JARA|HPC

Picture: Mathis Bode, ITV, RWTH

ANNUAL REPORT 2015

AN INITIATIVE OF

RWTH AACHEN UNIVERSITY

JÜLICH FORSCHUNGSZENTRUM

GLOSSAR

CSG	Cross-Sectional Group
CSG ImmVis	Cross-Sectional Group “Immersive Visualization”
CSG ParEff	Cross-Sectional Group “Parallel Efficiency”
RWTH	RWTH Aachen University
FZ Jülich	Forschungszentrum Jülich
GRS	German Research School for Simulation Sciences
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”
VGG	Vergabegremium

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. Wolfgang Dahmen	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 Kuhlen	RWTH
Prof. Werner Lehnert	FZ Jülich
Prof. Walter Leitner	RWTH
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Prof. Riccardo Mazzarello	RWTH
Prof. Ulf-G. Meißner	FZ Jülich
Prof. Abigail Morrison	FZ Jülich
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Prof. Uwe Naumann	RWTH
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Prof. Herbert Olivier	RWTH
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Prof. Stefan Pischinger	RWTH
Prof. Heinz Pitsch	RWTH
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Prof. Detlev Reiter	FZ Jülich
Prof. Martin Riese	FZ Jülich
Prof. James Ritman	FZ Jülich
Prof. Stefan Schael	RWTH
Prof. Wolfgang Schröder	RWTH
Prof. Ulrich Schwaneberg	RWTH
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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

1. JARA-HPC IN HEADLINES

> Modular Zonal Flow Solver (ZFS) becomes member of the High-Q Club

March 2015 – Following up on our JUQUEEN porting and scaling workshop and to promote the idea of exascale capability computing, JSC has established a showcase for codes that can utilise the entire 28-rack BlueGene/Q system at JSC. The aim is to encourage other developers to invest in tuning and scaling their codes and show that they are capable of using all 458,752 cores, aiming at more than 1 million concurrent threads on JUQUEEN. In 2015, two codes of JARA-HPC members and their institutes became members in the High-Q Club of codes scaling on the entire BlueGene/Q system:

- **CIAO:** Compressible/Incompressible Advanced reactive turbulent simulations with Overset (Institute for Combustion Technology, Prof. Pitsch)
- **ZFS:** A multiphysics framework for compressible and incompressible flow, aeroacoustics, and combustion phenomena. (Institute of Aerodynamics, Prof. Schröder)

> JARA-HPC Team Event


Picture: Bleiberger Fabrik

March 2015 – "Building bridges" was the theme of the first JARA-HPC Team event held at the Bleiberger Fabrik, Aachen, in March 2015. About 40 JARA-HPC employees participated and together they built a volcano landscape and created putty figurines and bridges out of pasta.

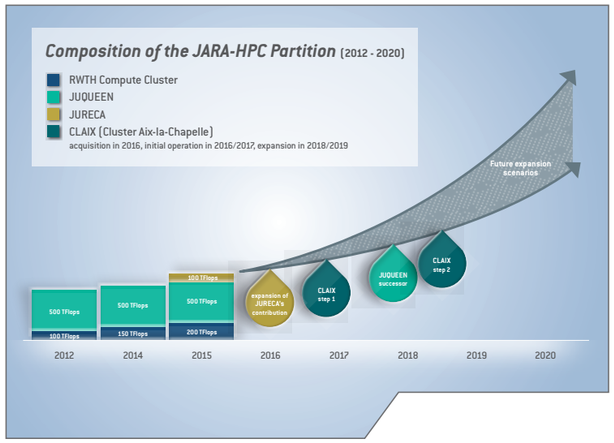
The workshop, planned as a team building activity, aimed at furthering the collaboration of the JARA-HPC employees using an unusual exercise and thereby improving the interdisciplinary collaboration in everyday research.

> Expansion of JARA-HPC Partition

May 2015 – Due to the great demand for computing capacity, especially for big projects the RWTH and FZ Jülich started increasing computing capacities on the JARA-HPC Partition reciprocally on November 01, 2014.

In a first step RWTH's IT Center doubled the Compute Cluster's contribution to the JARA-HPC Partition until May 01, 2015 successively up to 120 Mio. Core-h (about 200 TFlops). Starting in 2015 FZ Jülich provided users from Aachen and Jülich with additional computing capacity on JURECA of 18 Mio. Core-h (100 TFlops).

JUQUEEN's contribution remains unchanged at 288 Mio. Core-h (500 TFlops) so that since 2015 800 TFlops computing capacity are available on the JARA-HPC Partition for the exclusive use of Aachen's and Jülich's scientists.



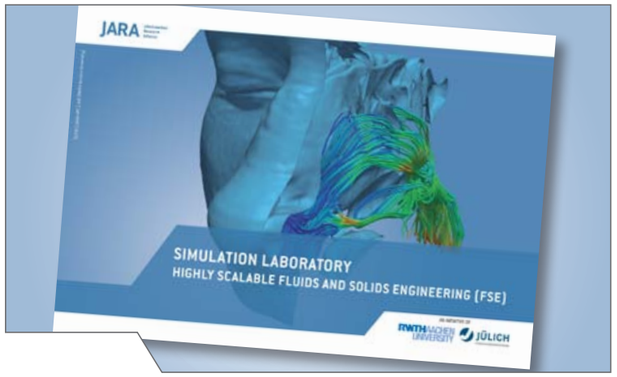
> Successful presentation at ISC'15

July 2015 – Scientists from JARA-HPC once again presented their current research at one of the largest and most important events dedicated to HPC – the ISC'15, which took place in Frankfurt am Main, Germany, from July 12-16, 2015.

Visitors had the opportunity to jump right into the world of JARA-HPC's new In Situ Visualization of Multiphase Jet Simulations (see detailed description on page 9). Furthermore, the staff reported on the latest developments in OpenMP and presented MUST, a correctness checker for parallel programs.

> New SimLab FSE information booklet

September 2015 – The SimLab FSE aims at supporting users of the engineering sciences who have already developed parallel codes but need support for the use of massively parallel systems regarding high scalability, memory optimization, programming of hierarchic computer architectures, and performance optimization on computer nodes.



An overview of all their current projects was recently published in an information booklet.

> JARA-FORUM 04

October 2015 – As part of the JARA-FORUM 04 "Simulation und Datenanalyse: Brücke über die Grenzen der Erkenntnis" on October 01, 2015, JARA-HPC scientists provided insights into potential applications of and concepts for computer simulations and massively parallel computing. The keynote speech was given by Andreas von Bechtolsheim, an informatics pioneer, co-founder of Sun Microsystems and one of the first to invest in Google. The forum was attended by politicians, industry experts, and representatives of the scientific community.

Picture: Phil Dera

During the reception members of JARA-HPC's CSG ImmVis presented their latest research results regarding the new In Situ Visualization of Multiphase Jet Simulations as well as the Visualization of Simulated Neural Brain Activity.

> JARA-HPC kicks off "JARA Ringvorlesung"

October 2015 – How does fine dust affect the flow in the human airways? How can chevron optimisation help reduce jet noise? These were just some of the questions that Andreas Lintermann (SimLab FSE) and Jens Henrik Göbbert (CSG ImmVis) tried to answer during the first "JARA Ringvorlesung" on October 30, 2015 at RWTH.

> RWTH Science Night

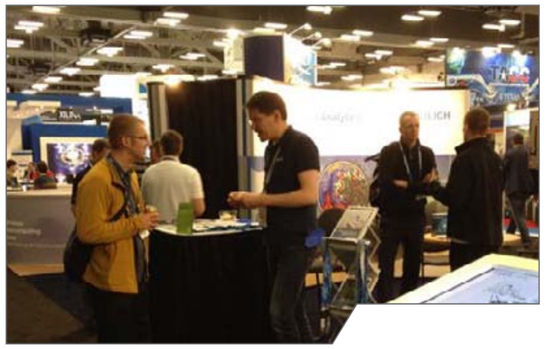

Picture: Martin Luk

November 2015 – The 13th "RWTH Science Night" took place on November 13, 2015 in the Kármán Auditorium at RWTH. The idea behind the "Science Night" is to present science in an unusual way and at an unusual time.

This year's program comprised over 40 talks and numerous exhibits and experiments. There were also various talks about the Excellence Initiative and JARA-HPC's scientists successfully presented their In Situ Visualization of Multiphase Jet Simulations.

> JARA-HPC at Supercomputing Conference (SC'15) in Austin

November 2015 – From November 15-20, 2015 JARA-HPC's scientists presented their current research from the fields of neuroscience and engineering at the JSC booth at the Supercomputing Conference (SC) in Austin, Texas.



> NESTML community workshop

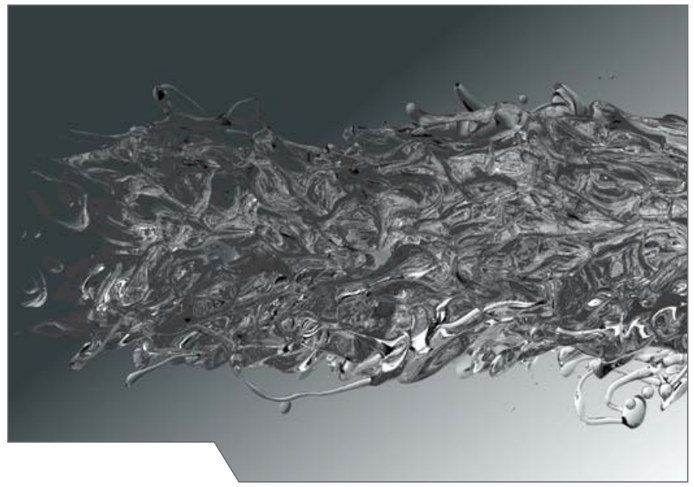
December 2015 – Since the beginning of 2015 scientists are working on the JARA-HPC Seed Fund Project "NESTML – A modeling language for spiking neuron and synapse models for NEST". The project aims at developing a special high-level description language and the infrastructure to create neuron models for the neuronal simulator NEST (http://www.nest-simulator.org).

With this novel language, neuroscientists using NEST can express their neuron models with domain concepts instead of formulating them in the general purpose programming language C++.

To evaluate the concepts and bring the tools to potential users, a community workshop with 15 participants was held from December 07-08, 2015. The feedback was generally very positive and has already been integrated into the current version of NESTML.

NESTML is a collaboration between the Chair of Software Engineering at RWTH and the Department Computational and Systems Neuroscience of the Institute of Neuroscience and Medicine (INM-6) at FZ Jülich.

> In Situ @ CSG ImmVis



For quite some time, our ability to generate data by large-scale simulations has by far outrun our ability to analyse this data. Today's HPC systems, however, are limited far earlier: they can produce data faster than it can be written to secondary storage.

In Situ visualization and analysis approaches address this situation. The idea behind In Situ is to integrate data analysis and visualization capabilities with the simulation code itself. In this way, data can be processed right after it has been produced. Ideally this utilizes the same resources, i.e. compute nodes that have been used for data generation, hence alleviating the need for costly data movement.

Recently, developers from JARA-HPC's CSG ImmVis took first steps towards an In Situ coupling of simulation and visualization methods. Particularly, the DNS codes CIAO and psOpen have been coupled to the open-source visualization software VisIt. The system's operability has been demonstrated in a full-system run on JUQUEEN's 458.752 cores.

