JARA | HPC

Picture: Conor Crowe

ANNUAL REPORT 2016

AN INITIATIVE OF

RWTH AACHEN UNIVERSITY

JÜLICH FORSCHUNGSZENTRUM

GLOSSAR

- **CSG** .... Cross-Sectional Group
- **CSG ImVis** .... Cross-Sectional Group "Immersive Visualization"
- **CSG ParE** .... Cross-Sectional Group "Parallel Efficiency"
- **RWTH** .... RWTH Aachen University
- **FZ Jülich** .... Forschungszentrum Jülich
- **HPC** .... High Performance Computing
- **JSC** .... Jülich Supercomputing Centre
- **SimLab** .... Simulation Laboratory
- **SimLab ab initio** .... Simulation Laboratory "ab initio Methods in Chemistry and Physics"
- **SimLab FSE** .... Simulation Laboratory "Highly Scalable Fluids & Solids Engineering"
- **SLNS** .... Simulation Lab Neuroscience

ANNUAL REPORT 2016

CONTENT

JARA-HPC MEMBERS

Prof. Marek Behr, Ph.D.	RWTH
Prof. Stefan Blügel	FZ Jülich
Prof. Dirk Bosbach	FZ Jülich
Prof. Paolo Carloni	FZ Jülich
Prof. Christoph Clauser	RWTH
Prof. Markus Diesmann	FZ Jülich
Prof. David DiVincenzo	RWTH
Prof. Richard Dronskowski	RWTH
Prof. Gerhard Gompper	FZ Jülich
Prof. Peter Jeschke	RWTH
Prof. Erik Koch	FZ Jülich
Prof. Torsten W. Kuhlen	RWTH
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Prof. Arne Lüchow	RWTH
Prof. Manfred Martin	RWTH
Prof. Riccardo Mazzarello	RWTH
Prof. Ulf-G. Meißner	FZ Jülich
Prof. Abigail Morrison	FZ Jülich
Prof. Matthias Müller	RWTH
Prof. Uwe Naumann	RWTH
Prof. Hermann Ney	RWTH
Prof. Herbert Olivier	RWTH
Prof. Eva Pavarini	FZ Jülich
Prof. Stefan Pischinger	RWTH
Prof. Heinz Pitsch	RWTH
Prof. Uwe Rau	FZ Jülich
Prof. Arnold Reusken	RWTH
Prof. Martin Riese	FZ Jülich
Prof. James Ritman	FZ Jülich
Prof. Stefan Schael	RWTH
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Prof. Ulrich Schwaneberg	RWTH
Prof. Bob Svendsen	RWTH
Prof. Harry Vereecken	FZ Jülich
Prof. Andreas Wahner	FZ Jülich
Prof. Stefan Wessel, Ph.D.	RWTH
Prof. Wolfgang Wiechert	FZ Jülich
Prof. Dieter Willbold	FZ Jülich
Prof. Manfred Wirsum	RWTH
Prof. Matthias Wuttig	RWTH

2016

1. JARA-HPC IN HEADLINES

JAN

> DR. BERND MOHR TO CHAIR SC17

Dr. Bernd Mohr from the JSC has been elected General Chair of the SC17 Conference in Denver. This is the first time that a computer scientist from outside the USA will chair the most important conference for high-performance computing.

SC17 General Chair Bernd Mohr introduced the theme of the upcoming conference with these words:

"One connection can change your life. Our community is making millions of connections every day: by bringing together people at workshops, conferences, in research teams and projects, by connecting extreme-scale supercomputers to instruments and visualization and data analytics systems, by inspiring collaborations between different fields of science and all with the goal of making the greatest impact on society and changing our world.

I invite you to continue on this journey of creating meaningful connections at SC17."

FEB

> RWTH INNOVATION AWARD FOR JARA-HPC MEMBER PROF. RICHARD DRONSKOWSKI

RWTH and FZ Jülich presented this year's RWTH Innovation Award. The prize honors outstanding projects at RWTH and FZ Jülich demonstrating promising innovation potential. First place, receiving 5,000 € in prize money, went to the CarboBat team headed by Prof. Richard Dronskowski (2nd from left in the picture), JARA-HPC member and member of the Steering Board for the SimLab "ab initio Methods in Chemistry and Physics".

Prof. Richard Dronskowski's team, working in close collaboration with FZ Jülich and the University of Montepellier, utilizes a novel class of materials of inorganic compounds, so-called carbodiimides, as anodes in rechargeable batteries. The technology makes it possible to produce highly powerful, cost-efficient, and non-toxic batteries.

FEB

> NEW MEMBER FOR THE JARA-HPC VERGABEGREMIUM

Since February 2016, Prof. Dr.-Ing. Heinz Pitsch from the Institute for Combustion Technology at RWTH (ITV), heads the JARA-HPC Vergabegremium (VGG) together with Prof. Dr. Gerhard Gompper.

The VGG determines detailed scientific and technical criteria for the assessment of proposals for computing time on the JARA-HPC Partition.

APR

> ERC GRANTS FOR JARA-HPC MEMBERS

On April 07, 2016, two JARA-HPC members received the Advanced Grants of the European Research Council (ERC): Prof. Heinz Pitsch, director of the Institute for Combustion Technology at RWTH and Prof. Hermann Ney, head of the Chair of Computer Science 6, are funded for their outstanding research for a maximum of five years.

The grants are considered one of the most prestigious funding instruments in Europe.

Prof. Heinz Pitsch

Prof. Hermann Ney

JUN

> JARA-HPC AT "OPEN DAY 2016 - 60 YEARS – RESEARCH AT THE CENTRE"

On June 05, 2016, almost 16.000 visitors of all ages had the opportunity to explore the campus of the FZ Jülich in marvelous sunshine, got a taste of research, and talked to the scientists. The institutes offered their visitors a glimpse into the world of supercomputers, electron microscopes, plants, proteins, molecules, and atoms.

"Past, Present, Future" was this year's motto for the Open Day. In the foyer of the lecture theatre of the Central Library, we looked back on the history and also at the current research and the research issues of the future.

JUN > JARA-HPC AT ISC 2016

From June 19 - 23, 2016, the International Supercomputing Conference (ISC), one of the biggest and most important events regarding HPC, took place once again in Frankfurt, Germany. At their booth, JARA-HPC's scientists presented current research activities like the In-Situ Visualization of Multiphase Jet Simulations. Furthermore, they showcased recent developments in the OpenMP standard and demonstrated their "Marmot Umpire Scalable Tool" (MUST), a correctness checker for parallel programs.

OCT > FIRST JARA-HPC SYMPOSIUM "JHPCS'16"

On October 04 and 05, 2016, JARA-HPC's scientists invited many local and international guests to the IT Center at RWTH for the first JARA-HPC Symposium JHPCS. First-class speakers from Germany, the US, Korea, Japan, France, Belgium, and the atten-dees looked especially forward to the Keynote by Victor Eijkhout from the Texas Advanced Supercomputing Center who talked about parallel programming for the 21st Century.

About 70 guests attended the six sessions and two Mini-Workshops with a total of 27 talks concerning various topics regarding HPC.

The Symposium aimed at providing a platform for discussions on the various aspects of the development of HPC applications between experts and young scientists from different research fields who make use of HPC in their daily work.

The symposium was concluded with a panel discussion on the topic 'Scaling applications: In-house development or cross-disciplinary work?'. Prof. Matthias Müller, deputy Director of JARA-HPC and Head of the IT Center at RWTH moderated the animated discussion. "It was interesting to see that all the panelists participated in such a lively exchange", he said afterwards.

Especially the different points of view of the attendees contributed to the success of the discussion. The mix of HPC-users from different fields of research, computer scientists, and a representative of the industry made sure the panel discussion was entertaining and effective.

Marie-Christine Sawley, manager for Intel at the ECR Lab Paris thanked the attendees for their numerous valuable contributions during the discussion. "They give me important clues on improving the cooperation between industry and science."

The next JARA-HPC Symposium will probably take place in 2018. The symposium's revised papers were published in March 2017 as a post-proceedings volume by the Springer Verlag in the prestigious LNCS (Lecture Notes in Computer Science).

OCT

> JARA-FORUM 05 „CAREER PATHS MADE BY JARA – CHANCES IN BRAIN RESEARCH AND DATA ANALYSIS"

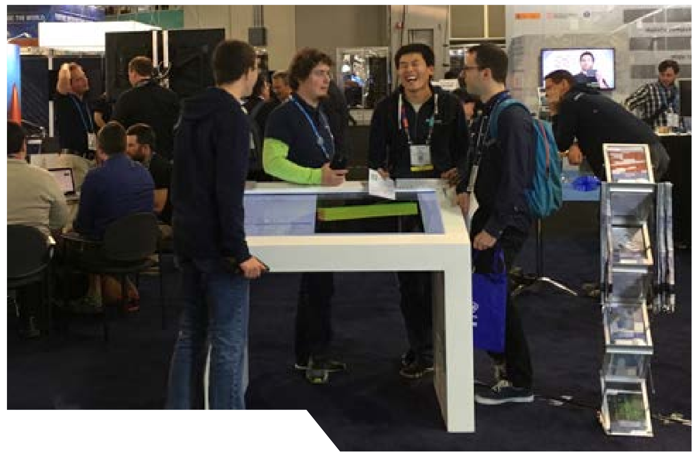
On October 18, 2016, for the fifth time the JARA FORUM 05 took place at the Representation of North Rhine-Westphalia in Berlin.

About 180 listeners from politics, academia, research and the public followed the presentations of the high-profile young speakers about their scientific work and latest research in the JARA-BRAIN and JARA-FIT sections.
They also gave information and showed prospects JARA can offer to young scientists.
Ralf Krauter, journalist at the "Deutschlandfunk", moderated the event.

NOV

> JARA-HPC AT SC16

From November 13 - 18, 2016, the "International Conference for High Performance Computing, Networking, Storage, and Analysis" (SC16) took place in Salt Lake City, USA. Scientists from RWTH and JARA-HPC participated in the conference, lead tutorials and also presented their current research at the JSC booth in the exhibition hall.



NOV > CLAIX – NEW HPC INFRASTRUCTURE AT RWTH

In November 2016 the RWTH Compute Cluster was replaced by the new compute cluster "CLAIX" in two stages. All computing nodes will continue to be equipped with processors of the x86_64 architecture and be operated under Linux. Because of the higher compute capacity of the new processors, more than 400 TFLops will be available for users of the JARA-HPC Partition after the installation of the first stage of CLAIX.
(see chapter 2.3 for detailed information on "CLAIX")

2. SCIENTIFIC WORK IN JARA-HPC

> 2.1. General overview

Scientists from JARA, and especially the section High-Performance Computing (JARA-HPC), unite the specialist know-how of highly parallel computing on supercomputers with the respective special knowledge of physicists, engineers, and other scientific researchers. In doing so they contribute considerably to making full use of the opportunities computer simulations offer to address current scientific issues.

JARA-HPC scientists are part of a unique organizational structure comprising so called Simulation Laboratories (SimLabs), Cross-Sectional Groups (CSGs), the JARA-HPC Partition and the Jülich Aachen Data Exchange (JADE).

> **JADE** aims at establishing a flexible and scalable data management tool that addresses the specific needs and requirement of domain scientists to exchange data in a convenient and efficient way.

> The **JARA-HPC Partition** consists of contingents of high-performance computers and supercomputers at RWTH (RWTH Compute Cluster / CLAIX) and FZ Jülich (JUQUEEN, JURECA) and provides researchers from Aachen and Jülich with local access to HPC resources on various architectures. (For detailed information on the Partition please see next chapter "The JARA-HPC Partition".)

> In the **SimLabs**, JARA-HPC addresses issues in interdisciplinary research and provides solutions with high scientific impact through the efficient use of high-end supercomputing resources. Since 2012, three SimLabs have been established:

- **SimLab "Highly Scalable Fluids and Solids Engineering"**
- **SimLab "Neuroscience"**
- **SimLab "ab initio Methods in Chemistry and Physics"**

> The **CSGs** comprise methodical activities that are relevant for the users of high-performance computers with utterly diverse scientific backgrounds. Currently two CSGs are established in the areas:

- **CSG "Immersive Visualization"**
  Development of algorithms for the immersive and interactive, as well as spatially distributed and cooperative visualization, and their application within the Vista software Framework.

- **CSG "Parallel Efficiency"**
  Development of algorithms for performance analysis and performance increase of parallel programs, and their application in tools such as Scalasca or SIONlib.

> 2.2. The JARA-HPC Partition

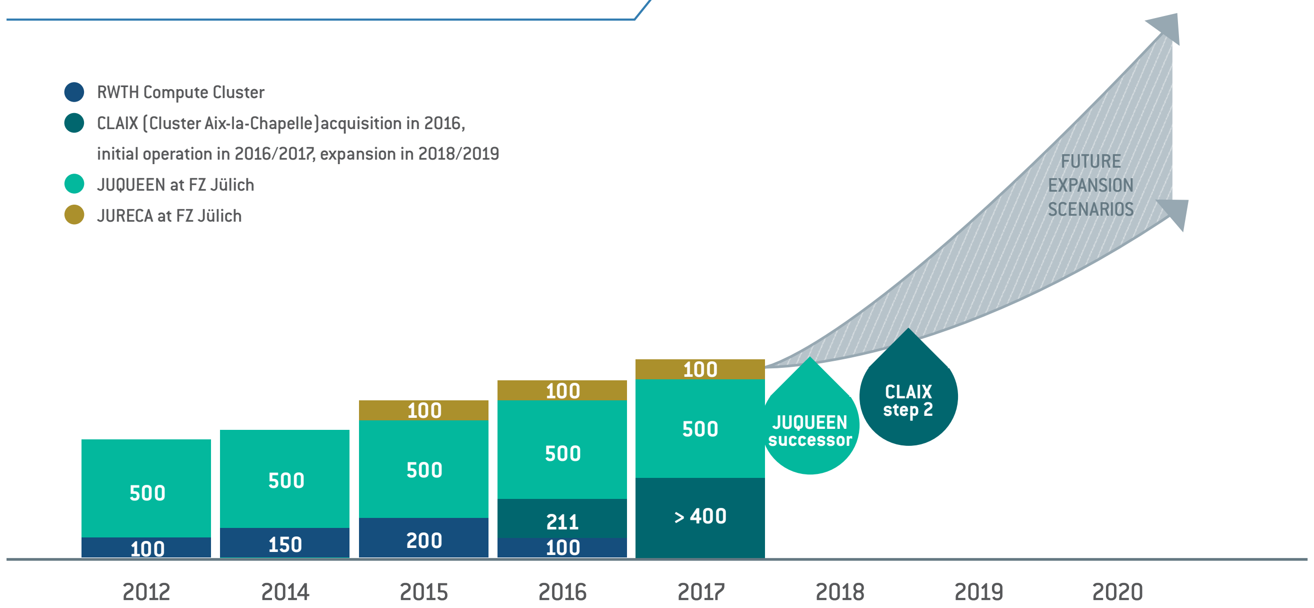
The JARA-HPC Partition is the merger of shares of HPC systems in Jülich and Aachen dedicated to researchers from FZ Jülich and RWTH. Main reasons to set up this Partition in 2012 were the guaranteed amount of computing time for projects from the two regional partners on latest HPC architectures, the reduced but highly efficient assignment procedure that fosters scientific excellence, and the requirements of the funding bodies BMBF and MIWF to arrange for larger and more efficiently used HPC infrastructures.

500 TFlops/s of the 5.9 PFlops/s IBM Blue Gene/Q JUQUEEN in Jülich and 100 TFlops/s of the 300 TFlops/s RWTH Compute Cluster formed the initial JARA-HPC Partition. Until end of 2015 the Partition has been extended due to the high demands for computing time. Aachen's part has been increased to 200 TFlops and Jülich has added 100 TFlop/s on the JUROPA cluster and, after its replacement, also 100 TFlop/s out of the 1.8 PFlop/s of the successor system JURECA.

RWTH and FZ Jülich have agreed to further increase computing capacities on the JARA-HPC Partition reciprocally in the future. Hence, in November 2016 Aachen's new high performance computer CLAIX has been made available to users of the JARA-HPC Partition. It will replace the Bull-Cluster installed in 2011. With 110 Mio core-hours Aachen's contribution to the JARA-HPC Partition will reach 400 TFlops/s, doubling the theoretical peak performance through the new processor architecture.

The accumulated computing capacity available on the JARA-HPC Partition for the exclusive use of Aachen's and Jülich's scientists in the JARA-HPC Partition exceeds 1 PFlops/s.

Composition of the JARA-HPC Partition (in TFlops)



Twice a year eligible scientists from the above mentioned institutions can submit applications for computing time on the Partition. The proposals undergo a scientific review by experienced researchers from the respective scientific fields, and a technical review with respect to their feasibility by HPC experts from the respective com¬puting centers. Based on these reviews, JARA-HPC Vergabegremium (VGG) finally decides in a comparative way about acceptance and volume of the computing time grants which are provided for one year periods. The VGG consists of the following scientists:

- Paul Gibbon / FZ Jülich
- Gerhard Gompper / FZ Jülich
- Gebhard Günther / FZ Jülich
- Robert Jones / FZ Jülich

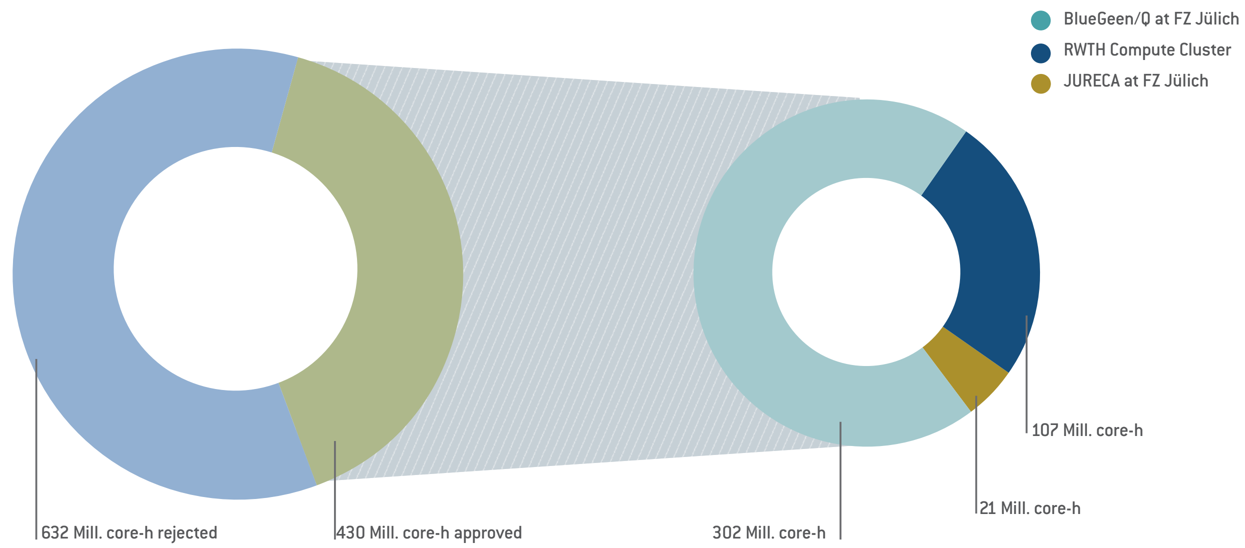
- Dieter an Mey / RWTH
- Paolo Bientinesi / RWTH
- Matthias Meinke / RWTH
- Heinz Pitsch / RWTH

All successful applicants are committed to submit reports on the project outcome and to deliver success stories that can be publicly promoted. Apart from applying for one-year standard quotas, applicants can also submit simplified proposals for trial quotas with a maximum duration of six months, supporting the porting and optimization of programs.

ALLOCATION

The allocation of computing time on the JARA-HPC Partition takes place twice per year, in April and in October, with computing time periods from May 01 to April 30, and from November 01 to October 30, respectively. On each occasion one half of the available computing time is allocated. Approximately, 55 million compute core-hours (core-h) on the RWTH system CLAIX, 145 million compute core-h on JUQUEEN, and 9 million compute core-h on JURECA are available for each compute time period.

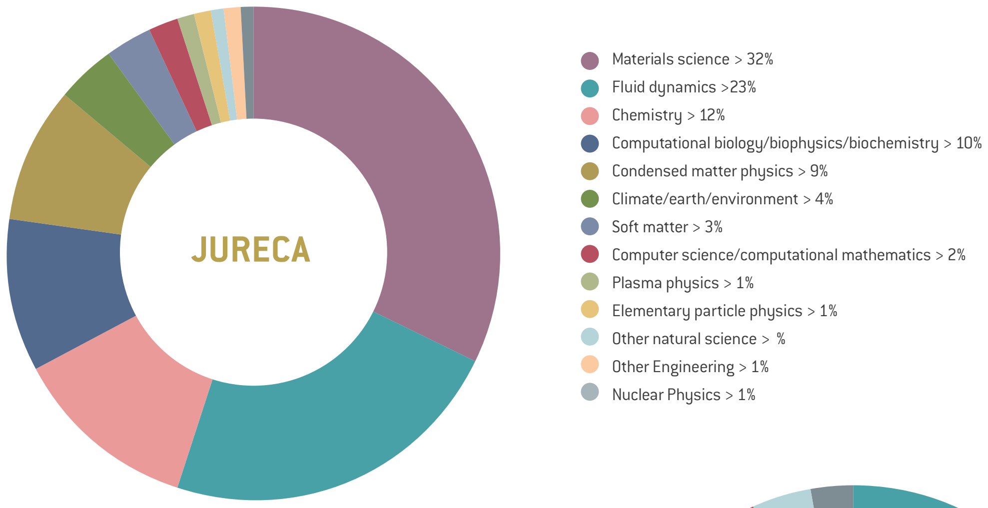
Allocation of computing time on the JARA-HPC Partition in 2016

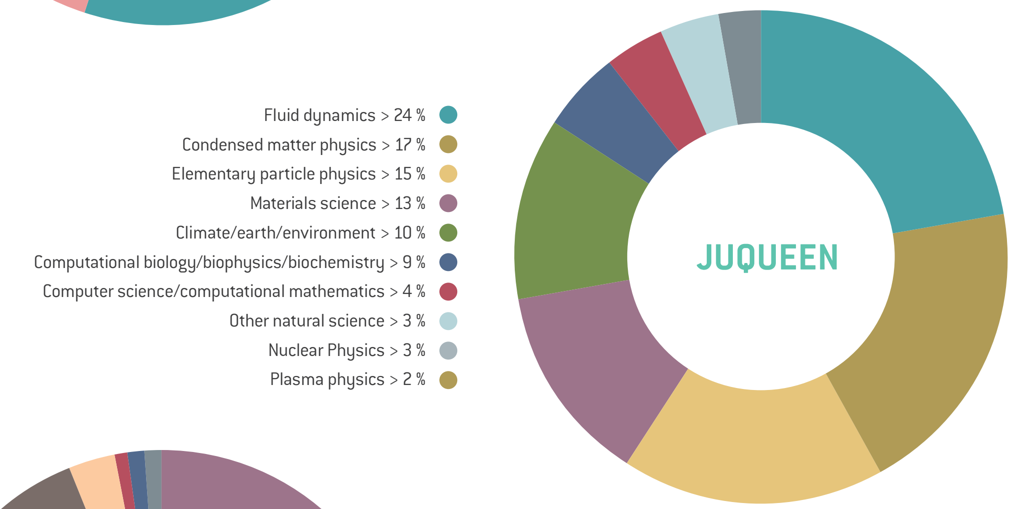


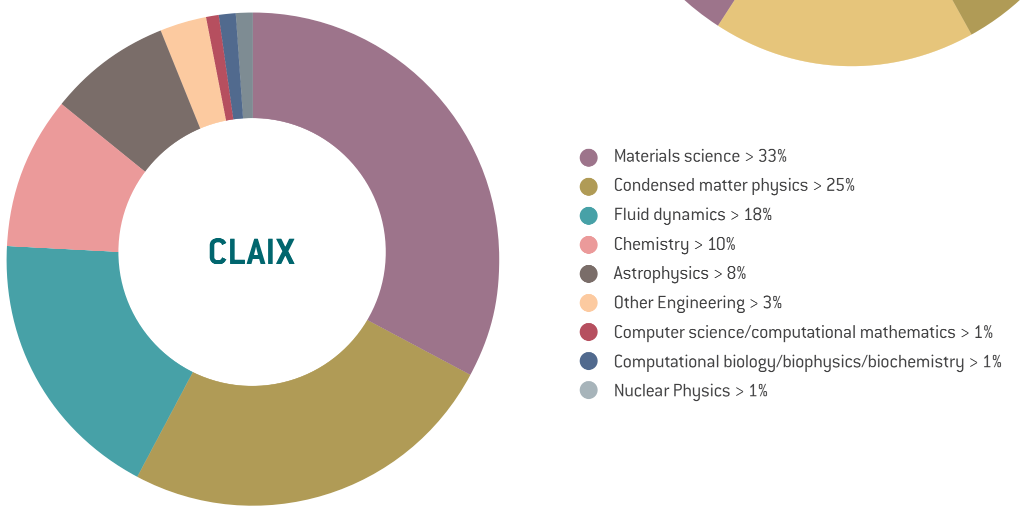
STATISTICS

In the two JARA-HPC calls of 2016 **174 proposals** were filed.
A total of **429 million core-h** have been approved which are distributed among the various research areas on the JUQUEEN and JURECA system and the RWTH Compute Cluster respectively as depicted in the following pie charts.

Distribution of research areas on the JARA-HPC Partition in 2016







In total, three fields of research account for 65% of the dedicated compute resources: Fluid dynamics, condensed matter physics, and materials science.

These fields of research also account for 55% of the number of accepted proposals.

Scientists from RWTH took the opportunity to heavily use not only the RWTH Compute Cluster but also the JUQUEEN in Jülich in the field of computational fluid dynamics, whereas scientists active in the area of condensed matter mainly from FZ Jülich use all three systems of the JARA-HPC Partition, showing that the new JURECA system was well received. This holds also for the field bio/life science, where the majority of the projects run on JURECA.

In materials science research groups from both locations are active on all three parts of the partition with a focus on the RWTH Compute Cluster and especially the JURECA System in Jülich.

Most research groups in elementary particle physics are located at FZ Jülich and employ the Jülich machinery, except for two, all research groups in chemistry remain on the Aachen machines.

This distribution of the users resembles the different characteristics of the three machines: the JUQUEEN offering very high scalability and the RWTH Compute Cluster and the JURECA system support large-memory applications with x86-compatibility. In consequence they complete each other in support of the wide range of computational sciences.

Contact:
Dr. Florian Janetzko, JSC, FZ Jülich
Dr. Christian Terboven, IT Center, RWTH

> 2.3. CLAIX – new HPC infrastructure at RWTH

In November 2016 the RWTH Compute Cluster was replaced by the new supercomputer CLAIX (Cluster Aix-la-Chapelle).

In a procurement system that emphasized the total-cost-of-ownership, the company NEC has been selected as the vendor of the new HPC system of RWTH. The system named CLAIX consists of two different node types, and over 90 % of the system's energy consumption is cooled by water. It started production in November 2016 and was ranked 309th in the corresponding Top500 list. Up to 80% of CLAIX are available within the JARA-HPC Partition.

CLAIX's main part comprises 625 dual-socket nodes with Intel Broadwell-EP processors, each with 12 cores and 2.2 GHz, and 128 GB main memory. The SMP section consists of eight nodes with 144 Intel Broadwell-EX cores and 1 TB main memory. Several nodes are equipped with two NVIDIA P100 (Pascal architecture) compute accelerators or local non-volatile memory devices. The Lustre-based parallel filesystem offers 3.3 PB of storage capacity and ZFS-based data integrity. The system interconnect is a 100 GigaBit/s Intel Omni-Path fabric.

RWTH and NEC agreed on a scientific collaboration to improve the efficiency and reliability of CLAIX and explore programming approaches for vector architectures.

Contact:
Dr. Christian Terboven, IT Center, RWTH

> 2.4. Simulation Laboratories (SimLabs)

2.4.1. SimLab "Highly Scalable Fluids & Solids Engineering" (SimLab FSE)

STEERING BOARD

Marek Behr / RWTH
Paul Gibbon / FZ Jülich
Wolfgang Schröder / RWTH

STAFF

Ole Baumeister / FZ Jülich
Metin Cakircali / FZ Jülich
Manuel Kosel / FZ Jülich
Andreas Lintermann / RWTH
Michael Schlottke-Lakemper / RWTH

> PROJECTS BEING SUPPORTED BY THE SIMLAB AND USING COMPUTING TIME ON THE JARA-HPC PARTITION:

>Simulation of the Flow and Fine-Dust Particle Deposition in the Human Respiratory System */ Lintermann*

Airborne fine dust particles like Diesel and coal aerosols are small and light enough to find their way through the human respiratory system during inspiration. Consequences of their deposition in the lung are coughing, allergic reactions, and even cancer. To investigate the particle deposition behavior, Computational Fluids Dynamics (CFD) methods using a coupled lattice-Boltzmann and Lagrange approach are applied in this study. $O(10^6)$ particles with varying sizes of 2.5-10μm and particle-to-air density ratios of 800-1300 are released at the left and right nostril and tracked down the airway. The simulation includes the nasal cavity, the pharynx, larynx, trachea, and the geometry of higher generations of the lung down to the bronchioles. By using the whole respiratory tract the filtering mechanism of the nasal cavity, the influence of the emerging jet in the larynx on the deposition likelihood in the trachea, and the deposition depth in the lung based on the particle size and density can be inferred to understand the cause of respiratory pathologies. To highly resolve the intricate flow in the human respiratory system it is necessary to simulate on computational meshes consisting of $O(10^9)$ cells. That is, to cover the small length scales of secondary flow structures in transitional flow regimes and to collect meaningful statistics a high resolution is necessary. Such an approach can only be followed by conducting the simulations on supercomputers like the JUQUEEN system at the JSC in Jülich, which offers the capability to massively parallelize the simulation problem to hundreds of thousands of CPUs and consequently reduces the overall simulation time.

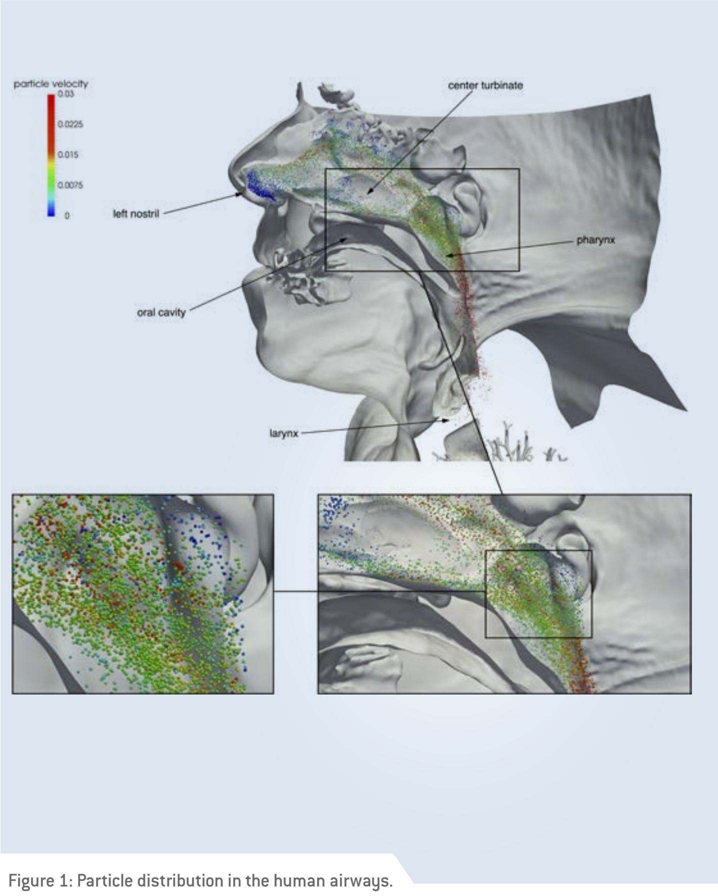
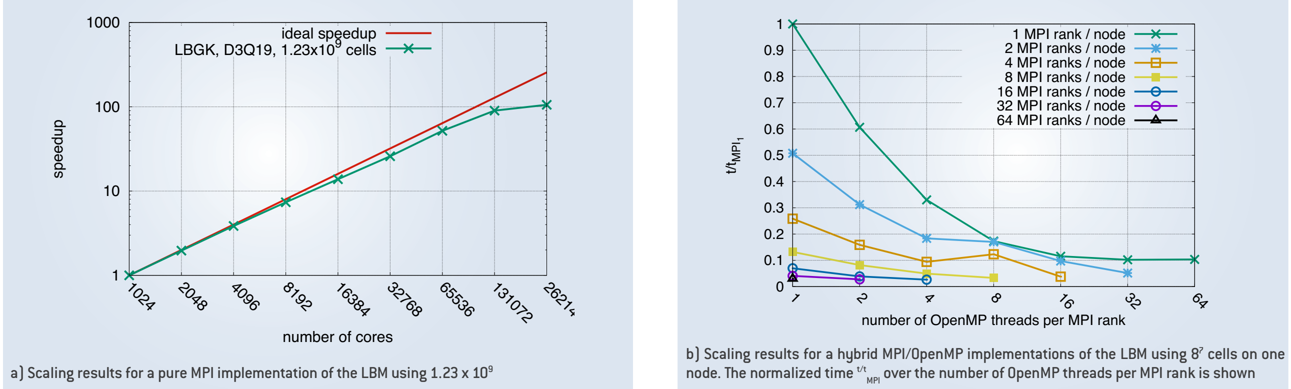


Figure 1: Particle distribution in the human airways.
The particles are colored by their velocity magnitude. The close-ups show the pharynx region in which the flows from the left and right nasal cavities mix.

JARA-HPC project with number: JHPC32



a) Scaling results for a pure MPI implementation of the LBM using 1.23 x 10^9

b) Scaling results for a hybrid MPI/OpenMP implementations of the LBM using 8^7 cells on one node. The normalized time $^{t/t}{}_{MPI}$ over the number of OpenMP threads per MPI rank is shown

Figure 2: Results of strong scaling experiments of the LBM on the JUQUEEN using different parallelization strategies.

>Development of Efficient Methods for Direct-Hybrid LES/ CAA Computations - JHPC23 */ Schlottke-Lakemper*

This project aims to predict the noise emissions of a jet engine using a new approach for scalable computational aeroacoustics (CAA). In classic hybrid computational fluid dynamics (CFD) CAA schemes, large volumes of source term data need to be transferred between the CFD and the CAA step, which is accomplished by storing the source information on disk. This poses a problem for large-scale simulations, as the required disk space for a single simulation reaches hundreds of terabytes, while the poor performance of the I/O subsystem in comparison to the CPUs slows down the overall computation. Therefore, a new direct-hybrid method is proposed and evaluated, in which both the flow and the acoustics simulations run simultaneously. That is, all data between the two solvers is transferred in-memory. Both solvers operate on a joint hierarchical Cartesian grid, which enables efficient parallelization and dynamic load balancing, and which inherently supports local mesh refinement. To demonstrate the capabilities of the new scheme, the flow-induced noise emissions of a turbulent, isothermal jet are predicted. The results show that the direct-hybrid method is able to accurately capture the sound pressure field and that it is particularly suitable for efficient, highly parallel simulations. Furthermore, in comparison to the classic hybrid method with data exchange via disk I/O, the novel approach shows superior performance when scaling to thousands of cores.

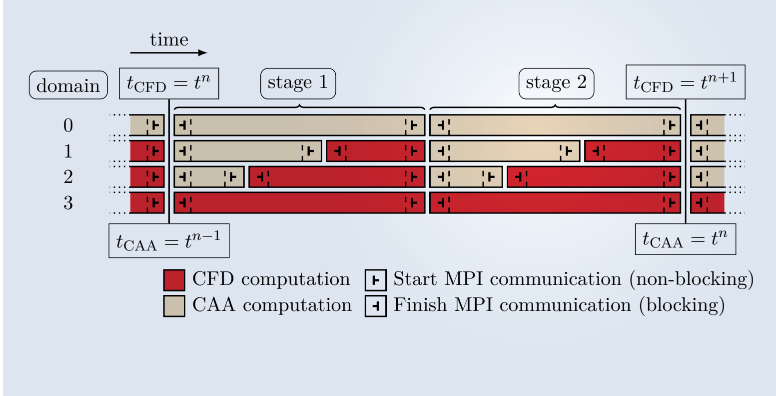


Figure 3: Time line for the direct-hybrid method on multiple domains. Each row represents a different MPI domain. A two-stage scheme is used for both the CFD and the CAA part, highlighting the interleaved execution of the solver stages.

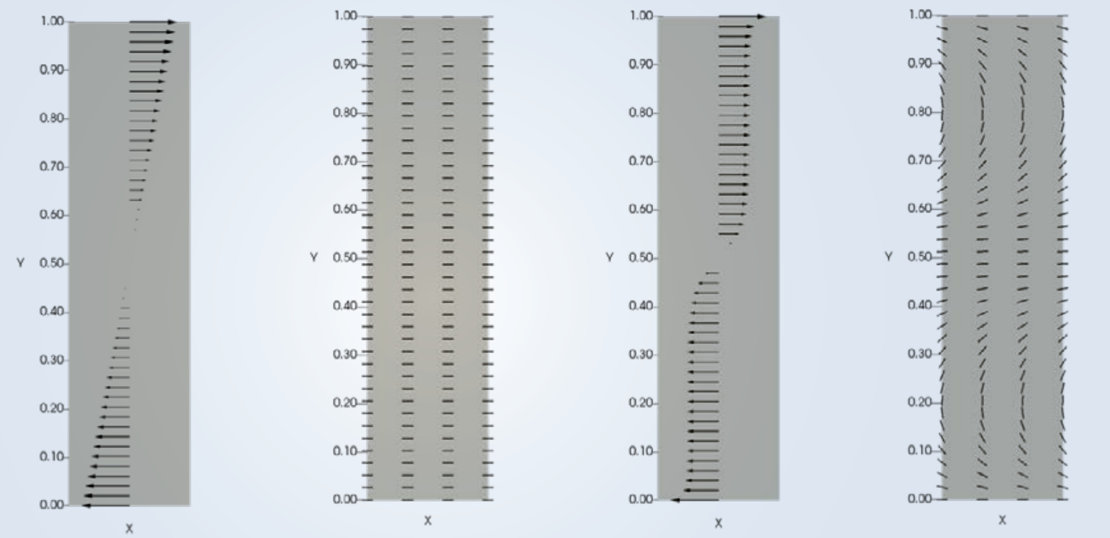
Figure 4: Acoustic pressure field of a jet in the x-y-plane.

