of discrete systems with a finite number of dynamical states [1]. This symmetry breaking – which partially affects the scale invariance property, although not totally destroying it – connects local and global scales in a subtle and generally undecidable way, leading to the systematic generation of universal Turing machines out of simple dynamical rules. A general theory for the local, nonlocal, and global dynamics of discrete systems has been accomplished following these results, and has been very recently submitted for publication. The theory is valid regardless of the number of dynamical states and/or range of the interactions, and has provided us with some interesting insights: The theory contains the means to achieve a coarse-graining of the microscopic dynamics of systems that are generally intractable, thus allowing for their approximation statistically with arbitrary precision. We are now looking forward to applying this mathematical formalism to the solution of specific physical problems.

Selected Publications

[1] V. García Morales, “Origin of complexity and conditional predictability in cellular automata,” *Phys. Rev. E*, vol. 88, no. 4, pp. 042814–042819, 2013.

[2] L. Schmidt, K. Schönleber, K. Krischer, and V. García Morales, “Coexistence of synchrony and incoherence in oscillatory media under nonlinear global coupling,” *Chaos*, to be published. arXiv:1312.3166v2 [nlin.CD]

More publications by this Focus Group can be found on page 130.



1 | (a)–(c) Transition to chimera states. Shown are snapshots of the spatial distribution for the real part of the complex order parameter Re (W) calculated from the complex Ginzburg-Landau equation with nonlinear global coupling. When changing the control parameter, two-phase clusters (a) lead through the subclustering of one of the phases to the formation of two-dimensional chimera states (c), with the stable coexistence of a homogeneous and strongly inhomogeneous and incoherent phase. In (d) the spatiotemporal evolution of Re (W) is shown for a 1D cut of the 2D sample. Perfectly synchronized motion coexists with asynchronous behavior, separated by a sharp boundary.

Publications

Publications

The number of scientific publications in high impact international journals, as well as contributions to conferences, is often used as a measure for the performance of an institute. The main goal of TUM-IAS is to initiate and support top-level research at TUM particularly in collaboration with selected guest scientists (Fellows), but further, to offer early-career scientists excellent conditions and an inspiring environment. The research topics are organized into Focus Groups; however the actual research is often performed in the laboratories of the TUM Host as well as in the Fellow's home institution. Therefore TUM-IAS does not always appear as author address in the publications. In such cases we asked the Hosts and Fellows to at least acknowledge TUM-IAS for supporting their work. In this Annual Report we present for the first time a nearly complete and quite impressive list of all the TUM-IAS-related publications of the past year. Quite a number of them have been published in high impact journals like *Science*, journals of the *Nature* family, *PNAS*, *PRL*, *Nano Letters*, *IEEE*, and so on. Some selected highlights are presented here.

PNAS PNAS

Five-vertex Archimedean surface
lanthanide-directed molecular se

David Écija[a,1], José I. Urgel[a], Anthoula C. Papageorgiou[a], Sushobhan Jo
Svetlana Klyatskaya[c], Mario Ruben[c,d], Sybille Fischer[a], Saranyan Vijaya
and Johannes V. Barth[a,1]

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Edited by Kenneth N. Raymond, University of California, Berkeley, CA, and approved March

The tessellation of the Euclidean plane by regular polygons has been contemplated since ancient times and presents intriguing aspects embracing mathematics, art, and crystallography. Significant efforts were devoted to engineer specific 2D interfacial tessellations at the molecular level, but periodic patterns with distinct five-vertex motifs remained elusive. Here, we report a direct scanning tunneling microscopy investigation on the cerium-directed assembly of linear polyphenyl molecular linkers with terminal carbonitrile groups on a smooth Ag(111) noble-metal surface. We demonstrate the spontaneous formation of fivefold Ce–ligand coordination motifs, which are planar and flexible, such that vertices connecting simultaneously trigonal and square polygons can be expressed. By tuning the concentration and the stoichiometric ratio of rare-earth metal centers to ligands, a hierarchic assembly with dodecameric units and a surface-confined metal–organic coordination network yielding the semiregular Archimedean snub square tiling could be fabricated.

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Global Change Biology

Global Change Biology (2014) 20, 170–182, doi: 10.1111/gcb.12360

Chilling outweighs photoperiod in preventing spring development

JULIA LAUBE*†, TIM H. SPARKS*†‡, NICOLE ESTRELLA*†, JOSEF HÖF
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München, Parkring 13, Garching-Hochbrück 85748, Germany

Abstract

It is well known that increased spring temperatures cause earlier onset dates of le
However, a temperature increase in winter may be associated with delayed develop
requirements are not fulfilled. Furthermore, photosensitivity is supposed to interfere
date, neither the relative importance nor possible interactions of these three factors have
we present a multispecies climate chamber experiment to test the effects of chilling
phenology of 36 woody species. Several hypotheses regarding their variation with spec