This software setup provides the basis for a scalable analysis of large-scale, DNS-based investigations of turbulent combustion processes. For example, fluid mechanics researchers from fluid mechanics aim to understand the mechanism underlying the breakup of ligaments into multiple droplets during the injection of fuel into a simulated Diesel engine. Since this process is characterized by sudden changes on different spatial scales, an In Situ approach is key to make the analysis feasible at the required spatiotemporal resolution; the raw data just could not be written out to disk for post hoc analysis. Thus, this example serves to demonstrate the contribution of In Situ strategies to next generation simulation-based workflows.

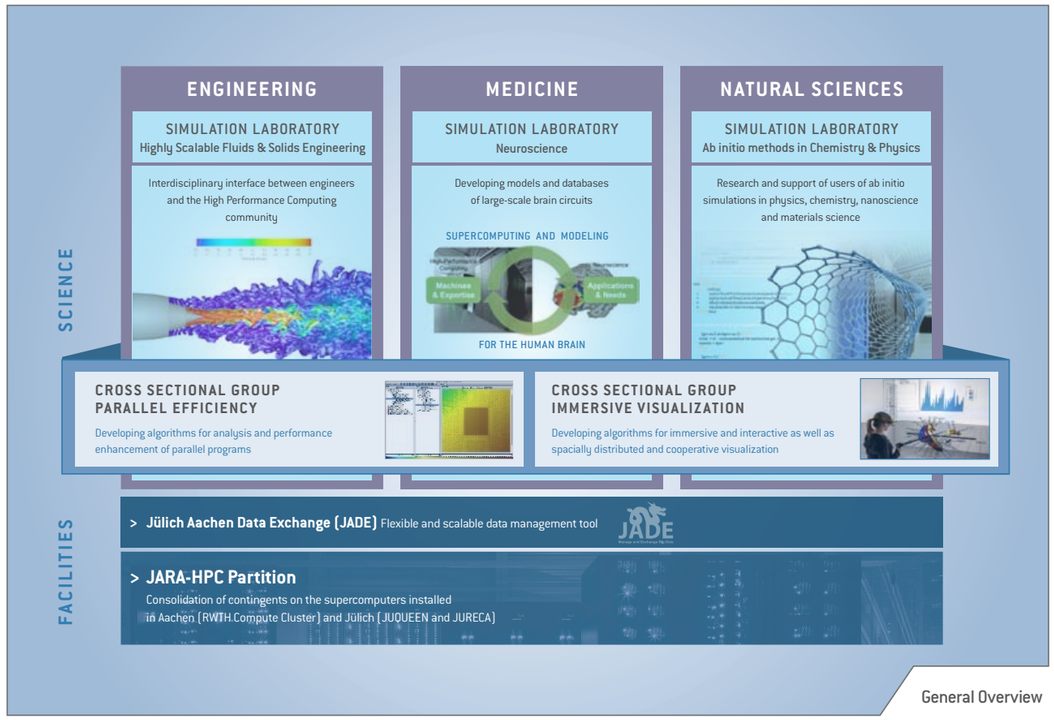
2. NEW COLLEAGUES IN JARA-HPC

3.1. CSG “Immersive Visualization”

DIPL.-INFORM. DOMINIK RAUSCH

3.2. SimLab “Neuroscience”

DR. ALEXANDER PEYSER



General Overview

3. SCIENTIFIC WORK IN JARA-HPC

> 3.1. General overview

Scientists from the Jülich Aachen Research Alliance, and especially the section 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) 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:

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

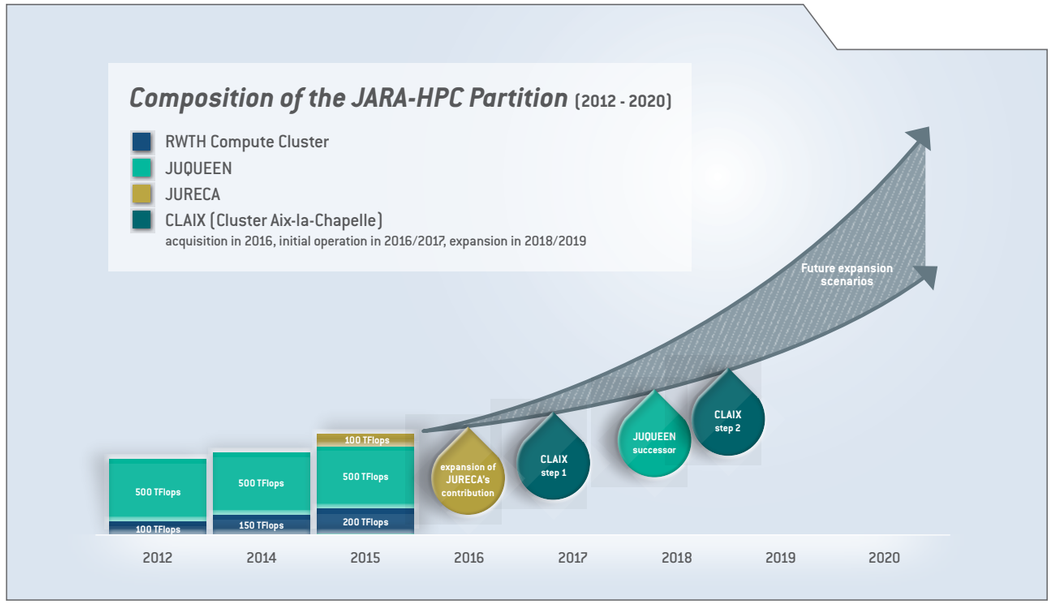
> The **CSGs** comprise methodical activities that are relevant for the users of high-performance computers with utterly diverse scientific backgrounds. Currently two CSGs are established in the areas:

- **”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.

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

> 3.2. 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 JARA-HPC Partition has been extended due to the high demands for compute 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 the summer of 2016 additional capacities of JURECA and in the beginning of 2017 Aachen's new high performance computer CLAIX will be available to users of the JARA-HPC Partition.

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 computing centers. Based on these reviews, an assignment board ("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:

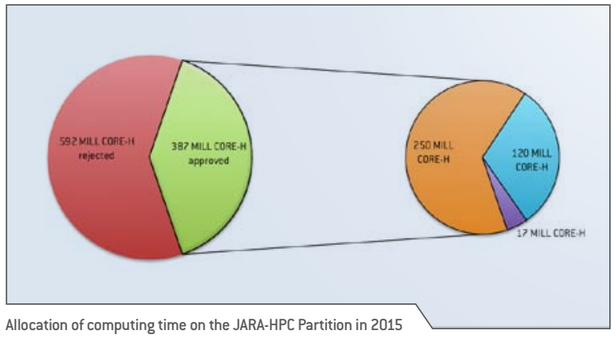
- Gerhard Gompper / FZ Jülich
- Robert Jones / FZ Jülich
- Paul Gibbon / FZ Jülich
- Gebhard Günther / FZ Jülich
- Paolo Bientinesi / RWTH
- Dieter an Mey / RWTH
- Matthias Meinke / RWTH

Sadly, Norbert Peters / RWTH who has been member of the VGG since the very beginning passed away in July 2015. As of February 2016, his successor will be Heinz Pitsch from the Institute for Combustion Technology at 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 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, 60 million compute core-hours (core-h) on the RWTH Compute Cluster (either on nodes with Westmere-EP processors or on nodes with Nehalem-EX processors), 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 2015

STATISTICS

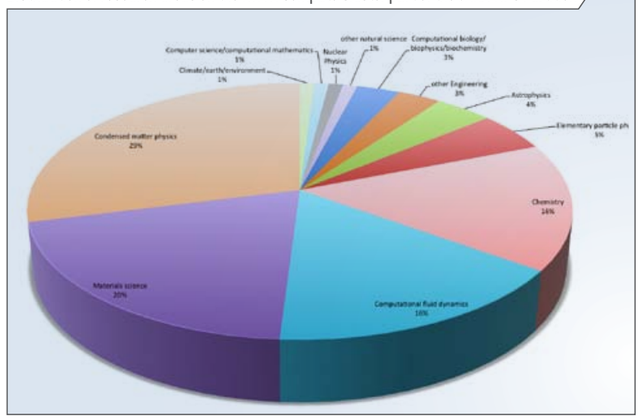
In the two JARA-HPC calls of 2015 170 proposals were filed.
A total of 387 million core-h have been approved which are distributed among the various research areas on the JUQUEEN and JURECA system and the RWTH Compute Cluster respectively as depicted in the following pie charts.

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

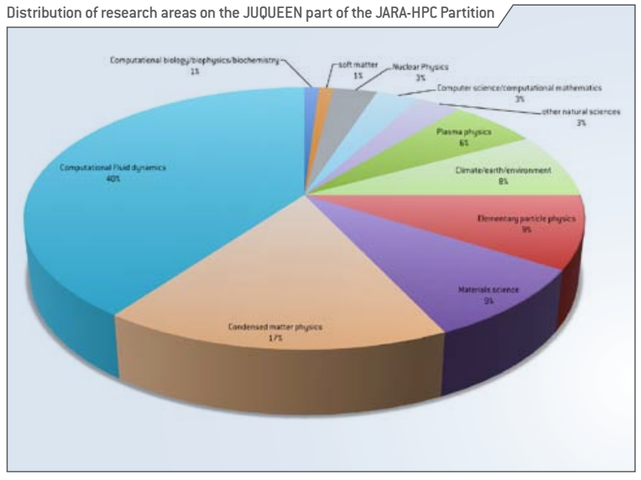
These fields of research also account for 55% of the number of accepted proposals.

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

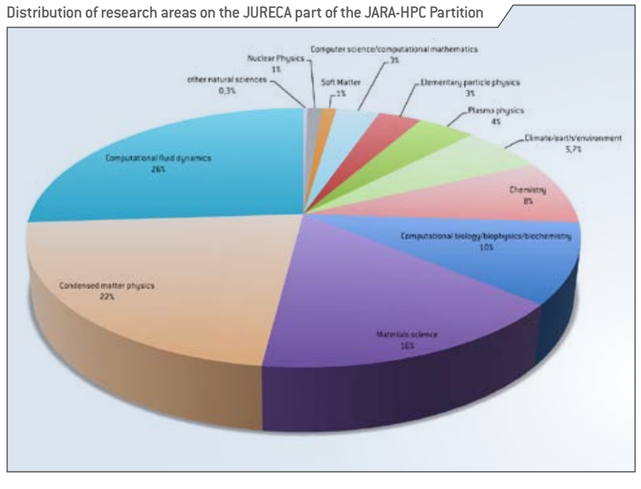
Distribution of research areas on the RWTH Compute Cluster part of the JARA-HPC Partition



Distribution of research areas on the JUQUEEN part of the JARA-HPC Partition



Distribution of research areas on the JURECA part of the JARA-HPC Partition



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, whereas 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 in Jülich offering very high scalability and the RWTH Compute Cluster in Aachen and the JURECA system in Jülich 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
Christian Terboven, IT Center, RWTH