JARA-HPC project with number: JHPC23

> Parallel Stabilized Finite Element Methods for Viscoelastic Fluid Simulations of Single-Walled Carbon Nanotube (SWNTs) */ Cakircali*

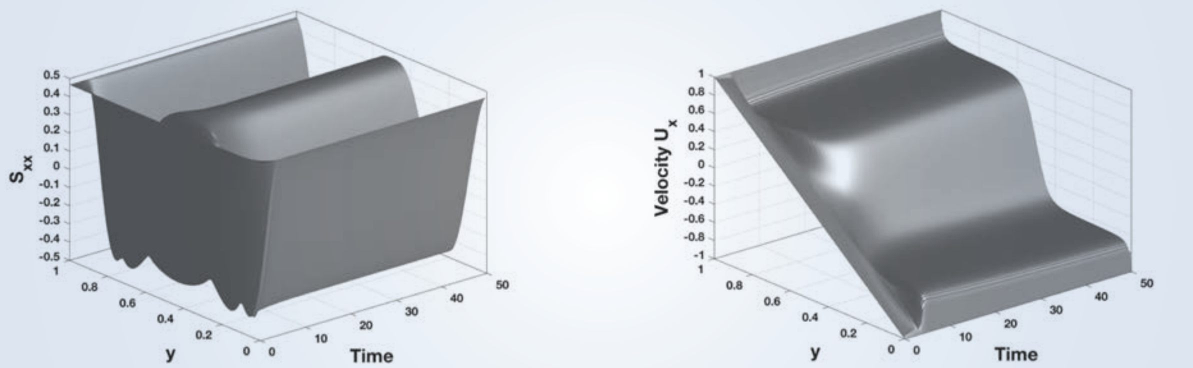
The objective of this project is to develop efficient numerical methods for the viscoelastic flows of micro-structured fluids; i.e., the Single-Walled Carbon Nanotube (SWNT) suspensions. SWNTs demonstrate unique properties in molecular scales, which make them ideal candidates as building blocks for multifunctional nano-materials. It is the aim to improve the understanding of material assembly processes (at macro scale) with the help of numerical methods. The complexity of the micro structural fluids results in highly nonlinear constitutive equations, which are usually derived from molecular and kinetic theories or via thermodynamic extensions in order to retain the micro-macro features of the flow. In this project, the constitutive model that was developed for the liquid-crystalline polymers (LCPs) is used. This model employs the mean-field potential that adds the non-local elasticity.

JARA-HPC project with number: JHPC34



(a) Velocity field at t = 0. (b) Orientation field at t = 0. (c) Velocity field at t = 50. (d) Orientation field at t = 50.

Figure 5: Results for a channel flow. The simulations employ a coupled incompressible Navier-Stokes and inhomogeneous nematic constitutive equations model. The images show the velocity and orientation fields at different time steps.



a) Order parameter tensor S_{xx} b) Velocity field

Figure 6: The transient coupled inhomogeneous model results for Reynolds number Re = 1, Deborah number De = 0.1, and Ericksen number Er = 100 are given. The results show that coupling the momentum and the constitutive equations affect the flow behavior; i.e., the flow reaches a steady state instead of showing periodic behavior.

> ADDITIONAL ACTIVITIES SIMLAB FSE

- Aeroacoustic simulation of jet noise */ Schlottke-Lakemper*
- Clang support */ Schlottke-Lakemper*
- Code performance analysis and tuning */ Cakircali, Kosel, Lintermann, Schlottke-Lakemper*
- Development of flow analysis tools */ Baumeister*
- GPU porting of ZFS (discontinuous Galerkin, Finite Volume) */ Schlottke-Lakemper*
- HPC consulting */ Lintermann*
- Industry relations team/ industry outreach */ Lintermann*
- JLESC: in charge of JSC applications */ Lintermann*
- Lattice-Boltzmann method (LBM) development */ Lintermann*
- MATSE studies */ Baumeister*
- Method development (discontinuous Galerkin) */ Schlottke-Lakemper*
- Method development (viscoelastic fluids) */ Cakircali*
- Nano-tube simulations */ Cakircali*
- Parallel geometry method development */ Lintermann*
- Respiratory tract simulations */ Lintermann*
- Shape optimization of chevrons for jet engines */ Kosel*
- System administration for SimLab servers & user support */ Cakircali, Kosel*

> Industry projects:

As a consequence of the 2014 Helmholtz PoF evaluation, an Industry Relations Team has recently been established at the JSC with Andreas Lintermann being in charge of research related simulation problems. In the following the industry activities are being reported. In 2016, the JSC sold 100,000 core-hours computing time on the JURECA system to an industry partner and delivers additional support. That is, the SimLab assisted the company in software installation and account management. / Lintermann

> Funding proposals:

Performance Engineering für wissenschaftliche Software im Bereich der Ingenieurswissenschaften (DFG)

Interested parties: AIA, CATS, SWL, ITV, IGPM, IFAM (all RWTH)

Status: not funded */ Lintermann*

> Computing time proposals

Prediction of jet engine noise, JARA-HPC, JURECA, requested 4.16 mio core-h, granted 1.66 mio core-h */ Lintermann*

> Refereeing for the following scientific journals and computing time applications

- Applied Mathematical Modeling
- European Journal of Mechanics B - Fluids
- RWTH IT Center Computing time proposals (technical & scientific)
- JARA-HPC/NIC/GCS computing time proposals (technical & scientific)

> Supervised student theses

- *Farrokhnezhad, F.,* **Implementation issues and benchmarking of lattice Boltzmann method for moving rigid simulations in a viscous flow, seminar Simulation Sciences**, RWTH
- *Krishnamurthy, K.,* **Computational study of Turbulence characteristics in a Natural Convective Flow,** master thesis, JSC, FZ Jülich

- *Seike, Y.,* **Experimental and Numerical Analysis of Horse Shoe Vortices Emanating from Pier Structures,** (ongoing) master thesis, AIA, RTWH Aachen University, Obi Laboratory, Keio University, Tokyo, Japan
- *Zechel, F.,* **Dissipations- und Dispersionseigenschaften der unstetigen Galerkin Spektrale Elemente Methode,** bachelor thesis, AIA, RWTH
- *Niemöller, A.,* **Spatial interpolation schemes for direct-hybrid computational aeroacoustics,** CES seminar thesis, AIA, RWTH
- *Peeters, B.* **Optimal time integration methods for computational aeroacoustics,** CES seminar thesis, AIA, RWTH
- *Mengel, A.,* **Investigation of the sound generated by the flow behind a rectangular cylinder with the direct-hybrid method for computational aeroacoustics,** master thesis, AIA, RWTH
- *Miller, J.,* **Software Cost Estimation for the Development Effort applied to Multi-node GPU Aeroacoustics Simulations,** master thesis, IT Center, AIA, RWTH

> NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE SIMLAB FSE

- Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH
- Chair for Computational Analysis of Technical Systems, RWTH
- IT Center, RWTH
- JSC, FZ Jülich
- The Laboratory for Biomaterials is part of the Institute for Biotechnology and the Helmholtz-Institute for Biomedical Engineering, RWTH
- Science and Technology Facilities Council, Daresbury Lab, U.K.
- Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZ Jülich
- Institute of Energy and Climate Research, Materials Synthesis and Processing, FZ Jülich
- Fire Simulation Team, FZ Jülich
- NVIDIA Application Lab, FZ Jülich
- Barcelona Supercomputing Center, Spain
- Department of Mechanical Engineering, Korea University, South Korea
- Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CAERFACS), France
- Complex Phenomena Unified Simulation Research Team, Riken Advanced Institute for Computational Science, Japan
- Obi Laboratory, Keio University, Japan
- Complex Flows of Complex Fluids, Rice University, Houston, Texas, U.S.

> SELECTED CONFERENCE PARTICIPATIONS WITHIN THE SIMLAB FSE

- DG Workshop, RWTH, January 18, 2016
- NIC Symposium, FZ Jülich, February 11-12, 2016
- ECCOMAS Congress, Crete Island, Greece, June 05-10, 2016
- Aachen Jülich Mathematics Workshop, FZ Jülich, June 15, 2016
- JLESC Lyon, Lyon, France, June 26-29, 2016
- EXA, invited talk, Stuttgart, Germany, June 07, 2016
- IISW 2016, Barcelona Supercomputing Center, Barcelona, Spain, September, 21-23, 2016
- JARA-HPC Symposium JHPCS'16, RWTH, October 04-05, 2016
- Riga RhinoDays, invited talk, Riga, Latvia, October 31-November 03, 2016

> WORKSHOPS / EVENTS ORGANIZED BY THE SIMLAB FSE

- DLR Workshop, FZ Jülich, May 25, 2016
- Program Committee:
  JARA-HPC Symposium (JHPCS'16), Aachen, Germany, October 4-5, 2016
- Organization of a talk by Dr.-Ing. Andrea Winzen from Oshima Laboratory, The University of Tokyo, Japan, at FZ Jülich, December 20, 2016
- Tour computing facilities JSC for JLESC guests from AICS, Riken, Japan, at FZ Jülich, July 16-17, 2016

> SELECTED HONORS, PRIZES AND AWARDS DURING REPORTING PERIOD

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2.4.2. SimLab " Simulation Lab Neuroscience" (SLNS)

SCIENTIFIC LEAD *Abigail Morrison / FZ Jülich*

STAFF
Rajalekshmi Deepu / FZ Jülich
Sandra Diaz / FZ Jülich
Steffen Graber / FZ Jülich
Jochen Martin Eppler / FZ Jülich
Fahad Khalid / FZ Jülich
Wouter Klijn / FZ Jülich
Anna Lührs (Westhoff) / FZ Jülich
Alexander Peyser / FZ Jülich
Meredith Peyser / FZ Jülich
Dimitri Plotnikov / FZ Jülich
Yachao Shao / FZ Jülich
Kim Sontheimer / FZ Jülich
Guido Trensch / FZ Jülich
Bastian Tweddell / FZ Jülich

> PROJECTS BEING SUPPORTED BY THE SIMLAB AND USING COMPUTING TIME ON THE JARA-HPC PARTITION:

- Modeling structural plasticity and self-organization of large-scale cortical networks in NEST. Ran from May 01, 2015 until April 30, 2016. - JIAS60

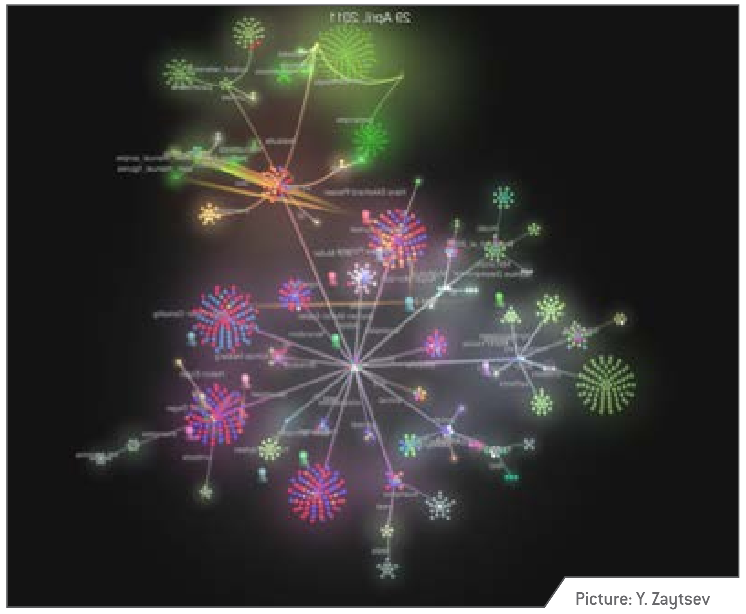
> ADDITIONAL ACTIVITIES SLNS

- Expertise in software engineering, software project management, and software development *Deepu, Diaz, Eppler, Khalid, Lührs, Peyser, Trensch*
- Infrastructure support for software development issues */ Deepu*
- HPC: Expertise in efficient parallelization and optimization of applications for supercomputers */ Deepu, Diaz, Eppler, Khalid, Klijn*
- High-performance neuronal multicompartment models (NestMC) */ Peyser, Shao*
- HPC architectures and storage systems */ Shao, Tweddell*
- Modeling and simulation of different features of neural networks, especially structural plasticity (VirtualConnectome, TVB for HPC) */ Diaz*
- NEST: Release management, coordination of (infrastructure) development, Seed Fund Project NESTML and support for the massively-parallel computer architecture SpiNNaker */ Eppler, Peyser, Plotnikov, Trensch*
- Research in applications of computer vision to problems in neuro-imaging */ Khalid*
- Scientific visualization */ Klijn, Peyser*
- Mathematical methods and nonlinear dynamics */ Klijn*
- VirtualConnectome for the VirtualBrain & TVB for HPC */ Peyser*
- Expertise in development of domain specific languages */ Plotnikov*
- Development and optimization of image processing software and development of quality control methods for 3D-PLI and its workflow */ Sontheimer*
- Development of programming models for the exchange of large data sets and tools for the solution of big data problems */ Tweddell*

> PROJECTS

> NEST – Neural Simulation Tool */ Deepu, Diaz, Eppler, Graber, Peyser, Trensch*

- Suitable for small-scale (notebook, workstation) and large-scale (super-computer) simulations
- Collaboration with Istitute for Neuroscience and Medicine (INM-6), FZ Jülich
- SLNS contributions:
  - > Development of the NEST kernel
  - > Performance modeling and tuning
  - > Python bindings (CyNEST)
  - > Input/Output routines
  - > Implementing Structural Plasticity in NEST
  - > Gap junctions


Picture: Y. Zaytsev

> NestMC multicompartment neuronal network simulation tool */ Klijn, Peyser, Shao*

- Simulation of neuronal networks with detailed morphology designed for new high performance computing architectures
- Backends: Serial/MPI/HPX, Serial/TBB/C++11 threads/HPX, CPU/KNL/GPU
- Developed in collaboration with the Swiss National Supercomputing Centre, CSCS
- SLNS contributions:
  - > Community outreach and use case development in neuroscience
  - > Software engineering, design, and scaling algorithms implementation
  - > Performance modeling and tuning

> HPC for TVB */ Diaz, Peyser*

- Neural mass model simulator for HPC computing architectures, mapping between fMRI and EEG experimental results and automated model kernel production for GPU backends
- Developed in collaboration with Viktor Jirsa, Aix-Marseille University, with use case support from Petra Ritter, Charité
- Includes frameworks for large scale parameter sweeps using adaptive searches such as evolutionary approaches

> ElePhAnT – ElectroPhysiological Analysis Toolkit */ Deepu, Klijn*

- Toolbox for the analysis of multi-scale, electrophysiological data from experiments and simulation
- Collaboration with Institute for Neuroscience and Medicine (INM-6), FZ Jülich

> Polarized Light Imaging (PLI) */ Khalid, Lührs, Sontheimer*

- HPC application for segmentation of very high resolution images of brain slices
- Research on the application of deep learning algorithms from computer vision to segmentation of PLI images
- Quality control tools for the PLI workflow
- Collaboration with Institute for Neuroscience and Medicine (INM-1), FZ Jülich

> NEST Modeling Language (NEST ML) */ Eppler, Plotnikov*

- Modeling language for spiking neurons
- JARA-HPC Seed Fund project in collaboration with Prof. Bernhard Rumpe, RWTH

> JADE – Jülich Aachen Data Exchange */ Deepu, Tweddell*

- Collaboration with the Virtual Reality Group, RWTH and Universidad Politécnica de Madrid

> NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE SLNS

- Participation in the Human Brain Project (FET Flagship Programme launched by the European Commission)
- Participation in the Helmholtz Portfolio Theme "Supercomputing and Modeling for the Human Brain" (SMHB)
- Member of the National Bernstein Network Computational Neuroscience (NNCN) as the "Bernstein Facility for Simulation and Database Technology"
- US - German Research Project entitled "Computational models linking connectomics and large-scale dynamics of the human brain" (funded by the BMBF in collaboration with the National Science Foundation)

> SELECTED CONFERENCE PARTICIPATIONS WITHIN THE SLNS

> Posters (after call)

- *Blundell, I., Plotnikov, Eppler, J.M., Diesmann, M., Rumpe, B., Morrison, A.*
  NESTML: a modeling language for spiking neurons
  IAS Symposium 2016, FZ Jülich, December 05-06, 2016
- *Klijn, W., Cumming, B., Karakas, V., Peyser, A., Yates, S.*
  NEST-MC: A morphologically detailed neural network simulator for many core high performance computer architectures
  IAS Symposium 2016, FZ Jülich, December 05-06, 2016
- *Klijn, W., Cumming, B., Karakasis, V., Peyser, A., Yates, S.*
  Nidus by NEST: A morphologically detailed neural network simulator for many core high performance computer architectures
  Bernstein Conference, Berlin, Germany, September 21-23, 2016
- *Yegenoglu, A., Senk, J., Amblet, O., Brukau, Y., Davison, A., Lester, D., Lührs, A., Quaglio, P., Rostami, V., Rowley, A., Schuller, B., Stokes, A., van Albada, S., Zielasko, D., Diesmann, M., Weyers, B., Denker, M., Grün, S.*
  Embedding Elephant in a Simulation-Validation Workflow within the HBP Collaboratory
  Human Brain Project Summit 2016, Florence, Italy, October 12-15, 2016

> Posters (other)

- *Bücker, O., Köhnen, S., Huynh, A. M., Tabbi, G., Lührs, A., Giesler, A., Hagemeier, B., Amunts, K., Lippert, T., Axer, M.*
  Automation and parallelization of a 3D Polarized Light Imaging workflow
  22nd Annual Meeting of the Organization for Human Brain Mapping (OHBM), Genf, Switzerland, June 26-30, 2016
- *Diaz, S., Nowke, C., Peyser, A., Hentschel, B., Weyers, B., Morrison, A., Kuhlen, T.*
  Multiscale approach to explore the relationships between connectivity and function in whole brain simulations
  Bernstein Conference 2016, Berlin, Germany, September 21, 2016
- *Diaz, S., Nowke, C., Peyser, A., Weyers, B., Hentschel, B., Morrison, A., Kuhlen, T.*
  Multiscale approach to explore the relationships between connectivity and function in whole brain simulations
  HBP Summit 2016, Florence, Italy, October 12-14, 2016
- *Klijn, W., Cumming, B., Karakasis, V., Peyser, A., Yates, S.*
  Nidus by NEST: A morphologically detailed neural network simulator for many core high performance computer architectures
  Human Brain Project Summit 2016, Florence, Italy, October 12-15, 2016

> Conference presentations (invited)

- *Peyser, A.*
  High Performance Analytics & Computing Platform
  Society for Neuroscience 2016, San Diego, CA, USA, November 11, 2016

> Conference presentations (other)

- *Peyser, A.*
  I/O for HPC: NEST case study
  SMHB General Assembly 2016, FZ Jülich, April 20-21, 2016
- *Peyser, A.*
  Simulation Lab Neuroscience
  JARA-HPC General Assembly, FZ Jülich, May 03, 2016
- *Senk, J., Yegenoglu, A., Amblet, O., Brukau, Y., Davison, A., Lester, D., Lührs, A., Quaglio, P., Rostami, V., Rowley, A., Schuller, B., Stokes, A., van Albada, S., Zielasko, D., Diesmann, M., Weyers, B., Denker, M., Grün, S.*
  Integrating HPC into a Collaborative Simulation-Analysis Workflow for Computational Neuroscience
  JARA-HPC Symposium (JHPCS'16), Aachen, Germany, October 04-05, 2016
- *Peyser, A., Yates, S.*
  NestMC: A new multi-compartment neuronal network simulator
  NEST Initiative User Workshop, Karlsruhe, Germany, November 03, 2016
- *Diaz, S., Nowke, C., Peyser, A.*
  Interactive visualization and steering of structural plasticity in NEST
  NEST User Workshop 2016, Karlsruhe, Germany, November 03-04, 2016
- *Diaz, S., Nowke, C., Peyser, A., Weyers, B., Hentschel, B., Kuhlen, T.*
  Multi-scale approach to explore the relationships between connectivity and function in whole brain simulations
  IAS Symposium 2016, FZ Jülich, December 05-06,2016

> Contribution to conference proceedings

- *Lührs, A., Bücker, O., Axer, M.*,
  Towards Large-Scale Fiber Orientation Models of the Brain – Automation and Parallelization of a Seeded Region Growing Segmentation of High-Resolution Brain Section Images
- *Amunts, K., Grandinetti, L., Lippert, T., Petkov, N. (eds),*
  Brain-Inspired Computing. BrainComp 2015
  Lecture Notes in Computer Science, vol 10087. Springer, Cham. Doi: 10.1007/978-3-319-50862-7_3 (2016)
- *Plotnikov, D., Blundell, I., Ippen, T., Eppler, J. M., Rumpe, B., Morrison, A.,*
  NESTML: a modeling language for spiking neurons
  Modellierung 2016, Karlsruhe, Germany, March 17-19, 2016
  Lecture Notes in Informatics (LNI) P-254, 93-108 (2016)

> WORKSHOPS / EVENTS ORGANIZED BY THE SLNS

- **SMHB General Assembly 2016**
  SMHB General Assembly 2016, FZ Jülich, April 20-21, 2016
- *Peyser, A., Morrison, A., Wachtler, T.,*
  HPC in Neuroscience Satellite Workshop
  Bernstein Conference 2016, Berlin, Germany, September 20-21, 2016
- *Napoli, E. D., Hentschel, B., Hermanns, M.-A., Iliev, H., Lintermann, A., Mohr, B., Orth, B., Peyser, A., Zilken, H.,*
  JARA-HPC Symposium (JHPCS'16), Aachen, Germany, October 04-05, 2016
- *Plotnikov, D., Blundell, I., Ippen, T., Eppler, J. M., Rumpe, B., Morrison, A.,*
  Code Generation from Model Description Languages II
  FZ Jülich, December 07-09, 2016

> TALKS BY THE SLNS

- *Diaz, S., Peyser, A.,*
  Virtual Connectome: Discovering the relationship between structural and functional connectivity during steady-states and transitions
  Aachen Jülich Mathematics Workshop, Germany, June 15, 2016
- *Klijn, W.,*
  Hardware Software Science Co-design in the Human Brain Project
  German-Indian Workshop on HPC Architectures and Applications, Pune, India, November 29 - 30, 2016
- *Plotnikov, D., Morrison, A., Trensch, G.,*
  Neuromorphic Systems - Running Neuron Models on SpiNNaker
  Jahresabschlusskolloquium des JSC 2016, FZ Jülich, December 13, 2016
- *Tweddell, B., Klijn, W.,*
  HBP Pilot Systems: Introduction and first Use-Case Experiences
  Jahresabschlusskolloquium des JSC 2016, FZ Jülich, December 13, 2016

> SELECTED HONORS, PRIZES AND AWARDS DURING REPORTING PERIOD

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2.4.3. SimLab "ab initio Methods in Chemistry and Physics" (Slai)

SCIENTIFIC LEAD
Stefan Blügel / FZ Jülich
Richard Dronskowski / RWTH

STAFF
Edoardo A. Di Napoli / FZ Jülich
Miriam Hinzen / FZ Jülich, RWTH
Sachin Nanavati / RWTH
Jan Winkelmann / RWTH

> PROJECTS

> High-performance algorithms in DFT simulations */ Di Napoli, Winkelmann*

In DFT codes based on the Linearized Augmented Plane Wave (LAPW) method, two are the computationally most expensive operations: matrix initialization and eigenproblem solution. We developed an alternative algorithm for the generation of the matrix entries in the FLEUR code, which is developed by the PGI-1 group in the FZ Jülich. The results of this work showed how by exposing the inner data structure it is possible to make the Hamiltonian and Overlap matrix generation performance portable. The newly designed algorithm achieved up to 2.5x speedup on shared memory processors and up to 12x on GPUs. Similarly we further developed an in-house eigensolver tailored for sequences of dense eigenvalue problems. The Chebyshev Accelerated Subspace iteration Eigensolver (ChASE) is coded in C++ and implemented in three separate versions targeting distinct parallel platforms: multi-cores with MPI, many-cores with both OpenMP and CUDA. [Partners: AICES/RWTH]

> HPC Tensor algebra */ Di Napoli*

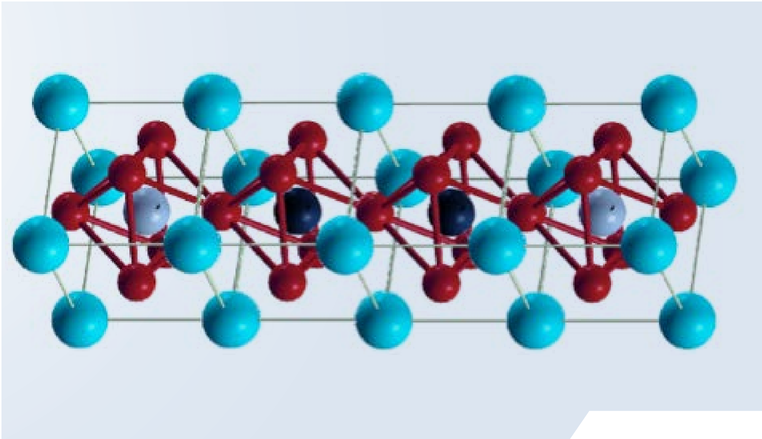
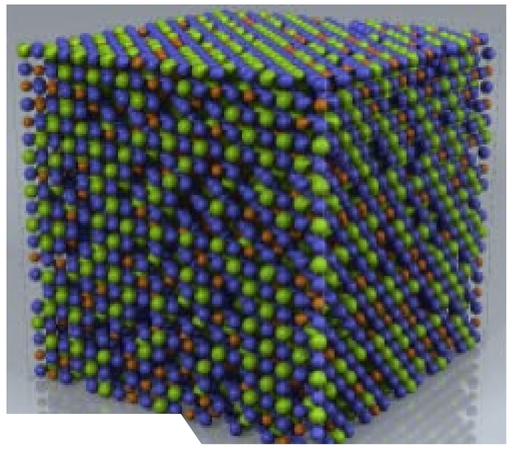
Multi-dimensional objects appear in many applications. In general such objects are parameterized by multi-index arrays called tensors. Contractions among two or more tensors are at the core of computations in Quantum Chemistry and fRG. We are involved in an on going project towards the development of specialized algorithms for high-performance multi-contraction operations between high dimensional tensors. We are in the process of extending a systematic approach to use the BLAS library to multiple contractions between multiple tensors and port it to GPUs. [Partners: Intel Corporation, AICES, RWTH]

> Rational approximation for generalized eigenproblems */ Di Napoli, Winkelmann*

Alternative methods in DFT make use of discretization strategies ending up in very large and sparse matrices. Contrary to LAPW methods, real-space methods require a completely different approach to the solution of eigenvalue problems. An on going research effort concentrates on the use of close to best rational approximation for the development of a novel iterative eigensolver for generalized eigenvalue problems. This algorithm is based on the slicing of the eigenspectrum in separate intervals using an approximate projector. We actively worked in the optimization of the rational filters at the base of this class of eigensolvers. The resulting filters are constructed through and elaborate process based on Non-Linear Least Squares minimization using the Levenberg-Marquardt method. [Partners: Department of Computer Science and Engineering, University of Minnesota, USA]

> High-performance methods in fRG */ Di Napoli, Winkelmann*

Functional Renormalization constitutes a very powerful framework capable of describing materials phase transition from weak to strong coupling. Together with a traditional DFT method, fRG promises to be the method of choice to simulate and screen future superconducting materials. In collaborations with RWTH, we developed a new highly scalable simulation code: TUfRG. In particular we have designed an adapted to the numerical algorithm for the adaptive quadrature, which is the most computationally expensive part of TUfRG, parallelized on many-cores. [Partners: ITSSP, RWTH]

> Adaptive preconditioner for DFT */ Di Napoli, Hinzen*

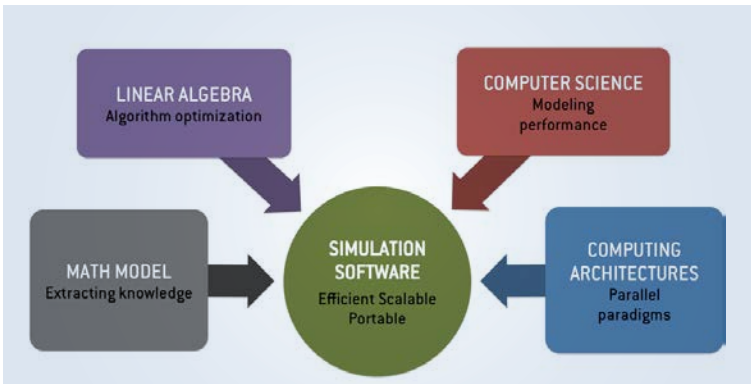
DFT calculations in the range of 10,000 atoms with cubic scaling algorithms can only be executed on large supercomputers to host the required memory footprint and to get to a reasonable time-to-solution for a single calculation. These runs are hardly affordable for production series. However, strong interest in disordered systems and broken symmetries is arising within the community motivated by the need of novel materials for data storage, energy storage and other functional materials designed for technology applications. Despite the advantages, large-scale DFT calculations suffer from a critical slowdown of the convergence of the self-consistency (SCF); the larger is a system the more evident this effect becomes. This repercussion is hardly seen in the range below a thousand atoms and has, therefore, not attracted much attention in the past. In the recent past, SCF convergence has been accelerated using Newton-Raphson-type algorithms, which are originally designed for a linear response behavior. However, the reoccupation dynamics occurring during the SCF iterations in a metal are far from being well described as a linear behavior. We are investigating and implementing an inexpensive approximations of the response density necessary to improve the convergence. Reaching such a target would allow codes to achieve N \log (N) which is the best achievable scaling inferred by the Poisson solver. [Partners: PGI-1, FZ Jülich]

> Integration of the Chase library in the FLEUR code */ Di Napoli, Hinzen*

Ongoing integration of the iterative eigensolver ChASE eigensolver within the FLEUR code. It is expected that ChASE will speed up the calculations for larger sized problems but also achieve faster convergence. Status: The main hurdle of integrating Chase (C++ code) with FLEUR (FORTRAN 77/90 code) through an interface code has been overcome. For some representative problems, the results from direct and iterative solvers match within numerical accuracy. Now, extensive tests have been planned for different physical systems by tweaking the algorithm parameters.[PGI-1, FZ Jülich]

> Inverse design of functional hetero-interfaces in photovoltaic applications */ Di Napoli*

Heterogeneous interfaces play an important role in a wide range of modern solar cell concepts. Despite this high relevance, charge carrier transport and recombination across such interfaces is, in many cases, difficult to handle and predict. Modeling charge transport across interfaces requires open boundary conditions for the underlying equations. Moreover, the interaction of charge carriers with photons and the lattice vibrations calls for a mathematical description that goes beyond the ballistic transport. We developed a code is based on the solution of two non-linearly-coupled equations describing charge transport and charge interactions using non-equilibrium Green's functions formalism. Since the equations are non-linearly coupled through self-energy terms, they have to be solved self-consistently. We proceeded



SimLab Strategy chart

to parallelize the code using OpenMP+ MPI and were able to scale the entire simulation of a diode over several thousands of processing units. Such a result is the first step towards the construction of a full-fledged 3-D optimized code which will be used to explore the complex parameter space necessary to describe photovoltaic materials. [Partners: IEK-5, FZ Jülich]

> ADDITIONAL ACTIVITIES SIMLAB SLAI

- Developing a Kerker pre-conditioner for the FLEUR code */ Hinzen*
- Developing and maintaining new codes developed under the SimLab */ Winkelmann*
- Developing a new data framework for Quantum Chemistry codes */ Nanavati*
- Developing a new algorithm and related code for the diagonalization of sparse eigenproblems in Density Functional Theory methods */ Winkelmann*
- Integrating libraries in existing ab initio codes */ Nanavati*
- Integrating the ChASE library into the FLEUR code */ Hinzen*
- Parallel programming in Fortran language */ Hinzen*
- Profiling and parallel programming new and legacy codes */ Di Napoli, Nanavati*
- Supervision of PhD, Masters, Guest Students, etc.

> Externally funded project */ Di Napoli*

- Materials Informatics - Preliminary study on materials properties using data mining techniques. Status: Study is still in its infancy. Initiated collaboration with IEK-6 and University of Minnesota. [Partners: IEK-6, FZJ. Department of Computer Science and Engineering, University of Minnesota, USA.]

> PhD project preparation

- Robust methods for achieving self-consistency in large-scale ab-initio quantum mechanical calculations
  The main target of this project is to build a universal pre-conditioner for Density Functional Theory methods that scales with the number of atoms and avoid stagnation of the SCF for metal and semiconductors.
- Inverse design of functional hetero-interfaces in photovoltaic applications
  > The objective of this project is to introduce algorithm optimizations in a recently developed code to simulate Photovoltaic cells with discrete anisotropies. In addition the code will be parallelized so as to be capable of running on massively parallel architectures. Eventually the goal is to simulate realistic materials in a relatively short amount of time using pre-esascale platforms.

> Refereeing for the following scientific journals:

- Journal of Computational and Applied Mathematics (Elsevier)
- SIAM journal on Matrix Analysis and Applications (SIAM)
- Parallel Computing (Elsevier)
- LNCS (Springer Verlag) for PPAM Conference

> Technical and administrative

- Co-organized the first JARA-HPC Symposium held on the 4-5th of October 2017. Co-chaired sessions of the symposium and acted as corresponding editor of the proceedings of the event
- General administrative tasks related to the management of the JARA-HPC ab initio SimLab activities
- Participating in bi-weekly meeting of the Young Research Group Leaders of AICES. Activities discussed are: admissions of new students, organization of academic and social activities, ordinary administrative AICES issues before they are passed on to the Steering Committee
- Performed technical and scientific evaluation of computing time applications for the initiated under JARA-HPC, RWTH RZ, NIC & VSR

> NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE SIMLAB SLAI

There are on going collaborations with the following groups and single researchers

- *Paolo Bientinesi's HPAC group,* AICES, RWTH
- *Carsten Honerkamp,* RWTH
- *Yousef Saad,* University of Minnesota, Minneapolis, USA
- *Stefan Blügel's group,* PGI-1, FZ Jülich
- *Mario Berljafa,* School of Mathematics, University of Manchester, Manchester, U.K.
- *Eric Polizzi,* University of Massachussetts, Amherst, USA
- *Matthieu Verstraete,* Univerity of Liege, Liege, Belgium
- *Markus Diesmann group,* INM-6, FZ Jülich
- *Ming Hu,* AICES, RWTH
- *Piotr Kowalski,* IEK-6, FZ Jülich
- *Davor Davidovic,* University of Zagreb, Zagreb, Croatia
- *Andre Schleife,* University of Illinois, Urbana-Champaign, USA

> SELECTED CONFERENCE PARTICIPATIONS WITHIN THE SIMLAB SLAI

- SIAM Conference on Parallel Processing (PP16)
  Chebyshev Accelerated Subspace iteration Eigensolver
  Contributed poster, Presenter: Edoardo Di Napoli, Paris, France, April 2016
- Aachen/Jülich Mathematics workshop
  Optimizing Algorithms for High-Performance Computations in Materials Science
  Speaker: Edoardo Di Napoli, Jülich, Germany, June 2016
- Joint Laboratory on Extreme Scale Computing (JLESC)
  Application of the ChASE Eigensolver to Excitonic Hamiltonians
  Speaker: Edoardo Di Napoli, Lyon, France, June 2016
- 9th International Workshop on Parallel Matrix Algorithms and Applications (PMAA 16)
  The ChASE library on distributed and heterogeneous platforms
  Speaker: Edoardo Di Napoli, Bordeaux, France, July 2016
- Joint Laboratory on Extreme Scale Computing (JLESC)
  An efficient Parallel Implementation of the ChASE Library on distributed CPU/GPU Architectures
  Speaker: Edoardo Di Napoli, Kobe, Japan, December 2016
- Joint Laboratory on Extreme Scale Computing (JLESC)
  HPC Generation of the Hamiltonian and Overlap matrices in DFT methods based on Linearized and Augmented Plane Waves
  Speaker: Edoardo Di Napoli, Kobe, Japan, December 2016

> WORKSHOPS / EVENTS ORGANIZED BY THE SIMLAB SLAI

- Program Committee:
  JARA-HPC Symposium (JHPCS'16), Aachen, Germany, October 04-05, 2016

> SELECTED HONORS, PRIZES AND AWARDS DURING REPORTING PERIOD

- -

> 2.5. Cross-Sectional Groups (CSGs)

2.5.1. CSG "Immersive Visualization (ImVis)"

SCIENTIFIC LEAD

Norbert Attig / FZ Jülich
Bernd Hentschel / RWTH
Torsten Kuhlen / RWTH
Herwig Zilken / FZ Jülich

CONTRIBUTORS

Jens Henrik Göbbert/ FZ Jülich
Joachim Herber / RWTH
Christian Nowke / RWTH
Heiko Overath / RWTH
Dominik Rausch / RWTH
Andrea Schnorr / RWTH
Tom Vierjahn / RWTH
Benjamin Weyers / RWTH

> PROJECTS

> Structural Plasticity Visualization and Steering in NEST */ Nowke*

A major goal of this year's research and development efforts has been to assist neuroscientists in the assessment of structural plasticity in simulated neural networks. Structural plasticity refers to the dynamic creation and deletion of synapses in a neural network and reflects the way the brain develops, learns, and heals. The relationship between anatomical connectivity and brain function is still unclear. To this end, our collaborators at the SimLab Neuroscience perform large-scale simulations of the brain in order to expose the connectivity between neurons by correlating simulations with experimental data. One driving challenge in the exploration of structural plasticity is the complexity of the underlying parameter space. In order to help domain scientists analyze this space effectively, we developed an interactive exploration tool that enables them to change parameters of a structural plasticity model while it is simulated. We built the tool on top the previously established methodology of the VisNEST project: loosely coupled and highly flexible coordinated, multiple views, linked to each other via inter-process communication. This approach allows the developed visualizations to run in conjunction with the supercomputer JURECA and visualizes calcium concentrations for brain regions as a proxy for their electrical activity and a region's connectivity (cf. Figure 1). The parameter steering accounts for several model parameters. For example, the rate at which new synapses form or old ones decay, or a minimum calcium concentration that regions should achieve in the simulation. In the future, we plan to extend this tool to gain a more detailed understanding of the yet unexplored parameter space.

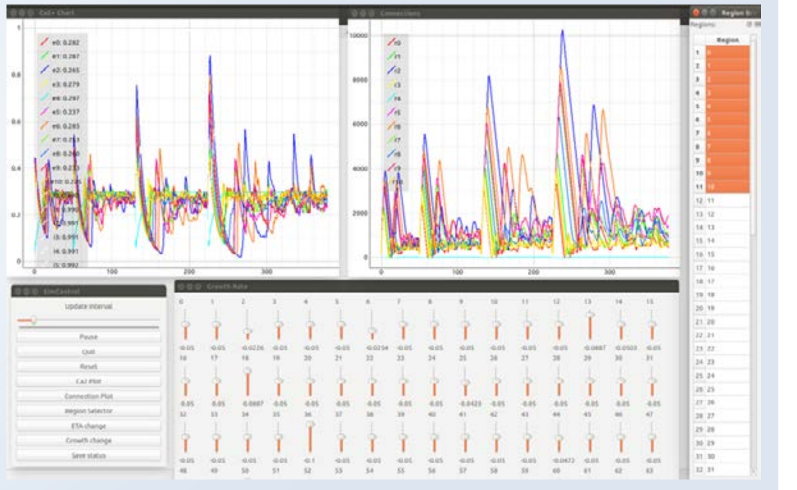


Figure 1: Calcium concentrations and connections are shown for brain regions (top left and right). A region selector allows users to focus on a subset of these (to the right). The steering panels (bottom middle) allow for interactive modification of model parameters while the simulation runs.

> Tracking Space-Filling Structures in Turbulent Flows */ Schnorr*

This project addresses the analysis of the temporal evolution of space-filling features in large-scale, turbulent flow datasets. This work is motivated by a collaboration with the Institute of Combustion Technology (ITV, RWTH) to track the temporal evolution of Dissipation Elements (DEs) which are space-filling by definition. Currently, the analysis of DEs is limited to individual snapshots of a simulation run. A stable tracking method would allow researchers to extend their analysis to the time dimension.

Recently, our research focus was on an event detection scheme, which enables the algorithmic identification of situations, where a feature either results from an interaction of multiple objects in the previous time step (merge) or separates into multiple objects in the subsequent time step (split). Figure 2 shows a representative situation taken from three successive time steps of a DNS simulation of isotropic turbulence. Tracking all features in a pre-process enables us to subsequently analyze and visualize the evolution of a single feature or a group of features. A corresponding publication which summarizes the main results is in preparation.