Global Change Biology

VOLUME 20
NUMBER 1
JANUARY 2014

- Influence of chilling and photoperiod on budburst
- Reconciling timber extraction with biodiversity conservation
- Forecasting the viability of sea turtle eggs
- Identifying threats and conservation priorities in the Great Plains

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Science Translational Medicine AAAS

RESEARCH ARTICLE

IMMUNOLOGY

TCR-Ligand k_{off} Rate Correlates with the Protective Capacity of Antigen-Specific CD8+ T Cells for Adoptive Transfer

Magdalena Nauerth,[1]* Bianca Weißbrich,[1]* Robert Knall,[1]* Tobias Franz,[1]
Georg Dössinger,[1] Jeannette Bet,[1,2] Paulina J. Paszkiewicz,[1,2] Lukas Pfeifer,[1]
Mario Bunse,[3,4] Wolfgang Uckert,[3,4] Rafaela Holtappels,[5] Dorothea Gillert-Marien,[5]
Michael Neuenhahn,[1,6,7] Angela Krackhardt,[6,8] Matthias J. Reddehase,[5,9]
Stanley R. Riddell,[2,10,11] Dirk H. Busch[1,2,6,7]†

Adoptive immunotherapy is a promising therapeuti
cancer. T cells within a certain range of high avidity
T cell receptor (TCR) transfer experiments indicate th
of the TCR. Unfortunately, rapid measurement of
veloped a technology where dissociation (k_{off}
complex (pMHC) molecules bound to surface-e
a highly reliable manner. A first evaluation of
T cell populations revealed unexpected differ
evaluated in clinical trials for efficacy in adop

the treatment of chronic infections and
d are believed to be most effective.
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nature COMMUNICATIONS

ARTICLE

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DOI: 10.1038/ncomms3931

Lasing from individual GaAs-AlGaAs core-shell nanowires up to room temperature

Benedikt Mayer[1], Daniel Rudolph[1], Joscha Schnell[1], Stefanie Morkötter[1], Julia Winnerl[1], Julian Treu[1], Kai Müller[1], Gregor Bracher[1], Gerhard Abstreiter[1,2], Gregor Koblmüller[1] & Jonathan J. Finley[1]

Semiconductor nanowires are widely considered to be the next frontier in the drive towards ultra-small, highly efficient coherent light sources. While NW lasers in the visible and ultraviolet have been widely demonstrated, the major role of surface and Auger recombination has hindered their development in the near infrared. Here we report infrared lasing up to room temperature from individual core-shell GaAs-AlGaAs nanowires. When subject to pulsed optical excitation, NWs exhibit lasing, characterized by single-mode emission at 10 K with a linewidth <60 GHz. The major role of non-radiative surface recombination is obviated by the presence of an AlGaAs shell around the GaAs-active region. Remarkably low threshold pump power densities down to ~ 760 W cm^{-2} are observed at 10 K, with a characteristic temperature of $T_0 = 109 \pm 12$ K and lasing operation up to room temperature. Our results show that, by carefully designing the materials properties, high performance infrared

e tessellation
elf-assembly

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8, 2013 (received for review December 28, 2012)

rfering laser beams, conceived to specifically address
tiling problem, yielded a distorted, 2D Archimedean-
ecture (24).
ast decade, the tools of supramolecular chemistry on
ve provided new ways to engineer a diversity of sur-
ed molecular architectures, mainly exploiting molecular
n of functional organic species or the metal-directed
f molecular linkers (5). Self-assembly protocols have
oped to achieve regular surface tessellations, includ-
niregular Kagomé lattice (11–13), and even more
ing patterns or surface decorations (25–30). Despite
advances, five-vertex structures remain a challenging
ting the lack of adequate complementary polygonal
modules and planar fivefold coordination nodes,
.
introduce an approach toward complex surface tes-
y the combination of rare earth metal centers with
r molecular linkers on a smooth Ag(111) substrate.