> 3.3. JADE – The new JARA-HPC facility

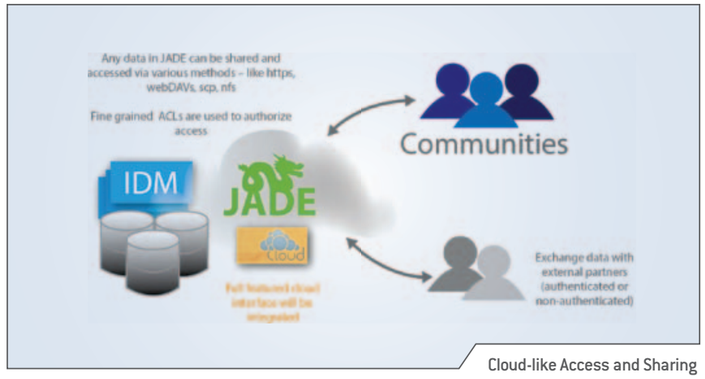
The Jülich Aachen Data Exchange (JADE) tries to establish a flexible and scalable data management tool that addresses the specific needs and requirements of domain scientists to exchange data in a convenient and efficient way. The main objectives of JADE were gained in close interaction with the intended user and the following requirements for JADE were derived:

- **Data exchange between distributed partners through data replication**
- **Archiving of stored data**
- **Flexible right management and access control**
- **Multi-level data access – from NFS mount to cloud-like access**
- **Flexible extension of partners and sites**

Therefore, the implementation of JADE addresses the following use cases:

USE CASE DATA ACCESS:

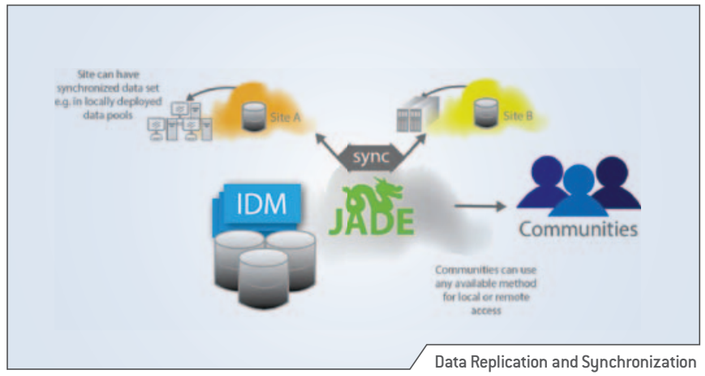
Any data in JADE can be accessed and shared using various methods, such as https, WebDAV, scp, or nfs. JADE further intends to provide a full featured cloud interface. Fine grained ACLs are used to authorize access to the data. Thus, JADE provides data access on various levels of abstraction: from file system mounting to web-based cloud access.



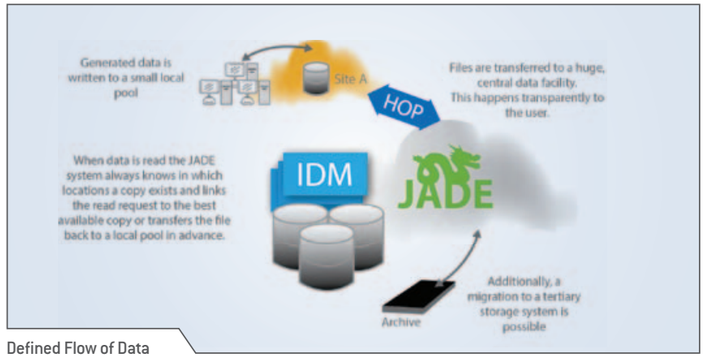
Cloud-like Access and Sharing

USE CASE DATA REPLICATION:

Sites can have synchronized data sets, e.g. in locally deployed data pools, where communities can use any available method for local or remote access. This offers a transparent data transport form data producers to data consumers and make this data accessible close to the place of usage and processing.



Data Replication and Synchronization



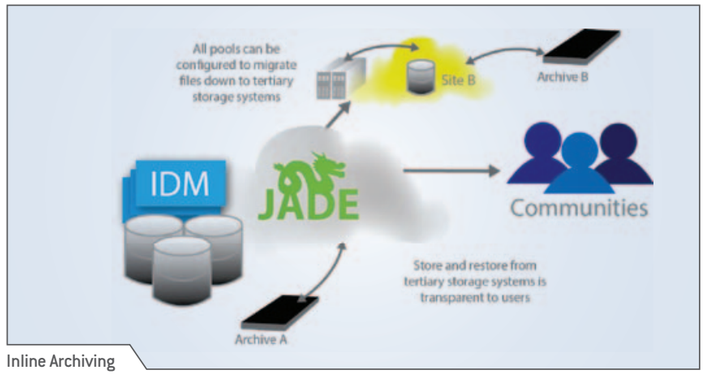
Defined Flow of Data

USE CASE DATA PROVIDING:

Generated data can be written to a local pool. These files get transferred to a huge and central data facility. This happens transparently to the user. When data is read, JADE always knows in which location a copy exists and links the read request to the best available copy or transfer the file back to the local pool in advance.

USE CASE DATA ARCHIVING:

A pool can be configured to migrate files down to tertiary storage systems. Store and restore from tertiary storage is transparent to the user. In JADE, JSC as central unit will provide tertiary storage and access to it.



Inline Archiving

In the middle of 2014, a first test bed based on dCache has been installed in the context of the SMHB project. dCache is a project to "provide a system for storing and retrieving huge amounts of data, distributed among a large number of heterogenous server nodes, under a single virtual filesystem tree with a variety of standard access methods" [http://www.dcache.org/].

JSC serves as JADE's central data center for storage and network resources. The embedding of resource at RWTH has shown the feasibility of the approach and initiates the JADE's inclusion into JARA.

The initial test bed of JADE contains 18TB storage at JSC and 30GB storage at RWTH. In its first operational phase, JADE will be installed in JSC with access to a multi TB storage connected to the JSC's archiving systems and at RWTH on an 80TB file server. The 30GbitE connection between Aachen and Jülich will be used to transfer data within JADE.

Beside the support of the service infrastructure for a distributed file system, JADE further investigates other software solutions, such as iRods and investigates actively in the development of these software solutions. Furthermore, JADE is in contact with other data communities, such as LSDMA or EUDAT.

CONTACT

Bastian Tweddell, FZ Jülich
Dr.-Ing. Benjamin Weyers, RWTH

> 3.4. Simulation Laboratories (SimLabs)

3.4.1. SimLab "Highly Scalable Fluids and Solids Engineering"

STEERING BOARD

Prof. Marek Behr, Ph.D. / RWTH
Prof. Paul Gibbon / FZ Jülich
Prof. Wolfgang Schröder / RWTH

STAFF

Ole Baumeister / FZ Jülich
Manuel Kosel / JARA-HPC, FZ Jülich
Metin Cakircali / FZ Jülich
Dr.-Ing. Andreas Lintermann / JARA-HPC, RWTH
Michael Schlottke-Lakemper / JARA-HPC, RWTH

PROJECTS

>Analysis of the flow in the human respiratory tract (Lintermann)

Since November 2015 the LBM of the Zonal Flow Solver (ZFS) of the Institute of Aerodynamics and Chair of Fluid Mechanics (AIA), RWTH, is used to analyze the flow in the human respiratory tract. That is, the inspiratory flow is computed and the impact of the deposition of fine-dust particles in the airways is investigated. Therefore, realistic geometries obtained from Computer Tomography (CT) images are used to model the upper airway down to the trachea. The lung geometry is generically generated using a space-filling algorithm. The highly resolved computations are performed on computational meshes containing 2 x 109 cells. Shared memory parallelization of the LBM lead to a scalability across half of the JUQUEEN and in October 2015 the project has been granted 23 million core hours on this system. Results have been presented at the 5th Korean-German Workshop (Jeju Island, South Korea, October 2015). New findings applying parallelized geometries will be presented at the ECCOMAS 2016 congress(Crete, Greece, June 2016).

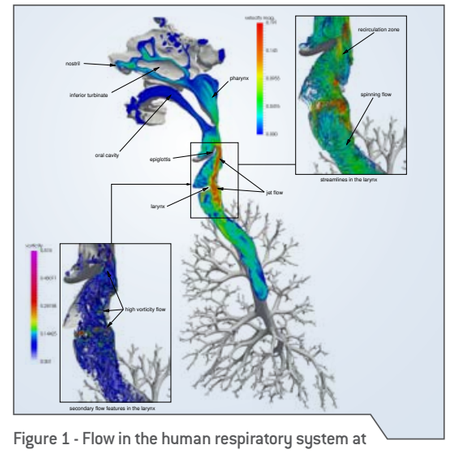


Figure 1 - Flow in the human respiratory system at inspiration. In the center, a cut-plane colored by the velocity magnitude is shown. The zooms in the left and right corner show contours of the Λ-criterion colored by the vorticity magnitude and streamlines colored by the velocity magnitude.

> Coupled-Parallel Simulation of Gas Turbines (COPA-GT) (Schlottke-Lakemper)

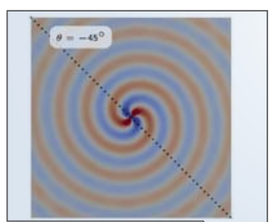


Figure 2 - Acoustic pressure waves excited by a spinning vortex pair.

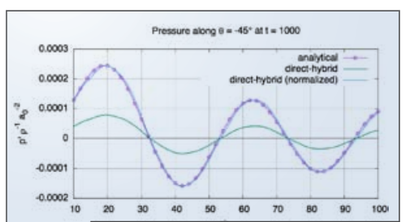


Figure 3 - Acoustic pressure along the line shown in Fig. 2.

Within the frame of this EU project, a discontinuous Galerkin (DG) solver for the prediction of aeroacoustic noise is developed in ZFS. This project aims at investigating turbojet engines with coupled, multiphysics simulations and at finding optimal designs for efficient and noise-reduced engines. After the presentation of

first results at the STAB Symposium in Munich in 2014 new developments involving a direct-hybrid approach have been presented at the 21st AIAA/CEAS Aeroacoustics Conference in Dallas, Texas, U.S., in 2015. The new implementations allow for increased execution performance as two solvers are directly coupled online during the simulation without exchanging information via I/O. In 2015 the according simulation code became a member of the High-Q Club and scaled across the complete Hornet system at the High Performance Computing Centre Stuttgart (HLRS).

> Noise Reduction through Chevron Nozzles via Multi-Point Optimization (Kosel)

Since February 2015, the SimLab supports this DFG-project by implementing shape optimization methods in ZFS to find optimal designs for chevron geometries. Therefore, the results of flow computations are used to directly evaluate objective functions, e.g. the noise production, the drag, or the thrust of an engine, by a local, gradient-based optimizer. The optimized shape that is given in T-spline representation is translated into a level-set that is used to adapt the computational mesh to a new and optimized geometry. First optimization results have been obtained for drag-reduced geometries of NACA 0012 airfoil profiles and further investigations will concentrate on the chevron geometries itself.

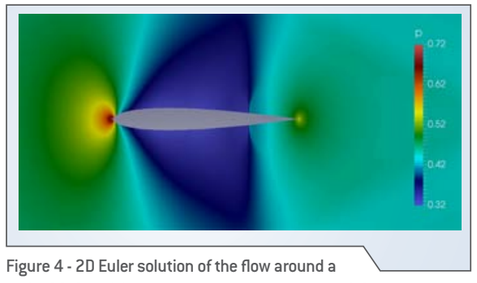


Figure 4 - 2D Euler solution of the flow around a NACA 0012 airfoil profile at Mach number Ma = 0.85 and an angle of attack of α = 0°.

> LES of the FDAs Centrifugal Blood Pump using HPC (Lintermann)

The SimLab is involved in a joint project investigating the blood-sensitivity of a centrifugal blood pump released by the U.S. Food and Drug Administration (FDA). The other project partners are the Biomaterials Lab of the University of Applied Sciences Aachen (PI), the Science and Technology Facilities Council, Daresbury Lab, U.K., and the JARA-HPC CSG "ImmVis". The project has been granted 9 million core hours on the JUQUEEN and uses Code Saturn (Elecricité de France) to perform the according Large-Eddy Simulations (LES).