Feature tracking will remain a focus area of research throughout 2017 because it addresses a key need in the analysis of time-varying, large-scale simulation data. As such, these developments immediately address a need highlighted by both reviewers in last year's JARA-HPC evaluation.

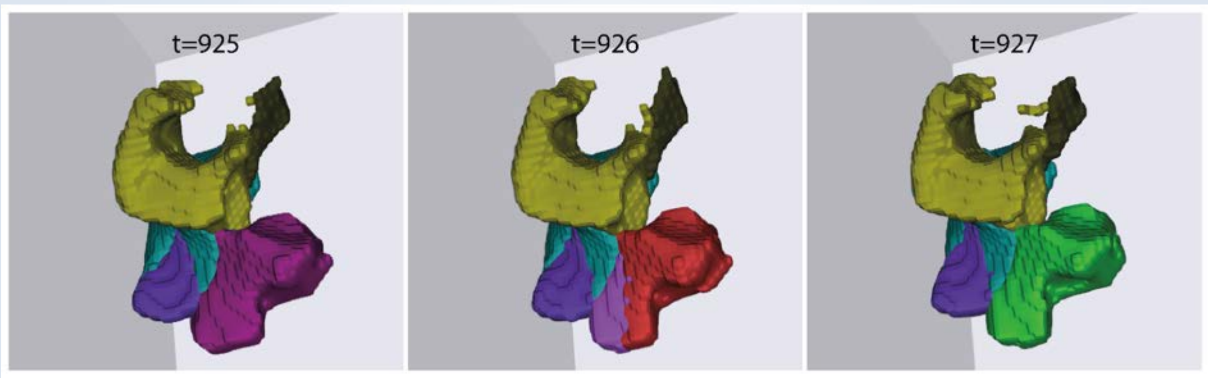


Figure 2: Depiction of the temporal evolution of selected dissipation elements in a 256^3 isotropic turbulence data set. The dense packing of the elements illustrates the space-filling characteristic.

> Modern Rendering Technology */ Herber*

Point clouds have become an increasingly common modality in modern computer graphics. To this end, we developed rendering algorithms for such data. One driving use case for this specific development has been a cooperation with the Police of NRW to visualize light detection and ranging (LiDAR) data representations of crime scenes. An application featuring the newly developed renderer has been successfully presented during the 13th International Police Workshop Photogrammetry / Laser Scanning which took place in Neuss, from July 11-15, 2016.

In addition, we launched an endeavor to modernize the current rendering infrastructure in the ViSTA eco-system in order to cater for the needs of large-data visualization. Specifically, integrated modern OpenGL features to enable rendering large-scale polygonal and volumetric data. Eventually, these developments will support a full replacement of the existing ViSTA rendering routines. Apart from significant performance improvements, the goal of this effort is to provide easy to use rendering facilities, which handle static and time varying geometry, particle, and volume data through a consistent, uniform interface. Finally, the API encapsulates dependencies to third party library, e.g., vtk, in order to allow for a seamless integration.

Virtual Sketching */ Kuhlen, Rausch*

Virtual Sketching is a cooperative teaching project of the Department for Visual Art (Prof. Schmitz) and the LuFG Virtual Reality and Immersive Visualization (Prof. Kuhlen).

Students of architecture have the possibility to sketch their own designs in 3D inside the aixCAVE.

Inspired by the creative, expressive and experimental design approach of 2D pen- and-paper sketches, Virtual Sketching allows similar design sessions in 3D. The students use virtual pens to draw three-dimensional strokes and shapes directly into 3D space. Different background models, brush types, colors and textures allow for a wide range of 3D drawings -- from architectural concepts to artistic designs - to be created and experienced in VR. Virtual Sketching recently won the RWTH's Teaching Award 2016 for best teaching project.

While 3D sketching was primarily motivated by the use case of teaching design students, the fundamental technology provides an innovative interface for adding sketch-based annotations to complex 3D data sets in order to aid their understanding.

> NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN CSG ImVis

- *Prof. C. Garth,* University of Kaiserslautern, Kaiserslautern, Germany
- *Prof. H. Childs,* University of Oregon, USA
- *Prof. Heinz Pitsch,* ITV, RWTH
- *Prof. A. Morrison,* SimLab Neuroscience, FZ Jülich
- *Prof. K. Amunts,* INM-1, FZ Jülich
- *Prof. M. Diesmann, Prof. S. Grün,* INM-6, FZ Jülich

> SELECTED CONFERENCE PARTICIPATIONS

-

> WORKSHOPS / EVENTS ORGANIZED BY THE CSG ImVis

-

> SELECTED HONORS, PRIZES AND AWARDS

- Best Poster Award LDAV 2016 for *Vierjahn, T., Hermanns, M.-A., Mohr, B., Kuhlen, T. W., Hentschel, B.,* Correlating Sub-Phenomena in Performance Data in the Frequency Domain

- RWTH Aachen University's Teaching Award 2016, *Schmitz, T. H., Groninger, H., Kuhlen, T. W., Rausch, D.,* Virtual Sketching

2.5.2. CSG "Parallel Efficiency (CSG ParE)"

SCIENTIFIC LEAD

Bernd Mohr / FZ Jülich
Matthias Müller / RWTH

CONTRIBUTORS

Dieter an Mey / RWTH
Uliana Alekseeva / RWTH
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Alesja Dammer / RWTH
Christian Feld / FZ Jülich
Markus Geimer / FZ Jülich
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Michael Knobloch / FZ Jülich
Julian Miller / RWTH
Jan Felix Münchhalfen / RWTH
Joachim Protze / RWTH
Dirk Schmidl / RWTH
Aamer Shah / RWTH
Alexandre Strube / FZ Jülich
Christian Terboven / RWTH
Sandra Wienke / RWTH
Bo Wang / RWTH
Brian Wylie / FZ Jülich
Ilya Zhukov / FZ Jülich

> PROJECTS BEING SUPPORTED BY THE CSG AND USING COMPUTING TIME ON THE JARA-HPC PARTITION

> User Support for Improved Scalability of Hybrid Parallel Codes (JARA0001)
an Mey, Cramer, Dammer, Iliev, Miller, Protze, Schmidl, Shah, Terboven, Wang, Wienke
Cooperation partners: IT Center, Chair I12, IKV, ITV, CATS, AIA (RWTH)

> Parallel Stabilized Finite Element Methods for Aero-, Hemo- and Hydrodynamics CATS, RWTH– code XNS) */ Iliev*
Cooperation partners: IT Center, CATS (RWTH)

> Scalable Performance Analysis of Large-Scale Parallel Applications (JZAM11) */ Hermanns, Iliev*
Cooperation partners: JSC, FZ Jülich, IT Center, RWTH

> Hybrid parallelism for the Jülich DFT code FLEUR (JARA-HPC Seed Fund Project) */ Alekseeva*
Cooperation partners: IT Center, RWTH, FZ Jülich

> Investigating the performance of the OpenMP programming paradigm on NUMA architectures
an Mey, Cramer, Schmidl, Terboven, Wang, Wienke

> POP (Performance, Optimization and Productivity Center of Excellence) */ Dammer, Knobloch, Shah, Wang, Wylie, Zhukov*
Cooperation partners: IT Center, RWTH, HLRS, Stuttgart JSC, FZ Jülich,
NAG (UK), BSC (Spain), TERATEC (France)

> Support of performance evaluation of the particle simulation code MP2C */ Hermanns*
Cooperation partners: JSC, FZ Jülich

> PROJECTS

> MUST */ Müller, Münchhalfen, Protze*
Description: Runtime error detection for parallel applications
Cooperation partners: IT Center, RWTH, ZIH, LANL (USA), LLNL (USA)

> Scalasca */ Hermanns, Mohr*
Cooperation partners: JSC, FZ Jülich
Description: Understanding application performance at scale

> Score-P – Scalable performance measurement infrastructure for parallel codes */ Feld, Geimer, Schmidl*
Cooperation partners: JSC, FZ Jülich, IT Center, RWTH, TUM, TUDA, TUD

> Cube */ Hermanns, Mohr*
Cooperation partners: JSC, FZ Jülich, IT Center, RWTH
Description: Intuitive performance profile exploration

> **Opari 2 – Source-level instrumentation for directive-based parallelization** */ Schmidl*
Cooperation partners: JSC, FZ Jülich

> ADDITIONAL ACTIVITIES CSG ParE

- Debugging support */ Strube*
- Innovative computing (GPU) */ Wienke, Cramer*
- Performance and power usage evaluation */ Wang*
- Performance Evaluation */ Hermanns, Schmidl, Wylie, Geimer, Zhukov, Knobloch*
- Performance Optimization */ Iliev*
- Programmer productivity */ Miller*
- Project ELP */ Cramer*
- Project ScaMPo */ Klinkenberg*
- Research and Development */ Hermanns*
- Training activities */ Wylie*

> NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE CSG ParE

- NUDT/NSCC, China on parallel performance tools
- RIKEN, Japan on parallel performance tools
- Lawrence Livermore National Laboratory, USA on performance tools
- EIC (Exascale innovation center) with IBM
- ECL (Exa Cluster Lab) with Intel and ParTec
- Virtual Institute – High Productivity Supercomputing (VI-HPS), 2007-2013, Helmholtz
- ELP (Effektive Laufzeitunterstützung für zukünftige Programmierstandards), 2013-2016, BMBF
- Mont-Blanc 2 (European approach towards energy efficient high performance), 2013-2016, EU
- Score-E (Scalable Tools for the Analysis and Optimization of Energy Consumption in HPC), 2013-2016, BMBF
- Human Brain Project, 2013-2016, EU OpenFET
- POP (Performance, Optimization and Productivity Center of Excellence), 2015-2018, EU H2020
- MYX (Scalable correctness checking methods for YvetteML, XcalableMP and selected features of MPI), 2016-2018, with RIKEN (Japan), University of Tsukuba (Japan), and Maison de la Simulation (France), DFG

> SELECTED CONFERENCE PARTICIPATIONS WITHIN THE CSG ParE

- Bernd Mohr, invited talk „**Multicore Performance at Scale: From two Embedded Cores to one Mittion HPC Cores**“ at Multicore@Siemens Konferenz 2016, Nürnberg, Germany, February 15, 2016
- Bernd, Mohr, invited talk „**Multicore Performance Debugging and Optimization at Scale: From Single Node to one Million HPC Cores**“ at Oak Ridge National Laboratory, Oakridge, TN, USA, August 08, 2016

> WORKSHOPS / EVENTS ORGANIZED BY THE CSG ParE

- Extreme Scaling on JUQUEEN, Jülich, Germany , February 01-03, 2016
- 20th VI-HPS Tuning Workshop, RIKEN AICS, Kobe, Japan, February 24-26, 2016
- PPCES 2016 – Parallel Programming in Computational Engineering and Science, Aachen, Germany, March 14-18, 2016
- 21st VI-HPS Tuning Workshop, LRZ, Garching, Germany, April 18-22, 2016
- JURECA Porting and Tuning Workshop, Jülich, Germany, June 06-08, 2016
- International Summer School on HPC Challenges in Computational Sciences Tutorial: Performance analysis and optimization, Ljubljana, Slovenia, June 30-July 01, 2016
- ISC16 Tutorial – Hands-on Practical Hybrid Parallel Application Performance Engineering, Frankfurt, Germany, June 19, 2016
- 22nd VI-HPS Tuning Workshop, Cambridge University, Cambridge, UK, July 06-08, 2016
- Score-P and Scalasca Performance Tools Training, Berkeley, CA, USA, July 26, 2016
- 23rd VI-HPS Tuning Workshop, LLNL, Livermore, CA, USA, July 27-29, 2016
- aiXvectorize Vectorization and Tuning Workshop, Aachen, Germany, September 21, 2016
- JARA-HPC Symposium 2016 (JHPCS'16), Aachen, Germany, October 04-05, 2016
- Practical Parallel Performance Analysis on Salomon, Ostrava, Czech Republic, October 20-21, 2016
- DKRZ 2016 Workshop: Program Analysis & Tools, Hamburg, Germany, October 25-27, 2016
- SC16 Tutorial – Efficient Parallel Debugging for MPI, Threads, and Beyond, Salt Lake City, UT, USA, November 13, 2016
- SC16 Tutorial – Advanced OpenMP: Performance and 4.5, Salt Lake City, UT, USA, November 14, 2016
- SC16 Tutorial – Practical Hybrid Parallel Application Performance Engineering, Salt Lake City, UT, USA, November 14, 2016,
- SC16 Workshop – 5th Workshop on Extreme-Scale Programming Tools, Salt Lake City, UT, USA, November 13, 2016
- aiXcelerate 2016 Tuning Workshop, Aachen, Germany, November 30-December 02, 2016,

> SELECTED HONORS, PRIZES AND AWARDS OF CSG ParE

- Best Poster Award:
  Vierjahn et al.: **"Correlating Sub-Phenomena in Performance Data in the Frequency Domain"**, LDAP 2016
- Best Paper Candidate:
  Rinke et al.: **"A Scalable Algorithm for Simulating the Structural Plasticity of the Brain"**, SBAC-PA

CHAIR FOR APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY (GGE) / E.ON ENERGY RESEARCH CENTER

RWTH / Prof. Christoph Clauser

> Water flow and permeability distribution in a tectonically limited hard-rock aquifer */ Johanna Bruckmann, M.Sc.*

In this project, we study water flow and permeability distribution in a tectonically complex hard-rock aquifer on reservoir scale by means of high-performance computing. We study a highly heterogeneous real-world aquifer as well as synthetic scenarios for improving groundwater (i.e. drinking water resources) management. This project is affiliated to the Centre for High Performance Scientific Computing in Terrestrial Systems (HPSC TerrSys) within the Geoverbund ABC/J.

A structural and conceptual reservoir model of the real-world aquifer near Eschweiler (Germany) (Burs et al. 2016) is the basis for the numerical reservoir model (see figure). We employ numerical simulations for analyzing experimental data, in particular piezometer time series. Field-scale, high-resolution simulations address groundwater flow and related permeability using an equivalent porous medium approach. Stochastic simulations based on the Monte Carlo approach enable estimating hydraulic model parameters and their uncertainties. Forward and inverse models of this size can be realized only with high-performance computing power. To this end, the GGE in-house code SHEMAT-Suite is used for flow and transport simulations and data assimilation that includes an MPI parallel Monte Carlo algorithm.

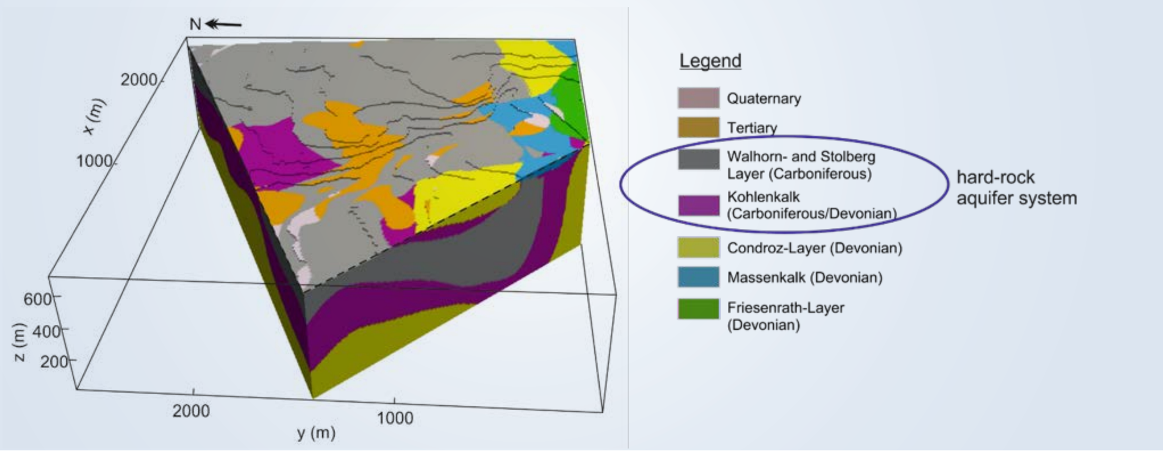
During the report period, we set up a stochastic model of the aquifer based on geostatistical analysis of permeability data from pumping tests. We simulated and analyzed 1000 realizations of a long term multiple step production test as performed in 2006. Comparing the simulated ensemble to monitoring data from six wells within the aquifer yields an average root mean square error of 2 m. The model's quality of fit could be improved by 1.4 m using stochastic simulations of a heterogeneous permeability field compared to using a homogeneous permeability field. In conclusion, we showed the applicability of an equivalent porous medium approach combined with stochastic parameter estimation for calibrating a heterogeneous hard-rock aquifer model to transient production test data.

References:

Burs, D., Bruckmann, J., Rüde, T.R., 2016. Developing a structural and conceptual model of a tectonically limited karst aquifer: a hydrogeological study of the Hastenrather Graben near Aachen, Germany, Environmental Earth Sciences, 75 (18), doi: 10.1007/s12665-016-6039-x.

PROJECT NUMBER JHPC28

Clip of the gridded three dimensional reservoir model of the Hastenrather Graben. A discretization of 10 m x 10 m x 10 m was necessary for resolving the complex geological structures such as the graben structure and folds. The legend describes the lithostratigraphy of model units. The Walhorn- and Stolberg Layer and the Kohlenkalk Formation build the hard-rock aquifer system that is the interest of our HPC simulations.



> Numerical Simulation of CO_2 Geo-Sequestration */ Dipl.-Math. Henrik Büsing*

The numerical simulation of geological CO_2 sequestration is computationally very demanding. On the one hand dissolution effects on a very small centimeter scale occur, while on the other hand CO_2 injection has pressure effects on a kilometer scale. This leads to the necessity to simulate on a reservoir scale while still maintaining a very high resolution of the computational grid.

Due to the strong coupling of the involved partial differential equations, often a fully implicit approach, relying on the implicit Euler method in time, is taken. Then in every time step in every Newton step a linear system needs to be solved.

We examined the performance of two different iterative solvers in a weak scaling test for the solution of these linear systems. Classical iterative solvers (such as ILU-preconditioned BiCGStab) might deteriorate in performance when increasing the resolution in space. In contrast algebraic multigrid methods (AMG) promise to have a stable number of iteration steps under refinement.

We compared a classical Constrained Pressure Residual approach (CPR-AMG) with a Schur complement reduction method (SCR-AMG) within PETSc (the Portable Extensible Toolkit for Scientific computation). This has the advantage of a fair comparison between the two methods. Both methods solve the two-phase flow equations in a very efficient way. Nevertheless, the efficiency in the weak scaling test was not optimal. Interestingly, this was not due to increased time for the linear solve, but rather due to an increase in the time to extract submatrices. The reason for this was a bad hashing algorithm for this specific problem. To finally judge, which method offers the better performance, at first this problem has to be resolved.

PROJECT NUMBER jara0128

CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)

RWTH / Prof. Marek Behr, Ph.D.

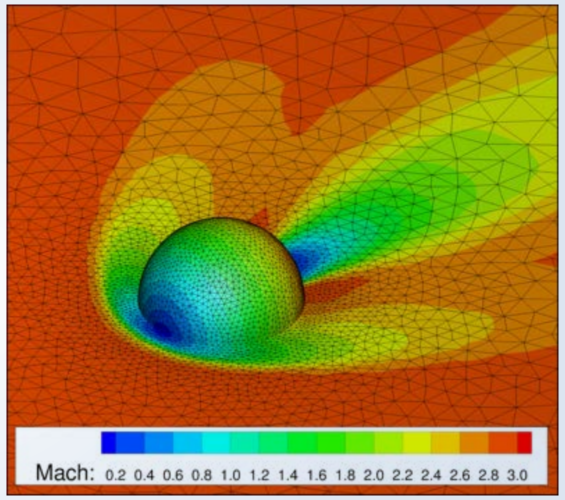
> Parallel Stabilized Finite Element Methods for Aero-, Hemo-, and Hydrodynamics

The objective of this project is the continued development of effective simulation methods for the unsteady flows of fluids.

The methods are based on the finite element technique using stabilized formulations. We use iterative solution strategies to solve nonlinearities and discretize the time by using either implicit time-stepping algorithms or space-time finite elements.

These methods enable simulations that include rotating, translating, and deforming domains.

Figure 1: Supersonic flow over a 3D sphere.



The main areas where novel computational methods are being developed are:

- simulation of rapidly translating and/or rotating boundaries, the Shear-Slip Mesh Update Method (SSMUM) and the multiple reference frames (MRF) method
- simulation of flows of microstructured liquids, the effect of flow on the microstructure in case of blood
- simulation of non-Newtonian fluids
- simulation of two-phase and free-surface flows
- fluid-structure interaction
- shape optimization of complex geometries, shear-thinning fluids and free-surface filling processes, and
- simulation of solidification.

PROJECT NUMBER JHPC07

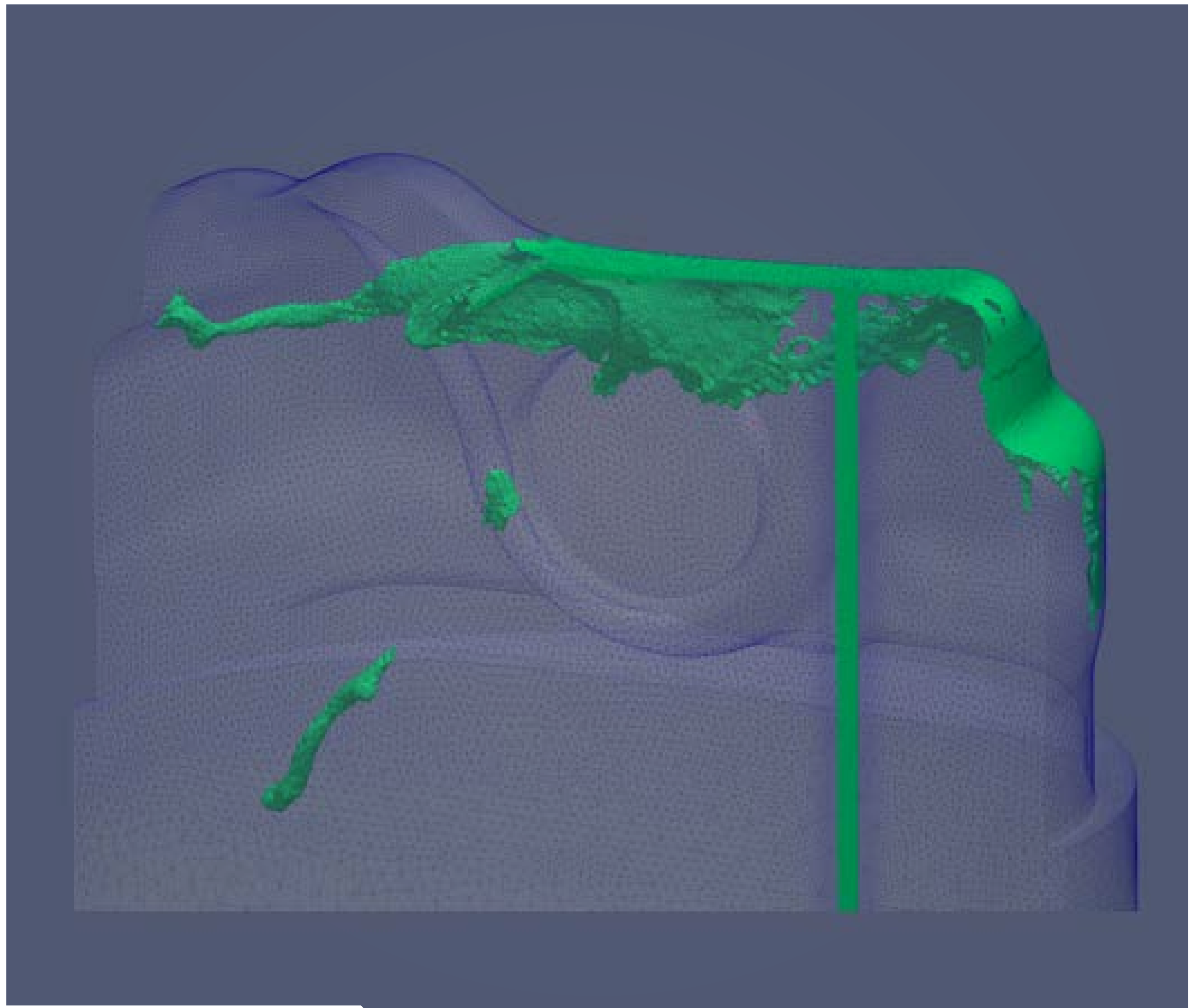


Figure 2: Oil spreading with real piston geometry.

> Parallel Stabilized Finite Element Methods for the Viscoelastic Flow Simulations of Microstructured Fluids

The objective of this project is to develop efficient numerical methods for the viscoelastic flows of microstructured fluids; i.e., the Single-Walled Carbon Nanotube (SWNT) suspensions. SWNTs demonstrate unique properties in molecular scales, which makes them ideal candidate as building blocks for multifunctional nano-materials. In this project, we aim to improve our understanding of material assembly processes (at macroscale) with the help of numerical methods. The complexity of the microstructural fluids results in highly nonlinear constitutive equations, which are usually derived from molecular and kinetic theories or via thermodynamic extensions in order to retain the micro-macro features of the flow. In this project, we use the constitutive model that was developed for the liquid-crystalline polymers (LCPs). This model employs the mean-field potential that adds the non-local elasticity.

PROJECT NUMBER JHPC34

CHAIR OF COMPUTER SCIENCE 6 / HUMAN LANGUAGE TECHNOLOGY AND PATTERN RECOGNITION

RWTH / Prof. Hermann Ney

> Deciphering Foreign Language

This project aims at treating translation of natural language as a decipherment problem. As opposed to the current state-of-the-art—which needs pairs of sentences that are translations of each other as training material—the decipherment approach is based only on (large) amounts of non-parallel data:

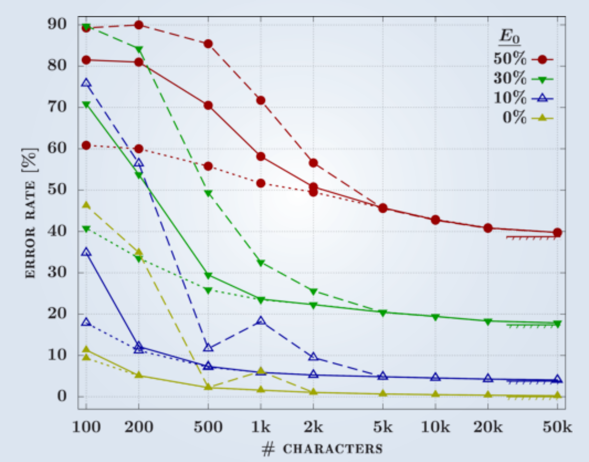
Just like cryptographers and archaeologists are able to decipher cryptograms by exploiting the statistical properties of the cryptograms and of the original plain text language, we aim at deciphering foreign language by exploiting the statistical properties of the source and target language. In this project we apply techniques developed in the field of statistical natural language processing to the decipherment problem and use the developed techniques to:

- Decipher ancient texts and previously unsolved ciphers
- Train automated natural language translation systems without parallel data

In order to determine the conditions which are necessary for decipherment methods to work successful, we conduct thorough simulation experiments, where we vary the most relevant conditions. The figure exemplarily presents the results of such a simulation experiment, where the analyzed conditions are the amount of cipher text, the noise ratio and the initialization of the decipherment method.

PROJECT NUMBER jara0040

Decipherment error rate in dependence of amount of available cipher text (#characters) and noise ratio E_0 of cipher text. Different linestyles indicate different initialization methods.



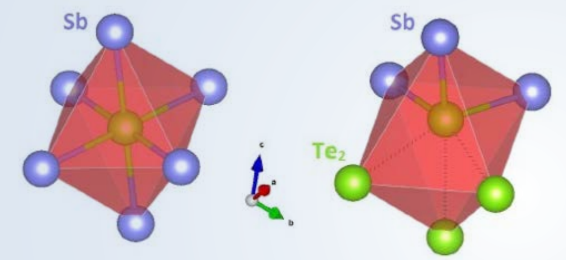
CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)

RWTH / Prof. Matthias Wuttig

> Breakdown of resonant bonding in Ge-Te-Se and Sb-Te-Se

Resonant bonding (RB) is identified as the most important feature in chalcogenide crystals, yet is a controversial idea in chemistry. Starting from GeTe and Sb_2Te_3, two different tellurides with RB, we demonstrate that such special bonding mechanism eventually breaks down by substituting Se for Te. Ab initio calculations have been performed to reveal the atomic and electronic structures accompanied with the transition. The atoms have been rearranged from an octahedral-like local motif to a less octahedral-like one (see figure). The calculated optical constants and Born effective charge also provide strong evidence for the breakdown of RB.

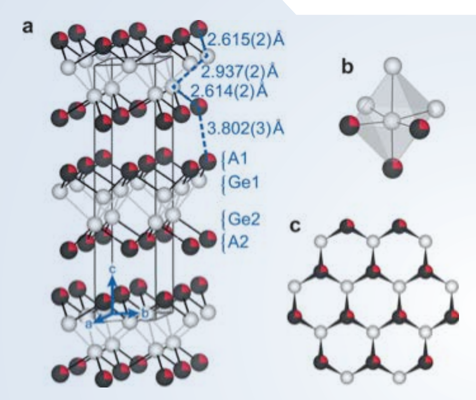
The local structure has changed from a octahedral-like cluster to a less octahedral-like one.



> Atomic structure and bonding nature of single crystalline Ge_4Se_3Te

A single crystal of Ge_4Se_3Te has been grown and the bonding nature has been studied using first principles calculations. The atomic structure of single crystal consists of layers that are held together by van der Waals type weak chalcogenide–chalcogenide interactions but also display unexpected Ge–Ge contacts (see figure). The nature of the electronic structure of Ge_4Se_3Te was characterized by chemical bonding analysis, in particular by the newly introduced density of energy (DOE) function. The results show that strong Ge-Ge contacts reshuffle electrons from antibonding Ge-Te into bonding Ge-Ge contacts. The analysis of the density of energy (DOE) function clarifies the importance of both off-site and on-site energetic contributions for phase stability. [1] These projects are done in collaboration with Prof. Richard Dronskowski.

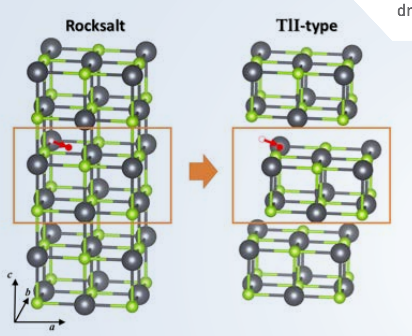
The atomic structure of Ge_4Se_3Te.



> Structural transition of GeSe and PbSe at high pressure

GeSe and PbSe were subjected to high pressure. Structural transitions have been identified under synchrotron x-ray diffraction and computer simulations. GeSe undergoes a transition from an orthorhombic structure to a more symmetric one under high pressure. Judging from the calculated optical constants and Born effective charge, we find that the resonant bonding is established in such more symmetric GeSe. In contrast, PbSe experiences an opposite transition from a highly symmetric cubic to a less symmetric orthorhombic structure, in which the resonant bonding is weakened (see figure). These projects are done in collaboration with Prof. Riccardo Mazzarello.

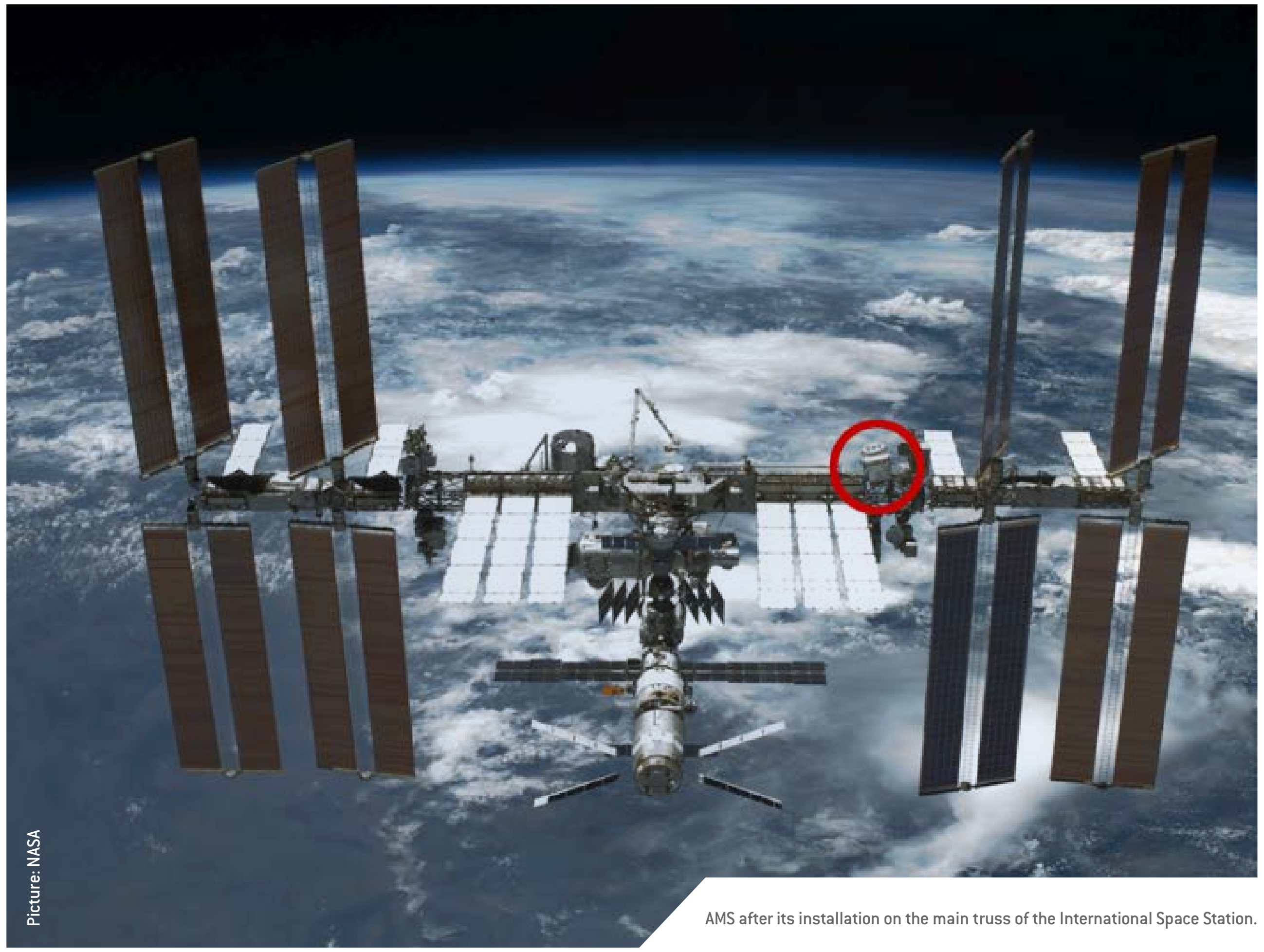
Structural transition of PbSe driven by high pressure.



CHAIR OF EXPERIMENTAL PHYSICS, I. PHYSICS INSTITUTE B

RWTH / Prof. Stefan Schael

> COSMIC-RAY PHYSICS WITH THE AMS EXPERIMENT ON THE INTERNATIONAL SPACE STATION



AMS after its installation on the main truss of the International Space Station.

AMS is a detector designed for precision spectroscopy of cosmic rays that was installed on the International Space Station in May 2011 (see figure). With dimensions of 5x4x3 m^3 and a weight of 7.5 tons, AMS is the largest cosmic-ray spectrometer ever built. Its construction began in 1995, and a successful prototype flight aboard the Space Shuttle Discovery proved the feasibility of the detector concept in 1998. Led by Nobel laureate Professor Samuel Ting from MIT, AMS has been constructed and is now operated by an international collaboration of more than 200 scientists and engineers, from Europe, America and Asia. The overall construction costs, including the flight of AMS to the Space Station aboard Space Shuttle Endeavour, have amounted to 1.5 billion US dollars. In Germany, RWTH has been strongly involved in the AMS project since its inception. One of the main components of AMS, the transition radiation detector (TRD), has been designed and constructed by the I. Physikalisches Institut B under the direction of Prof. Stefan Schael. Today, the Aachen group, comprising 20 scientists and students, plays a major role in the analysis of the data gathered by AMS and in the operation and calibration of the instrument.

Since their discovery in 1912, cosmic rays have held many surprises in stock for us, from the discovery of new elementary particles to the most violent processes taking place in the Universe and accelerating cosmic rays to enormous energies. As a multi-purpose instrument for the precision spectroscopy of cosmic rays, AMS was conceived to answer fundamental questions about our Universe: What is the nature of Dark Matter? What happened to the antimatter that must have been produced in the Big Bang? Where are cosmic rays accelerated and how do they propagate through the Milky Way? Answers to these questions will have a profound impact on our understanding about the inner workings of our Universe and help advance fundamental science. In particular, the search for dark matter complements the endeavour to search for new elementary particles at the Large Hadron Collider (LHC) at CERN, Geneva.

AMS so far has recorded more than 95 billion individual particle crossings (so called "events"). The raw data volume collected is on the order of 40 TB per year. AMS employs three different subdetectors for particle identification (the TRD, an electromagnetic calorimeter and a ring-imaging Cherenkov counter) and two subdetectors for energy or momentum measurements (a silicon tracker and a time-of-flight system). Before any physics analysis of the data can be performed, the information from all these subdetectors has to be pieced together and complicated reconstruction algorithms have to be run for each of them. The resulting high-level data serves as the input for physics analyses and occupies a volume of 160 TB per year of AMS flight on disk.

Several processing runs of AMS data have already been conducted successfully on the JUROPA and JUAMS clusters at JSC as the result of the cooperation within JARA.

Until 2016, eight publications from the AMS collaboration have appeared in the renowned Physical Review Letters, six of which have been selected as an Editor's suggestion. The findings have received considerable attention among astrophysicists and triggered an enormous amount of theoretical work. The two recent publications from 2016 deal with the cosmic-ray fluxes of anti-protons and the ratio of boron to carbon (B/C), respectively. The ratio of anti-protons to protons shows an unexpected flattening at high energies, possibly in excess of model calculations for the flux of background antiprotons, which originate in interactions of cosmic-ray primaries with interstellar matter. This may hint at an exotic contribution. In addition, the behaviour of the fluxes of protons, anti-protons, and positrons as a function of energy are found to be practically identical. This surprising observation challenges our understanding of the production and propagation of secondary cosmic rays. Remarkably, above 65 GV, the B/C ratio is well described by a single power law in rigidity (momentum per charge) with an index of 0.333 ± 0.014 (fit) $\pm$ 0.005 (syst), in good agreement with the Kolmogorov theory of turbulence which predicts a value of 1/3 asymptotically.

PROJECT NUMBER jara0052

CHAIR OF PHYSICAL CHEMISTRY I / PHYSICAL CHEMISTRY OF SOLIDS

RWTH / Prof. Manfred Martin

> Ab-initio study of composition, structure and conductivity in interstitial oxygen conductors

In classical oxygen ion conductors, like stabilized zirconia and doped ceria, the oxygen migration is enabled by a vacancy hopping mechanism. In contrast, oxygen ion conductors, where an interstitial mechanism is present, are not as well established although they are equally promising. In this project, starting from November 2016, materials with an oxygen interstitial mechanism are investigated.

In particular, the energies of formation and migration of defects in apatite-structured materials with the composition $A_8B_2Si_6O_{26}$ are calculated. First ab-initio calculations concerned the optimization of the crystal structure for various compositions and the estimation of the energy of formation of oxygen interstitials. Following computations will deal with the modeling of the migration path of oxygen ions.