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Engineering Sciences

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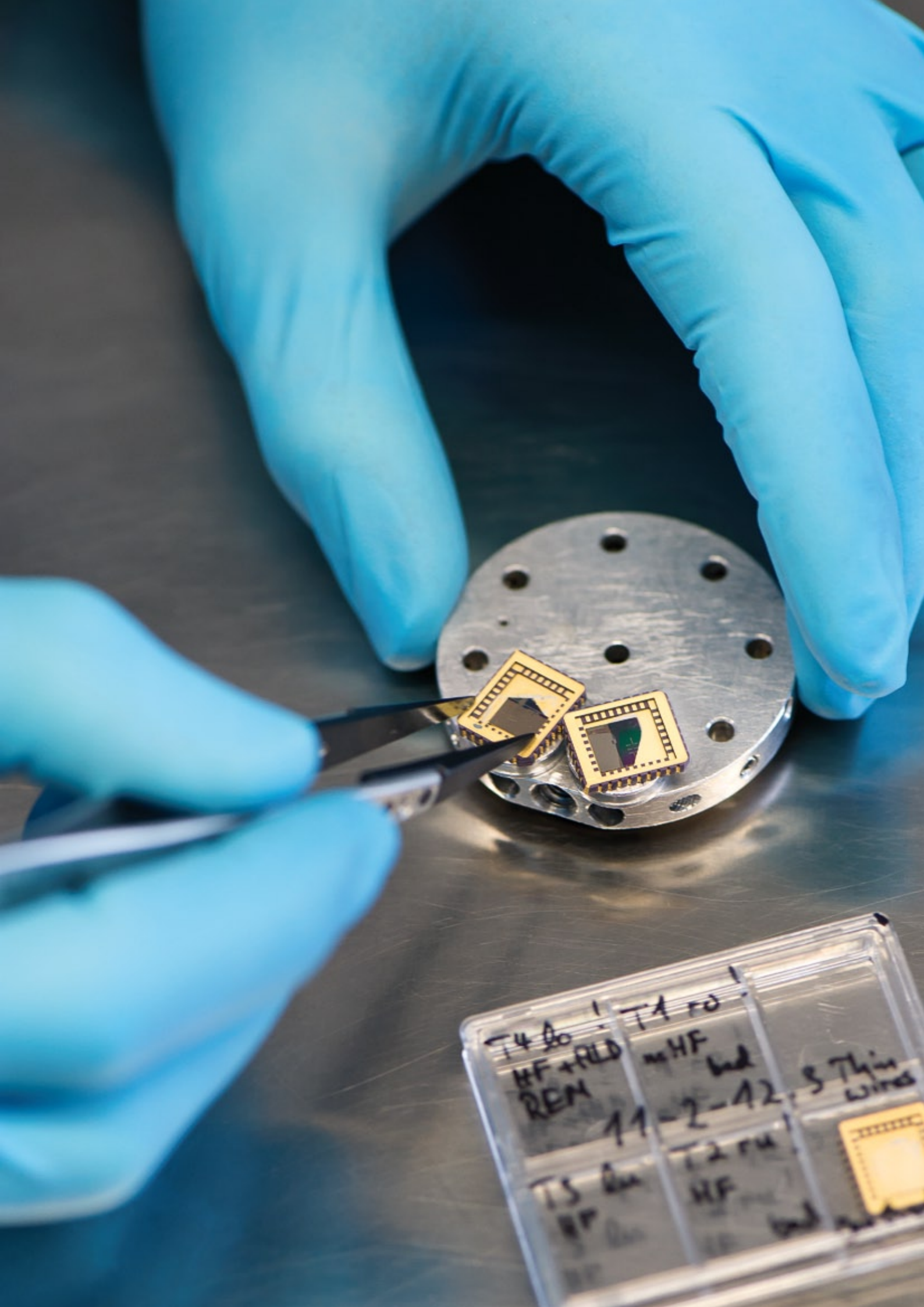