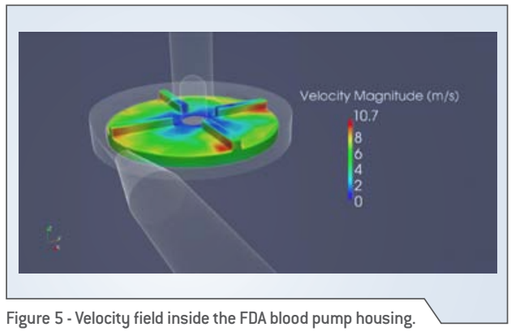


Figure 5 - Velocity field inside the FDA blood pump housing.

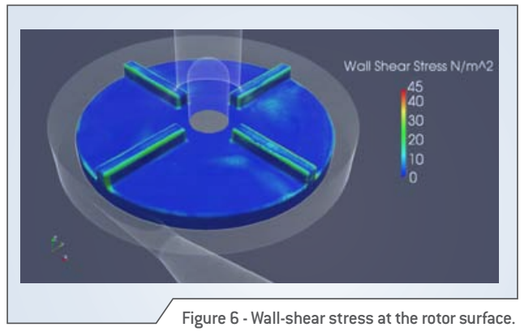


Figure 6 - Wall-shear stress at the rotor surface.

> Parallel Stabilized Finite Element Methods for Viscoelastic Fluid Simulations of Rigid Rod-like Polymers (SWNTs) (Cakircali)

Together with the Chair for Computational Analysis of Technical Systems (CATS), RWTH, and the Complex Flows of Complex Fluids group (Rice University, U.S.), the solver XNS from CATS is extended to allow for the simulation of viscoelastic fluids. The project started in Q1/2015 and aims at predicting fiber generation processes based on nano-tubes dissolved in acids. In contrast to Newtonian fluids, the shear stress tensor in the Navier-Stokes equations for viscoelastic fluids contains a non- linear part that is modeled by different approaches that are reformulated to be applicable in the Finite Element Method (FEM) which is used in XNS.

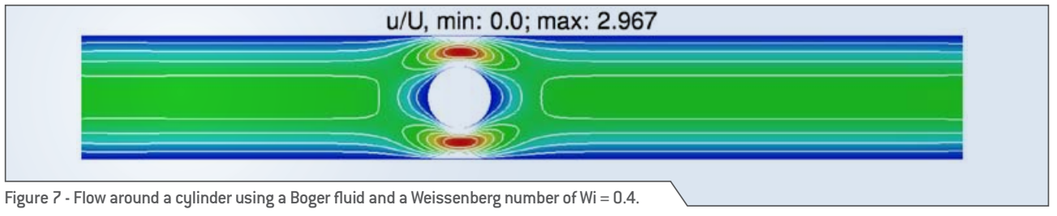


Figure 7 - Flow around a cylinder using a Boger fluid and a Weissenberg number of Wi = 0.4.

> 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 2015, 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.
- Currently, the conclusion of a contract with a second company on software performance optimization is pending.

ADDITIONAL ACTIVITIES

> Funding proposals

The first two following proposals have been submitted to the BMBF in the frame of the 4th HPC Call. Although not funded, both project have started and the implementations and findings will be used as a basis for future proposals w.r.t. to the ongoing work.

- **Entwicklung einer HPC-spezifischen parallelen Kopplungsstrategie zur Direktverar- beitung von Ergebnissen hochskalierender Simulationen (BMBF)**
  Project partners: SimLab FSE, CSG ImmVis (JARA-HPC), Application Optimization (JSC), SimLab Climate (JSC), SimLab TerrSys (JSC), AIA (associated), IT Center (associated), Ford GmbH (LOI), FEV GmbH (LOI)
  Status: not funded
- **Khyber: Einheitliche Kommunikationsarchitektur für hochgradig parallele, heterogene Rechensysteme (BMBF)**
  Project partners: SimLab FSE, Technology Div. (JSC), University of Heidelberg, DESY, NVIDIA, EXTOLL
  Status: not funded
- **Comparison of Meshing and CFD Methods for Accurate Flow Simulations on HPC Systems (JLESC)**
  Project partners: SimLab FSE, Complex Phenomena Unified Simulation Research Team (AICS, Riken, Japan)
  Status: submission in 02/2016

> Computing time proposals

- **Large-Eddy Simulation of the FDAs Centrifugal Blood Pump using High Performance Computing via Gauss Centre for Supercomputing**
  Requested / received [core-hours]: 11.35 · 106 / 9 · 106 on JUQUEEN
- **Simulation of the Flow and Fine-Dust Particle Deposition in the Human Respiratory System via JARA-HPC Partition**
  Requested / received [core-hours]: 28 · 106 / 23 · 106 on JUQUEEN
- **Prediction of jet engine noise via JARA-HPC Partition**
  Requested / received [core-hours]: 3.52 · 106 / 1.8 · 106 on JURECA

> **Teaching**

- Ringvorlesung JARA-HPC (RWTH extern) Interdisziplinäre Lösungsstrategien für Fragen der numerischen Strömungsmechanik (WS 2015/2016)
- invited lecture AIA: Biological and Medical Fluid Mechanics II (WS 2015/ 2016)

> **Refereeing**

- CFD2015 Minerals and Process Industries (Conference)
- Journal of Aerosol Science Aircraft Engineer and Aerospace Technology
- Annals of Biomechanical Engineering
- Computers in Biology and Medicine
- JARA Exzellenz
- RWTH IT Center Computing time proposals (technical & scientific)
- JARA-HPC/NIC/GCS computing time proposals (technical)

> **Supervised student theses**

- Comparison of different methods for solving the acoustic perturbation equations. Bachelor thesis, 2015 (Jul-Sep).
- Software Cost Estimation of GPU-accelerated Aeroacoustic Simulations with OpenACC. Bachelor thesis, 2015 (Apr-Sep).
- Simulating advection-diffusion problems with the discontinuous Galerkin method. Bachelor thesis, 2015 (Jan-Apr).
- Conservative interpolation methods for nodal discontinuous Galerkin schemes. Bachelor thesis, 2015 (Oct 14-Jan 15).

NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN SIMLAB

- Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH
- Chair for Computational Analysis of Technical Systems, RWTH
- Biomaterials Lab of the University of Applied Sciences Aachen
- 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 (CERFACS), 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, U.S.

SELECTED CONFERENCE PARTICIPATIONS

- Third JUQUEEN Porting and Tuning Workshop, February 02-04, 2015, JSC, Germany
- Siemens Workshop, February 18, 2015, JSC, Germany
- PPCES Workshop, March 18-20, 2015, IT Center, RWTH, Germany
- LSDMA Community Forum, March 25-26, 2015, Berlin, Germany
- AIAA Aviation, 21st AIAA/CEAS Aeroacoustics Conference, June 22-26, 2015, Dallas, Texas, USA
- JLESC Workshop, June 29 - July 01, 2015, Barcelona, Spain
- Workshop on conditional statistics along lines and trajectories in turbulence, June 29, 2015, RWTH, Germany
- JARA Forum 04, October 01, 2015, Berlin, Germany
- 5th Korean German Workshop, October 14-16, 2015, Jeju Island, South Korea
- Obi Lab Seminar, October 22, 2015, Obi Laboratory, Keio University, Tokyo, Japan
- FOR 1779 Symposium Active Drag Reduction, November 09-10, 2015
- ERC Starting Grant Workshop, November 20, 2015, RWTH, Germany
- JLESC Workshop, December 02-04, 2015, Bonn, Germany
- EoCoE-POP workshop, December 08-11, 2015, JSC, Germany

WORKSHOPS / EVENTS ORGANIZED BY THE SIMLAB / CSG

- Tour computing facilities JSC for guests from Rome, Italy; meeting with PRACE, July 30, 2015
- Organization of a talk by Prof. Makoto Tsubokura (AICS, Riken), tour computing facilities, August 21, 2015, AIA, RWTH, Germany
- JARA Forum 04, October 01, 2015, Berlin, Germany
- Tour of JSC computing facilities for guests from Kasach University, Kasach, November 26, 2015, JSC, Germany

SELECTED HONORS, PRIZES AND AWARDS

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3.3.2. SimLab "Neuroscience"

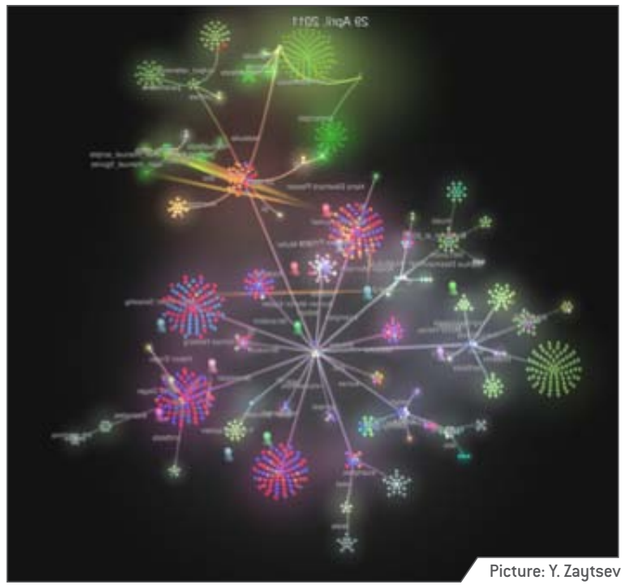
SCIENTIFIC LEAD *Prof. Abigail Morrison / FZ Jülich*

STAFF *Dr. Markus Butz-Ostendorf / JARA-HPC, FZ Jülich*
Rajalekshmi Deepu / FZ Jülich
Sandra Diaz / JARA-HPC, FZ Jülich
Dr. Jochen Martin Eppler / FZ Jülich
Steffen Graber / FZ Jülich
Susanne Kunkel / FZ Jülich
Wouter Klijn / FZ Jülich
Anna Lührs (Westhoff) / FZ Jülich
Dr. Mikaël Naveau / FZ Jülich
Alexander Peyser / FZ Jülich
Dr. Wolfram Schenck / FZ Jülich
Sven Strohmer / JARA-HPC, FZ Jülich
Guido Trensch / FZ Jülich
Bastian Tweddell / FZ Jülich
Yury V. Zaytsev / JARA-HPC, FZ Jülich

PROJECTS

> **NEST – Neural Simulation Tool** / *Butz-Ostendorf, Kunkel, Naveau, Peyser, Schenck, Trensch, Zaytsev*

- Simulation of neural networks focusing on their dynamics, size and structure
- Suitable for small-scale (notebook, workstation) and large-scale (supercomputer) simulations



Picture: Y. Zaytsev

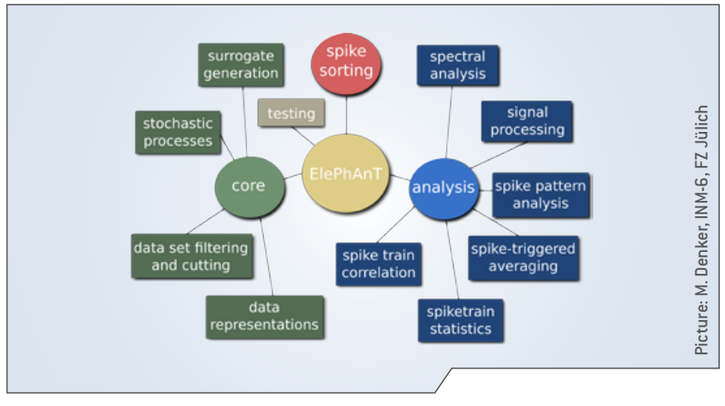
- SLNS contributions:
  > Development of the NEST kernel
  > Performance modeling and tuning
  > Python bindings (CyNEST)
  > Input/Output routines
  > Implementing the Model of Structural Plasticity in NEST
  > Gap junctions
- Structural plasticity during brain repair and memory formation
- Implementation within NEST for large-scale simulations