PROJECT NUMBER jara0156

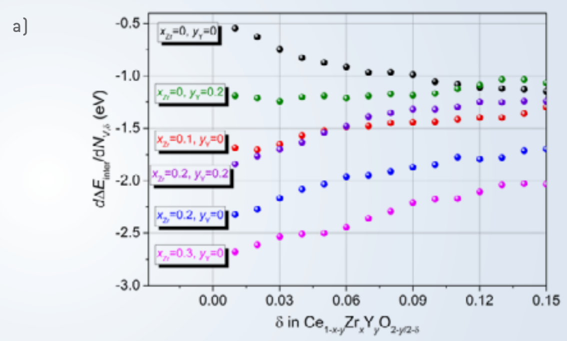
> Ab-initio study of structure, conductivity and thermodynamics of doped and non-stoichiometric ceria

Previously, we investigated the interactions of defects in rare-earth doped ceria. In this period extended this approach to ceria doped with zirconia and co-doped with zirconia and yttria.

Interaction energies were calculated for a pair of a zirconium ion and another Zr^{4+} ion (Zr-Zr), a Ce^{3+} ion (Zr-Ce'), a Y^{3+} ion (Zr-Y) or an oxygen vacancy (Zr-V). The pair interaction energies were applied in Metropolis Monte Carlo simulations in order to investigate the influence of Zr-doping on the energy of reduction. The simulations reveal a significant decrease of the lattice energy implying a decrease of the energy of reduction (Figure 1a).

This trend was already found for rare-earth doped ceria but is stronger in Zr-doped ceria due to the strong attraction of oxygen vacancies by Zr^{4+} ions. However, additional doping with yttria mitigates this effect as oxygen vacancies, which accompany the trivalent doping, are bound to the zirconium ions. The strong association between the zirconium ions and oxygen vacancies originates from the local relaxation of the ions around the defect pair (Figure 1b).

PROJECT NUMBER jara0035



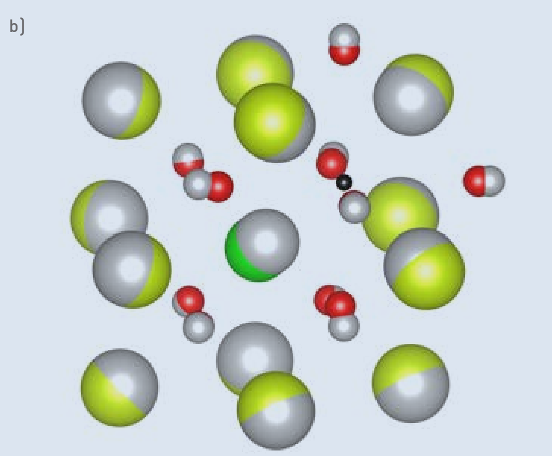


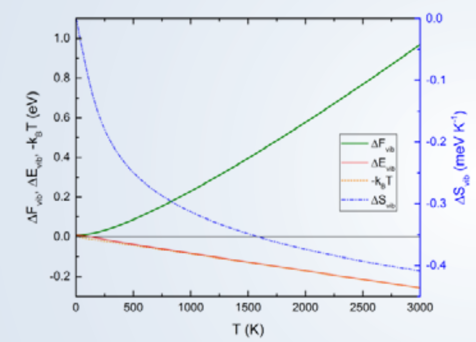
Figure 1a): Change of the energy of reduction due to defect interaction in pure ceria and ceria doped with yttria and zirconia. b) Lattice distortion around a pair of oxygen vacancy (black) and zirconium ion (green).

> Attempt frequency of oxygen ion jumps in doped ceria

The rate of oxygen ion jumps in a solid oxide depends not only on the activation energy but also on the pre-exponential factor of diffusion ν0. In order to allow a fully ab-initio prediction of the oxygen ion conductivity we calculated the attempt frequency for an oxygen ion jump from first principles using DFT+*U*, NEB, phonon calculations and the transition state theory.

For pure ceria, the vibrational free energy difference ΔF_{vib} and its components, the vibrational energy difference ΔE_{vib} and entropy difference ΔS_{vib}, in ceria in harmonic approximation for a 6×6×6 phonon mesh are shown in Figure 1. The vibrational energy difference is similar to $-k_B T$ as it differs less than 5 % for temperatures above 900 K.

Figure 1: Vibrational free energy difference ΔF_{vib}, vibrational energy difference ΔE_{vib} and entropy difference ΔS_{vib} of initial and transition state in ceria in harmonic approximation for a 6×6×6 phonon mesh. For comparison $-k_B T$ is shown which is similar to ΔE_{vib}.



Doping ceria with Sm increases the pre-factor for dopants both perpendicular to the oxygen migration path at the 'migration edge' and dopants in nearest neighbor position to the start position of the oxygen vacancy (Figure 2). However, a single Sm dopant at the migration edge has no influence on the attempt frequency. Reason for this is the oxygen migration path with deviates from the direct straight path found for the Ce-Ce and Sm-Sm edge between initial and final position. For the Ce-Sm edge the migrating oxygen follows a curved path by avoiding the steeper electronic energy curvature and a higher attempt frequency. Key properties are the distances of the edge cations in the transition state and the initial state. The electronic migration energies of the different edge configurations depend linearly on the difference of the distances of the edge cations between transition and initial state. Simply described, the cations at the edge must be pushed apart during an oxygen ion jump. This leads to a linear relationship between the widening of the edge cations and the migration energy. Likewise, the attempt frequency is majorly influenced by the edge cation distance in the transition state d_{TS}. For the Ce-Ce and Ce-Sm edge ν0 and d_{TS} are similar, respectively. Both values increase significantly for the Sm-Sm edge. In contrast, a single Sm dopant in nearest neighbor position to the start position of the oxygen vacancy has a larger attempt frequency than pure ceria or two Sm dopants at the same position.

Figure 2: Oxygen vacancy attempt frequency ν0 in harmonic approximation in samarium doped ceria with different number of dopants at the migration edge (black) or in nearest neighbor position to the start position of the oxygen vacancy (blue), using the generalized Vineyard method at a temperature of 900 K.

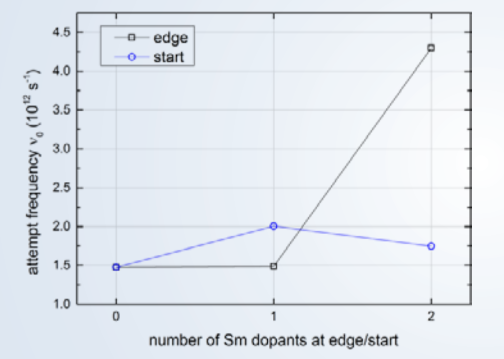


Figure 3: Assumed migration edge configurations in samarium doped ceria. Ce-Ce edge (left), Ce-Sm edge (middle) and Sm-Sm edge (right). Cerium ions (green), samarium ions (blue), oxygen ions (red spheres) and oxygen vacancies (red boxes).

We have studied the free energy migration barriers ΔF for oxygen diffusion in pure ceria and Sm doped ceria at 300 K. The migration of oxygen vacancies in fluorite structured ceria is considered between adjacent tetrahedral oxygen sites in <100> direction. Along this migration pathway two cations form a 'migration edge'. In pure CeO_2, only cerium ions are at the migration edge, while doping with samarium oxide leads to configurations with one or two Sm ions at the migration edge (compare Figure 3).

We used the density functional theory in the generalized gradient approximation and an additional Hubbard U parameter for the Ce 4f electronic states. We compare the results for the free energy deduced from two different methods. First, the total energy difference between the equilibrium state and the transition state is calculated using a static structure optimization for the equilibrium state and the improved dimer method. The vibrational contributions, energy and entropy, are deduced from the phonon frequencies. Second, the free energy is calculated by molecular dynamics using the metadynamics method.

The atomic relaxation of the ions for $(Ce_{32}O_{63})^{2+}$ shows that in the equilibrium state the migrating oxygen ion O_m is shifted from the equilibrium position in the ideal CeO_2 lattice by about 0.2 Å towards the oxygen vacancy. In the transition state the distance between O_m and the migration edge Ce ions is about 0.2 Å shorter than the Ce-O bonding distance in bulk ceria in accordance with an earlier work. We have calculated the free energy of activation or migration free energy $\Delta F_{a\to b}$, the results are summarized in Table 1. We have checked the accuracy by calculating $\Delta E_{el,a\to b}$ for a = 5.411 Å for different parameter settings. We found that the increase of the limit of the kinetic energy from 400 to 500 eV or the increase of the number of k-points changes the values for $\Delta E_{el,\ a\to b}$ by less than 0.002 eV.

Table 1: Migration energy, migration free energy (in eV) and migration entropy (in meV/K) in ceria and Sm doped ceria according to a static approximation for $\Delta E_{el,a\to b}$ & harmonic Γ-point approximation for $\Delta F_{vib,a\to b}$. Listed are the electronic (el) & vibrational (vib) contribution to the total free energy barrier $\Delta F_{a\to b}$.

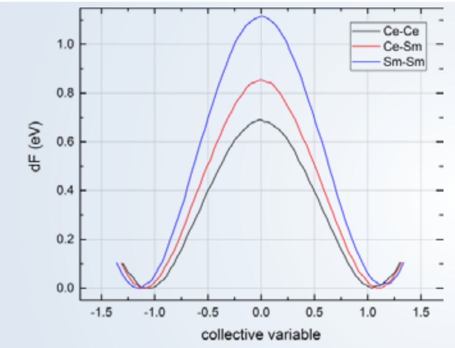
Migration edge	$\Delta E_{el,a\to b}$	$\Delta E_{vib,a\to b}$	$T\Delta S_{vib,a\to b}$	$\Delta F_{vib,a\to b}$	$\Delta F_{a\to b}$
Ce-Ce	0.70	-0.04	0.03	-0.07	0.63
Ce-Sm	0.85	-0.11	-0.05	-0.06	0.79
Sm-Sm	1.19	-0.03	0.01	-0.04	1.15

As expected, the influence of the vibrational energy and vibrational entropy on the migration free energy is small. Surprisingly, both positive and negative vibrational entropies have been found. The migration free energy is always smaller than the static, electronic energy as the sum of vibrational energy and entropy contributions is negative.

Figure 4 shows the free energy profile as a function of ξ for ceria determined using metadynamics. The simulation has been finished when the difference between the minimum and the maximum of $-\tilde{V}(\xi)$ was stable within 0.01 eV. We see that the metadynamics method gives the same trend for the free energy barrier as the static, harmonic calculation.

The influence of the supercell size is small. While for the static, electronic energy calculations the increase of the unit cell from 2×2×2 to 3×3×3 decreases $\Delta E_{el,\,a\rightarrow b}$ by 0.04 eV, the supercell size influence in the metadynamics calculations is even smaller.
The main aim of this work is to demonstrate that the metadynamics procedure is a powerful tool to study diffusion processes in oxides. Within this method, the restrictions of harmonic approximation,

Figure 4: Shape of the free energy along the y-axis of a migrating oxygen ion in ceria for the different migration edges given in Figure 3 at 300 K. Displayed is $-\tilde{V}(\xi) = \Delta F$ as a function of the collective variable ξ where $\tilde{V}(\xi)$ is the bias potential



such as the presumed shape of potential energy surface and decoupling of vibrational modes, are lifted and by choosing appropriate collective variables, even complex diffusion jumps can be taken into account. The metadynamics procedure might even be useful for amorphous systems if it is possible to clearly define the initial and final states in terms of one or a few structure descriptors or internal coordinates.

PROJECT NUMBER JHPC27

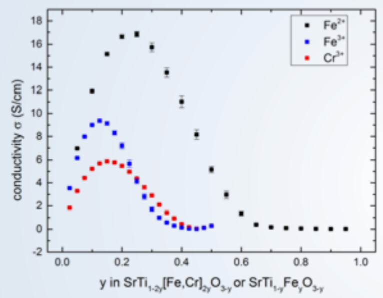
> Oxygen ion conductivity of doped $SrTiO_3$ and $CaTiO_3$ and beyond: A DFT and Kinetic Monte Carlo study

Migration energies in the perovskite Cr-doped $SrTiO_3$ and Fe^{3+}/Fe^{2+}-doped $SrTiO_3$ were calculated and all migration energies were used to perform Kinetic Monte Carlo simulations to obtain ionic conductivities (see Figure 1). The resulting conductivity curves show clear differences. By a thorough analysis of the jump frequencies these differences could be assigned to the influence of single migration energies and configurations.

Migration energies in undoped and doped $CaTiO_3$ were calculated. The analysis of the elemental cell of $CaTiO_3$ revealed that it is possible to halve the number of migration energies needed for jumps in 1NN due to geometrical reasons. It could also be shown that the influence of longer jumps is not negligible for high dopant concentrations. Looking forward to the future, more calculations will be necessary but we are confident that further geometrical analysis allows to calculate longer jumps with reasonable effort.

With the obtained migration energies, the oxygen conductivity in $CaTiO_3$ was simulated by means of Kinetic Monte Carlo calculations. To our best knowledge this was the first time these simulations were performed for this material. During these calculations an averaged activation energy for the oxygen migration in undoped $CaTiO_3$ was found as well as for doped $CaTiO_3$. In Figure 2 jumps with the same migration energy are marked in the same color. The migration energy is lower for green jumps than for red jumps. Trails of low migration energies through the crystal are built. As a result it was found that the conductivity is dependent of the direction of the ion flux.

Figure 1: Simulated conductivity of the oxygen ions in $SrTi_{1-2y}[Fe, Cr]_{2y}O_{3-y}$ (with Fe^{3+}) or $SrTi_{1-y}Fe_yO_{3-y}$ (with Fe^{2+}) at 1000 K in a 16x16x16 lattice with the migration energies obtained by the 333-supercell.



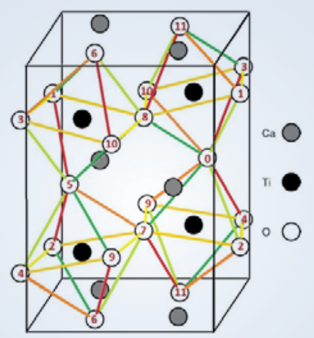


Figure 2: Elemental cell of $CaTiO_3$[1]. Equal jumps are marked in the same color.

References: E. Cockayne, B. P. Burton, Physical Review B 2000, 62(6), 3735 - 3743

PROJECT NUMBER jara0141

INSTITUTE FOR ADVANCED SIMULATION (IAS)

FZ Jülich / Theoretical Nanoelectronics (IAS-3) / Prof. David DiVincenzo / Prof. Eva Pavarini,

>Multiplet effects in strongly correlated material

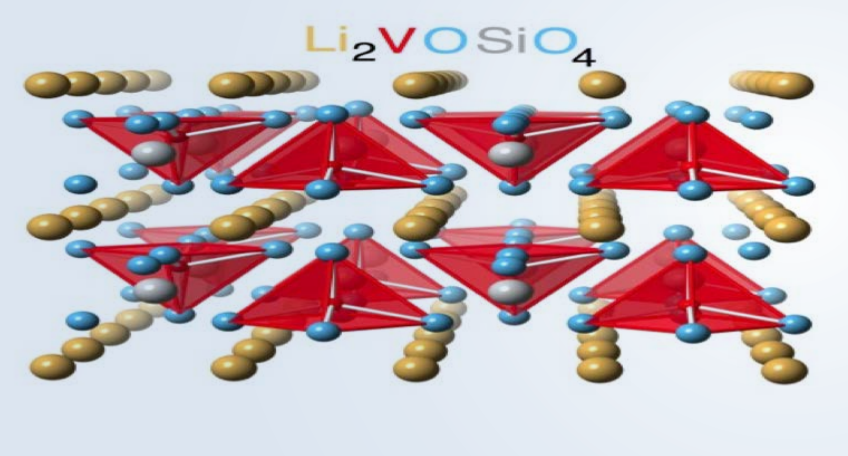
In the one-electron picture, completely filled or empty bands characterize insulators while metals have some partially filled bands. Strongly-correlated systems are different, however. Mott insulators would be band metals in the absence of electronic correlation, while strongly-correlated metals behave as Fermi-liquids only at low-energy and temperature. The bottleneck to study strongly correlated materials is the description of electronic many-body effects in a realistic setting. Density-functional theory in the local-density approximation (or its simple generalizations) fail even qualitatively for strongly correlated systems, predicting, e.g., a metallic ground state for Mott insulators.

The development of the LDA+DMFT method which merges DFT with a powerful many-body approach, dynamical mean-field theory (DMFT) has strongly advanced the field, but a lot remains to be done. The aim of this project is to address one of the major open problems, i.e., to unravel the role of multiplets in the physics of correlated transition-metal oxides. To this aim we have developed general DMFT solvers based on the continuous-time quantum Monte Carlo technique. In the last funding period we have studied in particular the interplay between spin-orbit coupling, crystal-field splitting, realistic multiplets and hoppings, in strongly correlated ruthenates.

> Spin-orbital order-disorder transitions in strongly correlated systems

Strongly-correlated materials exhibit spin and orbitally disordered phases, the nature of which is little understood. The main difficulty lies in the fact that, to address the issue, spin-orbital degrees of freedom, chemistry, strong correlations have to be treated on the same footing, and, at the same time, in large clusters might have to be considered. Paradigmatic systems are colossal magneto-resistance manganites, cuprates, and cobaltates. Conventional ab-initio or mean-field methods fail qualitatively. The aim of the project is to unravel the nature of spin-orbital order-disorder transitions and frustration phenomena in representative transition-metal oxides. In the last funding period we have studied in particular the nature of the Mott transition and spin-frustration phenomena in a family of strongly correlated materials, layered vanadates.

The structure of the strongly-correlated vanadate Li2VOSiO4. We have recently shown that, contrarily to early suggestions, this system is weakly frustrated [A. Kiani and E. Pavarini , Electronic correlation and magnetic frustration in Li2VOSiO4 and VOMoO4, Phys. Rev. B 94 , 075112 (2016)]



INSTITUTE FOR ADVANCED SIMULATION (IAS) / INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

FZ Jülich / Computational Biomedicine (IAS-5) & Computational Biomedicine (INM-9) / Prof. Paolo Carloni

> Allosteric effect of Na+ on the activation of μ-opioid receptors by enhanced sampling techniques

G-protein coupled receptors (GPCRs) allow cells to recognize diverse extracellular stimuli and transduce the signals across the plasma membrane to regulate central physiological processes. In addition to their canonical orthosteric ligands, several endogenous allosteric modulators (regulatory proteins, lipids, ions, etc.) can modulate the GPCR activation. For instance, sodium ions have been proved to play an important role in modulating μ-opioid receptors (μOR) activity. Specifically, it is known that sodium ions decrease the agonists binding affinity to μOR and the μOR basal activity (i.e. without binding an agonist), while promote agonist-induced responses. This dual opposing roles of sodium in modulating the receptor activation are still not understood.

In this project we have coupled accelerated MD (AMD) simulations and well-tempered (WT) metadynamics to fully characterize the effect of sodium on the conformational selection and kinetics of the activation process of mouse μOR, both in the apo form (i.e. without agonist, to mimic the basal activity of the receptor) and upon binding with the prototypical opioid agonist morphine. Our results will provide a molecular explanation that reconciles the contradictory observations of why sodium ions increase agonists effectiveness whilst decrease constitutive activity.

PROJECT NUMBER JARA01572016

> Predicting the apo-structure of a NEET protein involved in health and disease

The NAF-1 protein is an Fe-S protein belonging to the family of NEET proteins. This protein is composed by two intertwining monomers and each monomer contains an 2Fe-2S cluster coordinated to the protein by 3Cys:1His motif, which confers liability to the cluster. This protein is important for neuronal development, in particular it has been shown to be critical for the maintenance of skeletal muscle and for promoting longevity. It has also been reported to be involved in severe genetic disorders (e.g. Wolfram Syndrome). Although the relevant cellular pathways are still unknown, most likely they involve the release of the FeS cluster.

In this project we have used replica exchange solute tempering (REST)2 simulations in order to the structure of the protein in the two possible apo-states: the protein without one FeS (holo-apo state) and the protein without the two FeS (apo-apo state). Our results will be validated by comparison with the NMR experiments provided by our experimental collaborator Rachel Nechushtai (Hebrew University of Jerusalem).

PROJECT NUMBER JIAS57

> Towards the design of allosteric ligands binding to the human muscarinic receptor M2

Allosteric ligands (ALs) activate neuroreceptors by binding in a protein region topographically distinct from the canonical orthosteric site. They are usually more specific than the traditional agonist/antagonist molecules, making them highly amenable for brain imaging applications. In this project, we planned to identify new ALs targeting the five members of the muscarinic receptors subclass (M1-M5) of G-protein coupled receptors. Located mostly in the cerebral cortex, muscarinic receptors are implicated in many physiological brain functions.

In particular, we investigated the binding of different allosteric and orthosteric ligands to the M2 receptor using classical molecular dynamics. Our simulations allow to compare the differential protein-ligand interactions for each of the receptor-ligand pairs. This structural and dynamical information is essential to build a reliable 3D pharmacophore model. We plan to apply this model for structural-based virtual screening to identify novel potential candidates for allosteric modulation, which may be subsequently tested experimentally using receptor autoradiography.

PROJECT NUMBER JIAS59

> Ligand binding to the OR7D4 odorant receptor studied by multiscale molecular simulations

Olfactory receptors (ORs) are membrane proteins, which belong to the class A human G-protein coupled receptors (GPCRs) family. ORs bind volatile molecules, providing the first step in smell sensing. Moreover, it has been increasingly recognized that ORs are expressed in other tissues, besides the nose, where they play several physiological and pathological roles.

In this project, we have combined bioinformatics approaches and molecular mechanics /coarse grained simulations in order to characterize the structural determinants of the receptor OR7D4 in complex with the agonists androstenone and androstadienone. We will be able to pinpoint which residues are important for ligand binding and/or receptor activation. These predictions will be subsequently tested using molecular biology experiments.

In addition, we have run analogous simulations on a mutant of OR7D4 (more sensitive to both ligands) and on the paralog receptor OR2J2 (which has significant affinity for androstenone), in order to discriminate the key protein residues for ligand binding. The accuracy of our predictions will also be validated by comparison with site-directed mutagenesis experiments in the near future.

PROJECT NUMBER JARA0148

> Structural predictions of platinated DNA in complex with HMGB1A protein in quasi-in vivo conditions

Cisplatin is an effective anticancer drug in the treatment of several solid tumors. Cisplatin induces cell death by binding to DNA, inhibiting replication and transcription. Platinated lesions on DNA are recognized in vivo by the High mobility group box 1 (HMGB1). HMGB1 binding inhibits cisplatin–DNA damage repair in vitro and in cell, disfavoring drug resistance mechanisms. However, several factors limit the recognition of HMGB1 of platinated-DNA and that might, in turn, influence the efficacy of the drug, such as post-translational modifications (PTMs).

In this project, we have investigated the structural and functional effects of these PTMs, by means of classical molecular dynamics simulations in combination with enhanced sampling techniques (REST2). Our simulations show that the PTMs, as well as the presence of the protein tails, strongly affect the helical properties of the Pt-DNA and therefore its binding properties to HMGB1 box A.

PROJECT NUMBER JIAS56

> Copper binding to the physiological form of human alpha-synuclein

Parkinson's disease (PD) is the second most common neurodegenerative disease, affecting about 1.5 million people worldwide. Human protein α- synuclein (AS) is associated with the pathogenesis of the disease and the role of α-synuclein aggregation in the onset of PD is a subject of vivid debate. α-synuclein is a naturally unfolded monomeric protein, which is likely to be involved in the structural transitions of the protein to amyloid fibrils. Moreover, the protein's physiological form is acetylated on the N-terminus (AcAS), and acetylation affects the conformational ensemble on the protein, as well as its binding properties to membranes and to copper (II) ions. Copper (II) ions are present at high levels in the cerebrospinal fluid of PD brains and they are prominent group of α-synuclein aggregation modulators.

In this project, we have shed light into the the structural determinants of Cu(II) binding to the physiological form of α-synuclein, by means of extensive classical molecular simulations in combination with enhanced sampling techniques (REST2, see above).The accuracy of our predictions will be established by comparison with a variety of spectroscopic properties, such as NMR, X-ray absorption spectroscopy and circular dichroism (CD) spectroscopy, specifically measured for this project by our experimental collaborators (Prof. Fernández and Prof. Binolfi, Universidad Nacional de Rosario, Argentina).

PROJECT NUMBER JIAS54

> Molecular Simulation of the tRNA Cleavage Catalyzed by Human Angiogenin

Immunotoxins (ITs) are protein therapeutics for the treatment of malignant diseases, such as cancer. They are usually composed of a disease-specific binding moiety (antibodies or derivatives thereof) covalently linked to a catalytically active, cytotoxic effector domain (toxins, enzymes). Very encouragingly, the human angiogenin (HuAng)-containing IT exhibits (i) specific toxicity towards the targeted tumor cells after internalization; and (ii) promising cytotoxicity on tumor cells in vitro. HuAng is an RNase that cleaves cellular tRNAs to generate tiRNAs (or tiRNA halves). These events lead to the shutdown of translation, thereby promoting the induction of apoptosis. Nonetheless, the absence of structural and/or computational investigations of the enzymatic reaction of HuAng has hampered so far the rational design of more efficient HuAng variants, which are needed to improve ITs.

In this project, we have used Car-Parrinello based Quantum Mechanics/ Molecular Mechanics (QM/MM) simulations in order to investigate the reaction pathway of HuAng. Using metadynamics simulations, we have unraveled the molecular details of the phosphodiester cleavage reaction.

This information will allow us to design novel HuAng variants with enhanced catalytic activity, which will be validated in the near future by in vitro experiments conducted by the group of Prof. Stefan Barth (University of Cape Town, South Africa).

PROJECT NUMBER JIAS55

> Predicting the affinities of peptides binding to NEET proteins in Parkinson's disease

The NEET proteins mitoNEET (mNT) and NAF-1 are emerging as a potential therapeutic target for Parkinson's disease. These proteins belong to the NEET family of iron-sulfur (FeS) proteins, and feature a unique homo-dimeric structure, in which each monomer contains a labile 2Fe-2S cluster coordinated by 3Cys:1His. Upon non-physiological release of the cluster in the cytosol, the 2Fe-2S clusters dissociate, leading to an increase of reactive oxygen species. Remarkably, the liability of the cluster is affected by the binding of ligands, which has lead to the hypothesis that the development of specific ligands preventing cluster release may represent a promising route against the neuronal derangement associated with PD progression. Recently, our collaborators (Prof. Assaf Friedler and Prof. Rachel Nechushtai) have synthesized a small peptide YEWDA, which has been proved to be able to bind NAF-1 and mNT and affect the cluster release.

In this project, we will predict the binding pose of the peptide to the two NEET proteins by using docking approaches and molecular dynamics. Our calculations provide valuable structural information on the recognition process and on the specificity of the binding, which can be used to design novel binding compound with increased specificity for NAF-1 and mNT.

PROJECT NUMBER RWTH0092

> INSTITUTE FOR ADVANCED SIMULATION (IAS) / INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

Theoretical Neuroscience (IAS-6) & Computational and Systems Neuroscience (INM-6) /
Prof. Markus Diesmann

> Brain-Scale Simulations

The aim of this project is to simulate brain circuits at a scale where brain function occurs. The scope of the JINB33 project is two-fold: Models of large-scale cortical networks have to be constructed based on experimental data, simulated with the simulation tool NEST and analyzed by means of statistical analyses and analytical theory. These efforts are supported by the advancement of NEST in order to optimally exploit the resources of the JUQUEEN supercomputer.

In 2016, we made substantial progress on a manuscript entitled "Constructing neuronal network models in massively parallel environments" for the journal Frontiers in Neuroinformatics with the aim to describe the insights into the memory allocations in multi-process (MPI) multi-thread (OpenMP) simulations.

For the NEST simulator I/O performance the backend was generalized using SIONlib. After a first implementation and benchmarking tests in the last period, now code is in preparation for merging to the mainline and large-scale benchmarking across NEST behavior and SIONlib parameters has begun. Simulations have been conducted with the current code for 32 to 512 nodes with varying bandwidth loads over different portions of the simulation and show significant speedups.

For the runtime prediction for structured networks promising approaches for the dry-run mode exist and were implemented, but it is still necessary to collect data from a large set of real full simulations and to further refine and validate the dry-run-algorithms in a quantitative way on this data basis.

Full-scale models of cortical areas were simulated on JUQUEEN and both post-processing of simulation output and LFP predictions were carried out on JURECA. As one result, Figure 1 illustrates the relationship between spiking activity and LFP in our model.
An exploration of synaptic infrastructures for the exascale was performed using an implementation of the new connection infrastructure in the NEST simulator kernel. It was demonstrated that the new design has successfully removed the linear scaling of memory usage with network size that was present in the old simulation kernel (Figure 2).
A neural network model of deep brain stimulation was successfully ported to JUQUEEN. The testing of code performance for long-time simulations is currently starting from small scale simulations.

The Elephant[1] community-centered open-source Python library was used to compare and validate simulation data from NEST and SpiNNaker simulating the same $1x1mm^2$ micro-circuit model (Potjans-Diesmann, 2014, Celeb.Cortex).

[1] *ELEctroPHysiological ANalysis Toolkit*

PROJECT NUMBER JINB33

Figure 1: Instantaneous network and LFP activity in the 4×4 mm 2 spiking model. (A) Instantaneous spiking and LFP in a 4-layer network model covering 4×4 mm 2 at realistic cell and synapse density with distance-dependent connectivity. (B) Pairwise correlations between spike trains of excitatory and inhibitory layer 5 neurons as function of distance. (C) Distance-dependent LFP correlation computed for a 10×10 electrode grid in layer 5 (0.4 mm between contacts).

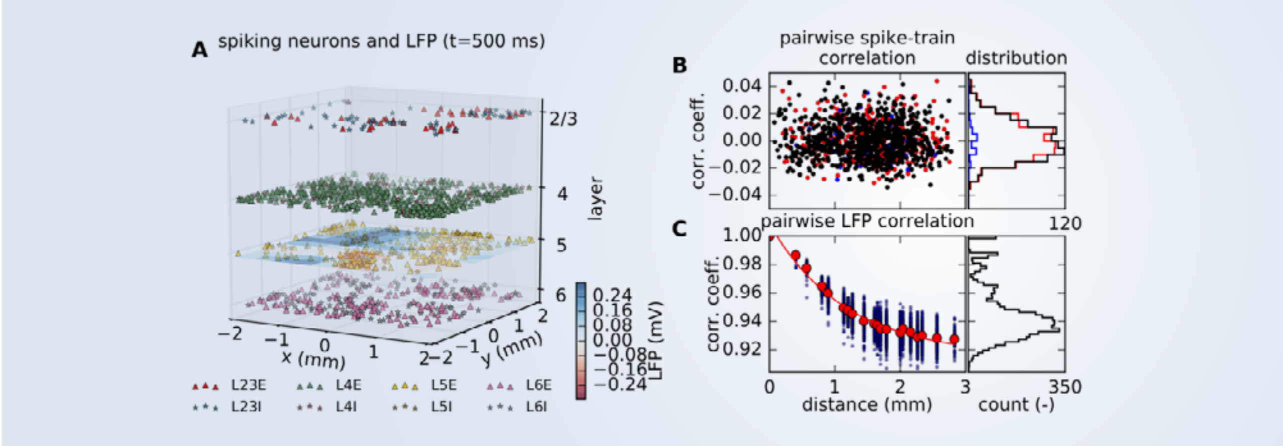
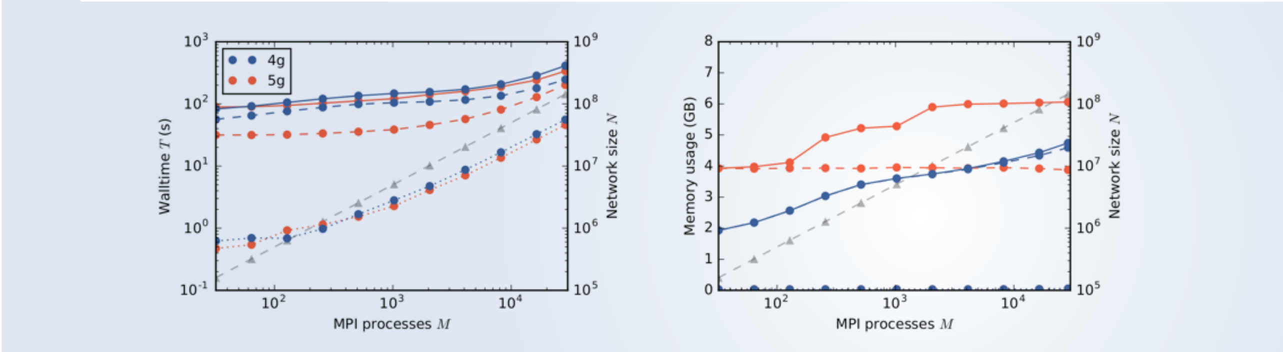


Figure 2: Cumulative wall-clock time (left) and memory usage (right) of the last generation simulation kernel ("4g", blue) and the new simulation kernel ("5g", red) for a weak scaling benchmark on JUQUEEN. Dotted lines: After node construction; dashed lines: after network construction; solid line: after simulation. Light gray: network size (right axis).



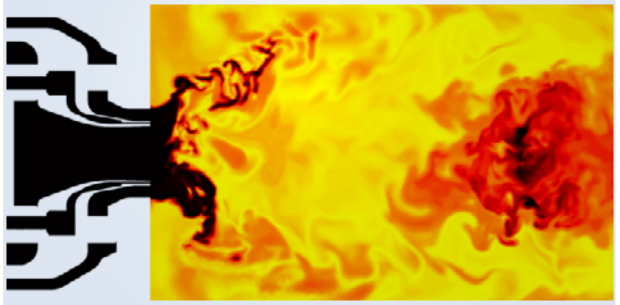
INSTITUTE FOR COMBUSTION TECHNOLOGY (ITV)

RWTH / Prof. Heinz Pitsch

> Large-Eddy Simulation of Soot Evolution at Elevated Pressure in a Model Aero Engine

To exploit the potential of computational modeling for the reduction of particulate emissions from aero engines, reliable modeling frameworks have to be developed and tested in system scale applications. Therefore, LES of soot formation in a model aero engine combustor experimentally investigated at the DLR are conducted using a flamelet-based combustion model and a detailed soot model. In a first set of LES, good results for the flow and temperature fields could be obtained, while soot was overpredicted, but qualitatively in good agreement with experimental data. To further improve the results, a combustion model for partially premixed combustion is currently being implemented and tested.

PROJECT NUMBER jara0159



Simulation of combustion and soot formation in a model aeronautic engine

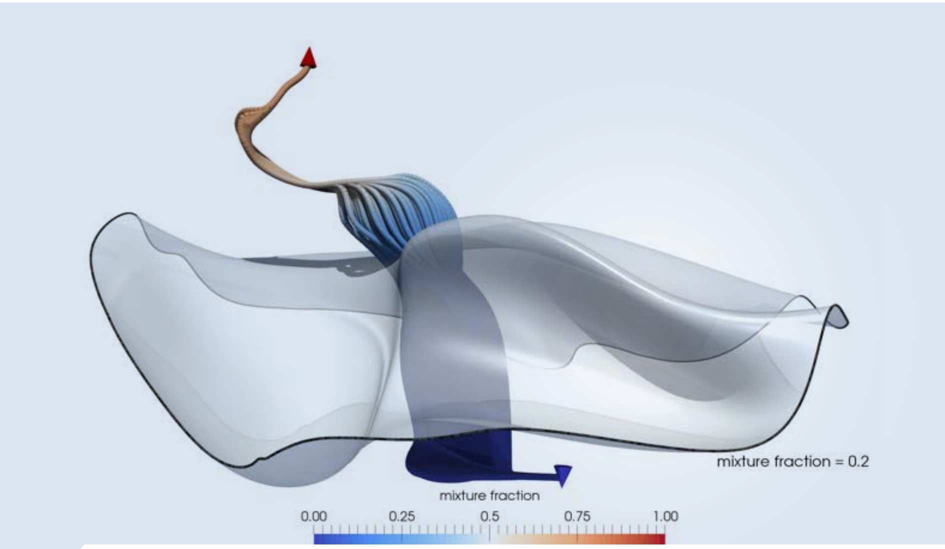
> Regimes in Turbulent Non-Premixed Combustion

Five highly resolved direct numerical simulations (DNS) of temporally evolving jet methane diffusion flames were conducted on the supercomputer JURECA.

The most prominent approach to modeling turbulent combustion is called the flamelet concept. The idea of this concept is that a turbulent flame is composed of an ensemble of thin laminar flamlets.

A promising and well tested method for measuring the local turbulent scales is the Dissipation Element (DE) Analysis. DEs are non-arbitrary space filling objects consisting of an ensemble of material points whose gradient trajectories share the same extremal points. Since the flamelet concept relies on the local smoothness of the chemical field, the attributes of the DEs encompassing the reaction zones will indicate whether the flamelet assumption is locally valid. Regions identified in this manner can then be thoroughly investigated and the effect of small scale mixing can be evaluated.

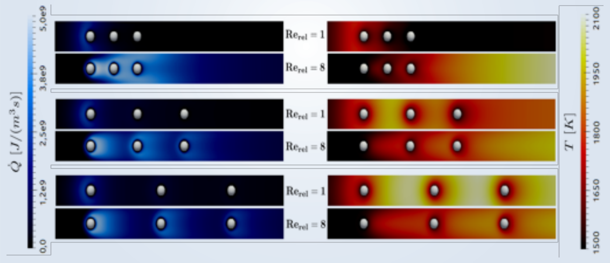
PROJECT NUMBER JHPC22



Interaction between a dissipation element and the local flame surface in a simulation of a turbulent non-premixed jet flame. Start and end points are indicated by cones. The grey surface represents the flame front which is wrinkled by turbulence.

> Direct numerical simulation and modeling of particle array combustion process

Char particle combustion is computed for an oxygen-enriched oxy-fuel environment. The main focus of this project pertains the influence of combustion on the drag force acting on a reactive char particle in a hot surrounding gas flow. The flow from the particle surface towards the gas phase affects the fluid flow around the reacting particle and yields a lower drag force on the reacting particle compared with non-reactive particles. This study provided a modified drag coefficient for reacting particles, which can be applied in point particle simulations to correct for the effect of the Stefan flow.



Distribution of heat release and temperature around particle array at various array configurations and Reynolds numbers.

A range of various parameters was considered, such as particle distance, oxygen levels in the incoming flow, particle Reynolds number, and the particle arrangement. The analysis showed a large dependence on the distance between the particles and the location of each particle within the array. Considering the temperature and the oxygen mass fraction around all the simulated particles in the parameter space provides insight towards the global relation between these variables, highlighting possible modeling directions.

PROJECT NUMBER jara0118

> Detailed Investigation of Liquid Sheet Breakup Using Direct Numerical Simulation and In-Situ Visualization

This project addresses the understanding of the mechanism underlying the breakup of ligaments into multiple droplet. Therefore, a Direct Numerical Simulation (DNS) of a temporal jet is performed resolving the breakup of ligaments temporally and spatially. The computation is visualized using in- situ visualization in order to identify areas of breaking up ligaments.