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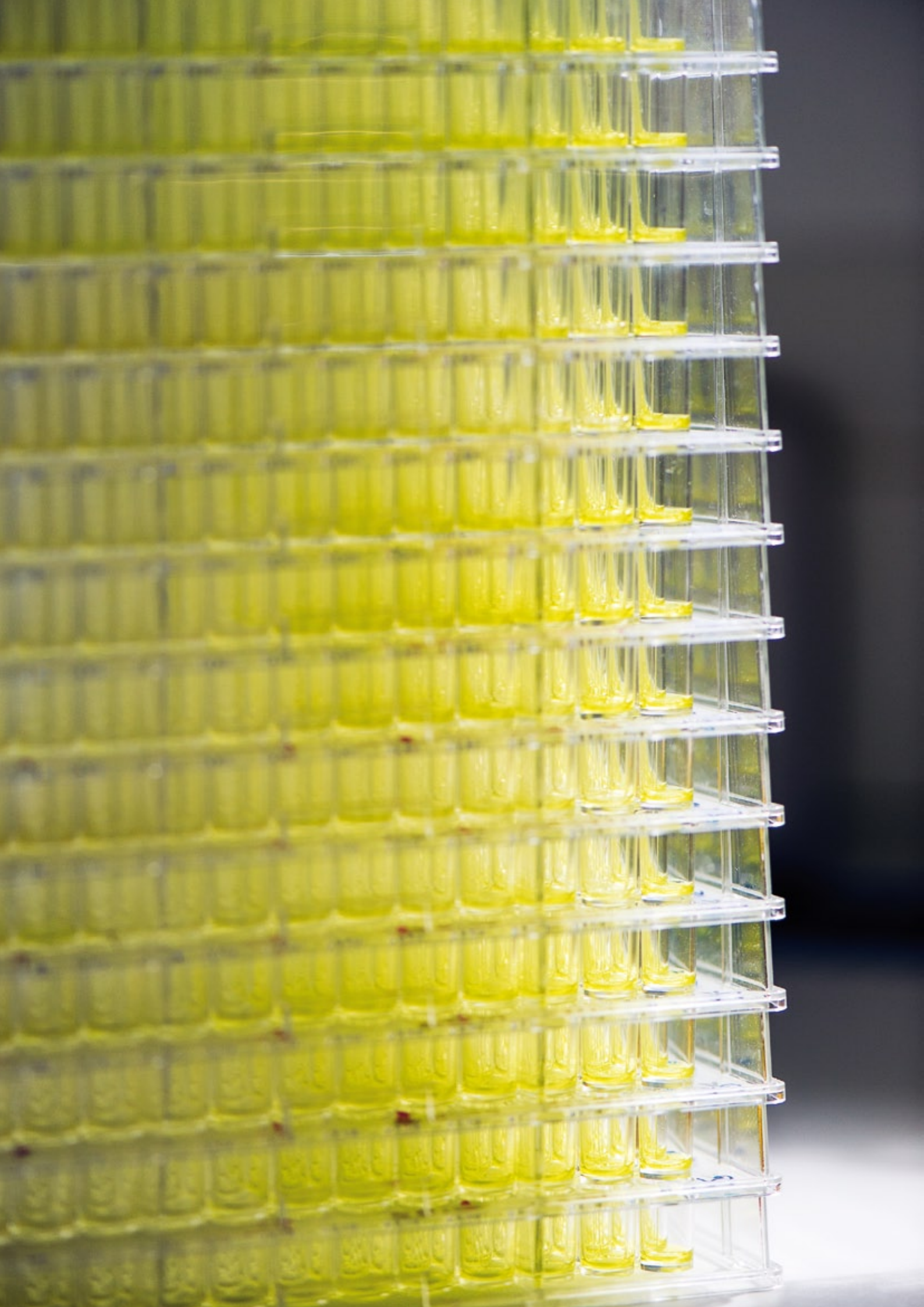
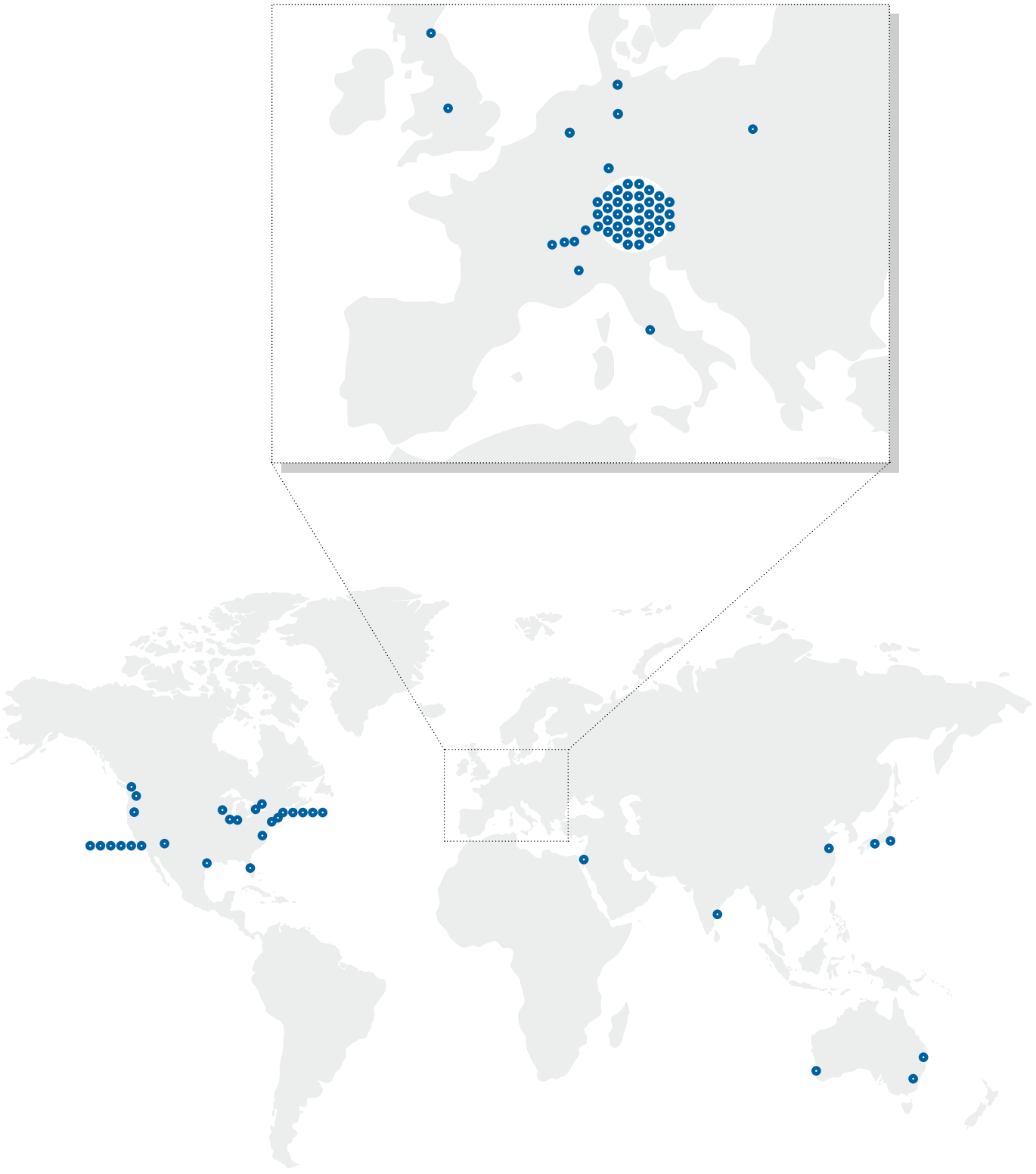
Facts and Figures