> **Analysis and modeling of receptor dynamics** / *Butz-Ostendorf*

- Developing a novel large-scale model accounting for and simulating changes in receptor densities in different brain areas
- Making the developed model ready for high parallel computing
- Collaboration with Prof. Karl Zilles, INM-1, FZ Jülich

> **JElePhAnT – Jülich ElectroPhysiological Analysis Toolkit** / *Deepu*

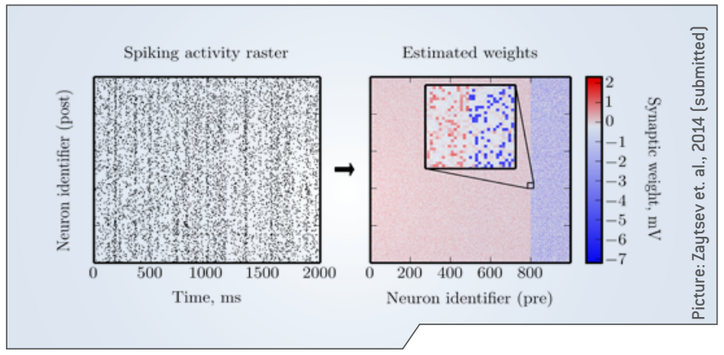
- Toolbox for the analysis of multi-scale electrophysiological data both from experiments and simulation
- Contribution to the Human Brain Project
- Collaboration with INM-6, FZ Jülich



Picture: M. Denker, INM-6, FZ Jülich

> **Connectivity reconstruction from spiking activity** / *Zaytsev*

- Input data: recordings of spike trains from thousands of neurons in parallel over extended periods of time
- Recovery of synaptic connectivity of large-scale neuronal networks from spiking dynamics, as direct experimental methods are unavailable for larger networks



Picture: Zaytsev et. al., 2014 (submitted)

> **Polarized Light Imaging** / *Lührs, Strohmer, Schenck*

- Reconstruction of the spatial structure of nerve fibers in the brain at the microscopic level
- Brain is cut into very thin slices which are recorded at different resolutions under varying polarizations of light
- Complex computational workflow to determine the fiber directions from the image data
- Image processing problems: calibration, noise reduction, stitching, registration, segmentation etc.
- Parallelized code running on JUROPA and JUDGE
- PLI is developed at Institute of INM-1, FZ Jülich

> **NEST Modeling Language (NEST ML)** / *Eppler*
- Modeling language for spiking neurons
- JARA Seed Fund in collaboration with Prof. Bernhard Rumpe, RWTH

> **Preparatory Access**
- Neuroimaging analytics workspace for large cohort data: Collaboration with INM-1
- Geant4 Application for Tomographic Emission (GATE) for neuroscience imaging development and applications: Collaboration with INM-4

> **JADE – Jülich Aachen Data Exchange** / *Tweddel*
- Collaboration with the Virtual Reality Group, RWTH
- Collaboration with Universidad Politécnica de Madrid

ADDITIONAL ACTIVITIES
- Assessing software development maturity in the SMHB / *Trensch*
- Development of programming models and tools for the solution of big data problems / *Tweddell*
- Development of programming models for the exchange of large data sets / *Tweddell*
- Efficient parallelization and optimization of applications for supercomputers / *Deepu, Diaz, Kunkel, Naveau, Schenck, Strohmer, Zaytsev*
- Development of websites and web-based services / *Graber*
- Expertise in agile software development and project management / *Trensch*
- Expertise in biophysics, software engineering, and numerical methods / *Peyser*
- Expertise in Development Operations / *Klijn*
- Expertise in parallel programming and HPC / *Diaz*
- Expertise in parallel programming for HPC and GPGPU / *Klijn*
- Expertise in software development / *Eppler*
- Expertise in software engineering / *Deepu, Diaz, Eppler, Klijn, Naveau, Schenck, Trensch, Zaytsev*
- Expertise in software project management / *Deepu, Zaytsev*
- HPC: Efficient parallelization and optimization of applications for supercomputers / *Deepu*
- HPC: High-performance neuronal multicompartment models / *Peyser*
- HPC: Modeling performance and memory footprints of large simulations / *Kunkel, Schenck*
- HPC: Modeling the performance of large simulations / *Zaytsev*
- HPC: Parallelization and optimization of large simulations for supercomputers / *Kunkel*
- HPC: Parallelization and optimization of software for supercomputers / *Lührs, Naveau, Schenck, Strohmer, Zaytsev*
- HPC: Parallelization for graphics cards and GPU clusters / *Lührs, Schenck*
- HPC: VirtualConnectome for the Virtual Brain / *Peyser*
- HPC systems architecture / *Tweddell*
- Image processing of medical images / *Lührs*
- Image processing and analysis (big data) / *Strohmer*
- Implementation and efficient parallelization of neuronal models in simulators / *Naveau*
- Infrastructure support for software development issues / *Deepu*
- Mathematical methods / *Lührs, Strohmer*
- Mathematical methods and nonlinear dynamics / *Klijn*
- Mathematical methods and statistical modeling / Zaytsev
- Modeling and simulation of different features of neural networks, especially structural plasticity / *Butz-Ostendorf, Diaz*
- Scientific visualization / *Klijn*

NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE SIMLAB
- 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 Grant "Computational models linking connectomics and large-scale dynamics of the human brain" (project funded by the BMBF in collaboration with the National Science Foundation)

SELECTED CONFERENCE PARTICIPATIONS
Posters (after call):
- Bachmann, C.; Tetzlaff, T.; Kunkel, S.; Morrison, A.
  Effect of Alzheimer disease on the dynamical and computational characteristics of recurrent neural networks
  11th Göttingen Meeting of the German Neuroscience Society, NWG, Göttingen, Germany, March 18-21, 2015
- Peyser, A.; Schenck, W.
  The NEST neuronal network simulator: Performance optimization techniques for high performance computing platforms
  Society for Neuroscience Annual Meeting, Chicago, USA, October 17-21, 2015

Posters (other):
- Do Lam-Ruschewski, A.; Lührs, A.; Morrison, A.; Orth, B.: **SimLab Neuroscience**
  JARA-Forum 04, Berlin, Germany, January 10, 2015
- Do Lam-Ruschewski, A.; Lührs, A.; Morrison, A.; Orth, B.: **SimLab Neuroscience**
  Bernstein Conference 2015, Heidelberg, Germany, September 15-17, 2015
- Do Lam-Ruschewski, A.; Lührs, A.; Morrison, A.; Orth, B.: **SimLab Neuroscience**
  11th Göttingen Meeting of the German Neuroscience Society, NWG, Göttingen, Germany, March 18-21, 2015
- Do Lam-Ruschewski, A.; Lührs, A.; Morrison, A.; Orth, B.: **SimLab Neuroscience – Ways of Collaborations**
  11th Göttingen Meeting of the German Neuroscience Society, NWG, Göttingen, Germany, March 18-21, 2015

Conference presentations (other):
- Kunkel, S.: **Replicable simulations with NEST**
  Workshop on replicability and reproducibility of neural network simulations, Bernstein Conference 2015, Heidelberg, Germany, September 15-17, 2015
- Schenck, W.: **NEST: Dry-run mode and performance modeling**
  SMHB General Assembly, Jülich, Germany, March 30-31, 2015
- Schenck, W.: **The Simulation Lab Neuroscience – A novel institution to support neuroscientists in using HPC infrastructure**

Workshop: “High-performance computing in neuroscience – from physiologically realistic neurons to full-scale brain models”, Annual Meeting of the Computational Neuroscience Society (CNS) 2015, Prague, Czech Republic, July 18-23, 2015

Contribution to a conference proceeding:

- Schumann, T., Frings, W.; Peyser, A.; Schenck, W.; Thust, K.; Eppler, J. M.
  Modeling the I/O behavior of the NEST simulator using a proxy
  Conference Proceedings of the YIC GACM 2015, Aachen, Germany, July 20-23, 2015
- Adinets, A.; Baumeister, P. F.; Böttiger, H.; Hater, T.; Maurer, T.; Pleiter, D.; Schenck, W.; Schifano, S. F.
  Performance evaluation of scientific applications on POWER8
  High Performance Computing Systems. Performance Modeling, Benchmarking and Simulation;
  Cham: Springer International Publishing, 2015, Chapter 2.
  5th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (held as part of SC14), PMBS 2014, New Orleans, LA, USA, November 16-21, 2014
  Lecture Notes in Computer Science 8966, 24 - 45 (2015) [10.1007/978-3-319-17248-4_2]

WORKSHOPS / EVENTS ORGANIZED BY THE SIMLAB

- Schenck, W.; Peyser, A.; Butz-Ostendorf, M.
  Workshop: “High-performance computing in neuroscience – from physiologically realistic neurons to full-scale brain models”, Annual Meeting of the Computational Neuroscience Society (CNS) 2015, Prague, Czech Republic, July 18-23, 2015
- SimLab “Neuroscience”
  “Supercomputing for Neuroscientists – How High-Performance Computing can help your neuroscience projects”, HPC Workshop, JSC, March 11, 2015

SELECTED HONORS, PRIZES AND AWARDS

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3.3.3. SimLab “ab Initio Methods in Chemistry and Physics”

STEERING BOARD *Prof. Stefan Blügel / FZ Jülich*
Prof. Richard Dronskowski / RWTH

STAFF *Edoardo Di Napoli, Ph.D. / JARA-HPC, FZ Jülich*
Dr. Sachin Nanavati /JARA-HPC, RWTH
Jan Winkelmann / AICES, RWTH

PROJECTS

> **ChASE eigensolver** / *Di Napoli, Winkelmann*

Development of a block iterative eigensolver for sequences of dense eigenvalue problems with application to DFT applications.

Status: Completed the development of a Chebyshev Accelerated Subspace iteration Eigensolver (ChASE). ChASE is now coded in C++ and implemented in three separate versions targeting distinct parallel platforms: multi-cores with MPI, many-cores with both OpenMP and CUDA. ChASE is bound to be publicly released at the end of March 2016 together with the submission of its two main characterizing papers. [Partners: School of Mathematics, University of Manchester, UK.]