PROJECT NUMBER JHPC18

Breakup of ligaments into multiple droplets

> Non-Universality Effects in Turbulent Combustion

Structure functions are statistics of the velocity difference evaluated at two points in space, separated by a distance r. They can be used to examine the multi-scale behavior of turbulent flows. Structure functions were first introduced in 1941 by Kolmogorov. As introduced by Kolmogorov, one can identify two distinct ranges when considering structure functions: The dissipative (viscous) range for small r and the inertial range situated in between the smallest and largest scales. For the viscous range, we have found that there are exact solutions for even-order longitudinal structure functions. This is an important result, as it can help shedding light in the intricated behavior of turbulent flows and help in formulating a more univesal understanding of the problem.

PROJECT NUMBER JHPC09

INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS

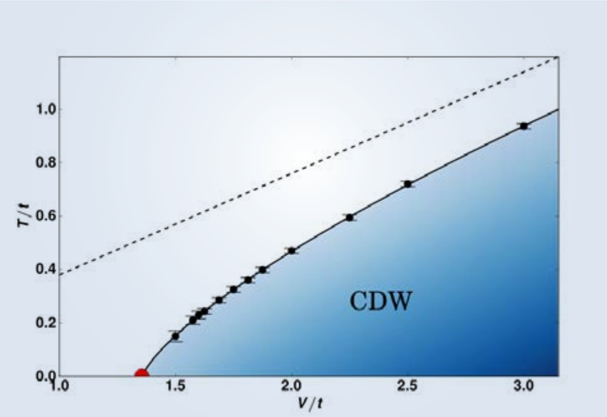
RWTH / Strongly Correlated Quantum Systems / Prof. Stefan Wessel, Ph.D.

> Quantum Monte Carlo Simulations of Emerging Many-Body

In our project we employ large-scale quantum Monte Carlo (QMC) simulations to in- vestigate collective quantum phenomena emerging in many-body quantum systems. These simulations span a wide range of physical systems and contribute to current research in different sub-fields. In one sub-project, we investigate an effective quantum spin model to describe the low-energy spin physics of the magnetic moments forming along the two edges of zig-zag graphene nanoribbons.

In contrast to various previous theoretical studies of the edge-magnetism in graphene nanoribbons, this effective model, containing long-ranged spin-interactions, allows for a systematic investigation of the magnetic properties on experimentally relevant length scales, while fully treating quantum fluctuations. In another sub-project, we perform a QMC-based level spectroscopy of the spinless fermion model on the honeycomb lattice. This model exhibits an interaction-driven quantum phase transition from a weak-coupling semimetal phase to a strong-coupling charge density wave (CDW) state.

Due to the importance of the coupling of the order parameter field to the microscopic fermions, this quantum phase transition belongs to the universality class of the Gross-Neveu-Yukawa theory. Only recently, it was found that this model can be analysed using large-scale, sign-problem free QMC simulations which we have previously employed to investigate the thermal phase diagram and the



Thermal phase diagram of the model of interacting spinless fermions on the honeycomb lattice in the vicinity of the chiral Ising quantum critical point.

scaling properties in the vicinity of the quantum critical point in this model. The thermal phase diagram is shown in the figure, where T denotes the temperature, t the hopping strenght and V the nearest-neighbor repulsion. We employ these QMC methods to analyse in more detail the excitation spectrum of this model near the quantum critical point. This approach will provide a distinct fingerprint for the chiral Ising criticality in this model and contrast it to the more conventional Ising model criticality. For this purpose, high quality numerical data are required for the imaginary-time dynamical correlation functions of appropriate operators that target specific quantum number sectors.

PROJECT NUMBER jhpc43 and jara0158

INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS

RWTH / Theoretical Nanoelectronics / Prof. Riccardo Mazzarello

> Metal-insulator transitions in crystalline GeSbTe compounds

Building on our previous work on disorder-driven metal-insulator transitions in phase-change materials, we recently demonstrated the existence of atomic and vacancy disorder on the Ge-Sb sublattice of rocksalt GeSbTe compounds obtained upon fast crystallization of the amorphous state [1]. The characterization was carried out by combining direct atomic scale chemical identification experiments and ab initio simulations. We also identified the gradual vacancy ordering process upon annealing, which was predicted to trigger the transition to extended electronic states. This work was done in close collaboration with Prof. Zhang and Prof. Evan Ma at Xi'an Jiaotong University (China).

We investigated the structural properties of highly-ordered GeSbTe models as well [2]. This work was done in collaboration with the experimental group of Dr. Raffaella Calarco (PDI Berlin). The experimental samples were obtained by engineering the complex stacking sequence of atoms and vacancies in the ternary alloy during epitaxial growth. Our simulations provided valuable information about the lattice symmetry and the distribution of vacancies. The samples were later employed in memory cells and demonstrated a superior electrical switching as compared to metastable disordered GeSbTe [2].

Finally, we studied the effects of ion irradiation on the structural and electronic properties of GeSbTe compounds [3], in collaboration with the experimental group of Prof. Emanuele Rimini (IMM and University of Catania, Italy). In the metastable rocksalt structure, the main effect of ion irradiation was found to be a progressive amorphization, whereas, for the stable trigonal structure, a metal-insulator transition and a crystalline transition were shown to occur prior to amorphization. We showed that, in the trigonal phase, the ion irradiation strongly affects the bonds of Te atoms close to the van der Waals gaps. Comparison between experiments and DFT simulations showed that ion irradiation leads to the gradual filling of the van der Waals gaps with displaced Ge and Sb lattice atoms, giving rise first to the metal-insulator transition (9% of displaced atoms) and then to the structural transition to the metastable rock-salt phase (15% of displaced atoms).

In summary, the results presented in these works showed new ways - including annealing, change of the growth conditions and ion irradiation - to tune the degree of order and, thus, the electrical properties of GeSbTe phase change materials. Our ab initio simulations provided a means to rationalize all of the experimental findings in terms of insulator-metal transitions induced by the ordering of vacancies.

References [1] to [10] please see page 65

> Structural, electronic and kinetic properties of liquid phase-change materials

We have investigated the structural and kinetic properties of liquid phase-change materials, including $Ge_2Sb_2Te_5$ [4] GeTe [5] and Ag, In-doped Sb_2Te [6], by a combined experimental and computational approach.

The study of the liquid state is important to elucidate the amorphization and crystallization processes, which occur in phase-change memory devices. We have shown that the structural properties of the models obtained from ab initio simulations (employing the so called van der Waals density functionals) and reverse Monte Carlo simulations are in good agreement with neutron and X-ray diffraction experiments. We have extracted the kinetic coefficients from the molecular dynamics trajectories and determined the activation energy for viscosity. The obtained values have been shown to be fully compatible with the viscosity measurements. This project has been done in close collaboration with the group of Dr. I. Kaban (IFF Dresden).

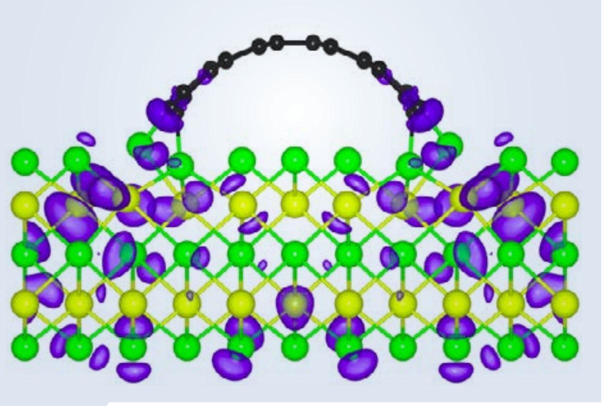
References [1] to [10] please see page 65

> Properties of graphene nanoribbons deposited on the topological insulator Sb_2Te_3

We investigated zigzag graphene nanoribbons (GNRs) deposited on Sb_2Te_3, a prototypical 3-dimensional topological insulator, by density functional theory [7]. We found that the interaction between monohydrogenated GNRs and the Sb_2Te_3 substrate is weak and, thus, the GNRs retain their edge magnetism and hardly affect the dispersion of the surface states of Sb_2Te_3. Nevertheless, the presence of the substrate affects significantly the magnitude of the exchange coupling constants between the magnetic moments of the edge states of the GNR.

More recently, we have considered unpassivated GNRs on Sb_2Te_3. Surprisingly, these GNRs retain their magnetism as well, in spite of the strong chemical interaction with the substrate [8]. Furthermore, a twisting of the spins of the two antiferromagnetically-coupled edge states of the GNR occurs due to the Dzyaloshinskii-Moriya interaction, which favours chiral configurations. The resulting net magnetization of the GNR shifts the Dirac point of the surface state of the topological insulator and opens a small gap. Besides their theoretical interests, these systems could have practical applications as spin filters in graphene-based spintronics devices.

References [1] to [10] please see page 65



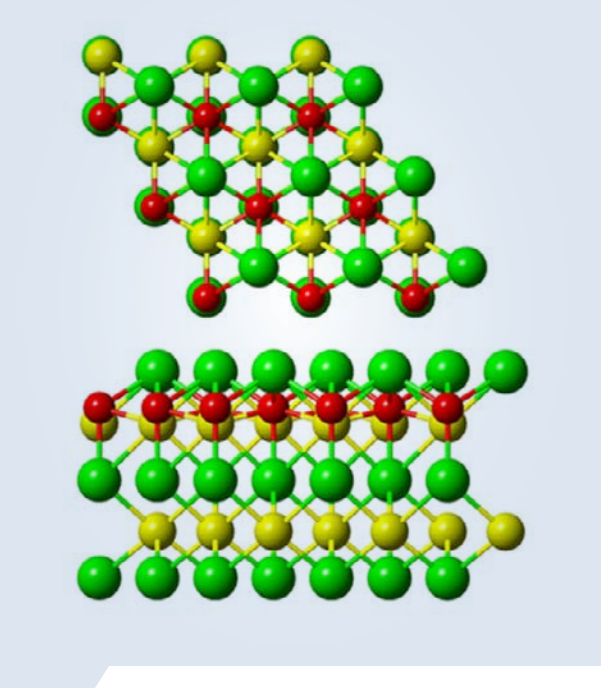
Structure of the unpassivated GNR deposited on Sb_2Te_3. C, Sb, and Te atoms are rendered with black, yellow, and green spheres. The blue surfaces are Isovalue surfaces of the charge density of a surface state of Sb_2Te_3. The state interacts with the dangling-bond orbitals of the edge C atoms.

> Effects of magnetic Fe monolayers on the surface states of Sb_2Te_3

We investigated the structural, electronic and magnetic properties of high-coverage Fe monolayers deposited on the (111) surface of the topological insulator Sb_2Te_3 by first-principles simulations [9]. We showed that, upon relaxation, the Fe atoms partly penetrate into the surface and that their magnetic moments are reduced due to the chemical interaction with the topmost layers of the substrate.

We computed the magnetic anisotropy energies and show that the easy axis is in-plane. We also investigated hexagonal warping effects and found that the clean Sb_2Te_3(111) displays a large warping term. In spite of this, the surface-state gap for in-plane magnetization is below 1 meV. Interestingly, no surface Dirac cones was observed for very high coverages (corresponding to three Fe atoms in the unit cell of Sb_2Te_3(111)), except for a metastable model consisting of a hexagonal Fe monolayer lying on top of the substrate, which also exhibits an out-of-plane easy axis.

References [1] to [10] please see page 65



Top and side view of the most stable model of the Fe monolayer on Sb_2Te_3(111). Fe, Sb, and Te atoms are rendered with red, yellow, and green spheres. Note that the Fe atoms partly penetrate into the substrate.

> Dithiocarbamate self-assembled monolayers on noble-metal surfaces

In this work, we showed that N,N-dialkyl dithiocarbamates (DTC) can be employed to lower the work function of Cu, Ag and Au metal electrodes [10]. Tuning the work function of the electrode is an effective way to improve charge extraction in organic electronic devices. Photoemission spectroscopy experiments revealed a maximum decrease in work function by 2.1 eV as compared to the bare metal surface. Our DFT calculations elucidated how the interplay between the dipoles induced by bond formation and the intrinsic dipoles of the molecules led to these work function shifts. The decrease in contact resistance of organic thin film transistor devices with DTC coated source and drain electrodes was also determined experimentally. Our work demonstrated that DTC molecules can be employed as universal surface modifiers to produce stable electrodes for electron injection in hybrid organic optoelectronic devices. This project was done in close collaboration with the group of Prof. Wuttig.

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INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)

RWTH / Prof. Wolfgang Schröder

> Simulation of Jet Engine Noise and Base-Flow Fields of Space Launchers

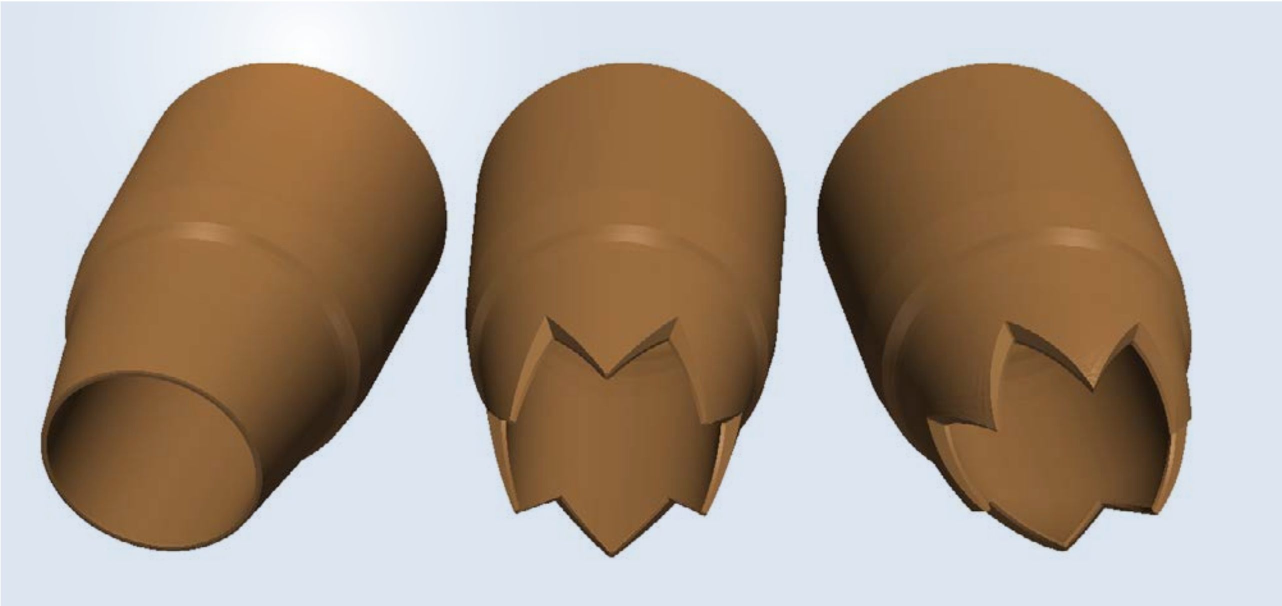


Figure 1: Three nozzle geometries: SMC000 (left, no chevrons), SMC001 (center, with chevrons), and SMC006 (right, with chevrons and higher penetration angle).

The aim of the first project is to reduce jet noise emissions, which are the major noise source of starting aircraft. One proposed measure is the use of serrated or chevron nozzles, since the turbulent jet structures strongly depend on the exit geometry of the nozzle and these flow structures define the noise sources of the jet. To investigate this idea, a hybrid method for computational aeroacoustics is used to analyze the flow and acoustic fields of three cold jet flows of the NASA Glenn nozzles SMC000, SMC001 and SMC006, as shown in Fig. 1.

The simulation results confirm that chevron nozzles enhance the mixing process by inducing stronger streamwise vorticity (Fig. 2). The excitation of pressure fluctuations is increased in the shear layer, leading to a distinct increase in the power spectral density (PSD) for the SMC006 configuration in the higher frequency range. Simultaneously, the PSD is damped in the lower frequency range, since the chevrons mitigate the formation of large-scale vortical structures. Furthermore, the overall sound pressure level in the near far field is higher for chevrons than for the baseline configuration. Therefore, the noise propagation into the far field has to be simulated and the influence of the synthetic turbulence inflow condition will be explored. The ultimate goal in chevron design is to decrease the low-frequency noise while preventing a significant increase in the high-frequency range.

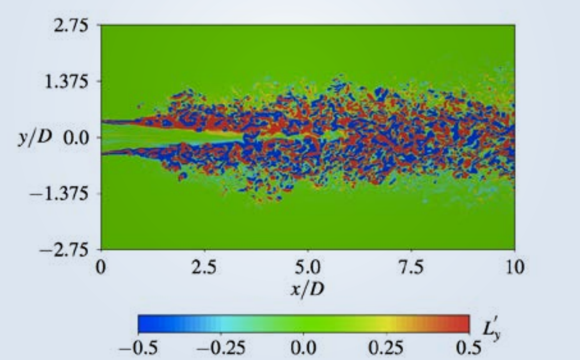


Figure 2: Instantaneous contours of the y-component of the Lamb vector L′ = (ω × u)′, which represents the acoustic noise source.

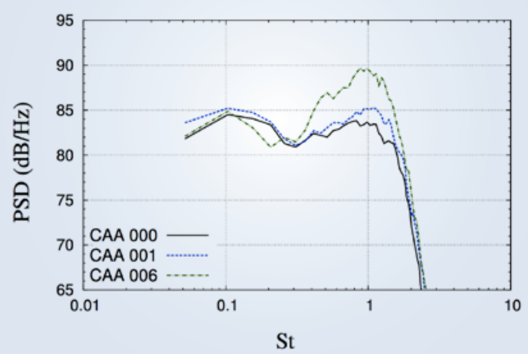


Figure 3: Power spectral density of the acoustic pressure field in the sideline direction for the three nozzles.

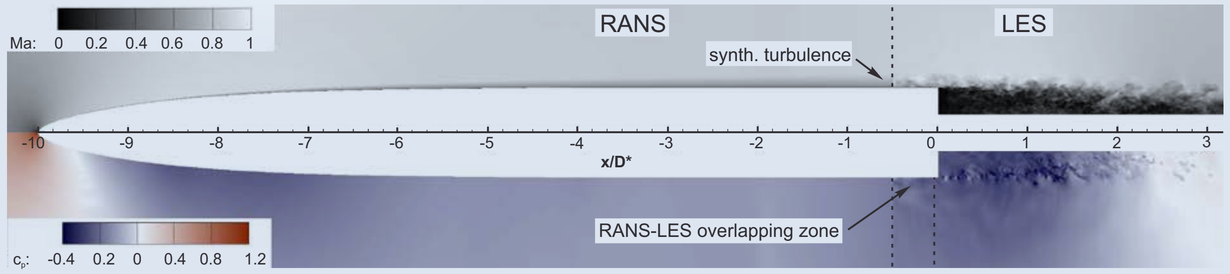


Figure 4: Velocity field (top) and pressure field (bottom) of the investigated space launcher configuration.

In the second project, the turbulent wake of a generic planar ARIANE 5-like configuration is investigated at transonic freestream conditions to detect characteristic wake flow modes responsible for the buffeting phenomenon of space launchers. The wake flow, which is examined using a zonal RANS-LES appraoch and dynamic mode decomposition (DMD), is characterized by a highly unsteady behavior of the shear layer shedding from the forebody and subsequently reattaching onto the splitter plate (Fig. 4). The results reveal that despite the quasi-two-dimensionality of the planar geometry, the wake is characterized by the formation of elongated wedge-shaped coherent structures.

Moreover, a pronounced periodicity of pressure oscillations and structural loads is detected at the splitter plate. To quantify the pressure oscillations, statistical analysis is applied to the numerical data. It reveals one spatial coherent scale with a spanwise wavelength of $\lambda z \approx 2h$ and two characteristic frequencies of Srh ≈0.034 and Srh ≈0.21 for the investigated wake flow problem (Fig. 5). To clarify the coherent fluid motion dominating the detected behavior, a DMD algorithm has been developed and applied to the streamwise velocity field. The analysis of the extracted DMD modes shows that the observed wake flow behavior is caused by a low-frequency cross-pumping motion of the recirculation region and a high-frequency cross-flapping motion of the shear layer.

PROJECT NUMBER number jhpc23

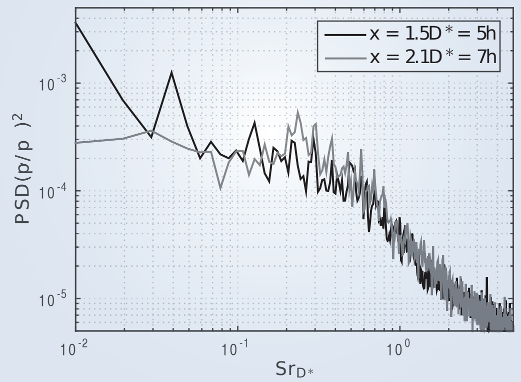


Figure 5: Power spectral density of the pressure signal at two downstream locations.

INSTITUTE OF BIO- AND GEOSCIENCES (IBG)

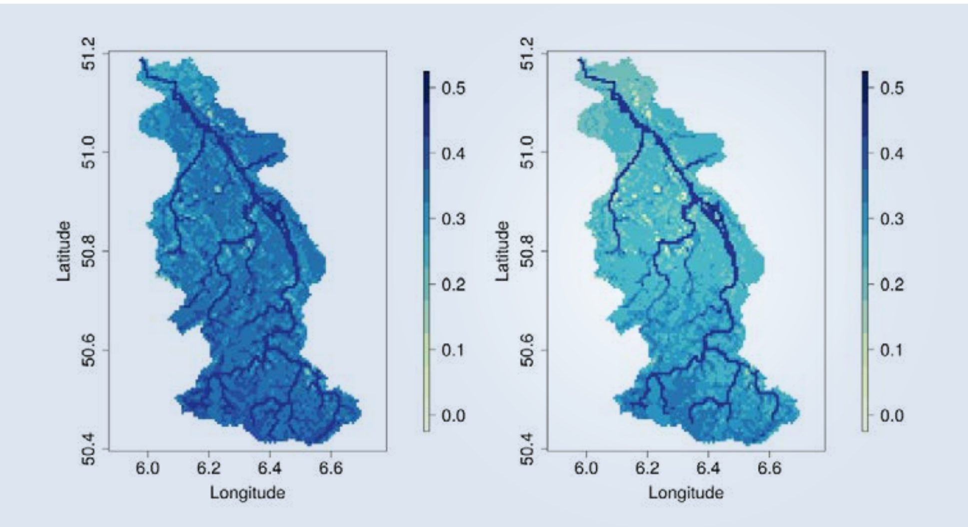
FZ Jülich / Agrosphere (IBG-3) / Prof. Harry Vereecken

> Assimilation of soil moisture data with integrated terrestrial modeling platform TerrSysMP at the catchment scale

Various studies have already shown that subsurface hydrology can have a profound influence on the estimation of land surface fluxes and the evolution of the atmospheric boundary layer (Kollet & Maxwell, 2008; Shrestha et al., 2014; Rahman et al., 2015). Such dynamic feedbacks can be taken into account by the application of integrated terrestrial modeling platforms which combine different compartment models for the subsurface, the land surface and the atmosphere and therefore allow a better physical representation of processes across compartments. However, model predictions with such highly sophisticated models are generally prone to uncertainties regarding the model input variables, like subsurface parameters, meteorological input variables or vegetation parameters. In this respect, data assimilation techniques can help to better constrain the model predictions and parameters and the associated uncertainties by merging the uncertain model predictions with field observations of the modelled quantities.

In this work, we perform data assimilation experiments with the integrated modeling platform TerrSysMP (Shrestha et al., 2014) consisting of individual component models for variably saturated subsurface flow (ParFlow), land surface processes (CLM3.5) and the atmosphere (COSMO). The component models are dynamically linked by the exchange of state variables and fluxes with the coupling software OASIS-MCT in a scale-consistent, modular manner. In a first step, we constructed a data assimilation framework for the land surface-subsurface part of TerrSysMP (CLM3.5 and ParFlow) by linking TerrSysMP with the PDAF (Parallel Data Assimilation Framework) software (Nerger & Hiller, 2013; Kurtz et al., 2016). The data assimilation framework uses a memory based communication between model and data assimilation routines and avoids frequent re-initializations of the model and is thus highly scalable and applicable to high-resolution hydrological models. The data assimilation system is also modular with respect to the model combination used in the forward simulations. Data assimilation experiments are performed with a hydrological model of the Rur catchment (TERENO/TR32-monitoring site, Germany) where a network of nine cosmic ray stations provides soil moisture data on a daily basis. These data are assimilated for a period of five months from April – August 2013. The effectiveness of the assimilation is assessed by performing jackknife experiments where data from eight stations were assimilated while the remaining station data were used for verification. This kind of experiments was performed with two different types of forward models which are both part of the terrestrial system model TerrSysMP: (I) the land surface model CLM and (II) CLM coupled to the groundwater model ParFlow. This comparison aims to provide more insight into the role of the hydrological process description on the assimilation performance. Results show that for all jackknife experiments the soil moisture prediction consistently improves for the corresponding verification sites. Additionally, certain differences were found for the two forward models with respect to spatial soil moisture pattern and the efficiency of the soil moisture assimilation.

PROJECT NUMBER jicg41



Ensemble mean of top soil moisture (0-2cm) for (left) an open-loop simulation without data assimilation and (right) for the assimilation of soil moisture data from eight cosmic-ray stations. Values are shown for May 01, 2013.

> High resolution river discharge modeling for hydropower energy applications

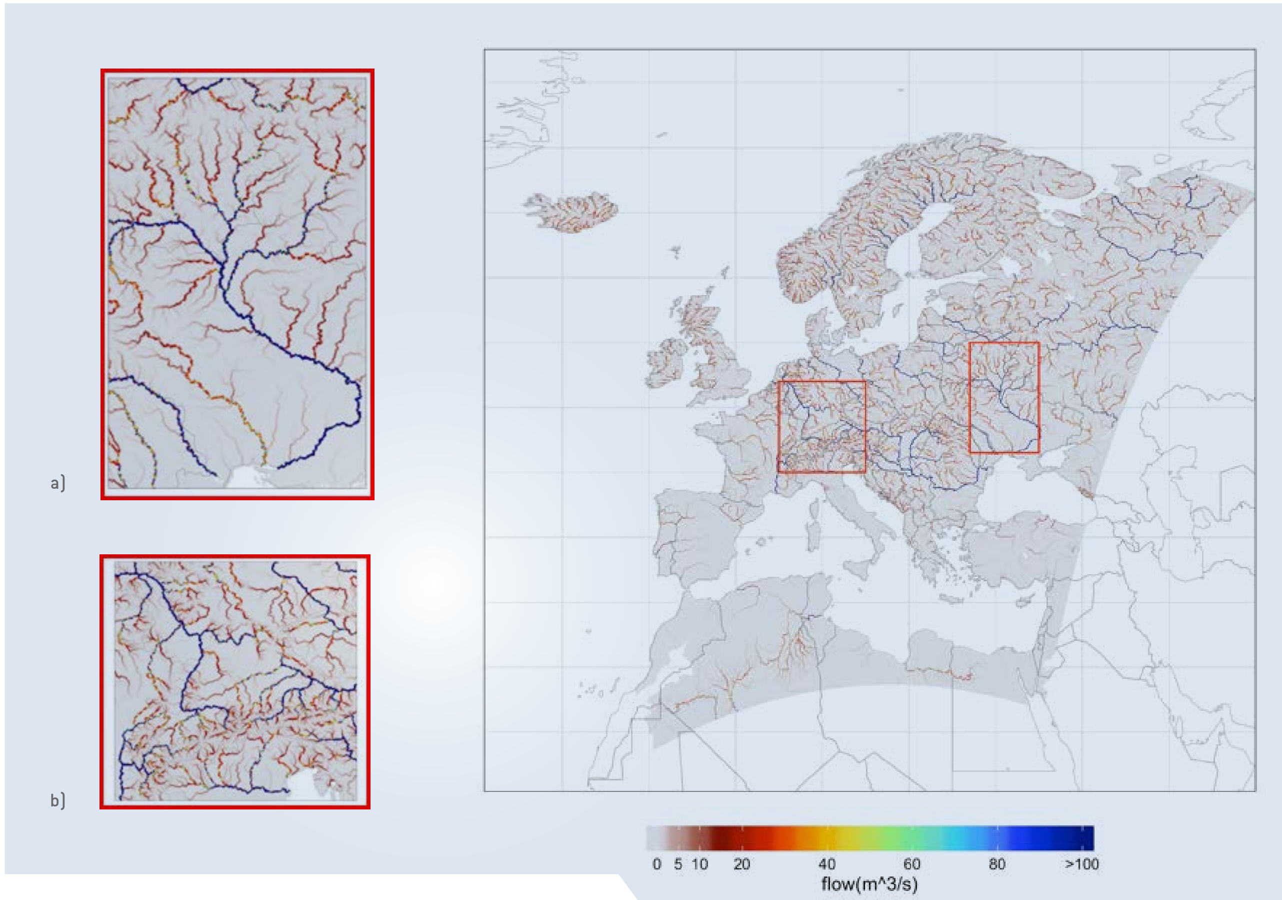
In the scope of EoCoE (Energy Oriented Centre Of Excellence), a continental scale hyper-resolution hydrologic modeling system for the investigation of hydropower potential in the continental European region is developed for use in hydrological models ParFlow and Common Land Model (CLM). ParFlow is a three dimensional watershed model which simulates surface and subsurface flow, where CLM combines runoff data generated from the model and a river routing algorithm.

Through these modeling systems, it will be possible to assess modeled time series data using visualization tools and post-processing analysis chains developed in collaboration with computer scientists. Comparisons of observed and modeled discharge data for a given geographic region and time frame will be made to assess the accuracy and suitability of each model.

These models will be used to simulate hydropower production within a framework that generates available streamflow

through a comprehensive analysis at continental scale by taking into account major factors influencing the production. This novel hyper-resolution continental scale approach to asses the large-scale hydropower potential over Europe, where simulations are run at climate time scales, will provide the current hydrologic status of the terrestrial system and predictions of all pertinent states and fluxes at the resolution relevant to the energy sector.

PROJECT NUMBER jibg31



Preliminary Results showing river flow (m) over continental Europe
with two insets zooming into the (a) Dnieper and (b) Rhine and Po River basins.

> Water cycle processes and land-atmosphere interactions in multi-scale regional climate change simulations with the WRF atmospheric model over Europe in the context of the WRCP EURO-CORDEX initiative

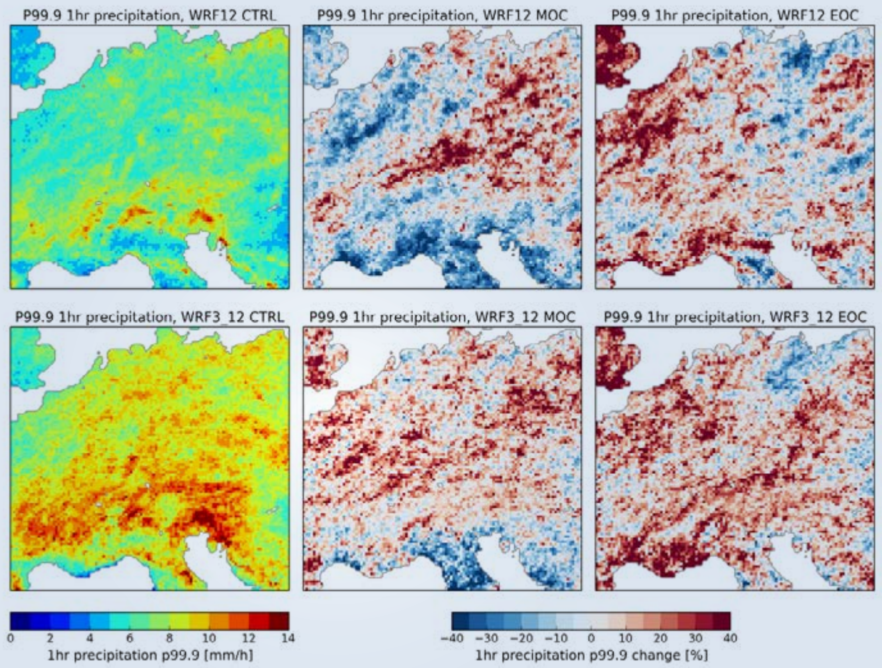
High-resolution regional climate models with a more detailed representation of heterogeneous land surface properties, as well as an explicit treatment of deep convection can lead to an improved simulation of meteorological processes and the climate system at the meso-gamma scale. Objectives of this project are the production and analysis of WRF RCM 10 years ERA-Interim driven evaluation runs and 3x12 years MPI-ESM-LR driven climate projection simulations at 3km convection-permitting spatial resolution for a central European model domain.

Science questions focusing on precipitation statistics are: How well can observations be reproduced? What is the added value of the high resolution runs? How do precipitation intensity distributions change in a future, projected climate? Evaluation simulations from both resolutions are compared and evaluated against sub-daily synop station data over three regions with a moderate, low mountain and high mountain topography. Added value in the 3km simulation is found especially at the sub-daily scale in the reproduction of intensity, diurnal cycle and spatial extent of precipitation. A positive precipitation bias found for both resolutions is more dominant in the 12km simulation, where too much light precipitation is generated. For different seasons, precipitation clearly differs between both simulations with largest differences over mountainous regions and during summer months with high convective activity.

In a second part, based on the MPI-ESM-LR RCP4.5 driven control and scenario time slices, we examine changes in precipitation intensity distributions as well as extreme precipitation indices, again for areas with different topographic variances and mean altitudes. With increasing mean temperature in the future climate the simulations reveal an increase in extreme precipitation that exceeds scaling rates of 7%/K according to the Clausius-Clapeyron relation while light and moderate precipitation decreases.

PROJECT NUMBER jjsc15

Hourly extreme precipitation sums (99.9th percentile) in summer (June-July-August) in the control simulation time period 1993-2005 (CTRL; left column) and its relative change in mid-of-century future 2038-2050 (MOC; middle column) and end-of-century future 2088-2100 (EOC; right column) for the WRF RCM simulation in 12 km resolution (WRF12; upper row) and 3 km resolution interpolated on 12 km grid (WRF3_12; lower row). Both resolutions run in a one-way nesting setup with the 3 km Middle European domain nested into the pan-European EURO-CORDEX domain. Boundary data is provided by the GCM MPI-ESM-LR with RCP4.5 greenhouse gas scenario.



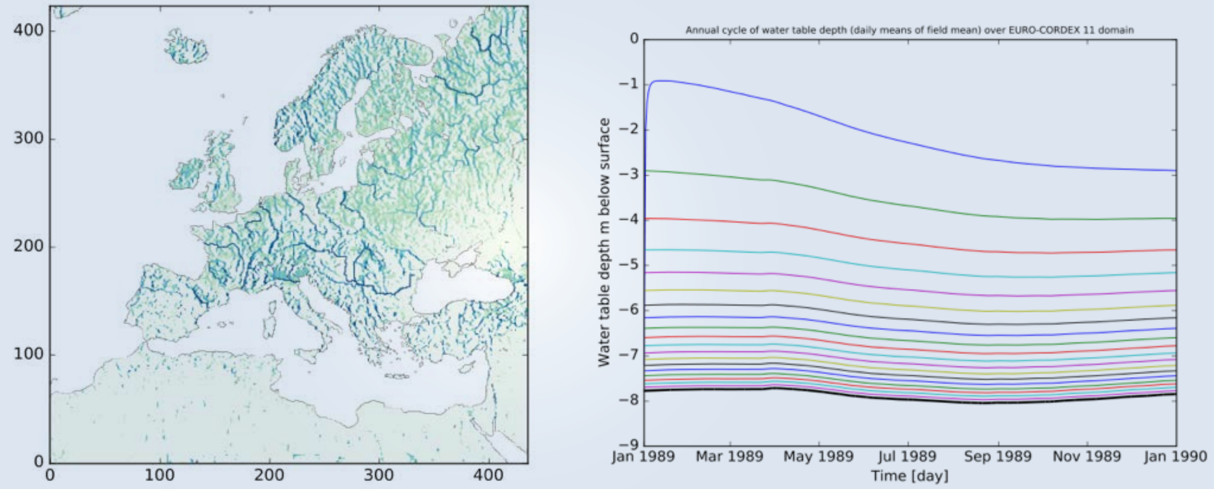
> Fully coupled water cycle EURO-CORDEX evaluation simulations with TerrSysMP from 1989-2008

Interactions and feedbacks between the sub-surface including groundwater, the land surface and the atmosphere are highly relevant for weather and the climate system. However, many state of the art global and regional earth system models do not consider the impacts of groundwater dynamics, which are critical for the closure of the hydrological cycle on different spatial and temporal scales. In this study we implement the coupled Terrestrial Systems Modelling Platform over the EURO-CORDEX domain for evaluation experiments in line with the CORDEX experiment design in order to study how the explicit treatment of groundwater affects states and fluxes of the terrestrial water and energy cycle over a continental domain on longer simulation time spans and in relation to existing uncoupled EURO-CORDEX RCM simulations.

The Terrestrial Systems Modelling Platform (TerrSysMP) is a fully coupled scale-consistent numerical modelling system, currently consisting of the COSMO NWP model, the Community Land Model (CLM) and the ParFlow variably saturated surface and subsurface hydrological model, coupled with the external coupler OASIS3(-MCT). TerrSysMP allows for a physically based representation of transport processes across scales down to sub-km resolution with explicit feedbacks between the individual compartments, including 3D groundwater dynamics and a full representation of the terrestrial hydrological cycle. The land surface-groundwater subsystem is spun up with a 1979-1989 cyclic climatological forcing derived from ERA-Interim reanalysis until an equilibrated groundwater state is achieved.

Using this as the initial conditions, the fully coupled simulation for the period from 1989 to 2008 are carried out over the EURO-CORDEX domain at 12 km resolution using ERA-Interim as lateral boundary forcing. COSMO physics settings are in line with the CCLM consortium runs done for EURO-CORDEX to allow for a better comparison. The JUBE2 (Juelich Benchmarking Environment) workflow engine is used to manage the complex operation of the simulations. In the analysis, we discuss the impact of groundwater on land atmosphere feedbacks and atmospheric boundary layer properties to demonstrate the added value of the coupled simulations. Several climate indices and performance metrics are used over PRUDENCE analysis regions in a comparison with observational data.

PROJECT NUMBER jjsc15



(Left) CLM-ParFlow spin up results showing evolution of river networks based on water table depth and (Right) annual cycle of average water table depth over EURO-CORDEX 11 domain over various spin up cycles.

INSTITUTE OF BIO- AND GEOSCIENCES (IBG)

FZ Jülich / Biotechnology (IBG-1) / Prof. Wolfgang Wiechert

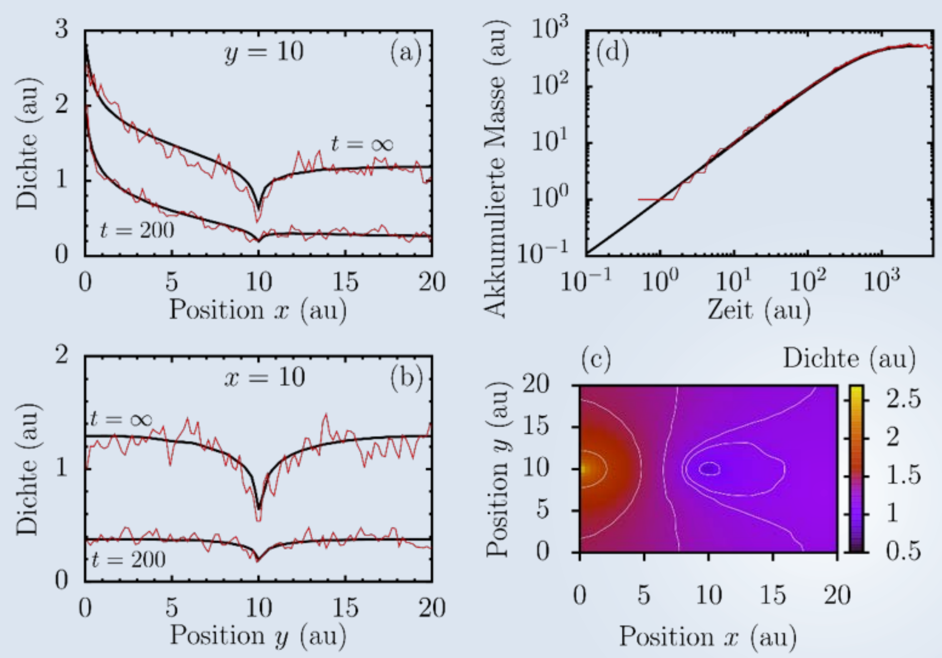
> Multiscale simulation of inhomogeneities in cellular biochemistry / Scaling BD_BOX for simulation of intracellular environments

We have developed a multiscale approach for spatially resolved reaction-diffusion systems.