Where do the TUM-IAS Fellows come from?



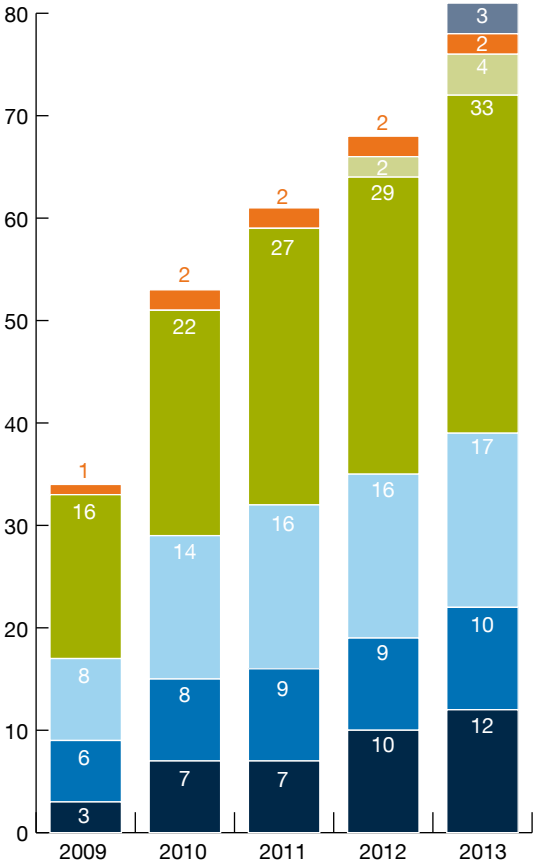
Fellow Distribution

In 2013, TUM-IAS has appointed 13 new Fellows in total: a Carl von Linde Senior and – for the last time - a Carl von Linde Junior Fellow, four Hans Fischer Senior and two Hans Fischer Fellows, two Rudolf Diesel Industry Fellows and three Rudolf Mößbauer Tenure Track Professors.

The new Fellows add to TUM-IAS's already diverse and interdisciplinary nature: The number of early-career scientists as well as researchers from industry has visibly increased, but the chart shows that TUM-IAS also continues to be a popular host to excellent experienced scientists from all over the world as well as from TUM.

While the engineering sciences are still going strong, the Fellows from the natural sciences have caught up, now amounting to more than a third of the total number's of Fellows. About a fifth comes from Life Sciences and Medicine, which strengthens the TUM-IAS's connection to the university hospital and the Weihenstephan campus. In total, nine of TUM's 13 faculties are currently involved with TUM-IAS by hosting at least one Fellow.