> **Matrix generation in LAPW-based methods** / *Di Napoli*

Study of the matrix entries generation in the FLEUR code. Status: completed the study of an alternative implementation of matrix generation enabling increased scalability and parallelism. Publication is in preparation. [Partners: AICES, RWTH]

> **Quantum Chemistry code development** / *Nanavati*

Code development for a quantum chemistry software that represents the different types of potentials between interacting atoms in an efficient data structure. In the current implementation, Slater type orbitals (STOs) were represented in a linked list format. [Partners: Lomonosov University, Moscow, Russia]

> **HPC Tensor algebra** / *Di Napoli*

On going project towards the development of libraries for high-performance multi-contractions between high dimensional tensors for quantum chemistry and fRG application. Status: planned the extension of high-performance multi-contraction between two generic tensors using effectively the BLAS library for GPUs. Working on an extension of the contraction analysis for general multiple contractions between multiple tensors as they appear in fRG methods. [Partners: Intel Corporation, AICES, RWTH]

> **Shared memory parallelization of KKR-imp code** / *Di Napoli, Nanavati*

Ongoing hybrid parallelization the KKRimpurity code. In particular shared memory parallelization of the Lippman-Schwinger equation to solve the radial wavefunctions. Status: after identifying the private and shared variables, the OpenMP parallelization of the routine implementing the Lippman-Schwinger eq. predicted correct results and a considerable speed-up. Future endeav-

ors, will integrate an additional layer of MPI over number of atoms. To demonstrate the efficacy of this method, a full simulation of about 2000 atoms would be conducted to demonstrate an interesting problem in magnetism. [Partners: PGI-1, FZ Jülich]

> **Rational approximation for generalized eigenproblems** / *Di Napoli, Winkelmann*
Ongoing research on the use of optimal rational approximation for the development of a novel iterative eigensolver for generalized eigenvalue problems appearing in real space ab initio Methods. Status: Ongoing PhD project studying rational approximations based on a combination of Least Squares combined with optimization methods (Levemberg-Marquardt, steepest descent). [Partners: Department of Computer Science and Engineering, University of Minnesota, USA]

> **Adaptive Integration** / *Di Napoli, Winkelmann*
Development of an adaptive integration method based on Clenshaw-Curtis numerical integration. Status: Preliminary study followed by the development of a C++ software for the adaptive integration of 2D domains parallelized using OpenMP directives. The code will be finalized to be integrated into the fRG code fRGdyn developed at the University of Tübingen and Wien.

> **Installation, benchmarking and usage of cudaVASP** / *Nanavati*
Porting and testing an experimental GPU version of VASP on two distinct testbeds: JSC machines with latest GPUs, viz., JUPP (IBM POWER8) and JURECA (Intel Xeon). Status: the installation on JUPP was particularly difficult due to an experimental compiler and the new architecture. The installation of host and GPU version of cudaVASP on JURECA was relatively straightforward. The GPU version was successfully tested for the performance of Davidson and RMM-DIIS diagonalisation routines, which are offloaded on GPUs. Based on this experience, a problem of interest would be chosen to effectively harness the capability of this code. [NVIDIA, France and JSC, FZ Jülich]

> **Integration of the Chase library in the FLEUR code** / *Di Napoli, Nanavati, Winkelmann*
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]

> **Non-equilibrium ab initio molecular dynamics** / *Di Napoli*
Development of a new methodology to compute the electronic contribution to thermal conductivity from ab initio principles. Status: Ongoing study using an extended VASP package. Numerical results indicate a great improvement with respect to methods based on the Boltzmann transport equation. Publication in preparation. [Partners: AICES/ RWTH]

> **Supporting ABINIT developers** / *Di Napoli*
Initiated a collaboration with the ABINIT developers in order to port the ABINIT code on JSC clusters and supercomputers, improve the algorithmic structure of the GW part of the code and its OpenMP parallelization. [Partners: Institute of Condensed Matter and Nanoscience, Université Catholique de Louvain]

EXTERNALLY FUNDED PROJECTS

> **High-performance methods in fRG** / *Di Napoli*
On-going collaboration with Dr. Rohe and prof. Honerkamp (RWTH) on how to introduce high-performance techniques in computations based on functional Renormalization Group (fRG). Monthly meetings with an RWTH-based PhD student (Julian Lichtenstein) are ongoing to determine the optimal method to implement the core of some fRG computations. Since September 2014 there is an ongoing collaboration with Dr. Ciro Taranto and the group of Prof. Karsten Held (TU Wien) for the optimization and parallelization of the fRGdyn code.

> **Materials Informatics** / *Di Napoli*
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, FZ Jülich. Department of Computer Science and Engineering, University of Minnesota, USA]

ADDITIONAL ACTIVITIES

- Supervision (of PhD, Masters, Guest Students, etc.)
  - JSC Guest Student Program 2015 – "Adaptive Integration on 2D complex domains for fRG methods", JSC, Jülich, August-September 2015 / Student supervised: Toni Vidovic
  - AICES Ph.D. Program – "Optimized solver for sequences of sparse eigenvalue problems arising in ab initio computations", August 2015-July 2018 / Student: Jan Winkelmann
  - AICES Ph.D. Program – "Ab Initio-Base Nanoscale interfacial heat transfer modeling", November 2014-October 2017 / Student: Sheng Ying Yue
  - AICES Ph.D. Program – "Detection of threshold crossings in the leaky integrate-and-fire neuron model with alfa-shaped postsynaptic currents in time driven-simulations" November 2014 – October 2017 / Student: Jeyashree Krishnan

- Grant proposal preparation
  - BMBF HPC software (Anwendungsorientierte HPC-Software für das Hoch- und Höchstleistungsrechnen) – Ten page skizze to fund two post-doctoral positions and two PhD positions shared between RWTH and FZ Jülich. Title: Architecture-driven algorithms in Materials Science. Pis: EDN, P. Bientinesi and D. Wortmann
  - IPCC proposal – Submitted a 30-page proposal to apply for an Intel Parallel Computing Center. Title: Moving scientific applications into the many-core age. Pis: EDN, Stefan Kollet, and S. Mohanty. Coordinated a confcall with Intel

- PhD project preparation
  - Optimized solver for sequences of sparse eigenvalue problems arising in ab initio computations – The main target of this project is to build on the experience of FEAST, and similar initiatives, and realize an intrinsically parallel spectrum-slicing eigensolver using optimization methods and advanced numerical linear algebra techniques.

- Refereeing (journal, proposals, evaluations, etc.)
  Acting as journal referee 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
  - Prepared a poster representing the activities of SLai and participated at the JARA-Forum 04, October 01, 2015, Berlin, Germany
  - 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.
  - Participated to the kick-off workshop for EoCoE project. Participated in profiling workshop. Mentoring the PVnegf code developed within the IEK-5 group by Urs Aeberhard.
  - Performed technical and scientific evaluation of computing time applications for the initiated under JARA-HPC, IT Center, RWTH, NIC and VSR.
  - Participated in the JSC preparatory access call by giving support to the ABINIT developers.
  - Participated in the PGI-1 retreat forum on software management and maintenance policies.

NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE SIMLAB

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

- Paolo Bientinesi's HPAC group, AICES, RWTH
- Matteo Giantomassi, Université Catholique de Louvain
- Yousef Saad, University of Minnesota, Minneapolis, USA
- Stefan Blügel's group, PGI-1, FZ Jülich
- Mario Berljafa, School of Mathematics, University of Manchester, UK
- Eric Polizzi, University of Massachussetts at Amherst, USA
- Matthieu Verstraete, Univerity of Liege, Belgium
- Markus Diesmann group, INM-6, FZ Jülich
- Ming Hu, AICES, RWTH
- Piotr Kowalski, IEK-6, FZ Jülich
- Alessandro Toschi, TU Wien, Austria
- Sabine Andergassen, Universität Tübingen
- Andrei Tchougreff, Lomonosoff State University, Moscow, Russia

SELECTED CONFERENCE PARTICIPATIONS

- SIAM Conference on Computational Science and Engineering (CSE15):
  "Enabling large scale LAPW DFT calculations by a scalable iterative eigensolver". Contributed talk at the First Principles methods and Applications for Computational Materials Science and Chemistry mini-symposium, CSE 15, March 2015, Salt Lake City, UTAH, USA

- 7th ABINIT developers workshop:
  "The inner workings of the Simulation Laboratory ab initio: algorithm development, parallel computing and performance efficiency"
  Invited talk at the 7th ABINIT developer workshop, April 2015, Liege, Belgium

- Deutsche Physikalischen Gesellschaft:
  "Towards high-performance functional renormalization group calculations for interacting fermions"
  Contributed poster, March 2015, Berlin, Germany

- Fermions 2015:
  "Frequency structures in 1PI vertex with fRGdyn"
  Contributed poster at International Conference at IWH, April 2015, Heidelberg, Germany

- Green's function method in electronic structure calculations:
  Workshop attended, February 2015, Bad Honnef, Bonn, Germany

- Psi-k conference:
  Conference attended, September 2015, San Sebastian, Spain

WORKSHOPS / EVENTS ORGANIZED BY THE SIMLAB

- Minisymposium organization:
  Minisymposium on Algorithms for the Eigenvalue Problem in Electronic Structure Computations.
  At the SIAM Conference on Computational Science and Engineering (CSE15, March 2015), Salt Lake City, Utah, USA

- Program Committee:
  Workshop on Numerical Algorithms on Hybrid Architectures 2015 (WNAHA15) – At the 11th International Conference on Parallel Processing and Applied Mathematics (PPAM 2015), September 06-09, 2015, Krakow, Poland

SELECTED HONORS, PRIZES AND AWARDS

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> 3.4. Cross-Sectional Groups (CSGs)

3.4.1. CSG "Immersive Visualization"

SCIENTIFIC LEAD

Dr. Norbert Attig / FZ Jülich, Steering Board
Prof. Dr. Torsten Kuhlen / RWTH, Steering Board
Dr. Bernd Hentschel, senior researcher, contact RWTH
Dr. Herwig Zilken, senior researcher, contact FZ Jülich

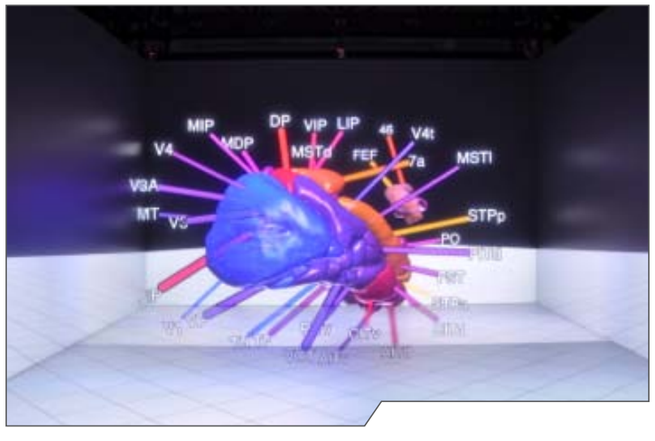
STAFF

Jens Henrik Göbbert / JARA-HPC, RWTH
Joachim Herber / JARA-HPC, RWTH
Christian Nowke / JARA-HPC, RWTH
Sven Porsche / JARA-HPC, RWTH
Stefan Selzer / JARA-HPC, RWTH
Dr.-Ing. Benjamin Weyers / RWTH

PROJECTS

> Visualization of Simulated Neural Activity from the NEST Solver – VisNEST / *Nowke*

One aspect in research and development focused on enabling hybrid visualization, namely the integrated use of 2D and 3D display systems. This aims at a seamless integration of VisNEST into the daily workflow of scientists. In order to enable hybrid visualization systems, we have developed a communication infrastructure which enables standalone views to be remotely linked and run on different platforms. This in turn enables semantically coordinated multiple views which users can dynamically configure to meet their current workflow needs. Decoupling views is essential in order to keep software complexity at bay and allow users to utilize external tools, e.g. the Electro Physiology Analysis Toolkit (Elephant), developed at the INM-6 at FZ Jülich. Eventually, this will enable scientists to synthesize custom-tailored tools which bridge the gap between their existing workflows and the VisNEST tool-chain, therefore extending the latter's usefulness to a broader user base.