This approach couples Brownian Dynamics simulations for macromolecules and the Finite Element Method for the evolution of metabolite densities. It can be used to study the influence of structural heterogeneity, e.g. in the cytosol of a cell, on the performance of biochemical reactions, and has been successfully applied by us to understand the effects of stochasticity, heterogeneity and discreteness on enzyme catalyzed reactions.

Our approach requires however certain input parameters, in particular macromolecular and metabolite diffusion coefficients. We have used BD_BOX to determine diffusion properties of macromolecules by modeling macromolecular environments with up to ~1000 particles. BD_BOX is also used to determine the properties of metabolic transport, and to validate our findings from the continuous simulations.

PROJECT NUMBER jibg11



Comparison of discrete BD simulations (red) and continuous reaction-diffusion-system (black). (a-b): metabolite concentration over position at time t=100 and in stationary state (t=∞). BD results averaged over 100 simulations. (c): accumulated mass in system over time. (d): contour plot of concentration over position in stationary state.

INSTITUTE OF BIOTECHNOLOGY

RWTH / Prof. Ulrich Schwaneberg

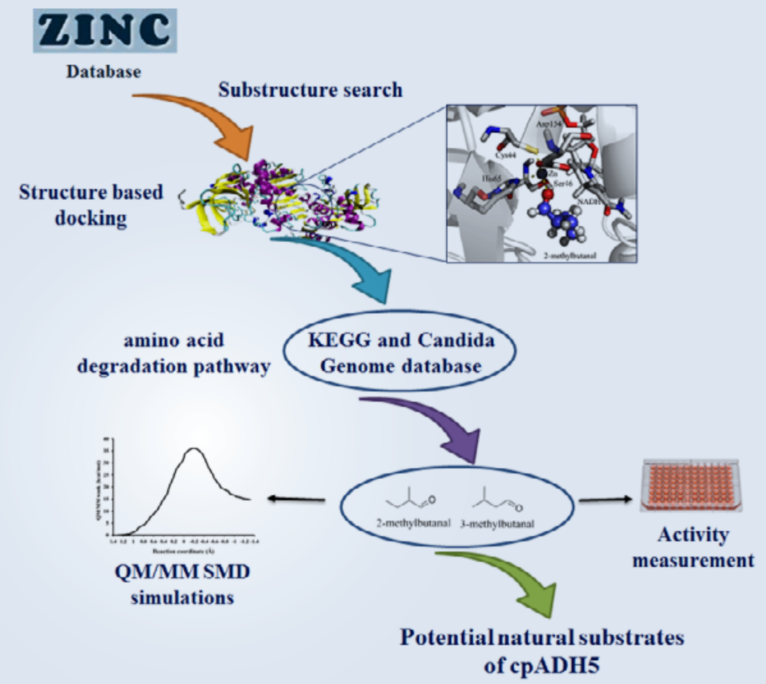
> Computational investigations on the substrate specificity of Carbonyl Reductases using hybrid quantum mechanics and molecular mechanics MD calculations

What's My Substrate? Computational Function Assignment of Candida parapsilosis ADH5 by Genome Database Search, Virtual Screening, and QM/MM Calculations

Zinc-dependent medium chain reductase from Candida parapsilosis can be used in the reduction of carbonyl compounds to pharmacologically important chiral secondary alcohols. To date, nomenclature of cpADH5 is differing (CPCR2/RCR/SADH) in the literature, and its natural substrate is not known. In this study, we utilized a substrate docking based virtual screening method combined with KEGG, MetaCyc pathway and Candida genome databases search for the discovery of naturalsubstrates of cpADH5. The virtual screening of 7834 carbonyl compounds from the ZINC database provided 94 aldehydes or methyl/ethyl ketones as putative carbonyl substrates. Out of which, 52 carbonyl substrates of cpADH5 with catalytically active docking pose were identified by employing mechanism based substrate docking protocol. Comparison of the virtual screening results with KEGG, MetaCyc database search and Candida genome pathway analysis suggest that cpADH5 might be involved in the Ehrlich pathway (reduction of fusel aldehydes in leucine, isoleucine and valine degradation). Our QM/MM calculations and experimental activity measurements affirmed that butyraldehyde substrates are the potential natural substrates of cpADH5, suggesting carbonyl reductase role for this enzyme in butyraldehyde reduction in aliphatic amino acid degradation pathways. Phylogenetic tree analysis of known ADHs from Candida albicans shows that cpADH5 is close to caADH5. We therefore propose according to the experimental substrate identification and sequence similarity, the common name butyraldehyde dehydrogenase cpADH5 for Candida parapsilosis CPCR2/RCR/SADH.

Published in: Journal of chemical information and modeling, 56 (7), 1313–1323, 2016, DOI: http://pubs.acs.org/doi/abs/10.1021/acs.jcim.6b00076

PROJECT NUMBER RWTH0015

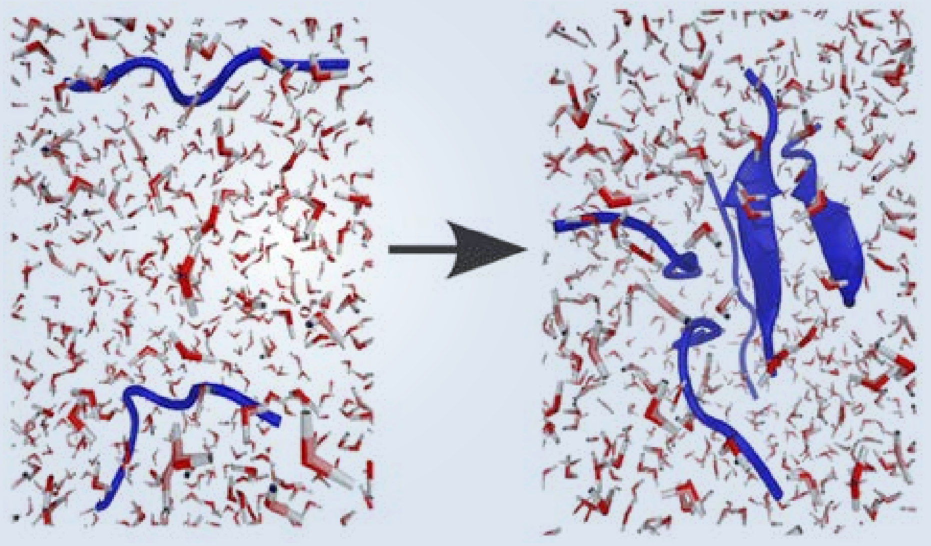


Workflow of our strategy for identification of potential substrates of cpADH5 using substrate docking based virtual screening protocol, KEGG and Candida Genome database search. The potential substrates obtained from virtual screening and KEEG pathway and Candida genome databases search were subjected to QM/MM SMD simulations to calculate the barriers involved in hydride transfer step and also to activity measurement of cpADH5 towards these candidate substrates using NADH consumption assay.

INSTITUTE OF COMPLEX SYSTEMS (ICS)

FZ Jülich / Structural Biochemistry (ICS-6) / Prof. Dieter Willbold

> Aggregation of Functional Amyloids



The aggregation of $A\beta_{16-22}$ into amyloid oligomers.

Protein aggregation into highly structured amyloid fibrils is associated both with devastating diseases, including Alzheimer's disease and type 2 diabetes, and functional roles, such as the storage of neuropeptides. Experimental evidence shows that the toxic species in amyloid diseases are small oligomers (see Figure).

These oligomers are transient and, hence, are hard to characterize experimentally. In this project, the aggregation of amyloidogenic peptides into oligomers is studied using classical molecular dynamics (MD) simulations. Most of the peptides simulated are variants of the amyloid-β peptide (Aβ), which is involved in the development of Alzheimer's disease. The quality of the results from MD simulations strongly depends on the accuracy of the force fields that are applied during the simulations.

To this end, the ability of different force fields in modeling intrinsically disordered proteins (IDPs), i.e, the class of proteins Aβ belongs to, and protein aggregation was tested. In recent years, new force fields were developed to balance the formation of secondary structures in protein folding simulations. In principle, these new force fields should also perform better than older ones for IDPs, which is confirmed by the simulations performed in this project.

The simulations of $A\beta_{1-42}$ revealed that the new force fields, particularly CHARMM22*, reproduce experimental nuclear magnetic resonance data better than the older force fields under study. However, in the force field benchmark of protein aggregation, none of the force fields was able to distinguish between slowly, fast and non-aggregating peptides. Yet, the force fields predict similar inter-peptide contacts for aggregating peptides, indicating that protein aggregation is driven by the same interactions with all force fields.

Thus, the conclusion is that the current force fields can be used to make predictions regarding the conformational ensemble of amyloid oligomers, but not for studying the aggregation kinetics. Finally, the monomer dynamics of multiple mutants of $A\beta_{16-22}$ with different aggre-gation propensities was investigated. The major finding of this study is that the implied time scale of the slowest process of the monomer dynamics correlates with aggregation propensity, which shows that amyloidogenic peptide aggregation is encoded, at least partially, in the dynamical properties of the monomer.

PROJECT NUMBER jara0095

INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)

FZ Jülich / Electrochemical Process Engineering (IEK-3) / Prof. Werner Lehnert

> Flexible Simulation of Fuel Cells with OpenFOAM

A high-temperature polymer electrolyte fuel cell (HT-PEFC) model was developed for the OpenFOAM CFD software. The geometry of a fuel cell is shown in Figure 1.

The efficiency of HT-PEFCs depends strongly on the presence of water. It was experimentally shown that water appears on both anode and cathode side of the membrane. This effect is recognized by the electrochemical model of the OpenFOAM implementation. Figure 2 shows the steam distribution across the active area on anode and cathode side of a HT-PEFC at typical operating conditions.

PROJECT NUMBER jara0070

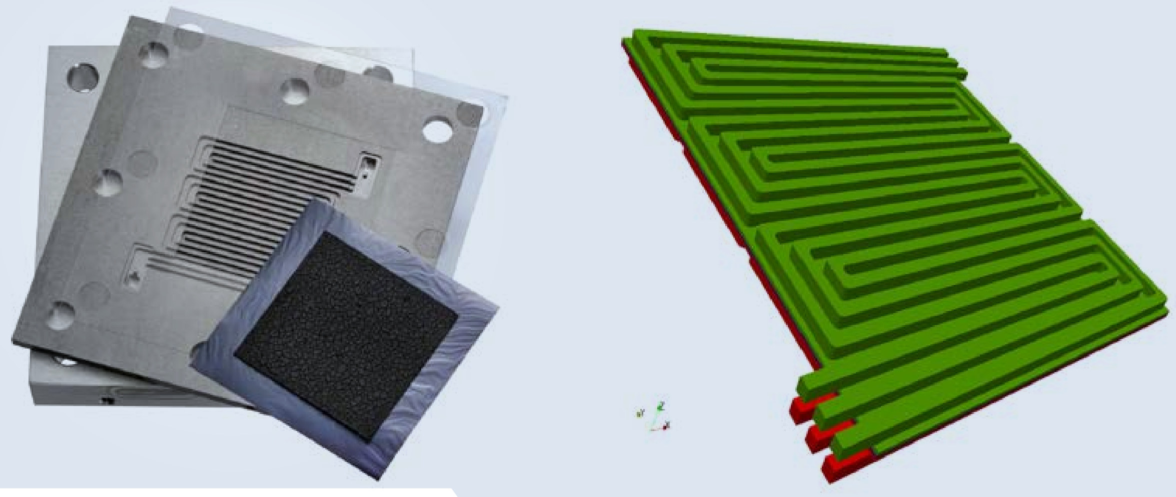
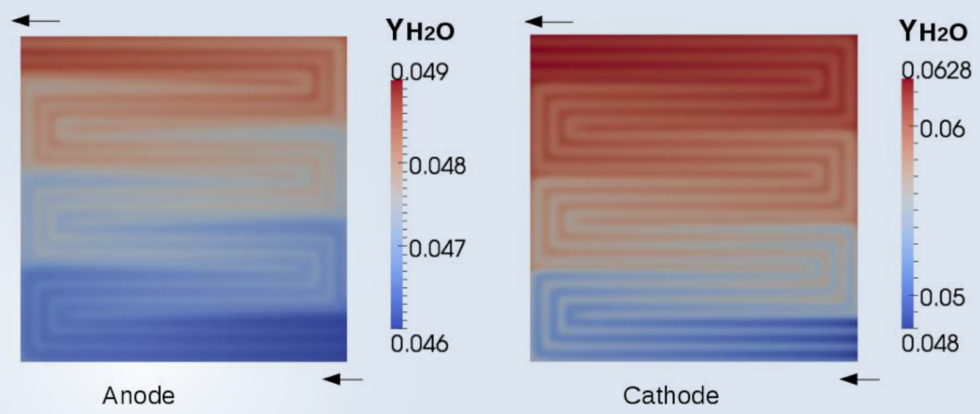


Figure 1:Components of a HT-PEFC (left) and mesh of the flow field (right)

Figure 2: Local distribution oft he H_2O mole fraction at 160 °C 101325 Pa and stoichiometry of air/H_2 =2/2.



INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)

FZ Jülich / Stratosphere (IEK-7) / Prof. Martin Riese

> Air Mass Origin in the Lower Stratosphere in the Asian Monsoon region based on Measurements and CLaMS Simulations

Global simulations by the Chemical Lagrangian Model of the Stratosphere (CLaMS) using artificial tracers of air mass origin are used to analyze transport mechanisms from the Asian monsoon region into the lower stratosphere.

In a case study, the transport of air masses from the Asian monsoon anticyclone originating in India/China by an eastward-migrating anticyclone which broke off from the main anticyclone on 20 September 2012 and filaments separated at the north-eastern flank of the anticyclone are analyzed Vogel et al. (2016). Enhanced contributions of young air masses (younger than 5 months) are found within the separated anticyclone confined at the top by the thermal tropopause. Further, these air masses are confined by the anticyclonic circulation and, on the polar side, by the subtropical jet such that the vertical structure resembles a bubble within the upper troposphere. Subsequently, these air masses are transported eastwards along the subtropical jet and enter the lower stratosphere by quasi-horizontal transport in a region of double tropopauses most likely associated with Rossby wave breaking events. As a result, thin filaments with enhanced signatures of tropospheric trace gases were measured in the lower stratosphere over Europe during the TACTS/ESMVal campaign in September 2012 in very good agreement with CLaMS simulations.

Our simulations demonstrate that source regions in Asia and in the Pacific Ocean have a significant impact on the chemical composition of the lower stratosphere of the Northern Hemisphere. Young, moist air masses, in particular at the end of the monsoon season in September/October 2012, flooded the extra-tropical lower stratosphere in the Northern Hemisphere with contributions of up to ≈ 30 % at 380 K (with the remaining fraction being aged air). In contrast, the contribution of young air masses to the Southern Hemisphere is much lower. At the end of October 2012, approximately 1.5 ppmv water vapor is found in the lower Northern Hemisphere stratosphere (at 380 K) from source regions both in Asia and in the tropical Pacific compared to a mean water vapor content of ≈ 5 ppmv. In addition to this main transport pathway from the Asian monsoon anticyclone to the east along the subtropical jet and subsequent transport into the northern lower stratosphere, a second horizontal transport pathway out of the anticyclone to the west into the tropics (TTL) is found in agreement with MIPAS HCFC-22 measurements.

INSTITUTE OF INORGANIC CHEMISTRY (IAC)

RWTH / Chair of Solid-State and Quantum Chemistry / Prof. Richard Dronskowski

> Quantum-chemical studies of chalcogenide nanocrystals for phase-change memories and other applications

In this project, we model surfaces of telluride-based phase-change materials. The oxidation of GeTe(111) is simulated, in straightforward extension of our previous work. This is expected to give new insights into the technologically important oxidation (i.e., failure) mechanism of more complex telluride alloys.

Furthermore, other telluride surfaces such as $Ge_2Sb_2Te_5$(0001) have been successfully described by comparable DFT techniques, extending the scope of our work further.

PROJECT NUMBER jara0033

> Metastable Transition-Metal Oxides of the Vanadium and Chromium Group

In this project, density-functional theory methods are used in order to search for potential candidates of metastable oxides of the metals of the vanadium and chromium group. Subsequent high-pressure and temperature simulations will provide experimentalists with appropriate synthetic conditions.

PROJECT NUMBER jara0034

> Interstitials in high-manganese steels

The project is concerned with simulations of high-manganese steels. Processes such as crystallization and melting, vacancy formation and vacancy migration as well as the formation of ordered structures in steels will be investigated.

PROJECT NUMBER jara0057

> Ab initio investigations of ϰ-carbides in high-manganese steels

This project is concerned with first-principles calculations of iron-based materials. The focus in this period will be ϰ-carbides in high-manganese steels.

PROJECT NUMBER jara0058

> Quantum chemistry and structural exploration of crystalline molecular networks

The project is concerned with first-principles calculations of nitrogen-based crystal networks. The focus is on testing emerging new software with evolutionary structure-prediction algorithms, used on weakly bound crystals. The chemical systems under study incorporate ionic molecular fragments, for which new structures are predicted. Furthermore, phonon computations on the ground-state structures found with minimum-energy searches are used to determine the dynamic stability of these new crystalline networks.

PROJECT NUMBER jara0069

> Exploration of the Silicon-Tellurium System: On the Search for the Mysterious SiTe

Binary AB materials of main-group IV elements (A = Ge, Sn, Pb) and tellurium (= B) are of interest due to their commercial applications in energy and data storage technologies.

While the structures and the properties of GeTe, SnTe and PbTe are well characterized, there are no reports on a SiTe in the solid state. In a lack of full knowledge of the causes for the non-existence of a SiTe and the actual compositions and properties for the detected single-phase material, there is a critical need to resolve the controversy for the single-phase material and to identify the source for the absence of SiTe. The goals of this project will be accomplished through examinations of the electronic and the vibrational properties for diverse models representing the structures of SiTe, $SiTe_2$ and Si_2Te_3.

PROJECT NUMBER jara0144

INSTITUTE OF JET PROPULSION AND TURBOMACHINERY (IST)

RWTH / Prof. Peter Jeschke

> Noise generation and propagation in a radial compressor

The primary goal of this project is to develop a robust, flexible applicable and low costly acoustic measurement system and to validate it experimentally. The target of this measurement system is to determine the in-duct sound power level emitted by a radial compressor into its discharge pipe. This measurement system is developed based on results obtained from extensive aeroacoustic simulations described in the following.

In the numerical part of this project the noise generation and propagation mechanisms in a centrifugal compressor coupled with a vaneless diffuser and a volute are investigated. In a first step single passage RANS-simulations of the impeller, diffuser and volute, connected with a mixing plane, were conducted in order to evaluate the aerodynamic behaviour of the stage. For the unsteady simulations however, the simulation of a single passage is not sufficient and due to the lack of symmetry of the volute geometry, full annulus 360° URANS-simulations are required.

The initialisation was obtained from a frozen rotor simulation, where the relative position of the impeller is held constant and unsteady effects are neglected. Based on this initialisation, the unsteady simulations were started.

In order to evaluate the sound source mechanisms and to identify the dominant sound sources, the pressure fluctuations in the vaneless diffuser and volute were analysed. The CFD-code TRACE allows for storing the Fourier-coefficients for various harmonics of the rotor speed. The pressure fluctuations can therefore easily be analysed. Figure 1 shows the pressure fluctuations on the impeller blades. Due to its geometry the volute induces asymmetries upstream in the flow region of the impeller. Considering all of the 13 impeller passages provides the possibility to capture these asymmetries and therefore obtain a different pressure pattern for each of the blades.

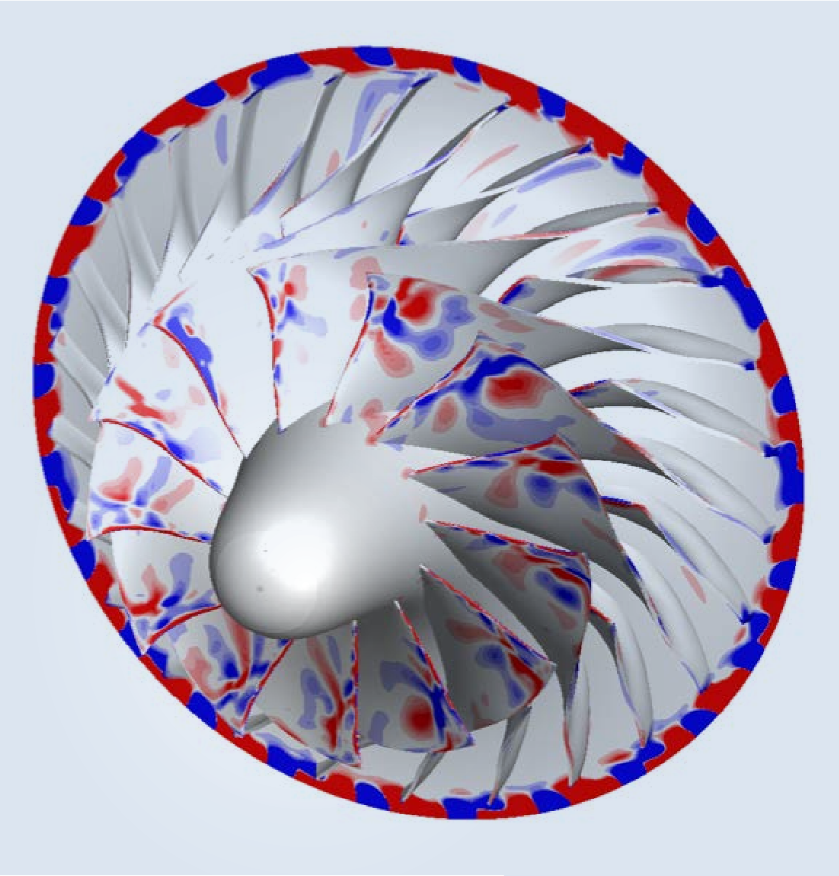


Figure 1: Pressure fluctuations on impeller blades

Besides the sound source mechanisms in the compressor and the volute the sound pressure field at the volute outlet is investigated in this project. With the results of the URANS-simulations conducted on the JARA partition the sound pressure field can be decomposed in different acoustic modes. These acoustic modes show a symmetric flow pattern each, an example given by the (3,1)-mode shown in Figure 2.

The sound pressure field can fully be described by the modes and their corresponding amplitudes. Since only a limited number of modes are capable of propagation, the number of analysis points required is predefined. Given the flow simulation results the pressure fluctuations can easily be obtained at any point in the flow region and the mode analysis thus be conducted. When measurements are conducted, however, the number of sensors is crucial for financial and practical reasons. Hence different approaches are investigated to develop feasible measurement techniques. The simulations conducted on the JARA-HPC Partition form the foundation of these investigations.

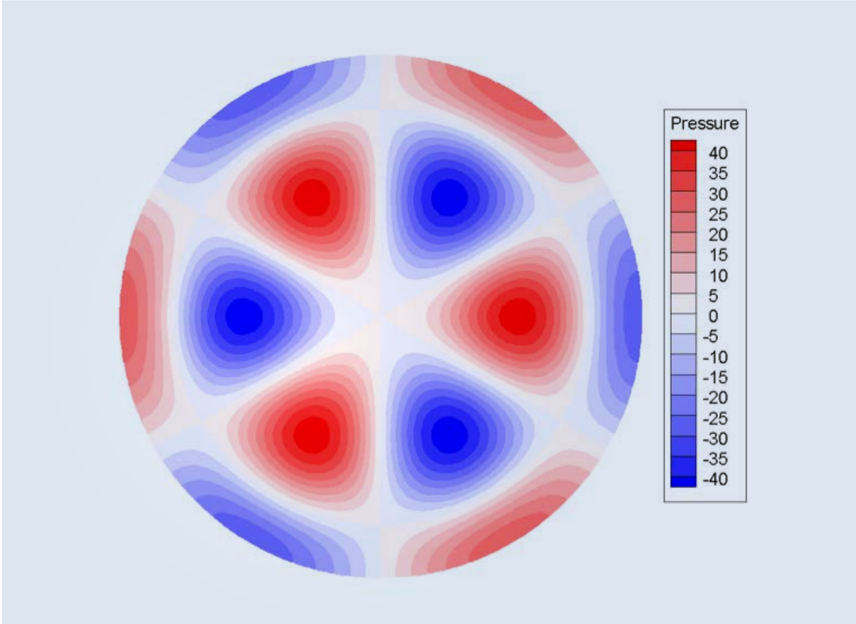


Figure 2: (3,1) sound mode in a circular duct

PROJECT NUMBER jara0033

> Numerical investigation of circumferential flow distortion at the exit of multistage compressors and stall mechanisms due to upstream stator and rotor wakes

In the current running project full annulus URANS simulations of the IDAC compressor were conducted. Three operation points were simulated at the midspan streamtrace which results are presented below. Furthermore the aerodynamic design point was simulated in full 3D with 200mio. grid points. These simulations are the first that confirm these reasons and amount of non-uniform flow with numerical results.

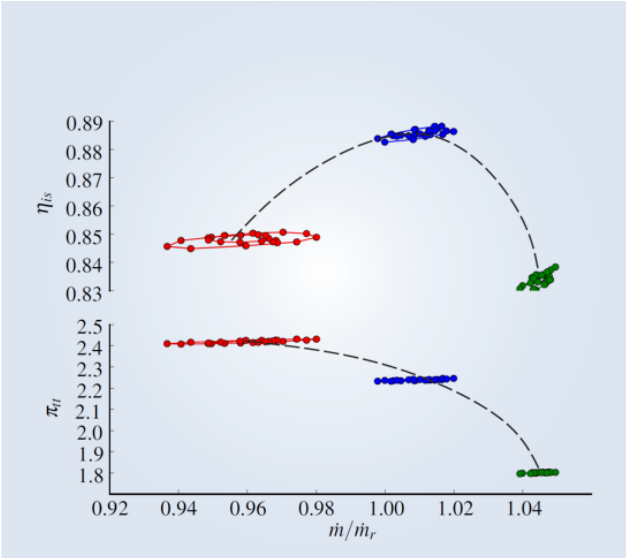


Figure 1: Performance map of the compressor with significant amount of non-uniform flow

The flow in multistage compressors is inherently unsteady. A primary source of unsteadiness is the interaction between wakes and downstream blades. Unsteady wake interaction and wake convection influences local flow condition as well as performance. In addition to stator-rotor interaction, the interaction between two stators and, accordingly, two rotors lead to different local flow conditions. The stator-stator positioning affects the flow on suction as well as the pressure side. Even more for rows with the same blade count, each airfoil has the same clocking position, which can be adjusted to optimize the performance. For rows with the same blade count, the influence of clocking on the performance is experimentally and numerically well examined. The stator positioning showed changes in efficiency of a multistage compressor. For different blade counts, each airfoil of a downstream row has a different clocking position causing inhomogeneous inflow conditions. Interference of wakes and circumferential varying clocking occurs. For the same blade count the performance varies with the clocking position. The results of this project show the effects of airfoil interaction with a different blade count, including circumferential non-uniform flow for the simulated multistage compressor. A strong impact of superposition and interaction of wakes from different rows occurs at the outlet. The quasi 3D simulations show also an influence on the off design operating points. In particular the important surge line is influenced by this effect.

Each airfoil has a different flow condition depending on the upstream wake interference. This is visible in the performance map shown in figure 1 for the design speedline. The flow after each airfoil is averaged over one pitch. The lines connect the flow condition of neighboring pitches for stator 3, while the points represent the pitch-averaged flow conditions. Matching the common divisor of two in the stators, the flow conditions occur at two ellipses for all operating points. Conspicuous is the pitch-average deviation of massflow that increases from choke to surge. At the surge operating point, the pitch-averaged massflow changes over more than 4 %. The pitch-averaged changes in efficiency are more than a half percentage point, while the total pressure ratio changes most at the surge operating point by 2%.

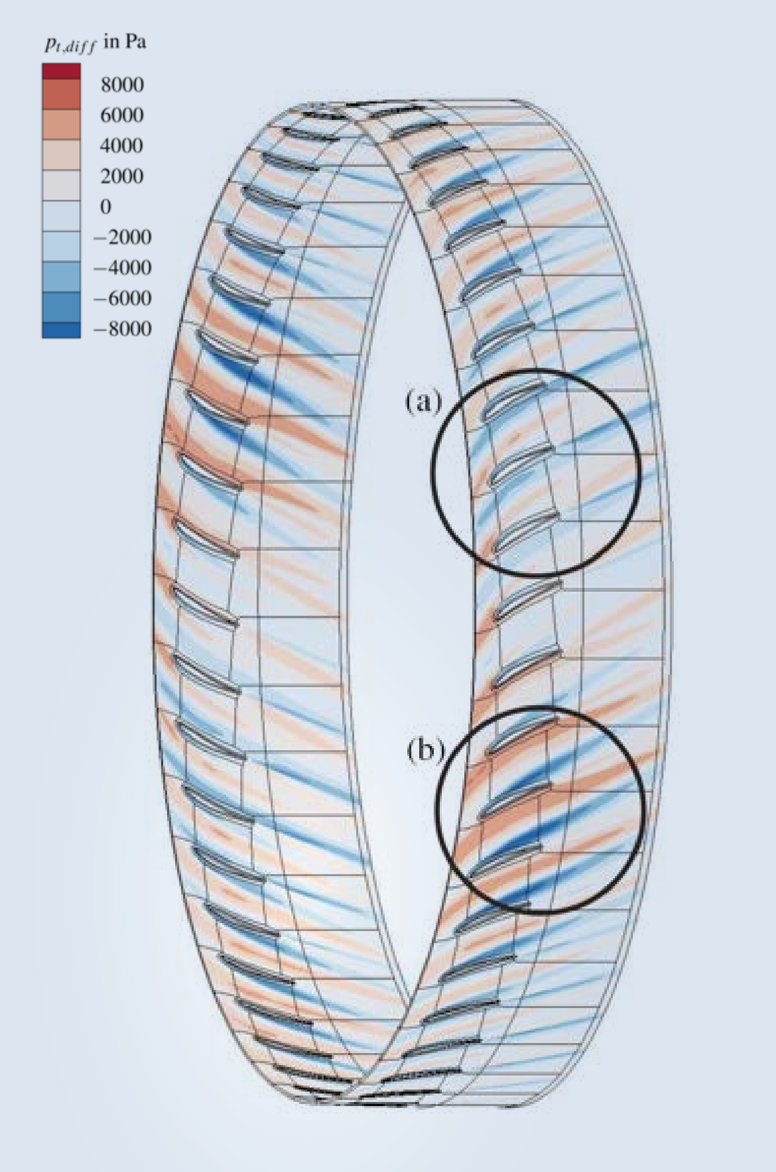


Figure 2: Flow separation at several vanes of the last stator

The detailed analysis of the different operation points shows different aerodynamic effects for the surge and the stall operation point that lead to circumferential non-uniform flow. In figure 2 the last stator is visible for the surge operation point. At the circle marked with (a) the wakes of upstream stators pass along the pressure side. For these configurations a high pressure rise is visible. For the vanes marked with (b) the wakes pass along the suction side. Due to the wake the flow separates at these vanes. Hence this leads to undesirable, unstable flow conditions like rotating stall or surging of the compressor. For the stall operation point are also a undesirable high amount of deviations from periodic flow visible.

PROJECT NUMBER jara0090

INSTITUTE OF TECHNICAL AND MACROMOLECULAR CHEMISTRY

RWTH / Prof. Walter Leitner

> Manganese based catalysts for the oxygen evolution reaction

The identification of suitable molecular catalysts for an efficient electrocatalytical oxygen evolution reaction is the aim of this research project. The generation of oxygen in the oxidation of water suffers from high overpotentials limiting strongly the possibility to introduce this enormously important reaction to produce energy carriers on the industrial scale. While efficient molecular electrocatalytically active compounds mainly consist of noble metals like iridium a search for cheaper catalysts focuses on 4^{th} row metals like manganese, as manganese is an active and efficient component of corresponding naturally occurring photosystems.

In this context it is important to support experimental research by theoretical methods in order to understand the various chemical reaction steps on the molecular level. As the systems under investigation are too large to be treated computationally by highly accurate ab-initio methods like coupled cluster computations an alternative method of choice might be density functional theory. Prior to investigating any chemical steps of a given catalyst a thorough screening of density functionals is necessary to ensure the reliable reproduction of experimentally observed geometries and spin states.

In this project a variety of experimentally known and well characterized manganese complexes were investigated by means of DFT computations. The aim was to obtain information about the quality of various density functionals with regard to describing the geometries and spin states of these complexes correctly. We investigated DFs B3LYP, BP86, M06, MN12L, mPWPW91, PBE0 and TPSSh. The results show that BP86, mPWPW91, and especially MN12L, tend to yield the wrong spin states. The usage of these functionals for such compounds is, thus, discouraged. All the functionals considered deliver accurate geometries. The results also show, however, that B3LYP delivers geometries deviating substantially from experimental values when compared to the other functionals of the set. M06, PBE0 and TPSSh deliver geometries of similar accuracy, PBE0 outstanding slightly with respect to the other two DFs.

As a result we conclude that DFT can certainly be used to investigate unknown mononuclear manganese complexes when the necessary care is taken in chosing the density functional.

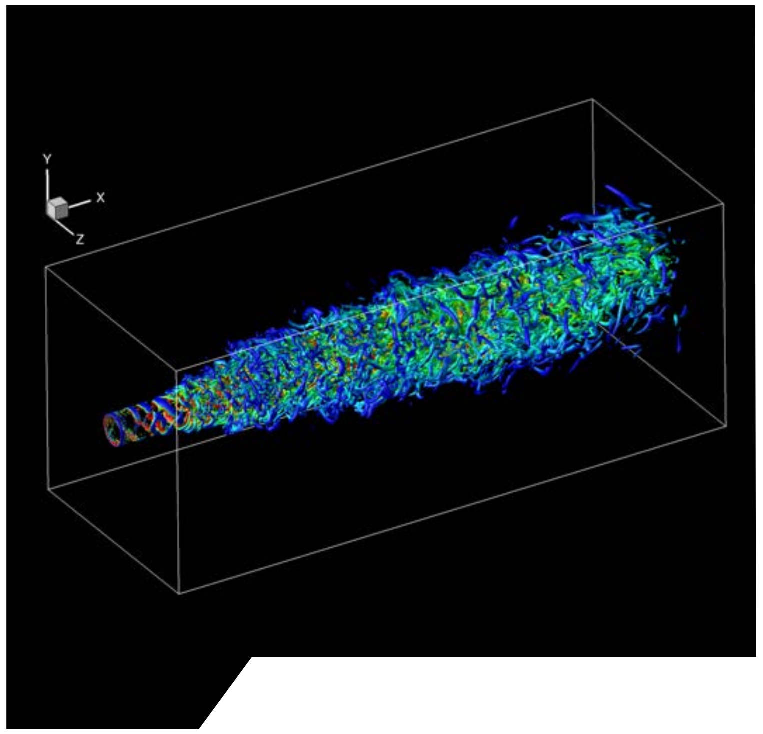
SHOCK WAVE LABORATORY

RWTH / Prof. Herbert Olivier

> Shear layer instability of coaxial jets in cold and hot environments

Coaxial jets with and without a supersonic core flow are typical for many technical applications and therefore of general interest. These jets show a lot of unsteady phenomena such as shear layer instability and transition to turbulence. Their accurate numerical simulation is still challenging despite todays available computing resources. The strategy of using high-fidelity numerical methods and a high spatial resolution helps to increase the range of resolved scales of the flow. This project focuses on the numerical simulation of coaxial jets entering into cold and hot environments. Based on these results a new correlation model and optimisation criteria is proposed to predict the potential core- and supersonic length of the coaxial jet and leading to a significantly increased jet length. In particular, the enlarged supersonic jet length is of interest for special industrial applications.

PROJECT NUMBER jara0142



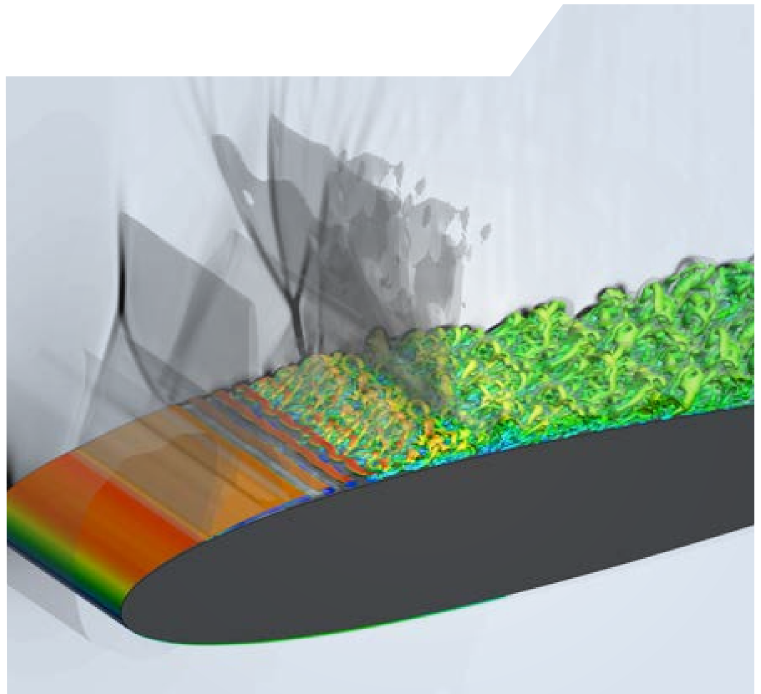
> Direct numerical simulation of the transonic airfoil flow and study of pressure wave sources at the trailing-edge

Within this project, two focuses have been set:

- Mesh study for DNS (Sub-project A),
- Pressure wave phenomena in transonic airfoil flow (Sub-project B).

For the flow around the NACA 0012 airfoil at a transonic flow condition an extensive mesh study was performed. Evaluations of the transient processes allowed a detailed view of the complex wave phenomena. A phenomenon to be emphasized here is the reflection of waves at the sound line of the supersonic region above the detached boundary layer. Complex wave structures and interactions with upstream pressure waves were described. Another focus of the project was the review of the tonal noise phenomenon in transonic flows. Furthermore, the effect of vortex generators on tonal noise was investigated.