Total Number of Fellows and Alumni Fellows



Hans Fischer Tenure Track Professors

Hans Fischer Fellows

Hans Fischer Senior Fellows

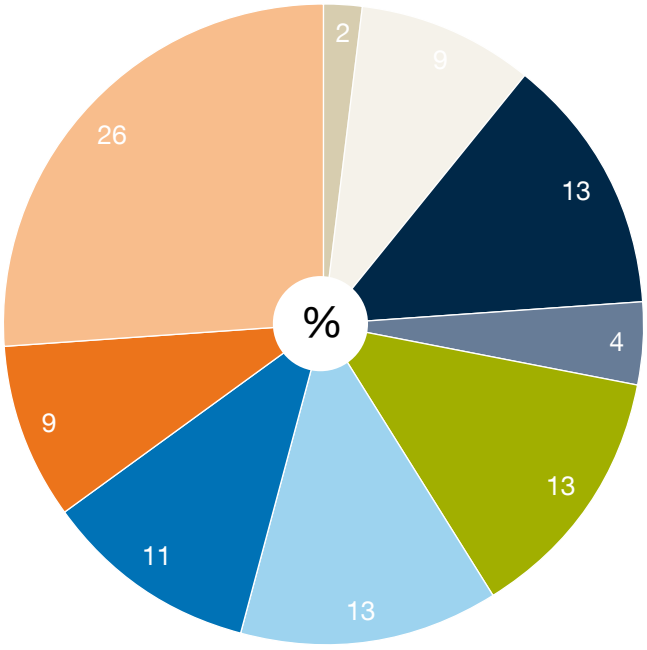
Carl von Linde Junior Fellows

Carl von Linde Senior Fellows

Rudolf Diesel Industry Fellows

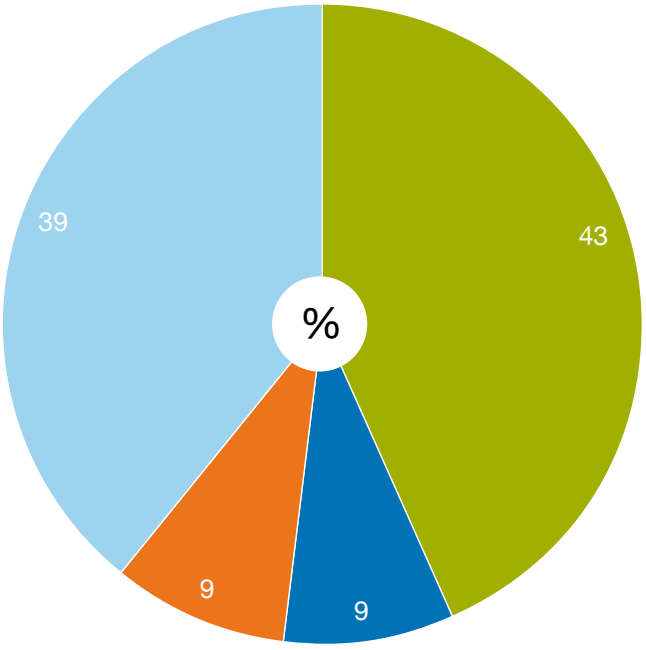
Rudolf Mößbauer Tenure Track Professors

Distribution of Active Fellows According to Faculties



- Architecture
- Center of Life and Food Sciences Weihenstephan
- Chemistry
- Civil, Geo and Environmental Engineering
- Electrical Engineering and Information Technology
- Informatics
- Mechanical Engineering
- Medicine
- Physics

Distribution According to Main Scientific Fields

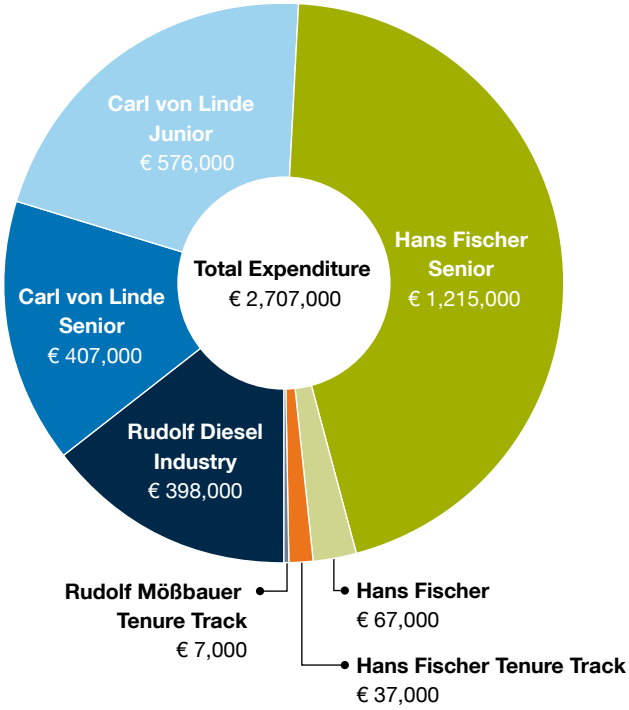


- Engineering
- Life Sciences
- Medicine
- Natural Sciences

Finances

In this section we present a brief survey of the financial data of TUM-IAS. The expenditures of TUM-IAS are covered by the “third funding line” of the German Excellence Initiative as well as the European Union Seventh Framework Program (Marie Curie COFUND).

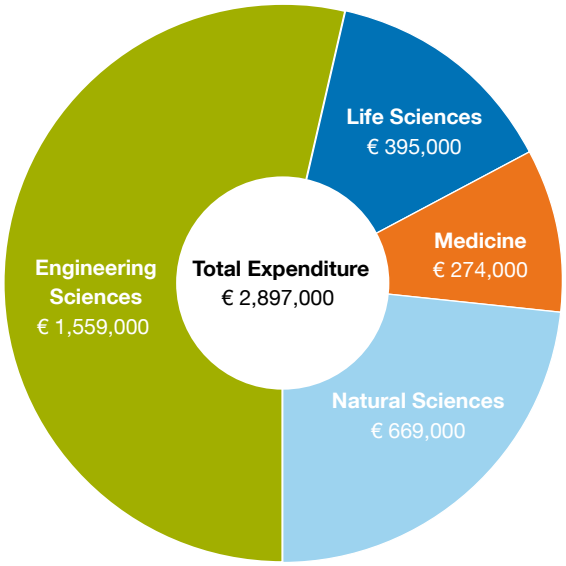
Expenditures per Fellowship Category in 2013



This chart illustrates expenditure in 2013 for each Fellowship category. Most dominant in terms of costs – with 45% of the total expenditure – is the Hans Fischer Senior Fellowship; these Fellowships are an integral part of the TUM internationalization strategy and are immensely valuable in terms of the exchange of complementary expertise and the grooming of emerging fields. Continuing on, expenditure for the Rudolf Diesel Industry Fellowship underwent approximately no change this year, as the recent recipients are fully active and operational, with stable funding, and have been for some time.