> In Situ Visualization – real-time processing of large-scale simulations / *Göbbert*

Saving the results of large-scale simulation runs at full spatiotemporal resolution has become prohibitive. Traditional post-processing workflows are therefore severely limited by the amount of data they have access to. In order to address this challenge, we have taken first steps in order to enable In Situ visualization, i.e. the immediate execution of visualization and data analysis capabilities at simulation runtime. In cooperation with the Institute of Combustion Technology (ITV, RWTH) In Situ functionality from the open source visualization tool VisIt has been coupled to the multi-physics simulation code CIAO. Recently (as of February 2016) the setup has successfully been run on the full JUQUEEN system utilizing all 458,752 cores. The ongoing cooperation is supported by compute time on the JARA partition (see above). In cooperation with the SimLab "Highly Scalable Fluids & Solids Engineering" In Situ functionality are currently being added to the simulation code ZFS of the Institute of Aerodynamics (AIA). In the future, we plan to extend the coupling to multiple visualization tools and simulation codes via an HDF5-based IO interface.

> JADE – flexible and scalable data management intrastructure / *Weyers*

The "Juelich Aachen Data Exchange (JADE)" has established a flexible and scalable data management infrastructure which addresses the specific needs of domain scientists to exchange data between both sites in a convenient and efficient way. In addition to supporting the service infrastructure for a distributed file system, JADE further investigates software solutions beyond the currently used dCache stack, such as iRods. Among other things, we are actively looking into the ongoing development of these software solutions. JADE originates from a direct collaboration between the JSC at FZ Jülich and RWTH's Virtual Reality and Immersive Visualization Group in the context of the Helholtz Portfolio "Simulation and Modelling for the Human Brain". Eventually, we evolved it into an additional piece of JARA HPC Infrastructure complementing the JARA HPC Partition. In current work, we aim at using dCache as a means for integrating data source, e.g. simulation codes, to data consumers, e.g. a visualization tool. This loose, file-based coupling augments the In Situ work outlined above and is part of ongoing developments in the EU flagship The Human Brain Project.

>Seed Fund "Volume Rendering on BGAS / *Herber, Porsche*

For an effective use of Virtual-Reality (VR)-systems and techniques combined with scientific visualization active development of a software stack is necessary. In particular a generic application enabling users to bring their data in to VR in an uncomplicated manner, as well as tools used to prepare simulation data to meet the requirements given by the VR-software are developed and maintained. This software is considered as basic software for the JARA-HPC VR-installations.

ADDITIONAL ACTIVITIES

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NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE CSG

Prof. Torsten W. Kuhlen got appointed full professor (W2) at RWTH's department for computer science.

SELECTED CONFERENCE PARTICIPATIONS

–

WORKSHOPS / EVENTS ORGANIZED BY THE CSG

–

SELECTED HONORS, PRIZES AND AWARDS

–

3.4.2. CSG "Parallel Efficiency"

SCIENTIFIC LEAD

Dr. Bernd Mohr / FZ Jülich
Prof. Dr. Matthias Müller / RWTH
Prof. Dr. Felix Wolf / GRS (left group on January 31, 2015)

STAFF

Marc-André Hermanns / JARA-HPC, RWTH
Hristo Iliev, Ph.D. / JARA-HPC, RWTH

CONTRIBUTORS

Uliana Alekseeva / Project FLEUR, FZ Jülich
Dieter an Mey / HPC group leader at IT Center, RWTH
Tim Cramer / Innovative computing (Intel MIC), RWTH
Alesja Dammer / Project POP, RWTH
Christian Feld / Score-P infrastructure, FZ Jülich
Markus Geimer / Performance evaluation, FZ Jülich
Jan Felix Münchhalfen / Project MUST, RWTH
Joachim Protze / Project MUST, RWTH
Dirk Schmidl / Performance evaluation, RWTH
Aamer Shah / Project POP, RWTH
Alexandre Strube / Debugging support, FZ Jülich
Christian Terboven / HPC group deputy leader at IT Center, RWTH
Sandra Wienke / Innovative computing (GPU), RWTH
Bo Wang / Performance and power usage evaluation, RWTH
Brian Wylie / Training activities, Performance evaluation, FZ Jülich
Ilya Zhukov / Research & Development; Performance evaluation, FZ Jülich

PROJECTS:

> 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)
  Involved staff: Hristo Iliev, Dieter an Mey, Christian Terboven, Dirk Schmidl, Sandra Wienke, Tim Cramer, Bo Wang, Alesja Dammer
  Cooperation partners: IT Center, Chair I12, IKV, ITV, CATS
- Parallel Stabilized Finite Element Methods for Aero-, Hemo- and Hydrodynamics (CATS, RWTH – code XNS)
  Involved staff: Hristo Iliev
  Cooperation partners: IT Center, CATS
- Scalable Performance Analysis of Large-Scale Parallel Applications (JZAM11)
  Involved staff: Hristo Iliev, Marc-André Hermanns
  Cooperation partners: JSC, RWTH (IT Center)
- Hybrid parallelism for the Jülich DFT code FLEUR (JARA-HPC Seed Fund Project)
  Involved staff: Uliana Alekseeva
  Cooperation partners: RWTH (IT Center), FZ Jülich
- Investigating the performance of the OpenMP programming paradigm on NUMA architectures
  Involved staff: Dirk Schmidl, Christian Terboven, Dieter an Mey, Bo Wang, Tim Crammer, Sandra Wienke
- POP (Performance, Optimization and Productivity Center of Excellence)
  Involved staff: Alesja Dammer, Aamer Shah, Bo Wang, Ilya Zhukov, Brian Wylie
  Cooperation partners: RWTH, HLRS, JSC, NAG (UK), BSC (Spain), TERATEC (France)
- Continued support for the performance evaluation of a fully-coupled simulation code (SimLab TerrSys)
  Involved staff: Markus Geimer, Brian Wylie, Marc-Andre Hermanns
- Support of performance evaluation of the parallel-in-time C++ code PFASST++ (CSG Methods & Algorithms)
  Involved staff: Marc-André Hermanns

> Other relevant projects/ long-term software projects:

- MUST – Runtime error detection for parallel applications
  Involved staff: Matthias Müller
  Cooperation partners: RWTH (IT Center), ZIH, LANL (USA), LLNL (USA)
- Scalasca – Understanding application performance at scale
  Involved staff: Bernd Mohr, Marc-André Hermanns
  Cooperation partners: JSC
- Score-P – Scalable performance measurement infrastructure for parallel codes
  Involved staff: Dirk Schmidl, Markus Geimer
  Cooperation partners: JSC, RWTH (IT Center), TUM, TUDA, TUD
- Cube – Intuitive performance profile exploration
  Involved staff: Bernd Mohr, Marc-André Hermanns
  Cooperation partners: JSC, RWTH (IT Center)
- Opari 2 – Source-level instrumentation for directive-based parallelization
  Involved staff: Dirk Schmidl
  Cooperation partners: JSC, RWTH (IT Center)

ADDITIONAL ACTIVITIES

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NATIONAL AND INTERNATIONAL COOPERATIONS WITHIN THE CSG

- 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
- Mont-Blanc (European approach towards energy efficient high performance), 2011 – 2015, EU
- Catwalk (A quick development path for performance models), 2013 – 2015, DFG & SNSF
- 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
- POP (Performance, Optimization and Productivity Center of Excellence), 2015-2018, EU H2020

SELECTED CONFERENCE PARTICIPATIONS

- Bernd Mohr, invited talk "Jülich on the way to Exascale" at IHPCF 2015, Tianjin, China, May 21, 2015
- Bernd, Mohr, invited talk "Multicore Performance Debugging and Optimization at Scale: From two Embedded Cores to one Million HPC Cores" at SICS Multicore Day 2015, Stockholm, Schweden, October 20, 2015
- Matthias Müller, invited talk "TSM for Research Data Management" at TSM Symposium 2015, Cologne, Germany, September 23, 2015

WORKSHOPS / EVENTS ORGANIZED BY THE CSG

- Extreme Scaling on JUQUEEN, Jülich, Germany, February 05-06, 2015
- 17th VI-HPS Tuning Workshop, HLRS, Stuttgart, German, February 23-27, 2015
- Parallel Programming in Computational Engineering and Science 2015, Aachen, Germany, March 16-20, 2015
- 18th VI-HPS Tuning Workshop, UGA, Grenoble, France, May 18-22, 2015
- ISC15 Tutorial – Advanced OpenMP: Performance & 4.0 Features, Frankfurt am Main, Germany, July 12, 2015
- ISC15 Tutorial – Hands-on Practical Hybrid Parallel Application Performance Engineering, Frankfurt am Main, Germany, Jul 12, 2015
- OpenMPCon 2015 OpenMP developer conference, Aachen, Germany, September 28-30, 2015
- aiXcelerate 2015 Tuning Workshop, Aachen, Germany, October 09, 2015
- 19th VI-HPS Tuning Workshop, NLHPC, Santiago, Chile, October 27-29, 2015
- aiXvectorize Vectorization and Tuning Workshop, Aachen, Germany, November 02, 2015
- SC15 Tutorial – Towards Comprehensive System Comparison: Using the SPEC HPG Benchmarks for Better Analysis, Evaluation, and Procurement of Next-Generation HPC Systems, Austin, TX, USA, November 15, 2015
- SC15 Tutorial – Efficient Parallel Debugging for MPI, Threads, and Beyond, Austin, TX, USA, November 15, 2015
- SC15 Tutorial – Advanced OpenMP: Performance and 4.1 Features, Austin, TX, USA, November 16, 2015
- SC15 Tutorial – Practical Hybrid Parallel Application Performance Engineering, Austin, TX, USA, November 15, 2015
- SC15 Tutorial – Debugging and Performance Tools for MPI and OpenMP 4.0 Applications for CPU and Accelerators/ Coprocessors, Austin, TX, USA, November 16, 2015
- EoCoE/POP Training Workshop, Jülich, Germany, December 08-11, 2015

SELECTED HONORS, PRIZES AND AWARDS

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4. SCIENTIFIC REPORTS

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

> AG-Turbo 2020 Vorhaben 4.1.7 – Profiles with advanced tangential end wall contouring

Prof. Dr. Manfred Wirsum / Dipl.-Wirt. Ing. Oliver Curkovic, M.Sc. / Dipl.-Ing. Mathias Diefenthal / Piotr Luczynski, M.Sc

The current investigation focuses on a 2D and 3D blade design with tangential end wall contouring (TEWC) and uses a reference design without TEWC (BASE), see Figure 2. Main focus of the research project is the study of flow phenomena and the leakage flow for both blade types depending on operating parameters and axial distance using CFD simulation. The structure of the numerical part of the investigation of the previous project "COORETEC-turbo" and the current project "AG Turbo 2020" is given in Figure 1.

To enhance the impact of the TEWC, the cavities of the rotors are sealed by means of combined brush- and labyrinth seals, whereas the stator cavities are sealed by labyrinth seals only. The brush seals are modeled as porous bodies (see Figure 2) whose porosity values are calibrated with pressure drop measurements across the rotor cavities.