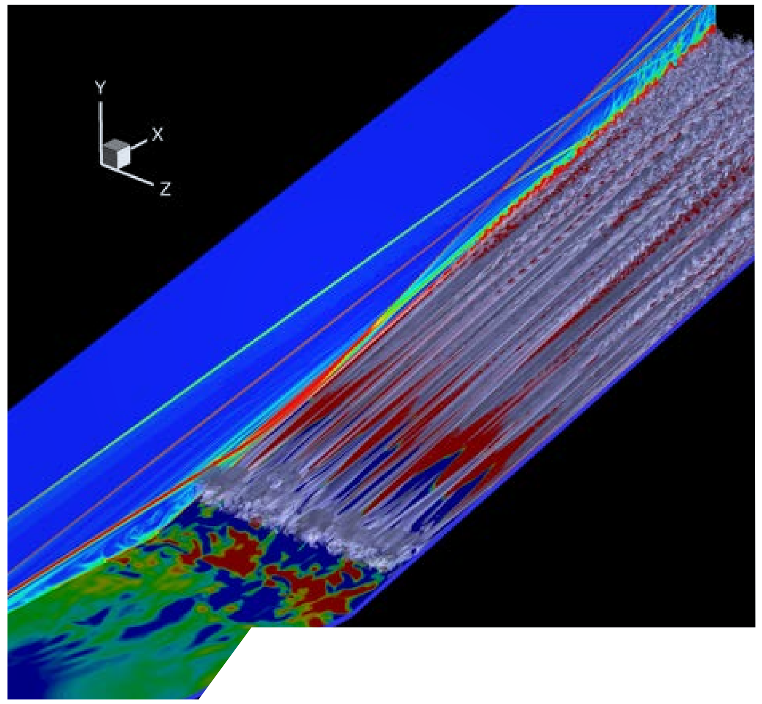
PROJECT NUMBERJHPC13



> Direct numerical simulation of Görtler vortices in hypersonic flows over compression ramps

Hypersonic corner flows show a lot of unsteady phenomena such as local separation regions, shock-boundary layer interaction, boundary layer transition and turbulence. DNS of three-dimensional hypersonic corner flows were performed using 262144 ranks on a JUQUEEN. The results obtained with 4096x512x512 mesh points show a very good resolution in the region of the separation shock, the separation bubble, up to the region of the appearance of Görtler vortices. Depending on the flow condition, the Görtler vortices show some unsteady features. The development and the detailed structure of Görtler vortices downstream of the reattachment region is shown. The Görtler vortices produce strong spanwise heat transfer variations with significant peak heating.

PROJECT NUMBER JHPC30



4. SELECTED HONORS, PRIZES, AWARDS, OFFERS OF PROFESSORSHIP

> CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)

RWTH / Prof. Marek Behr, Ph.D.

- *Dr. Stefanie Elgeti*, elected Co-Chair of ECCOMAS Young Investigator's Committee (EYIC)
- *Linda Gesenhues*, Friedrich-Wilhelm-Prize 2016 of RWTH for Master thesis **"Strain-Based Blood Damage Estimations for Computational Design of Ventricular Assist Devices"**

> CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)

RWTH / Prof. Manfred Martin

- *Prof. Manfred Martin* was invited as Adjunct Professor in the Department of Materials Science and Engineering of Seoul National University, Seoul, Korea
- *Dr. Steffen Grieshammer* became Young Investigator Group Leader within the Helmholtz-Institut Münster (HI MS) Ionics in Energy Storage

> INSTITUTE FOR ADVANCED SIMULATION (IAS) / INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

FZ Jülich / Computational Biomedicine (IAS-5) & Computational Biomedicine (INM-9) / Prof. Paolo Carloni

- Appointment of *Prof. Paolo Carloni* as co-director of the Key Science Laboratory on Multiscale Simulations of Complex Systems (VNU-KeyLab)
- W1 Jr.-Prof. appointment to *Dr. Mercedes Alfonso Prieto*, shared between FZ Jülich and Heinrich Heine Universität Düsseldorf. The position is funded for the 50% by the 'Ernesto Illy Fundation'

> INSTITUTE FOR COMBUSTION ENGINES (VKA)
RWTH / Prof. Stefan Pischinger

- RWTH Fellow

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS
RWTH / Theoretical Nanoelectronics / Prof. Riccardo Mazzarello

- *Mazzarello, R.:* Head of the organizing committee of the MRS Symposium "Phase-Change Materials and Applications", which was held at the 2016 MRS Spring Meeting, Phoenix (USA), March 28-April 1, 2016

> INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)
RWTH / Prof. Wolfgang Schröder

- Membre de l'Académie de l'Air et de l'Espace

> INSTITUTE OF BIOTECHNOLOGY
RWTH / Prof. Ulrich Schwaneberg

- Forschungspreis 2016, BMBF Research Award
- Gold medals for iGEM2016 RWTH team

> INSTITUTE OF COMPLEX SYSTEMS (ICS)
FZ Jülich / Structural Biochemistry (ICS-6) / Prof. Dieter Willbold

- *Xue Wang:* Chinese Scholarship Council fellowship for her PhD studies
- *Birgit Strodel:* Appointment as Associate Editor for RSC Advances (Royal Society of Chemistry)

> INSTITUTE OF INORGANIC CHEMISTRY (IAC), CHAIR OF SOLID-STATE AND QUANTUM CHEMISTRY
RWTH / Prof. Richard Dronskowski

- PhD Scholarship (Fonds der chemischen Industrie) to *Janine George*
- Innovation Award, RWTH, to *Prof. Dr. R. Dronskowski*

5. SELECTED CONFERENCE PARTICIPATIONS

> CHAIR AND INSTITUTE FOR POWER PLANT TECHNOLOGY, STEAM AND GAS TURBINES (IKDG)
RWTH / Prof. Manfred Wirsum

- **TURBO EXPO 2016 – Turbomachinery Technical Conference & Exposition, Seoul, South Korea,** June 13-17, 2016
- **16th International Symposium on Transport Phenomena and Dynamics of Rotating Machinery, Honolulu, Hawaii, USA,** April 10-15, 2016

> CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)
RWTH / Prof. Marek Behr, Ph.D.

- *Behr, M.,* **Complex Fluids in Production and Biomedical Engineering**, Plenary lecture at the World Congress on Computational Mechanics XII, Seoul, South Korea, July 25, 2016

> CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)
RWTH / Prof. Matthias Wuttig

- **Phasenwechselmaterialien: Neue Materialien durch Defektkontrolle?** Kolloquium, Universität Dortmund, Germany, January 26, 2016
- **Novel Phase Change Materials by Design: The Tragedy of Resonance Bonding**, (invited talk), Micron Technology, Boise, USA, March 25, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), CINaM Marseille, Marseille, France, May 27, 2015
- **Novel Phase Change Materials by Design: The Tragedy of Resonance Bonding**, (invited talk), Paris, France, June 09, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), Micron Agrate, Italy, June 21, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), FZ Jülich, July 08, 2016
- **Functional Thin Films By Design: Employing Resonance Bonding To Tailor Thermoelectric And Phase Change Materials** (invited talk), ICSFS 18: International Conference on Solid Films and Surfaces, Chemnitz, Germany, August 30, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), European Symposium on Phase-Change and Ovonic Science, Cambridge, UK, September 05, 2016
- **Novel Phase Change Materials by Design: The Role of Stoichiometry and Disorder**, (invited talk), 20th International Conference on Ternary and Multinary Compounds (ICTMC20), Halle, Germany, September 09, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), MEMRIOX International Workshop 2016, Dresden, Germany, September 27, 2016

- **Advanced functional materials by design: the mystery of resonance Bonding**, Plenary Talk at the National Congress, Italian Physical Society, Padua, Italy, September 29, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, (invited talk), Non-Volatile Memory Technolgy Symposium (NVMTS), Pittsburgh, USA, October 18, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, IMEC, Leuven, Belgium, November 18, 2016
- **Novel Phase Change Materials by Design: The Mystery of Resonance Bonding**, Universita di Catania, Italy, December 06, 2016

> CHAIR OF EXPERIMENTAL PHYSICS, I. PHYSICS INSTITUTE B

RWTH / Prof. Stefan Schael

Invited plenary talks / *Prof. Schael:*

- **New results from the AMS experiment on the ISS**, Physikalisches Kolloquium Universität Kiel, Germany, January 12, 2016
- **New results from the AMS experiment on the ISS**, GSI Winterschule, Schleching, Germany, February 22, 2016
- **Primary spectra of light nuclei in cosmic rays – new results from the AMS experiment**, La Thuile, France, March 21, 2016
- **New Results from the AMS Experiment**, Heidelberg International Symposium on High Energy Gamma-Ray Astronomy, Heidelberg, Germany, July 13, 2016
- **New Results from the AMS Experiment**, TeV Particle Astrophysics, CERN, Switzerland, September 14, 2016
- **New Results from the AMS Experiment**, Physikalisches Kolloquium Universität Kiel, Germany, November 18, 2016

Invited plenary talk / *Dr. Gast:*

- **New results from the AMS experiment on the International Space Station**, DESY Kolloquium Hamburg, Zeuthen, Germany, November 08-09, 2016

> CHAIR OF MATERIAL MECHANICS (CMM)

RWTH / Prof. Bob Svendsen

- **Discrete and coarse-grained Continuum Thermodynamic Models for Dislocation**, Plasticity 2016, USA, January 03-09, 2016
- **Atomistic and phase-field modelling of nanoscopic dislocation processes**, Dislocation based Plasticity, Kloster Schöntal, Germany, February 28-March 03, 2016
- **A laminate-based framework for switching and microstructure evolution in Polycrystalline ferroelectrics**, 87th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Braunschweig, Germany, March 07-10, 2016
- **Stochastic and projection-operator methods for spatio-temporal coarse-grained thermodynamic modeling of multiscale material behavior**, Mechanics of Materials: Mechanics of Interfaces and Evolving Microstructure, Oberwohlfach, Germany, March 13-19, 2016
- **Comparison of algorithms and solution methods for classic and phase-field-based periodic inhomogeneous elastostatics**, ECCOMAS Congress 2016, Crete, Greece, June 05-10, 2016
- **Two-scale FE-FFT phase-field-based computational modeling of bulk microstructural evolution and nanolaminates**, 12th World Congress on Computational Mechanics, Seoul, South Korea, July 24-29, 2016
- **Comparison of Methods for Discontinuous and Smooth Inhomogeneous Elastostatics**, 24th International Congress of Theoretical and Applied Mechanics, Montreal, Canada, August, 21-26, 2016
- **Strongly versus weakly non-local dislocation transport and Pile-up**, 24th International Congress of Theoretical and Applied Mechanics, Montreal, Canada, August 21-26, 2016
- **Atomistic and continuum modelling of nanoscopic dislocation processes**, Recent Advances in Computational Methods for Nanoscale Phenomena, Ann Arbor, USA, August 29-31, 2016
- **Phase field modeling of dislocation cross slip**, European Mechanics of Materials Conference, Brussels, Belgium, September 07-09, 2016
- **A multiscale FE-FFT-and phase-field-based computational approach to predict the structural and local response of polycrystalline materials**, European Mechanics of Materials Conference, Brussels, Belgium, September 07-09, 2016
- **Multiscale FE-FFT-based analysis of macroscopic material behavior and microstructural modifications in polycrystalline materials**, Special Workshop Multiscale modeling of Heterogeneous Structures, Dubrovnik, Croatia, September 21-23, 2016
- **GENERIC-based coarse-graining of the dynamics of discrete dislocation line ensembles with variable orientation**, Dislocation 2016, USA, September 19-23, 2016
- **Linking macroscopic deformation processes to microstructure evolution using an FE-FFT-based micro-macro transition and non-conserved phase-fields**, 87th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Braunschweig, Germany, October 07-10, 2016

> CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS

RWTH / Prof. Manfred Martin

- 2016 EMN Spring, Taipei Sunworld Dynasty Hotel, Taipei, Taiwan, March 08-11, 2016
- DSL 2016, Split, Croatia, June 26-30, 2016
- E-MRS Spring Meeting, Lille, France, Mai 02-06, 2016
- Nonstoichiometric Compounds VI, Santa Fe, New Mexico, USA, September 04-08, 2016

> INSTITUTE FOR ADVANCED SIMULATION (IAS)

FZ Jülich / Theoretical Nanoelectronics (IAS-3) – Prof. Eva Pavarini

- Strong correlations and the LDA+DMFT approach Hands-on workshop and Humboldt-Kolleg: **Density-Functional Theory and Beyond – Basic Principles and Modern Insights**, Isfahan University of Technology, Iran, May 02-13, 2016

> INSTITUTE FOR ADVANCED SIMULATION (IAS), INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

FZ Jülich / Computational Biomedicine (IAS-5) & Computational Biomedicine (INM-9) / Prof. Paolo Carloni

- *Carloni, P.,* Minerva Mühlheim Conference, Mühlheim, Germany, February 15-16, 2016
- *Carloni, P.,* **Biomolecular Simulations across Scales**, Workshop, University of Shanghai, China, May 26-30, 2016
- *Giorgetti, A.,* **Evidence for a Transient Additional Ligand Binding Site in the TAS2R46 Bitter Taste Receptor**, 6th International Conference on the Development of Biomedical Engineering, Ho Chi Min City, Vietnam, June 27-29, 2016
- *Rossetti, G.,* **Molecular View of Ligands Specificity for CAG Repeats: targeting Huntington**, 6th International Conference on the Development of Biomedical Engineering, Ho Chi Min City, Vietnam, June 27-29, 2016
- *Carloni, P.,* **Advanced molecular simulation and experimental biophysical approaches for drug design**, Ho Chi Min City, Vietnam, June 30-July 01, 2016
- *Calandrini, V.,* **Charge Transport at Biological Interfaces: Insights from Molecular Dynamics Simulations**, Interactions and Transport of Charged Species in Bulk and at Interfaces, Vienna, Austria, July 04-07, 2016
- *Carloni, P.,* Shanghai Workshop on **Frontiers in Molecular Biophysics**, University of Shanghai, China, July 23-25, 2016
- *Carloni, P.,* ACS Philadelphia National Meeting, Philadelphia, USA, August 21-25, 2016
- *Rossetti, G.,* **Binding of antagonist to Human Adenosine Receptor A2A in Nearly Physiological Condition**, EuroQSAR: Where Molecular Simulations Meet Drug Discovery, Verona, Italy, September 05-07, 2016
- *Carloni, P.,* Erice Free Energy Landscapes, Erice, Italy, October 07-12, 2016

- *Calandrini, V.,* **Mesoscale physics modelling of protein-protein interactions**, Workshop in Computational biology and applications in human health, Cyprus, October 24-November 04, 2016
- *Giorgetti, A.,* **Membrane Protein Modelling: Bitter taste receptors**, Biophysics-colloquium of the Institute of Biophysics, Johannes Kepler University, Linz, Austria, November 09, 2016

> INSTITUTE FOR ADVANCED SIMULATION (IAS) / INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

FZ Jülich / Theoretical Neuroscience (IAS-6) & Computational and Systems Neuroscience (INM-6)
Prof. M. Diesmann

- *Jordan, J., Kunkel, S., Ippen, T., et al,* **NEST 5g: a simulation kernel for the exascale Seminar**, Talk (Invited), Germany
- Diesmann, M., **Multi-area multi-layer models of cortical networks**, Talk (Invited), EITN, HBP SP3-SP4 meeting, Paris, France, February 04, 2016
- *Diesmann, M.,* **Multi-area multi-layer models of cortical networks T4.2.1**, Talk (Invited) HBP SP3 - SP4 Meeting, Paris, France, February 04, 2016
- *Grün, S.,* Present and Future Role in the HBP, SP3 -SP4 Meeting, EITN, Paris, France, February 04, 2016
- *Diesmann, M.,* **Brain-scale simulations of cortical networks at cellular and synaptic resolution**, Talk (Invited), SFB 936 Multi-Site Communication in the Brain, University Medical Center Hamburg-Eppendorf (UKE), Hamburg, Germany, February 15, 2016
- *Grün, S.,* **Multi-Scale Neuron Recordings and Analysis of Network Interaction**, Talk (Invited), Neuro Data Analysis Workshop, Kyoto University, Japan, February 22, 2016
- *Grün, S.,* **Towards reproducible Analysis of electrophysiological data**, Talk (Invited), Neuro Data Analysis Workshop, Kyoto, Japan, February 22, 2016
- *Diesmann, M.,* **Necessity and feasibility of brain-scale simulations at cellular and synaptic resolution**, Talk (Invited) 6th AICS International Symposium, RIKEN AICS, Kobe, Japan, February 22-23, 2016
- *Diesmann, M.,* **Simulations of macaque cortical networks at cellular and synaptic resolution**, Talk (Invited), Graduate School of Frontier Biosciences, Osaka University, Japan, February 24, 2016
- *Diesmann, M.,* **Simulations of macaque cortical networks at cellular and synaptic resolution**, Talk (Invited), Laboratory for Cognitive Neuroscience, Graduate School of Frontier Biosciences, Osaka University, Japan, February 24, 2016
- *Grün, S., Ohl, F., Schmidt, B.,* **Causative mechanisms of mesoscopic activity patterns in auditory category discrimination**, Talk (Invited), SPP 1665: Resolving and manipulating neuronal networks in the mammalian brain - from correlative to causal analysis, Frankfurt, Germany, February 29-March 02, 2016
- *Diesmann, M.,* **Necessity and feasibility of brain-scale simulation at cellular and synaptic resolution**, Talk (Invited, Workshop on High-Performance Computing, Stochastic Modeling and Databases in Neuroscience NeuroMat, Sao Paulo, Brazil, April 24-29, 2016
- *Diesmann, M.,* **Technology for Brain Scale Simulation at Cellular Resolution**, PASC16 Conference, Ms28 Level of Detail in Brain Modeling, Lausanne, Switzerland, Jun 08-10, 2016
- *Grün, S., Denker, M.,* **The Electrophysiology Analysis Toolkit 'Elephant'**, CDP4 Kickoff meeting, EITN, Paris, France, June 13-14, 2016
- *Grün, S.,* **Progress and Challenges in Analysis of Massively Parallel Spike Data**, Conference Presentation (Invited), MONA2 - Modeling Neural Activity: Statistics, dynamical Systems and Networks, Waikoloa, Hawaii, June 23-25, 2016
- *Grün, S.,* **Analysis of large-scale recordings of neural activity in vivo and in silico**, Conference Presentation (Invited), Introduction to the HBP Collaboratory, Copenhagen, Denmark, July 01-02, 2016
- *Grün, S.,* **Behavioral related synchronous spike patterns in macaque motor cortex during an instructed-delay reach-to-grasp task**, Conference Presentation (Invited), Neural Coding Workshop, Cologne, Germany, August 29-September 01, 2016
- *Grün, S.,* **Behavioral related synchronous spike patterns in macaque motor cortex during an instructed-delay reach-to-grasp task**, Conference Presentation (Invited), Neural Coding Workshop, Cologne, Germany, September 01, 2016
- *Grün, S.,* **Free Viewing in Monkeys - Relating Neuronal Activity and Eye Movements**, Conference Presentation (Invited), International Workshop Vision Over vision, Osaka University, Japan, September 29-October 07, 2016
- *Grün, S.,* **Analysis of Massively Parallel Spike Data: Progress and Challenges**, Conference Presentation (Invited), Intern. Vision for Vision Workshop, Osaka University, Japan, October 03, 2016
- *Senk, J., Yegenoglu, A., Amblet, O., et al,* **Integrating HPC into a Collaborative Simulation-Analysis Workflow for Computational Neuroscience**, Conference Presentation (After Call), JARA-HPC Symposium, Aachen, Germany, Oct 04-05, 2016
- *Grün, S., Rostami, V., Ito, J., et al,* **ReScience – Replication of Riehle et al, 1997**, Conference Presentation (Invited), 9th Vision for Action Meeting, Marseille, France, October 24-26, 2016
- *Grün, S.,* **Framework for the Analysis of Activity Data: Concepts and Use Cases**, Conference Presentation (Invited), SP3-based Meeting: current science, plans, and collaborations across HBP, Congress Centre Amsterdam Science Park, Netherlands, November 30-December 01, 2016
- *Grün, S.,* **Framework for the Analysis of Activity Data: Concepts and Use Cases**, Conference Presentation (Invited), 3rd Brain Initiative Investigators Meeting, Bethesda, USA, December 09-14, 2016

> INSTITUTE FOR COMBUSTION ENGINES (VKA)

RWTH / Prof. Stefan Pischinger

- **Fuel Design for Future Combustion Engines – A View from the Cluster "Tailor-Made Fuels from Biomass"**, Vienna Engine Symposium, Vienna, Austria, April 28, 2016

> INSTITUTE FOR COMBUSTION TECHNOLOGY (ITV)

RWTH / Prof. Heinz Pitsch

- *Jocher, A., Foo, K. K., Sun, Z., Dally, B., Pitsch, H., Alwahabi, Z., Nathan, G.,* **Impact of acoustic forcing on soot evolution and temperature in ethylene-air flames**, 36th International Symposium on Combustion, Seoul, South Korea, July 31-August 05, 2016
- *Jocher, A.,* **Control of Soot Formation in Flames – Effects of Magnetic Fields and Acoustic Waves**, KAUST Clean Combustion Research Center, Thuwal, Saudi-Arabia, 2016
- *Göbbert, J.H., Bode, M.,* **Case Study: Multiphase Flow Simulation Analysis with VisIt/LibSim**, Scalable HPC Visualization and Data Analysis using VisIt, Supercomputing, Salt Lake City, USA, November 13-18, 2016
- *Bode, M., Göbbert, J.H., Pitsch, H.,* **High-Fidelity Multiphase Simulations and In-Situ Visualization Using CIAO**, NIC Symposium, Jülich, Germany, February 11-12, 2016
- *Bode, M., Pitsch, H.,* **Novel simulations of fuel injection systems investigating spray characteristics by use of high-fidelity multiphase methods and supercomputers**, PRACEdays16, Prague, Czech Republic, May 10-12, 2016
- *Göbbert, J.H., Bode, M., Wylie, B.J.N.,* **Extreme-Scale In Situ Visualization of Turbulent Flows on IBM Blue Gene/Q JUQUEEN**. International Supercomputing Conference (ISC) 2016, International Workshops ExaComm, E-MuCoCoS, HPC-IODC, IXPUG, IWOPH, P3MA, VHPC, WOPSSS, Frankfurt, Germany, June 19-23, 2016
- *Göbbert, J.H., Bode, M., Wylie, B.J.N.,* **Extreme-Scale In-Situ Visualization of Turbulent Flows on IBM Blue Gene/Q JUQUEEN**, International Supercomputing Conference (ISC) 2016, Frankfurt, Germany, June 19-23, 2016
- *Göbbert, J.H., Bode, M., Lintermann, A., Zilken, H.,* **Lowering the Barriers to In-Situ Visualization**, ISC Workshop on In-Situ Visualization WOIV, Frankfurt, Germany, June 23, 2016
- *Bode, M., Davidovic, M., Pitsch, H.,* **Multi-scale Coupling for Predictive Injector Simulations**, First JARA-HPC Symposium (JHPCS 2016), Aachen, Germany, October 04-05, 2016

- *Denker, D., Boschung, J., Hennig, F., Pitsch, H.,* **Dissipation Element Analysis of Reacting- and Non-Reacting Flows**, 69th Annual Meeting of the APS Division of Fluid Dynamics, Portland, Oregon, USA, November 2016
- *Boschung, J., Gauding, M., Hennig, F., Denker, D., Pitsch, H.,* **Corrections to the 4/5-law for decaying turbulence**, 69th Annual Meeting of the APS Division of Fluid Dynamics, Portland, Oregon, USA, November 2016
- *Davidovic, M., Bode, M., Falkenstein, T., Cai, L., Pitsch, H.,* **LES of n-dodecane spray combustion and pollutant formation using a Multiple Representative Interactive Flamelet model**, LES for Internal Combustion Engine Flows LES4ICE, France, November 30-December 1, 2016

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS

RWTH / Strongly Correlated Quantum Systems - Prof. Stefan Wessel, Ph.D.

- **Correlations, integrability, and criticality in quantum systems**, Évora, Portugal, October 24-28, 2016
- **Recent progress in low-dimensional quantum magnetism**, Lausanne, Switzerland, September 05-16, 2016
- **International Summer School on Computational Approaches for Quantum-Many-Body Systems**, Beijing, China, August 01-20, 2016

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS

RWTH / Theoretical Nanoelectronics / Prof. Riccardo Mazzarello

- **Phase change materials for universal memory**, IIT Indore - TU9 Research Workshop, Berlin, Germany, November 02-03, 2016
- **First-principles simulations of phase-change materials**, EU-JAPAN Workshop on Computational Materials Design, Jülich, Germany, September 18-30, 2016
- **Interfacial phase-change materials**, 47th IFF Spring School "Memristive phenomena", Jülich, Germany, February 22- March 04, 2016

> INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)

RWTH / Prof. Wolfgang Schröder

- *Schröder, W., et al.,* **Cut-Cell Based Analysis of Moving Particles in Viscous Flows**, ETH Zürich, Switzerland, 2016
- *Schröder. W., et al.,* **Development and Application of Cut-Cell Methods**, Moscow HPC Workshop, Russia, 2016

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)

FZ Jülich / Biotechnology (IBG-1) / Prof. Wolfgang Wiechert

- *Kondrat, S., Zimmermann, O., von Lieres, E.,* **Multiscale modelling of reaction-diffusion processes in living systems**, 18. Heiligen-städter Kolloquium, Technische Systeme für die Lebenswissenschaften, Heilbad Heiligenstadt, Germany, September 19-21, 2016

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)

FZ Jülich / Agrosphere (IBG-3) / Prof. Harry Vereecken

- *Knist S.,* **Added value and land-atmosphere coupling in convection-permitting WRF climate simulations over a Middle Eurpean domain**, International Conference on Regional Climate (ICRC)-CORDEX 2016, Stockholm, Sweden, May 17-20, 2016
- *Kulkarni, K.,* Fully coupled terrestrial water cycle simulations with TerrSysMP: Technical aspects and applications, 4th ENES Workshop on High Performance Computing for Climate and Weather, Toulouse, France, April 06-07, 2016

> INSTITUTE OF BIOTECHNOLOGY

RWTH / Prof. Ulrich Schwaneberg

- **Directed evolution of binding proteins for functionalization of fibers**, CLIB International Conference 2016, Düsseldorf, Germany, January 21, 2016
- **Ankerpeptides and application**, Thai-German Bioeconomy Conference: Cooperation Opportunities for a Sustainable Bioeconomy, Bankok, Thailand, January 28, 2016
- **KnowVolution: Redesigning enzymes for innovations**, Toulouse White Biotechnology Center of Excellence, National Institute for Applied Sciences, University of Toulouse, France, February 11, 2016
- **Directed Enzyme Evolution: Concepts and Lessons**, Industrial Biotechnology Forum 2016, TUM, München-Garching, Germany, March 14, 2016
- **Hybrid Catalysts**, JSPS Japanese-German Graduate Externship International Symposium "Biotechnology and Chemistry for Green Growth", Japan, March 09, 2016
- **"Pioneering the „Integrated Bioeconomy": The BioSC Paradigm Grand Challenges: Answers from North Rhine-Westphalia"**, conference on "Innovation Pathways for Bioeconomic Solutions", Brussels, Belgium, April 07, 2016
- **Wirtschaft mit Zukunft - Wege zur nachhaltigen Produktion in Nordrhein-Westfalen**, Landtag NRW, Düsseldorf, Germany, May 25, 2016
- **Selektive P450- und Ganzzellhybridkatalysatoren in synthetischen Biofilmen**, BMBF Vortrag zum Forschungspreis "Nächste Generation biotechnologischer Verfahren", Berlin, Germany, July 04, 2016
- **KnowVolution: Redesigning enzymes for innovations**, Zheijian University, Hangzhou, China, August 10, 2016
- BMBF Statusseminar in Rahmen des Heiligenstädter Kolloquiums, Heiligenstadt, Germany, September 21, 2016

> INSTITUTE OF COMPLEX SYSTEMS (ICS)

FZ Jülich / Structural Biochemistry (ICS-6) – Prof. Dieter Willbold

- *Strodel, B.,* **Mechanism of amyloid beta-protein oligomerization determined using molecular simulations**, Invited Talk, Sino-German Workshop 1292: Biomolecular Simulations across Scales, Shanghai, China, May 2016
- *Strodel, B.,* **Thermodynamics and kinetics of protein aggregation from atomistic simulations**, Invited Talk, Conference on Energy Landscapes: Theory and Applications, Porquerolles, France, June 2016
- *Strodel, B.,* **Advances and challenges in the simulation of protein aggregation at the atomistic scale**, Keynote talk, 15th Swedish Bioinformatics Workshop, Linköping, Sweden, October 2016
- *Strodel, B.,* **Advances in the simulation of protein aggregation at the atomistic scale**, Keynote talk, Conference on the Future of Chemical Physics, Oxford, UK, September 2016

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)

FZ Jülich / Electrochemical Process Engineering (IEK-3) / Prof. Werner Lehnert

- *Lehnert, W., Reimer, U., Janßen, H., Froning, D., Stolten, D.,* **Water distribution in high temperature polymer electrolyte fuel cells**, invited keynote lecture, Symposium for Fuel Cell and Battery Modeling and Experimental Validation, EPFL (SwissTech Convention Center), Lausanne, Switzerland, March 22-23, 2016

> INSTITUTE OF INORGANIC CHEMISTRY (IAC), CHAIR OF SOLID-STATE AND QUANTUM CHEMISTRY

RWTH / Prof. Richard Dronskowski

- **Chemical Bonding (in Solids) from Local Orbitals and Plane Waves**, Spring Meeting of the American Chemical Society, San Diego, USA, March 2016
- **Complex Inorganic Polymorphs and the Synergy between Quantum Chemistry and Advanced Synthesis**, iPolymorphs Workshop on Novel Routes to Inorganic Polymorphs, San Sebastian, Spain, June 2016
- **A Chemical (Bonding) Perspective on Phase-change and Related Materials**, International Symposium on Structure-Property Relationships in Solid State Materials, Nantes, France, July 2016
- **Chemistry and Neutrons**, Baker Laboratory, Cornell University, Ithaca, USA, July 2016
- **Solid State Chemistry and Neutron Powder Diffraction**, German Conference on Neutron Scattering, Kiel, Germany, September 2016

> INSTITUTE OF JET PROPULSION AND TURBOMACHINERY (IST)

RWTH / Prof. Peter Jeschke

- *Bexten, T., Roscher, B., Weintraub, D., Bachmann, R., Schelenz, R., Jacobs, G., Jeschke, P.,* **Modellbasierte Analyse der Auslegung und des Betriebs kommunaler Energieversorgungssysteme**, 14. Symposium Energieinnovation (EnInnov2016), Graz, Austria, February 10-12, 2016
- *Hölle, M., Bartsch, C., Jeschke, P.,* **Evaluation of measurement uncertainties for pneumatic multi-hole probes using a monte carlo method**, GT2016-56626, ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016
- *Hösgen, C., Behre, S., Hönen, H., Jeschke, P.,* **Analytical uncertainty analysis for hot-wire measurements**, GT2016-56623, ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016
- *Bartsch, C., Hölle, M., Jeschke, P., Metzler, T.,* **Quasi 2D flow-adaptive algorithm for pneumatic probe measurements**, GT2016-56624, ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016
- *Kluxen, R., Behre, S., Jeschke, P., Guendogdu, Y.,* **Loss mechanisms of inter-platform steps in a 1.5 stage axial flow turbine**, GT2016-56940, ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016
- *Fruth, F., Jeschke, P., Franz, H.,* **On the scaling of aeroelastic parameters for high pressure applications in centrifugal compressors**, GT2016-57409, ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016
- *Kaluza, P., Landgraf, C., Schwarz, P., Jeschke, P., Smythe, C.,* **On the influence of a hubside exducer cavity and bleed air in a close-coupled centrifugal compressor stage**, GT2016-58082, Proceedings of ASME Turbo Expo 2016, Seoul, South Korea, June 13-17, 2016

> JÜLICH SUPERCOMPUTING CENTRE (JSC)

FZ Jülich / Prof. Erik Koch

- Scientific Program Committee member of the series of International Workshops on Computational Physics and Materials Science: Total Energy and Force Methods, Luxemburg, January 11-13, 2016

6. SELECTED NATIONAL & INTERNATIONAL COOPERATIONS

> CHAIR AND INSTITUTE FOR POWER PLANT TECHNOLOGY, STEAM AND GAS TURBINES (IKDG)

RWTH / Prof. Manfred Wirsum

- GE Power AG, Mannheim, Germany
- GE Power AG, Rugby, United Kingdom

> CHAIR FOR APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY (GGE)

E.ON Energy Research Center / RWTH / Prof. Christoph Clauser

- *Prof. Thomas R. Rüde,* Lehr- und Forschungsgebiet Hydrogeologie, RWTH
- Centre for High-Performance Scientific Computing in Terrestrial Systems, Geoverbund ABC/J, Germany
- *Prof. Martin Bücker,* Chair for Computer Architecture and Advanced Computing, Friedrich Schiller University, Jena, Germany
- JSC, FZ Jülich

> CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)

RWTH / Prof. Marek Behr, Ph.D.

- *Matteo Pasquali*/Cf2 Complex Flows of Complex Liquids, Rice University, USA
- *Jaewook Nam,* SungKyunKwan University, Korea
- Ford Research Center Aachen, Germany
- ReinVAD GmbH, Aachen, Germany
- SIG Combibloc GmbH, Aachen, Germany

> CHAIR OF COMPUTER SCIENCE 6, HUMAN LANGUAGE TECHNOLOGY AND PATTERN RECOGNITION

RWTH / Prof. Hermann Ney

- Nuance Foundation Inc., Burlington, Massachusetts, USA

> CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)

RWTH / Prof. Matthias Wuttig

- *Dr. Jean-Yves Raty,* Université de Liège, Belgium
- *Dr. Christophe Bichara,* CINaM, CNRS and Aix-Marseille Université, France

> CHAIR OF EXPERIMENTAL PHYSICS, I. PHYSICS INSTITUTE B

RWTH / Prof. Stefan Schael

- *Prof. Dr. Samuel C. C. Ting,* Massachusetts Institute of Technology, Cambridge, Massachusetts, USA
- *Prof. Dr. Bruna Bertucci,* INFN and University of Perugia, Perugia, Italy
- *Dr. Iris Gebauer,* Karlsruhe Insitute of Technology, Karlsruhe, Germany

> CHAIR OF MATERIAL MECHANICS (CMM)

RWTH / Prof. Bob Svendsen

- *Prof. Robert Spatschek,* FZ Jülich and RWTH
- *Prof. Irene Beyerlein,* Los Alamos National Lab, UC Santa Barbara, USA
- *Prof. Markus Hütter,* Polymer Technology, TU Eindhoven, Netherlands
- *Prof. Dierk Raabe,* Max-Planck-Institut für Eisenhüttenkunde, Düsseldorf, Germany
- *Prof. Marc Geers,* Material Mechanics, TU Eindhoven, Netherlands

> CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS

RWTH / Prof. Manfred Martin

- *Prof. P.C. Schmidt,* Technical University of Darmstadt, Darmstadt, Germany
- *Prof. H.-I. Yoo,* Seoul National University, Seoul, Korea
- *Prof. Y. Aoki,* Hokkaido University, Sapporo, Japan
- *Prof. M. Nakayama,* Nagoya Institute of Technology, Nagoya, Japan
- *Prof. S. Ebbinghaus,* Halle University, Germany

> INSTITUTE FOR ADVANCED SIMULATION (IAS)

FZ Jülich / Theoretical Nanoelectronics (IAS-3) / Prof. Eva Pavarini

- Running projects:
- DFG Research Unit Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials
  http://www.physik.uni-augsburg.de/for1346/
- DFT Research Training Group Quantum many-body methods in condensed matter systems
  http://www.physik.rwth-aachen.de/institute/institut-fuer-theorie-der-statistischen-physik/rtg1995/

> INSTITUTE FOR ADVANCED SIMULATION (IAS), INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM),

FZ Jülich / Computational Biomedicine (IAS-5) & Computational Biomedicine (INM-9) / Prof. Paolo Carloni

- Key Science Laboratory on Multiscale Simulations of Complex Systems (VNU-KeyLab), Vietnam National University, University of Science, Hanoi, Vietnam. The VNU-KeyLab is an international initiative between German and Vietnamese scientists, which will offer a unique chance to do outstanding research in computational neuromedicine for highly selected students with an excellent theoretical physics background.

- European Joint PhD program HPC-LEAP (Grant received from the RWTH). HPC-LEAP (www.hpc-leap.eu) is a highly interdisciplinary joint doctorate program realized by bringing together world-leading experts in applied mathematics, high performance computing technologies, particle and nuclear physics, fluid dynamics and life sciences to appropriately train researchers in Europe to exploit high performance computing, advance science and promote innovation. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 642069.

- Centre of Excellence for Computational Biomolecular Research BioExcel. BioExcel (www.bioexcel.eu) is an international European initiative for provision of support to academic and industrial researchers in the use of high-performance computing (HPC) and high-throughput computing (HTC) in biomolecular research. It will provide the necessary solutions for long-term support of the bio-molecular research communities: fast and scalable software, user-friendly automation workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code and personalized consultancy support.

- Internal collaboration within the FZ Jülich to create a transverse group between the Institute of Neuroscience and Medicine INM9 and the Institute of Complex System ICS3, at the FZ Jülich. The group works on the mesoscale modeling of post-synaptic signaling events. This approach aims at bridging the gap between the molecular description and a more systemic-oriented modeling, in order to correctly describe downstream signaling in response to different neuromodulators or diseases-linked mutations.

> INSTITUTE FOR ADVANCED SIMULATION (IAS), INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)

FZ Jülich / Theoretical Neuroscience (IAS-6) & Computational and Systems Neuroscience (INM-6)
Prof. Markus Diesmann

- **Human Brain Project:**
  http://www.humanbrainproject.eu
  > *Prof. Markus Diesmann* is leader of work package 7.1 (SGA1) / Simulation Technology
  > *Prof. Markus Diesmann* is leader of Task 6.3.5 (SGA1) / Tools for network simulation
  > *Sonja Grün* is leader of work package 4.5 (SGA1) / Linking Model Activity and Function to Experimental Data
- **Helmholtz Portfolio Theme - Supercomputing and Modeling for the Human Brain (SMHB):**
  http://www.fz-juelich.de/inm/inm-1/EN/Forschung/JuBrain/Helmholtz%20Portfolio.html
- **Memorandum of Understanding** between FZ Jülich and RIKEN Advanced Institute for Computational Science, Kobe, Japan, February 2013

> INSTITUTE FOR COMBUSTION ENGINES (VKA)
RWTH / Prof. Stefan Pischinger

- Universidad Politécnica de Valencia, CMT, Valencia, Spain
- Technische Universität München, LVK, Munich, Germany
- Universität Kassel, Kassel, Germany
- TU Hamburg-Harburg, Hamburg, Germany
- Tsinghua University, Peking, China

> INSTITUTE FOR COMBUSTION TECHNOLOGY (ITV)
RWTH / Prof. Heinz Pitsch

- *Schiemann, M., Vorobiev, N., Scherer, V.,* Ruhr University of Bochum, Bochum, Germany
- *Kang, S.,* Sogang University, South Korea
- *Dally, B., Alwahabi, Z., Nathan, G.,* University of Adelaide, Adelaide, Australia
- *Geigle K.P.,* German Aerospace Center (DLR), Stuttgart, Germany
- Cooperation with other researchers within the International Sooting Flame (ISF) Workshop, which is co-organized by Prof. H. Pitsch

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS
RWTH / Strongly Correlated Quantum Systems / Prof. Stefan Wessel, Ph.D.