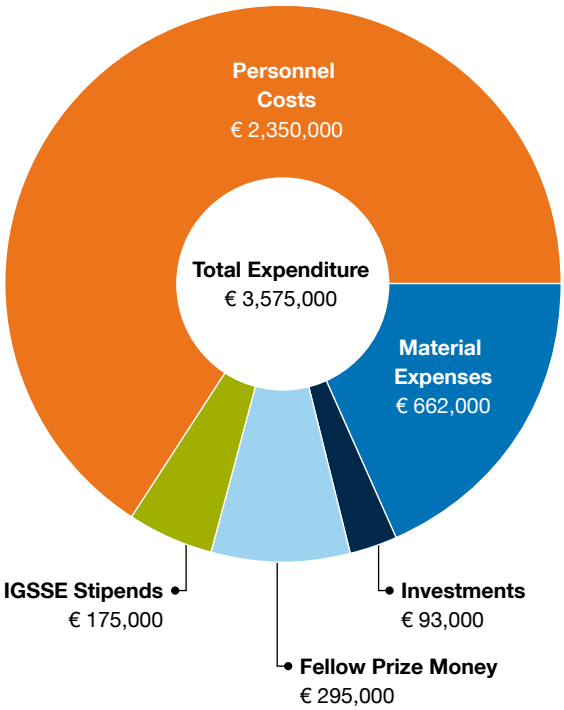
In contrast, the Carl von Linde Senior Fellowship category received less than before, the primary reason being that in 2010, it was established that only one of these Fellowships was to be awarded per year. Likewise, expenditure for the Carl von Linde Junior Fellowships also decreased this year, as a number of Fellows terminated their tenure in 2012; further the new Rudolf Mößbauer Tenure Track Professorship was established in 2013, replacing the Carl von Linde Junior Fellowship. TUM-IAS’s goal with regards to this new Professorship is the funding of outstanding, high-potential early-career scientists who have the ambition of developing a new field of endeavor when joining as Tenure Track Assistant Professors.

Expenditures per Main Scientific Field in 2013



This chart shows the expenditure of the TUM-IAS 'Fellowships grouped into the TUM scientific fields, as well as the expenditures from the Start-up and Visiting Fellowship programs, also according to scientific fields. Interdisciplinary projects were classed according to their most dominant field. As last year, engineering is the most strongly represented field in terms of costs, with more than half of the total expenditure. The remaining 50% is divided between life sciences, medicine, and natural sciences. Expenditure per main scientific field is virtually identical to the distribution of Fellows according to the same divisions (see page 137).

Total Expenditures in 2013



On this chart, total expenditure of TUM-IAS is displayed, including Fellowships, Start-up funding, Visiting Fellowships, events, and management. Total expenditure decreased in 2013 as fewer Fellows were nominated in 2012 because of the transition phase between Excellence Initiatives I and II.

Finally, it has become a policy of the Institute to offer working contracts to doctoral candidates instead of stipends, and this is reflected in an increase in personnel costs and a decrease in IGSSE stipends.

4, 5, 11 (Abstreiter, Hofmann, Steinberger, Fischer, Jelinek), 48, 68, 70, 72 (Hegland, Mehl), 74 (Friebe), 78, 82, 84, 86, 88, 90, 92, 94 (Misgeld), 100, 131, 134: A. Eckert.

8, 11 (Sturm, Schmid), 12, 24, 25, 58, 60 (Lee), 62 (Peer), 63, 94 (Konnerth), 96 (Kuhn), 102 (Hirata), 110, 112, 114: A. Heddergott.

76 (Werthmann), 106 (Kessler): facesbyfrank.

27, 28, 29 (photographs), 36 (photographs), 38 (photographs ”Tag der offenen Tür“): TUM-IAS.

29 (Poster), 33, 34, 35 (Science and Society), 39: J. Rousset.

38 (banner „Tag der offenen Tür“), 66 (figure 1), 67: TUM.

85, 119 (cover Global Change Biology): J. Laube, T. Sparks, N. Estrella, J. Höfler, D. Ankerst, and A. Menzel, “Chilling outweighs photoperiod in preventing precocious spring development,” *Global Change Biology*, vol. 20, no. 1, pp. 170–182, 2014 (reproduced with permission of the journal).

31: B. Steinbüchler.

36 (top center): S. Matich (WSI-ZNN, TUM) and R. Hoffmann (NIM); (bottom left): J. I. Urgel, D. Écija, W. Auwärter, and J. V. Barth (Molecular Nanoscience and Chemical Physics of Interfaces, TUM); (bottom center): P. Fernandez and A. R. Bausch (Molecular and Cellular Biophysics, TUM); (bottom right): D. Baierl, M. Schmidt, G. Scarpa, and P. Lugli (Nanoelectronics, TUM/NIM).

43–45: J. Peisl.

52 (figure 1): Focus Group Advanced Computation.

54 (figure 1): Focus Group Advanced Cardiacs Emulator.

54 (figure 2): T. Studeny (Computational Mechanics, TUM); (figure 3): J. Hörmann (Computational Mechanics, TUM); (figure 3): S. Heyden (Caltech).

60 (figure 1): S. An and D. Lee, “Prioritized Inverse Kinematics using QR and Cholesky Decompositions,” in *IEEE International Conference on Robotics and Automation (ICRA)*, 2014, accepted.

61 (figure 2): K. Hu, C. Ott, and D. Lee, “Online Human Walking Imitation in Task and Joint Space based on Quadratic Programming,” in IEEE Int. Conf. on Robotics and Automation (ICRA), 2014, accepted.

63 (figure 2): MOBOT.

64 (Braungart): E. Stenhuys.

65 (figure 2): M. Kulik (Energy Efficient and Sustainable Design and Building, TUM).

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69 (figure 1): W. Betz, C.M. Mok, I. Papaioannou, and D. Straub, “Bayesian Model Calibration using Structural Reliability Methods: Application to the simple hydrological abc model,” *Proc. 2nd Int. Conf. on Vulnerability and Risk Analysis and Management*, Liverpool, 2014, to be published; (figure 2): Google Earth.

73: C. Kowitz (Scientific Computing, TUM).

74 (figures 1–2): Focus Group Intra-Operative Therapy.

75: Focus Group Intra-Operative Therapy and KAIST.

76 (figure 1): J. C. Hannemann.

77: R. Guin.

87: Focus Group Soil Science.

93: S. Aime (University of Turin).

95: M. Leischner-Brill (Neuroscience, TUM).

96 (figure 1)/97 (figure 2): Focus Group Proteomics.

102 (figure 1): Focus Group Advanced Construction Chemicals and Materials.

103 (Arnold): The University of Edinburgh.

105: F. Hagn (Harvard Medical School).

106 (figure 1)/107: 2013 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

113 (figure 2): adapted from S. Joshi, F. Bischoff, R. Koitz, D. Ecija, K. Seufert, A. P. Seitsonen, J. Hutter, K. Diller, J. I. Urgel, H. Sachdev, J. V. Barth, and W. Auwärter, “Control of molecular organization and energy level alignment by an electronically nanopatterned boron nitride template,” *ACS Nano*, vol. 8, no. 1, pp. 430–442, 2014.

115: L. Schmid.

118: D. Ecija, J. I. Urgel, A. C. Papageorgiou, S. Joshi, W. Auwärter, S. Klyatskaya, M. Ruben, S. Fischer, S. Vijayaraghavan, J. Reichert, and J. V. Barth, “Five-vertex Archimedean surface tessalation by lanthanide directed molecular self-assembly,” *PNAS*, vol. 110, no. 17, pp. 6678–6681, 2013.

119 (top): J. Laube, T. Sparks, N. Estrella, J. Höfler, D. Ankerst, and A. Menzel, “Chilling outweighs photoperiod in preventing precocious spring development,” *Glob. Change Biol.*, vol. 20, no. 1, pp. 170–182, 2014. doi: 10.1111/gcb.12360; (center): M. Nauerth, B. Weißbrich, R. Knall, T. Franz, G. Dössinger, J. Bet, P. J. Paszkiewicz, L. Pfeifer, M. Bunse, W. Uckert, R. Holtappels, D. Gillert-Marien, M. Neuenhahn, A. Krackhardt, M. J. Reddehase, S. R. Riddell, and D. H. Busch, “TCR-ligand koff rate correlates with the protective capacity of antigen-specific CD8+ T cells for adoptive transfer,” *Sci. Transl. Med.*, vol. 5, no. 192, pp. 192ra87, 2013; bottom: D. Rudolph, L. Schweickert, S. Morkötter, L. Hanschke, S. Hertenberger, M. Bichler, G. Koblmüller, G. Abstreiter, and J. J. Finley, “Probing the trapping and thermal activation dynamics of excitons at single twin defects in GaAs–AlGaAs core–shell nanowires,” in *New J. Phys.*, vol. 15, pp. 113032/1-13, 2013.

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Self-organisation at the nanometer-scale: Filaments of cellular cytoskeletons with diameters of a few nanometers ordered in circles.
V. Schaller and A. R. Bausch (TUM Physics Department and Nanosystems Initiative Munich), PNAS (2011) 108. 19183–19188.

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