- *Prof. Zi Yang Meng,* IOP, CAS, China
- *Prof. F. Mila,* EPFL Lausanne, Switzerland
- *Prof. A. Honecker,* Universite de Cergy-Pontoise, Cergy-Pontoise, France

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS
RWTH / Theoretical Nanoelectronics / Prof. Riccardo Mazzarello

- *Prof. Wei Zhang and Prof. Evan Ma,* Xi'an Jiaotong University, Shanghai, China
- *Prof. Anbarasu Manivannan,* IIT Indore, India
- *Dr. Ivan Kaban,* IFF Dresden, Germany
- *Dr. Raffaella Calarco,* PDI Berlin, Germany
- *Dr. Jean-Yves Raty,* Université de Liège, Liège, Belgium

> INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)
RWTH / Prof. Wolfgang Schröder

- Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS), Toulouse, France
- NVIDIA Application Lab, Jülich, Germany
- Institut Pprime, Université de Poitiers, France
- Laboratoire d'Hydrodynamique de l'X (LadHyX), École Polytechnique, France
- Fachgebiet Energie- und Kraftwerkstechnik, TU Darmstadt, Darmstadt, Germany

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)
FZ Jülich / Biotechnology (IBG-1) / Prof. Wolfgang Wiechert

- *Prof. Charles Haynes,* University of British Columbia (UBC), Vancouver, Canada
- *Prof. Matthias Weiss,* Bayreuth University, Bayreuth, Germany
- *Prof. Marek Behr,* RWTH
- *Prof. Jörg Fitter,* RWTH
- *Dr. Marco Bocola,* RWTH

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)
FZ Jülich / Agrosphere (IBG-3) / Prof. Harry Vereecken

- Reed Maxwell, Colorado School of Mines: International Groundwater Modeling Center, Golden, Colorado, USA
- Eric Wood, Princeton University and Marc Bierkens: Hyperresolution global Hydrological Modeling Project, Princeton, New Jersey, USA
- FOR 2131, DFG: Data Assimilation for Improved Characterization of Fluxes across Compartmental Interfaces
- SFB/TR32: Patterns in soil-vegetation-atmosphere systems: monitoring, modeling and data assimilation
- World Climate Research Programme (WCRP) Coordinated Regional Downscaling Experiment European Initiative (EURO-CORDEX)

> INSTITUTE OF BIOTECHNOLOGY
RWTH / Prof. Ulrich Schwaneberg

- DFG, SFB 985, Funktionelle Mikrogele und Mikrogelsysteme, DWI - Leibniz-Institut für Interaktive Materialien e.V., Germany
- DFG, Gradiertenkolleg GRK 1628/1, Selectivity in Chemo-and Biocatalysis, Prof. Takashi Hayashi, Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Osaka, Japan
- Cooperation for a sustainable bioeconomy with several institutes from Heinrich Heine University (Düsseldorf), Friedrich Wilhelms University, Bonn and Jülich Research Center in the frame of Bioeconomy Science Center (www.biosc.de), Germany
- Cooparation with Henkel, Düsseldorf, Henkel Innovation Campus for Advanced Sustainable Technologies (HICAST) at RWTH
- Tianjin Institute of Biotechnology (TIB), Chinese Academy of Science, Tianjin, China
- EU Project ROBOX

> INSTITUTE OF COMPLEX SYSTEMS (ICS)
FZ Jülich / Structural Biochemistry (ICS-6) – Prof. Dieter Willbold

- *Prof. Dr. Lynn Kamerlin,* Uppsala University, Uppsala, Sweden
- *Dr. Sebastian Wärmländer,* Stockholm University, Stockholm, Sweden
- *Prof. Dr. Bettina Keller,* Free University of Berlin, Berlin, Germany

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)
FZ Jülich / Stratosphere (IEK-7) / Prof. Martin Riese

- *Prof. Dr. Y. Liu,* Institute of Atmospheric Physics (IAP), Chinese Academy of Sciences, Beijing, China,

> INSTITUTE OF INORGANIC CHEMISTRY (IAC), CHAIR OF SOLID-STATE AND QUANTUM CHEMISTRY

RWTH / Prof. Richard Dronskowski

- all corresponding colleagues of RWTH and MPI for Iron Research, Düsseldorf within Sonderforschungsbereich 761, "Steel ab initio"
- all corresponding colleagues of RWTH and FZ Jülich within Sonderforschungsbereich 917, "Nanoswitches"
- *Prof. Martin Lerch*, TU Berlin, within Priority Programme 1415, "Crystalline Non-Equilibrium Phases"
- *Prof. Shinichi Kikkawa*, Hokkaido University, Sapporo, Japan, on the characterization of complex oxides and oxide nitrides
- *Prof. Andrei Tchougréeff*, Lomonosov State University, Moscow, Russia, on the many-body theory of nitrogen-based pseudo-oxides

> INSTITUTE OF JET PROPULSION AND TURBOMACHINERY (IST)

RWTH / Prof. Peter Jeschke

- MTU Aero Engines,
- MAN Diesel & Turbo, Augsburg, Germany
- GE Aviation, Evendale, Ohio, USA
- Deutsches Zentrum für Luft- und Raumfahrt (DLR), Cologne, Germany
- Forschungsvereinigung Verbrennungskraftmaschinen (FVV), Frankfurt a.M., Germany

J

> JÜLICH SUPERCOMPUTING CENTRE (JSC)

FZ Jülich / Prof. Erik Koch

- DFG Research Training Group 1346/2: Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials
- DFG Graduiertenkolleg 1995/1: Quantum many-body methods in condensed matter systems

7. VISITING SCIENTISTS

C

> CHAIR FOR APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY (GGE)

E.ON Energy Research Center / RWTH / Prof. Christoph Clauser

- *Dr. Lucas Pimienta,* Ecole Normale Supérieure of Paris, Paris, France

> CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)

RWTH / Prof. Marek Behr, Ph.D.

- *Prof. Jaewook Nam,* SungKyunKwan University, Seoul, South Korea
- *Prof. Alessandro Reali,* University of Pavia, Italy
- *Prof. Tom Hughes,* University of Texas at Austin, USA
- *Prof. Matthias Heinkenschloss,* Rice University, Houston, Texas, USA
- *Prof. Matteo Pasquali,* Rice University, Houston, Texas, USA
- *Prof. Kazuo Kashiyama,* Chuo University, Japan
- *Prof. Kenjiro Terada,* Tohoku University, Sendai, Japan

> CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)

RWTH / Prof. Matthias Wuttig

- *Prof. Dr. T. Siegrist,* Florida, USA
- *Prof . X. Gonze, Louvain,* Belgium
- *Dr. Konstantyn Shportko,* Physics department of NAS Ukraine
- *Prof. Anbarasu Manivannan,* India

> CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS

RWTH / Prof. Manfred Martin

- *Prof. P.C. Schmidt,* Technical University of Darmstadt, Darmstadt, Germany
- *Dr. P. Mchedlov,* National Science Center Kharkov Institite for Physics & Technology, Kharkiv, Ukraine

> INSTITUTE FOR ADVANCED SIMULATION (IAS)
FZ Jülich / Theoretical Nanoelectronics (IAS-3) / Prof. Eva Pavarini

- Our institute, together with the GRS hosts the Autumn School on Correlated Electrons, Local organizers: E. Pavarini (IAS/PGI) and E. Koch (GRS). You can find the list of lecturers and photos of the school here: http://www.cond-mat.de/events/correl.html
This school every year attracts internationally very well known scientists at the FZJ, highly increasing the visibility of the FZJ in the field of strongly correlated materials.

> INSTITUTE FOR ADVANCED SIMULATION (IAS), INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM),
FZ Jülich / Computational Biomedicine (IAS-5) & Computational Biomedicine (INM-9) / Prof. Paolo Carloni

- *Ass. Prof. Anne Grünewald,* Université du Luxembourg, Luxembourg
- *Prof. Dr. Simon Bernèche,* University of Basel, Basel, Switzerland
- *Dr. Albert Konijnenberg,* University of Antwerp, Antwerp, Belgium
- *Prof. Dr. Tiago Outeiro,* University of Göttingen, Göttingen, Germany
- *Prof. Claudio Fernández,* Max-Planck Institute, Rosario, Argentina
- *Prof. Dr. Jörg Schulz,* RWTH and University Hospital Aachen, Germany
- *Dr. Ralf Biehl,* JCNS-1/ICS-1 FZ Jülich
- *Dr. Reiner Zorn,* JCNS-1/ICS-1 FZ Jülich
- *Prof. Dr. Raimund Dutzler,* University of Zurich, Zurich, Switzerland
- *Dr. Daniël van den Hove,* PhD, Maastricht University, Maastricht, The Netherlands
- *Jun-Prof. Dr. Bettina Keller,* Freie Universität Berlin, Germany
- *Dr. Daniele Dimarino,* Universitá della Svizzera Italiana, Lugano, Switzerland
- *Prof. Dr. Inga D. Neumann,* University of Regensburg, Regensburg, Germany
- *Dr. Kyong Kang,* ICS-3, FZ Jülich
- *Prof. Rachel Nechushtai,* The Hebrew University of Jerusalem, Israel
- *Dr. Theo Rein,* Max Planck Institute of Psychiatry, München, Germany
- *Dr. Francesco Colizzi,* IRB Barcelona, Spain
- *Prof. Oded Livnah,* The Hebrew University, Israel
- *Prof. Rafal E. Dunin-Borkowski,* Institute for Microstructure Research, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, and Peter Gruenberg Institute, Germany
- *Dr. Ulrich Zachariae,* University of Dundee, Dundee, UK

> INSTITUTE FOR ADVANCED SIMULATION (IAS), INSTITUTE OF NEUROSCIENCE AND MEDICINE (INM)
FZ Jülich / Theoretical Neuroscience (IAS-6) & Computational and Systems Neuroscience (INM-6)
Prof. Markus Diesmann

- *Hans Ekkehard Plesser,* Department of Mathematical Sciences and Technology, Norwegian University of Life Sciences, Norway (since 2013)

> INSTITUTE FOR COMBUSTION ENGINES (VKA)
RWTH / Prof. Stefan Pischinger

- *Jorge Valero Marco,* Universidad Politécnica de Valencia, CMT, Valencia, Spain

> INSTITUTE FOR COMBUSTION TECHNOLOGY (ITV)
RWTH / Prof. Heinz Pitsch

- *Dr. Zhenxun Gao,* Beihang University, Beijing Shi, China

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS
RWTH / Strongly Correlated Quantum Systems / Prof. Stefan Wessel, Ph.D.

- *Prof. A. Honecker,* Universite de Cergy-Pontoise, Cergy-Pontoise, France

> INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)
RWTH / Prof. Wolfgang Schröder

- *Claus-Dieter Munz,* University of Stuttgart, Stuttgart, Germany
- *Gregor Gassner,* University of Cologne, Cologne, Germany
- *Uwe Küster,* HLRS Stuttgart, Stuttgart, Germany
- *Shinnosuke Obi,* Keio University, Japan
- *Henrik Alfredsson,* KTH Royal Institute of Technology, Stockholm, Sweden
- *Mihai Mihaescu,* KTH Royal Institute of Technology, Stockholm, Sweden
- *Luca Brandt,* KTH Royal Institute of Technology, Stockholm, Sweden
- *Rainald Löhner,* George Mason University, Fairfax, VA, USA
- *Hans Hornung,* Caltech, California Institute of Technology, Pasadena, CA, USA

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)

FZ Jülich / Agrosphere (IBG-3) / Prof. Harry Vereecken

· *Robert Walko,* University of Miami/RSMAS, Miami, Florida, USA

> INSTITUTE OF BIOTECHNOLOGY

RWTH / Prof. Ulrich Schwaneberg

- *Prof. Joery de Kock and Jessi Neuckermans,* In Vitro Toxicology and Dermato-Cosmetology (IVTD), Vrije Universiteit Brussel, Brussels, Belgium
- *Prof. Zhimin Li,* State Key Lab of Bioreactor Engineering, East China University of Science and Technology, Shanghai, China
- *Hao Cao,* Beijing University of Chemical Technology, Beijing, China

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)

FZ Jülich/ Electrochemical Process Engineering (IEK-3) / Prof. Werner Lehnert

- *Prof. Martin Andersson,* Lund University, Faculty of Engineering, Lund, Sweden
- *Prof. Liangfei Xu,* Automotive Engineering Department, Tsinghua University, China
- *Prof. Dirk Henkensmeier,* Korea Institute of Science and Technology, Seoul, South Korea

> INSTITUTE OF INORGANIC CHEMISTRY (IAC), CHAIR OF SOLID-STATE AND QUANTUM CHEMISTRY

RWTH / Prof. Richard Dronskowski

- *Prof. Dr. Andrei Tchougréeff,* Lomonosov State University, Moscow, Russia
- *Dr. Ryky Nelson,* Louisiana State University, Baton Rouge, Louisiana, USA

8. YOUNG RESEARCHER GROUPS ESTABLISHED IN JARA-HPC INSTITUTES

A

Ab initio description of double and charge transfer excitations: from solvable models to complex systems / Dr. Nicole Helbig
Institute for Advanced Simulation (IAS), FZ Jülich
Quantum Theory of Materials (IAS-1) / *Prof. Stefan Blügel*

Actinide Solid State Chemistry - A direct Link from fundamental Science to the safe Management of high-level nuclear waste / Prof. Dr. Evgeny Alekseev
Institute of Energy and Climate Research (IEK), FZ Jülich
Nuclear Waste Management and Reactor Safety (IEK-6) / *Prof. Dirk Bosbach*

Active-Materials: Cell tissues in silico / PD Dr. Jens Elgeti
Institute for Advanced Simulation (IAS), FZ Jülich
Theoretical Soft Matter and Biophysics (IAS-2) / *Prof. Gerhard Gompper*

C

Computational modeling of materials for nuclear technology / Dr. Piotr Kowalski
Institute of Energy and Climate Research (IEK), FZ Jülich
Nuclear Waste Management and Reactor Safety (IEK-6) / *Prof. Dirk Bosbach*

I

Instrumental and Data-driven Approaches to Source-Partitioning of Greenhouse Gas Fluxes: Comparison, Combination, Advancement (IDAS-GHG) / Dr. Alexander Graf
Institute of Bio- and Geosciences (IBG), FZ Jülich
Agrosphere (IBG-3) / *Prof. Harry Vereecken*

M

Modellierung klimarelevanter Prozesse / Dr. Felix Plöger
Institute of Energy and Climate Research (IEK), FZ Jülich
Stratosphere (IEK-7) / *Prof. Martin Riese*

Microcirculation in Health and in Cancer: Blood Flow and Drug Delivery in Silicio / Dr. Dmitry Fedosov

Institute for Advanced Simulation (IAS), FZ Jülich

Theoretical Soft Matter and Biophysics (IAS-2) / *Prof. Gerhard Gompper*

Microscale Bioengineering / Dr. Dietrich Kohlheyer

Institute of Bio- and Geosciences (IBG), FZ Jülich

Biotechnology (IBG-1) / *Prof. Wolfgang Wiechert*

Modular Synthetic Enzyme Cascades / Juniorprof. Dr. Dörte Rother

Institute of Bio- and Geosciences (IBG), FZ Jülich

Biotechnology (IBG-1) / *Prof. Wolfgang Wiechert*

Multiscale Modelling and Simulation of Macromolecules / Dr. Benedikt Sabass

Institute for Advanced Simulation (IAS), FZ Jülich

Theoretical Soft Matter and Biophysics (ICS-2 / IAS-2) / *Prof. Gerhard Gompper*

Theory of Multi-scale neuronal networks / Prof. Dr. Moritz Helias

Institute of Neuroscience and Medicine, FZ Jülich

Computational and Systems Neuroscience (INM-6) / *Prof. Markus Diesmann*

9. GENERAL INFORMATION

> 9.1 JARA-HPC members

On 31 December 2016, 42 scientists and their institutes were members of JARA-HPC:

MEMBER	INSTITUTE
Prof. Marek Behr, Ph.D.	SimLab FSE Chair for Computational Analysis of Technical Systems (CATS), RWTH
Prof. Stefan Blügel	SimLab ab initio Peter Grünberg Institute / Institute for Advanced Simulation, Quantum Theory of Materials (PGI-1 / IAS-1), FZ Jülich
Prof. Dirk Bosbach	Institute of Energy and Climate Research, Nuclear Waste Management and Reactor Safety (IEK-6), FZ Jülich
Prof. Paolo Carloni	Deputy Director JARA-HPC Institute of Neuroscience and Medicine, Computational Biomedicine (IAS-5 / INM-9), FZ Jülich
Prof. Christoph Clauser	Chair for Applied Geophysics and Geothermal Energy (GGE), E.ON Energy Research Center, RWTH
Prof. Markus Diesmann	Institute for Advanced Simulation, Theoretical Neuroscience (IAS-6), Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), FZ Jülich
Prof. David DiVincenzo	Peter Grünberg Institute, Theoretical Nanoelectronics (PGI-2 / IAS-3), FZ Jülich Department of Physics, Institute for Quantum Information (IQI), RWTH
Prof. Richard Dronskowski	SimLab ab initio Institute of Inorganic Chemistry (IAC), Chair of Solid-State and Quantum Chemistry, RWTH
Prof. Gerhard Gompper	Institute of Complex Systems, Theoretical Soft Matter and Biophysics (ICS-2 / IAS-2), FZ Jülich
Prof. Peter Jeschke	Institute of Jet Propulsion and Turbomachinery (IST), RWTH
Prof. Erik Koch	Jülich Supercomputing Centre (JSC), FZ Jülich
Prof. Torsten W. Kuhlen	CSG ImVis Virtual Reality and Immersive Visualization, IT Center, RWTH
Prof. Werner Lehnert	Institute of Energy and Climate Research, Electrochemical Process Engineering (IEK-3), FZ Jülich
Prof. Walter Leitner	Institute of Technical and Macromolecular Chemistry (ITMC), RWTH
Prof. Thomas Lippert	Director JARA-HPC, Jülich Supercomputing Centre (JSC), Institute for Advanced Simulation (IAS), FZ Jülich

Prof. Arne Lüchow	Institute of Physical Chemistry (IPC), Theoretical Chemistry, RWTH
Prof. Manfred Martin	Chair of Physical Chemistry I, Physical Chemistry of Solids, RWTH
Prof. Riccardo Mazzarello	Institute for Theoretical Solid State Physics, Theoretical Nanoelectronics, RWTH
Prof. Ulf-G. Meißner	Institute for Nuclear Physics, Theory of the strong interactions (IKP-3 / IAS-4), FZ Jülich
Prof. Abigail Morrison	SimLab Neuroscience Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), Institute for Advanced Simulation, Theoretical Neuroscience (IAS-6), FZ Jülich
Prof. Matthias Müller	Deputy Director JARA-HPC, CSG ParE Chair for Computer Science 12, IT Center, RWTH
Prof. Uwe Naumann	Software and Tools for Computational Engineering (STCE), LufG Informatik, RWTH
Prof. Hermann Ney	Chair of Computer Science 6, Human Language Technology and Pattern Recognition, RWTH
Prof. Herbert Olivier	Shock Wave Laboratory, RWTH
Prof. Eva Pavarini	Peter Grünberg Institute / Institute for Advanced Simulation, Theoretical Nanoelectronics (PGI-2 / IAS-3), FZ Jülich
Prof. Stefan Pischinger	Institute for Combustion Engines (VKA), RWTH
Prof. Heinz Pitsch	Institute for Combustion Technology (ITV), RWTH
Prof. Uwe Rau	Institute of Energy and Climate Research, Photovoltaics (IEK-5), FZ Jülich
Prof. Arnold Reusken	Institute for Geometry and Practical Mathematics (IGPM), RWTH
Prof. Martin Riese	Institute of Energy and Climate Research, Stratosphere (IEK-7), FZ Jülich
Prof. James Ritman	Institute for Nuclear Physics, Experimental Hadron Structure (IKP-1), FZ Jülich
Prof. Stefan Schael	Chair of Experimental Physics, I. Physics Institute B, RWTH
Prof. Wolfgang Schröder	Director JARA-HPC, SimLab FSE Institute of Aerodynamics and Chair of Fluid Mechanics (AIA), RWTH
Prof. Ulrich Schwaneberg	Institute of Biotechnology, RWTH
Prof. Bob Svendsen	Chair of Material Mechanics (CMM), RWTH
Prof. Harry Vereecken	Institute of Bio- and Geosciences, Agrosphere (IBG-3), FZ Jülich
Prof. Andreas Wahner	Institute of Energy and Climate Research, Troposphere (IEK-8), FZ Jülich
Prof. Stefan Wessel, Ph.D.	Institute for Theoretical Solid State Physics, Strongly Correlated Quantum Systems, RWTH
Prof. Wolfgang Wiechert	Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZ Jülich
Prof. Dieter Willbold	Institute of Complex Systems, Structural Biochemistry (ICS-6), FZ Jülich
Prof. Manfred Wirsum	Chair and Institute of Power Plant Engineering, Steam and Gas Turbines (IKDG), RWTH
Prof. Matthias Wuttig	Chair of Experimental Physics, I. Institute of Physics (IA) , RWTH

> 9.2 Involved institudes

> CHAIR AND INSTITUTE FOR POWER PLANT TECHNOLOGY, STEAM AND GAS TURBINES (IKDG)

RWTH / Prof. Manfred Wirsum

The Institute for Power Plant Technology, Steam and Gas Turbines (IKDG) deals with the analysis and assessment of energy conversion systems, with the investigation and optimization of steam and gas turbines and valves for power plant applications and their integration into the power plant process.

The IKDG has several large test rigs, in which combustion processes in gas turbine combustion chambers or flow phenomena in steam and gas turbines, such as secondary flows in the blade channel and leakage flows in the shroud cavity and their interaction can be investigated. The aim of this research is optimization of the turbine aerodynamics and characterization of loss mechanisms. The increasing of power plants efficiencies is associated with the increase of the process parameters of turbines which requires the application of porous materials and improved cooling technologies.

The investigations of combustion processes aim at reducing of pollutant emissions and combustion instabilities. The latter induce combustion chamber humming in premix burners which is a threat to the safe operation of the gas turbine plant. These burners are in comparison to diffusion burners characterized by significantly lower NOx emissions.

Furthermore the Institute is concerned with power plant simulations. The interaction of the individual machines in a complex energy conversion system is analyzed in order to derive strategies for the optimization of the overall system and the components. Besides decentralized and hybrid technologies can be evaluated.

> CHAIR FOR APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY (GGE) / E.ON ENERGY RESEARCH CENTER

RWTH / Prof. Christoph Clauser

Within the framework of the establishment of the E.ON ERC, the Institute for Applied Geophysics and Geothermal Energy (GGE) at RWTH has evolved from the former institute for Applied Geophysics. The research at GGE focuses on geophysical and hydrodynamic reservoir engineering (e.g. for geothermal energy, CO_2-sequestration, hydrocarbons) by using numerical simulation technology, petrophysics and borehole geophysics. GGE's research profile is characterized by an application-oriented approach.

> CHAIR FOR COMPUTATIONAL ANALYSIS OF TECHNICAL SYSTEMS (CATS)

RWTH / Prof. Marek Behr, Ph.D.

The focus of our research lies on the development of numerical methods and on modeling. All activities can be broadly related to fluid flow. Basis is our in-house flow solver. In recent years, topics in the area of numerical shape optimization have been treated, the flow solver now being a component of an optimization framework. The latter contains a geometry kernel based on T-splines as well as a variety of optimization algorithms. So far, the framework has been applied to profile extrusion dies and medical devices. However, shape optimization can only be as good as the underlying simulation. In order to improve the simulationquality, we conduct extensive research in material modeling of various materials (e.g. thermoplastics or blood). In order to cope with simulations of this size, highly parallel solvers are indispensable, leading to the development of parallelization techniques as one of our further research fields.

> CHAIR OF COMPUTER SCIENCE 6, HUMAN LANGUAGE TECHNOLOGY AND PATTERN RECOGNITION

RWTH / Prof. Hermann Ney

The Chair of Computer Science 6 is concerned with research on advanced methods for statistical pattern recognition. The main application of these methods is in the field of automatic processing of human language, i.e. the recognition of speech, the translation of spoken and written language, the understanding of natural language and spoken dialogue systems. The general framework for the research activities is based on statistical decision theory and problem specific modeling. The prototypical area where this approach has been pushed forward is speech recognition.

> CHAIR OF EXPERIMENTAL PHYSICS, I. INSTITUTE OF PHYSICS (IA)

RWTH / Prof. Matthias Wuttig

In our institute several groups investigate the properties of novel materials. Professor Matthias Wuttig, head of the institute, is engaged in the understanding and design of materials that are suitable for non-volatile memory applications based on phase change technology. Moreover, he researches organic films that can be applied in the field of opto-electronics, e.g. organic LEDs. Finally, his third group looks into the physical processes involved in sputter deposition techniques.

- Professor Gero von Plessen and his group are active in the field of Nano-optics, involving photonic crystals and excitations of metallic nano-particles.
- The group lead by Professor Thomas Taubner, Professor of Metamaterials and Nanooptics, focuses on new materials and systems for imaging and sensing at infrared wavelengths.
- The research activities of Professor Jörg Fitter are focused on fluorescence based single molecule studies exploring functional conformational dynamics of proteins and protein folding.
- Professor Heidrun Heinke concentrates on the education of young scientists and didactics.

> CHAIR OF EXPERIMENTAL PHYSICS, I. PHYSICS INSTITUTE B

RWTH / Prof. Stefan Schael

The research groups of the I. Physics Institute B of the RWTH are involved in projects in experimental particle and astro-particle physics. The activities cover new particle detector development, the construction of large particle physics detectors, the integration, commissioning and operation of particle physics experiments, software development and scientific data analysis. A special focus is the nature of Dark Matter.

> CHAIR OF MATERIAL MECHANICS (CMM)

RWTH / Prof. Bob Svendsen

Current research topics of the CMM are

- Modeling of microstructure evolution based on phase field approach
- Modeling and simulation of process chains in sheet metal forming and processing
- Characterization of microstructure in aluminum alloys and generation of associated synthetic microstructures
- Analysis and determination of the inhomogeneous material behavior in heterogeneous materials
- Molecular dynamic based simulations of twinning induced plasticity in steel

> CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS

RWTH / Prof. Manfred Martin

Oxides play an ever increasing role as advanced functional materials. Examples are tarnishing layers during high temperature oxidation, oxygen ion conducting oxides in high temperature fuel cells, mixed conducting oxides in oxygen permeation membranes, lithiumoxides for batteries, high temperature superconductors, ferroelectrics, catalysts etc.

The oxides that are used are complex oxides, i.e. they contain normally several cations and they exist in complicated crystal structures with several sublattices. The properties of these oxides are determined to a large extent by the thermodynamics and kinetics of point defects. Basic research concerning defect chemistry, transport properties and chemical reactivity is the basis for the improvement and optimization of functional materials.

> INSTITUTE FOR ADVANCED SIMULATION (IAS)

FZ Jülich / Quantum Theory of Materials (IAS-1) / Prof. Stefan Blügel
Theoretical Soft Matter and Biophysics (IAS-2) / Prof. Gerhard Gompper
Theoretical Nanoelectronics (IAS-3) / Prof. Eva Pavarini, Prof. David DiVincenzo
Theory of the strong interactions (IAS-4) / Prof. Ulf-G. Meißner
Computational Biomedicine (IAS-5) / Prof. Paolo Carloni
Theoretical Neuroscience (IAS-6) / Prof. Markus Diesmann, Prof. Abigail Morrison

The IAS unites Simulation Sciences and supercomputing under one roof. Thus, disciplinary, methodic and technological competences can be combined to manage the future challenges in the Simulation Sciences.

The close cooperation of the scientific users with the staff of the JSC leads to a prolific usage of the highly attractive European supercomputing centre in Jülich - especially in method development and scientific visualization. The institute consists of the JSC and six sections (IAS 1-6).

> INSTITUTE FOR COMBUSTION ENGINES (VKA)

RWTH / Prof. Stefan Pischinger

The Institute for combustion engines (VKA) covers classical engine topics like innovative engine constructions and research and development of new more efficient and clean combustion processes. Further on topics with more and more rising importance like the virtual engine development, research at the complete powertrain of hybrid powertrain and engine electronics are considered.

All this is associated with the ongoing development of intelligent methods for test procedures and engine cali-bration, e.g. by "Design of Experiment" (DoE).

> INSTITUTE FOR COMBUSTION TECHNOLOGY (ITV)
RWTH / Prof. Heinz Pitsch

Research in the fields of turbulent combustion and its applications in engines, gas turbines and furnaces, chemical kinetics of combustion, turbulence theory, multiphase flows and electrochemistry with applications to fuel cells. The approach is the combination of simultaneous theoretical model development, numerical simulation, and experimental validation. Within the Collaborative Research Center (SFB 686) "Model-Based Control of Homogenized Low-Temperature Combustion", aspects from the field of automatic control are also considered.
A further emphasis is on "Tailor-Made Fuels from Biomass" within the cluster of excellence under the same title. Diesel engines are operated at the institute and measurements are conducted in different flow reactors, high-pressure combustion chambers and open flames. For numerical simulations, in-house codes for direct numerical simulation (DNS), large eddy simulation (LES), Reynolds-averaged Navier-Stokes (RANS), and 1-D flame calculations are available.

> INSTITUTE FOR GEOMETRY AND PRACTICAL MATHEMATICS (IGPM)
RWTH / Prof. Arnold Reusken

The IGPM provides basic and advanced training in Numerical Analysis to students of Mathematics, Computer Sciences, Natural and Engineering Sciences.

The research conducted at IGPM covers a wide range of topics in Numerical Mathematics, from its analytical foundations to applications in the Engineering and Natural Sciences. Both in teaching and research, we collaborate closely with the RWTH computational science and engineering groups CCES, AICES and GRS.

> INSTITUTE FOR NUCLEAR PHYSICS (IKP)
FZ Jülich / Experimental Hadron Structure (IKP-1) / Prof. James Ritman
Theory of the strong interactions (IKP-3) / Prof. Ulf-G. Meißner

The institute as a member of the Jülich Centre for Hadron Physics (JCHP) is dedicated to fundamental research in the field of hadron, particle, and nuclear physics. The aim is to study the properties and behavior of hadrons in an energy range that resides between the nuclear and the high energy regime.

> INSTITUTE FOR QUANTUM INFORMATION (IQI)
RWTH / Prof. David DiVincenzo

Founded in 2011, the institute pursues a variety of topics in both practical and fundamental quantum information science. Solid state quantum information processing devices, either based on spins or superconductors, are a real possibility for the future.

Our theoretical work seeks to find improved ways for these qubits to function and to work together in a system. These goals motivate very fundamental studies in a diverse set of areas, including many-body physics, the theory of quantum error correction codes, the theory of quantum control, and quantum computational complexity. The institute has both theoretical and experimental directions. It functions within the larger research environment of condensed matter theory and experiment at the department of physics of the RWTH. It is also closely tied to the department of theoretical nanoelectronics at the FZ Jülich under the umbrella of JARA.

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS
RWTH / Strongly Correlated Quantum Systems / Prof. Stefan Wessel, Ph.D.
Theoretical Nanoelectronics / Prof. Riccardo Mazzarello

The research groups in this institute study many-particle interactions in solids, ranging from quantum effects in magnetic systems over electron correlation effects leading to unconventional superconductivity and magnetism to the dynamics of structural phase transitions. Recent work has focused on interaction effects in graphene systems, topological insulators, pnictide high-temperature superconductors and chalcogenide phase-change materials.

The powerful theoretical methods employed and developed here comprise quantum Monte Carlo techniques, the functional renormalization group, density-functional theory and molecular dynamics.

> INSTITUTE OF AERODYNAMICS AND CHAIR OF FLUID MECHANICS (AIA)
RWTH / Prof. Wolfgang Schröder

The Institute of Aerodynamics and the Chair of Fluid Mechanics belong to the department of mechanical engineering of the RWTH. The experimental and numerical units plus the laboratory for biomedical flows constitute the main departments of the institute. Several subsonic, transonic, and supersonic wind tunnels and water tunnels are the essential experimental facilities. In addition, there are special test rigs to study flow fields, e.g., within piston engines, through safety valves, and artificial heart valve prostheses. The measurement methods consist of, e.g., particle-image and particle-tracking velocimetry, laser-, doppler- and hot-wire anemometry, multisensor hot films, differential and Mach-Zehnder interferometry, and schlieren methods. Continuous as well as pulse lasers and high-speed cameras are part of the experimental setups. Measuring equipment such as hot wires and hot films is inhouse manufactured.

> INSTITUTE OF BIO- AND GEOSCIENCES (IBG)
FZ Jülich / Biotechnology (IBG-1) / Prof. Wolfgang Wiechert
Agrosphere (IBG-3) / Prof. Harry Vereecken

The IBG focuses on research for the sustainable production of food, biological energy carriers, chemicals, pharmaceuticals, and materials based on plant and microbial processes or principles, the sustainable use of the natural resources soil and water, and the analysis and optimization of matter cycles and energy use. This cross-process approach is a promising solution for long-term relief of the central problems associated with today's fossil-resource-based economy.

> INSTITUTE OF BIOTECHNOLOGY
RWTH / Prof. Ulrich Schwaneberg

The Schwaneberg Group seeks to be at the research frontier in the interdisciplinary field of directed protein evolution by developing novel methods for generating diversity at the gene level, analyzing consequence of mutational biases on the protein level and developing novel high-throughput screening systems that will ultimately lead to tailored-biocatalysts for significant applications in industry. We train our students in the cutting edge technologies of laboratory evolution, biocatalyst engineering and high throughput screening methodologies. We believe in integrating fundamental principles of protein design with environmental awareness in our research and seek to promote international scientific collaborations.

> INSTITUTE OF COMPLEX SYSTEMS (ICS)

FZ Jülich / Theoretical Soft Matter and Biophysics (ICS-2) / Prof. Gebhard Gompper
Structural Biochemistry (ICS-6) / Prof. Dieter Willbold

In ICS, physicists, biologists and chemists together explore the principles forming the basis of the fascinating properties of living cells and macromolecular functional systems. By means of basic research in soft matter, structural biology and cell biophysics, we are able to contribute to visionary applications in the fields of medicine, biotechnology and chemical technology.

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH (IEK)

FZ Jülich / Electrochemical Process Engineering (IEK-3) – Prof. Werner Lehnert
Photovoltaics (IEK-5) /Prof. Uwe Rau
Nuclear Waste Management and Reactor Safety (IEK-6) / Prof. Dirk Bosbach
Stratosphere (IEK-7) / Prof. Martin Riese
Troposphere (IEK-8) / Prof. Andreas Wahner

The IEK investigates modern energy conversion technologies within the framework of climate and environmental protection. The topics it covers in the energy sector range from photovoltaics and fuel cells, through nuclear fusion and nuclear safety research, right up to innovative coal and gas power plants as well as an overarching systems analysis.

> INSTITUTE OF INORGANIC CHEMISTRY (IAC) / CHAIR OF SOLID-STATE AND QUANTUM CHEMISTRY

RWTH / Prof. Richard Dronskowski

The institute is specialized in the fields of synthetic and quantum-theoretical solid-state chemistry, bordering with materials science, solid-state and theoretical physics, crystallography, as well as quantum and computational chemistry. In detail, we synthesize novel, sometimes extremely sensitive, compounds and elucidate their compositions and crystal structures by means of X-ray and neutron diffractional techniques. The characterization of their physical properties, that is electronic transport and magnetism, also plays a very important role.

We regularly perform solid-state quantum-chemical calculations from first principles to yield the electronic (band) structures and, in particular, to extract the important chemical bonding information needed to thoroughly understand the interplay between chemistry and physics. Syntheses are theory-driven and experiments challenge theories.

> INSTITUTE OF JET PROPULSION AND TURBOMACHINERY (IST)

RWTH / Prof. Peter Jeschke

For more than fifty years, the Institute for Jet Propulsion and Turbomachinery (IST) has been working in the field of teaching and experimental and analytical/numerical research. Teaching and research activities at the institute focus on jet engines used in the aviation and aeronautics industry and turbo machines in general, including stationary gas and steam-powered turbines. We cover the whole technological spectrum, from basic principles to specific applications for our industrial partners.

> INSTITUTE OF NEUROSCIENCE AND MEDICINE

FZ Jülich / Computational and Systems Neuroscience (INM-6) / Prof. Markus Diesmann
Computational Biomedicine (INM-9) / Prof. Paolo Carloni

The Institute of Neuroscience and Medicine addresses under the program "Decoding the Human Brain" human brain organization on its different temporal and spatial scales. Due to the complexity of the brain and its extensive changes during the life span and in neuropsychiatric disorders, this can only be achieved by using advanced neuroimaging techniques and high-performance computing. Basic neuroscience goes hand in hand with modeling/simulation to face the challenges Brain Complexity and Big Data Analytics and to develop robust control techniques. This knowledge enables translational medicine to understand, diagnose and cure neurological and mental disorders, which become increasingly relevant in an aging society.

> INSTITUTE OF PHYSICAL CHEMISTRY (IPC), THEORETICAL CHEMISTRY

RWTH / Prof. Arne Lüchow

Our research interest is the accurate theoretical calculation of electronic and vibrational states of molecules and molecular clusters. We employ standard methods and develop new methods based on the quantum Monte Carlo approach.

> INSTITUTE OF TECHNICAL AND MACROMOLECULAR CHEMISTRY (ITMC)

RWTH / Prof. Walter Leitner

Our group's research is concerned mainly with homogeneous catalysis of chemical processes using transition metal complexes. Particular emphasis is placed on the use of supercritical carbon dioxide as an environmentally benign solvent for sustainable synthetic chemistry. Over the last decade, homogeneous catalysis with transition metal complexes has led to revolutionary new synthetic possibilities not only on a laboratory scale, but has also established itself in many different technical applications. Efficient homogeneous catalysts are nowadays known in virtually all areas of synthesis, from bulk chemicals and commodities, through fine chemicals and pharmaceuticals, to polymers and specialist materials.

Enantioselective catalysis is growing in importance for the preparation of biologically active compounds Important goals of the present research in the area of homogeneous catalysis are the synthesis of new or improved catalysts, the search for new catalytic reactions, and the development of innovative processes for the application of catalytic reactions.

> IT Center

RWTH / Chair for Computer Science 12 / Prof. Matthias Müller
Virtual Reality and Immersive Visualization / Prof. Torsten W. Kuhlen

The Center for Computing and Communication at RWTH is a centralized body providing computing and communication services and resources to all the university's institutes, personnel and students. In particular, the center is responsible for planning, operating and making available centralized computing, visualization and communication facilities, and providing additional services where it would be impossible or inappropriate for a single institute to do so. The Center also supports users and advises them on how they can make the most of the tools it offers.

> JÜLICH SUPERCOMPUTING CENTRE (JSC)

FZ Jülich / Prof. Erik Koch
Prof. Thomas Lippert

JSC's research and development concentrates on mathematical modeling and numerical, especially parallel algorithms for quantum chemistry, molecular dynamics and Monte-Carlo simulations.

The focus in the computer sciences is on cluster computing, performance analysis of parallel programs, visualization, computational steering and grid computing.

> SHOCK WAVE LABORATORY

RWTH / Prof. Herbert Olivier

- High temperature gas dynamics
- Hypersonic and supersonic flows
- Shock wave phenomena

The delivery of industry solutions as well as the education of students and the ongoing scientific qualification of our Ph.D. students are the main ambitions of our work.

> SOFTWARE AND TOOLS FOR COMPUTATIONAL ENGINEERING (STCE) / LUFG INFORMATIK

RWTH / Prof. Uwe Naumann

Research and software development at STCE are inspired by derivative-based methods in Computational Science, Engineering, and Finance (CSEF). The following topics are covered:

- (adjoint) algorithmic differentiation algorithms and software
- numerical (optimization) algorithms and software
- parallel algorithms and software
- combinatorial (graph) algorithms and software
- complexity of (discrete) algorithms
- domain-specific compilers and program analyses
- simulation software engineering
- applications of the above in CSEF

10. JOINT PUBLICATIONS

Reported by involved institutes (FZ Jülich and RWTH)

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Picture: Conor Crowe

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