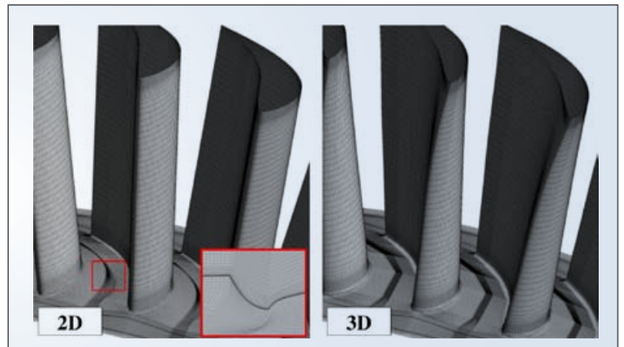
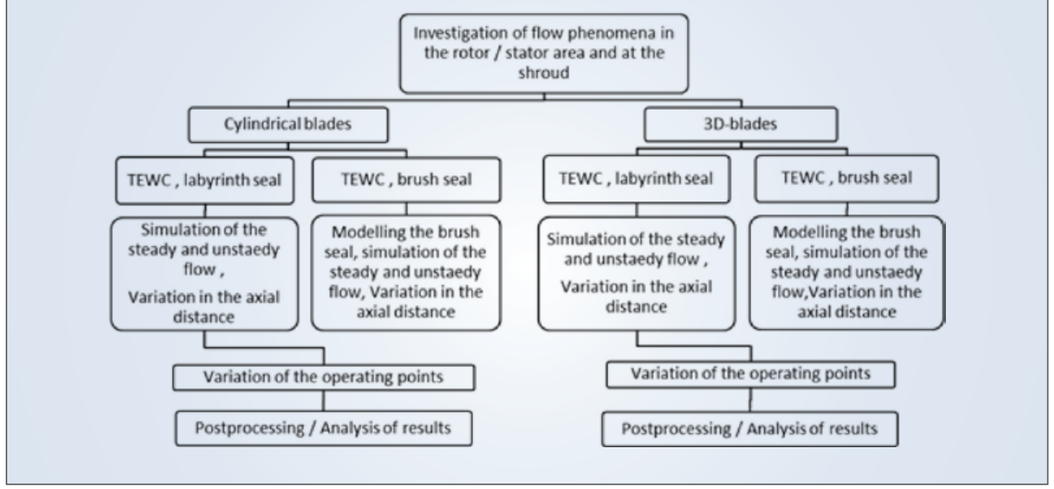


Figure 2: Computational mesh of rotor 1 for 2D TEWC (l.) and 3D BASE (r.) blading (©IKDG)

Figure 1: Breakdown of the numeric portion into subtasks (©IKDG)



> COOREFLEX-turbo – Vorhaben 4.3.10 – Pre-warming of steam turbine components

Prof. Dr. Manfred Wirsum / Dipl.-Wirt. Ing. Oliver Curkovic, M.Sc. / Dipl.-Ing. Mathias Diefenthal / Piotr Luczynski, M.Sc.

The main goal of the project is to identify the vortex effects in the fluid state which are mainly responsible for the heat transfer (see Figure) in the turbine and to develop phenomenological equations to predict the steady temperature distribution inside a high pressure or intermediate pressure turbine. These equations should be applicable without any prior numerical CHT calculations. For this model to work, the heat flows between solid-solid and solid-fluid components need to be considered with sufficient accuracy.

To achieve this goal, the project is divided into two branches – the phenomenological branch and the numerical branch. The numerical investigation provides the phenomenological branch with important influencing factors and servers as a validation method for the phenomenological model.

The working packages (WP) are as followed:

WP 1: Numerical preparation of a repetitive stage

WP 2: Development of a phenomenological model and steady CHT calculation of a repetitive stage

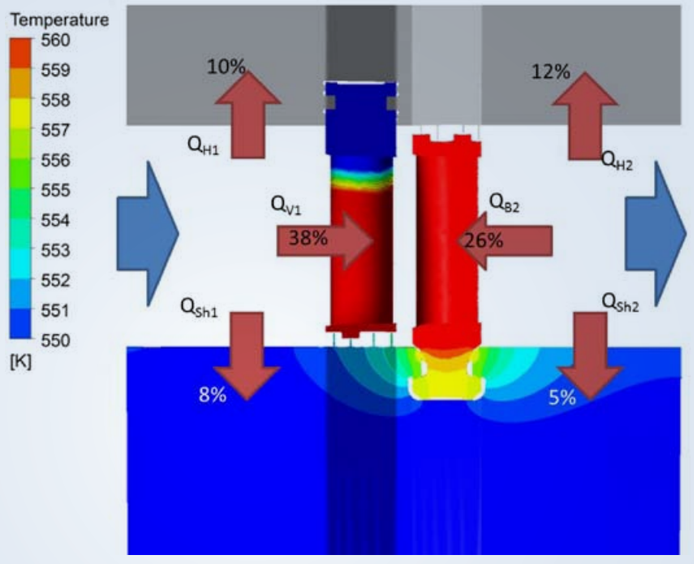
WP 3: Comparison between the phenomenological model and the CHT calculation and identification of relevant influencing factors

WP 4: Upgrading the numerical model to a multi-stage axial turbine

WP5: Upgrading the phenomenological model to a multi-stage model and adjustment of the model's parameters

WP 6: Concept development for rotor temperature prediction

WP 7: Validation concept development for the phenomenological model



Heat fluxes in a single stage at low volume flow (©IKDG)

CHAIR FOR APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY (GGE), E.ON ENERGY RESEARCH CENTER / RWTH / Prof. Christoph Clauser

> Water flow and permeability distribution in a textonically limited hard-rock aquifer

Johanny Buckmann, 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 a hydrogeological reservoir model of the real-world reservoir near Eschweiler (Germany) are being developed by our project partners at the Lehr- und Forschungsgebiet Hydrogeologie, RWTH, as basis for the numerical reservoir model. 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. Hydraulic parameters and their uncertainties are estimated by simulations based on Monte-Carlo (MC) and Ensemble-Kalman-Filter (EnKF) approaches. 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 which includes an MPI parallel Monte Carlo algorithm.

During the report period we applied successfully for computing time on the JARA HPC Partition part of the supercomputer JURECA at JSC. The three dimensional structural subsurface model of the structurally complex and heterogeneous aquifer system in the study area provides the basis for numerical simulations. A subset of around 3.6 km in E-W direction, 2.9 km in N-S direction and 720 m depth is divided into a rectilinear grid with a uniform cell size of 10 m x 10 m x 10 m, resulting in nearly 7.5 Million grid cells. This discretization is necessary for resolving the folded hard-rock aquifer and its structural limitations sufficiently.

> Numerical Simulation of CO_2 Geo-Sequestration

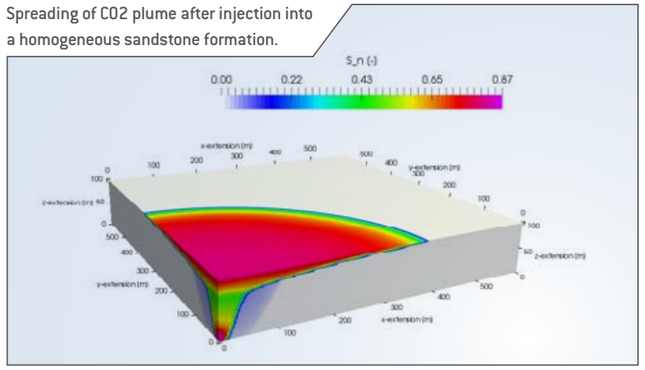
Dipl.-Math. Henrik Büsing

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.

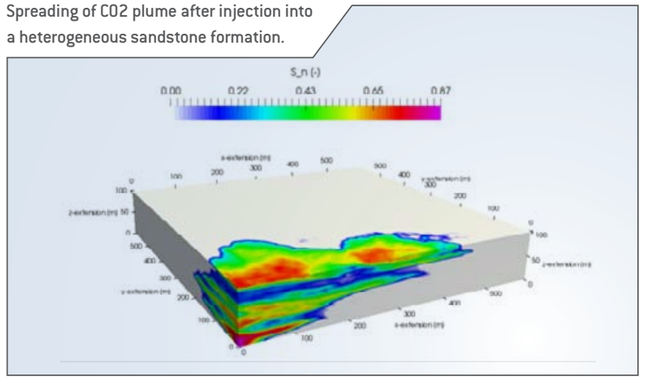
We examine the influence of heterogeneities in the permeability field on the formation of fingers due to dissolution processes. Additionally we are interested in the different spreading behavior of the CO_2 plume due to the heterogeneity and the amount of trapped CO_2. Coarse grid resolution might overestimate, e.g., the spreading of the CO_2 plume thus making these studies, though inaccurate, a conservative approach in terms of risk assessment.

The different behavior of a CO_2-brine system during and after injection becomes also apparent in the occurring systems of equations. In the beginning advective forces dominate and the system is hyperbolic in nature. Later when dissolution processes dominate the system becomes parabolic. Therefore, different solution algorithms in the different phases might be advantageous.

Spreading of CO2 plume after injection into a homogeneous sandstone formation.



Spreading of CO2 plume after injection into a heterogeneous sandstone formation.



To this end, we examine classical BiCGStab with ILU0 preconditioning in contrast to algebraic multigrid and sparse direct solvers.

We are also interested in the performance of the different solvers with respect to the heterogeneity in permeability. Classical iterative solvers might deteriorate in performance and the number of steps until convergence increases due to increasing heterogeneity. Here, sparse direct solvers can be a better choice

Finally, automatic differentiation (AD) as an alternative to the standard finite difference (FD) approach can help during the solution process. On the one hand, this ensures that always the correct derivative is taken, but additionally liberates the user from the obligation of choosing an FD step size. The exact (up to machine precision) derivative is always available.

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

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

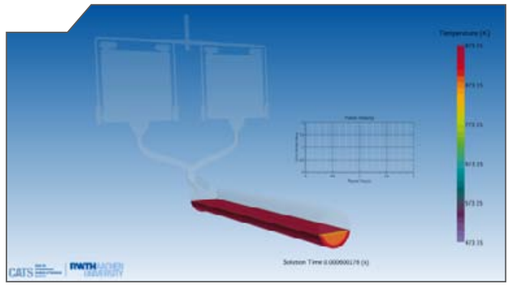
The objective is the continued development of simulation methods for unsteady flows of fluids and gases, in situations involving significant deformations of the computational domain.

These methods are based on stabilized FE formulations, unstructured 3D meshes, and parallel iterative solvers. The main application areas are: microstructured fluids such as blood and plastic melts, flows in the presence of rotating components such as turbine rotors, and free-surface flows.

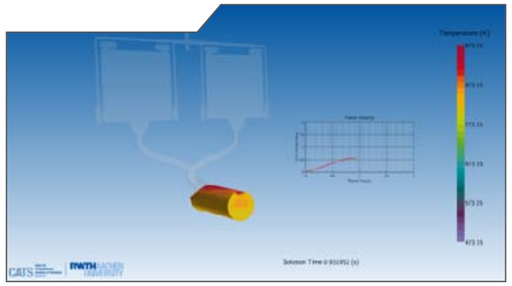
Of immediate concern are the simulation of blood flow in ventricular assist pumps and other medical devices, the simulation of wind turbine aerodynamics, and simulation of fluid-based production processes, e.g., plastics extrusion.

The long-term goal is to perform shape optimization of complex geometries improving in a significant way the biocompatibility of biomedical devices, the precision of the production tools such as extrusion dies, and the efficiency of the wind-based or ocean-current-based energy generation.

> Parallel Stabilized FEM for Viscoelastic Fluid Simulations of Rigid Rod-Like Polymers



Molten metal flow in aluminum die casting: begin (top) and end of the slow shot phase (bottom).

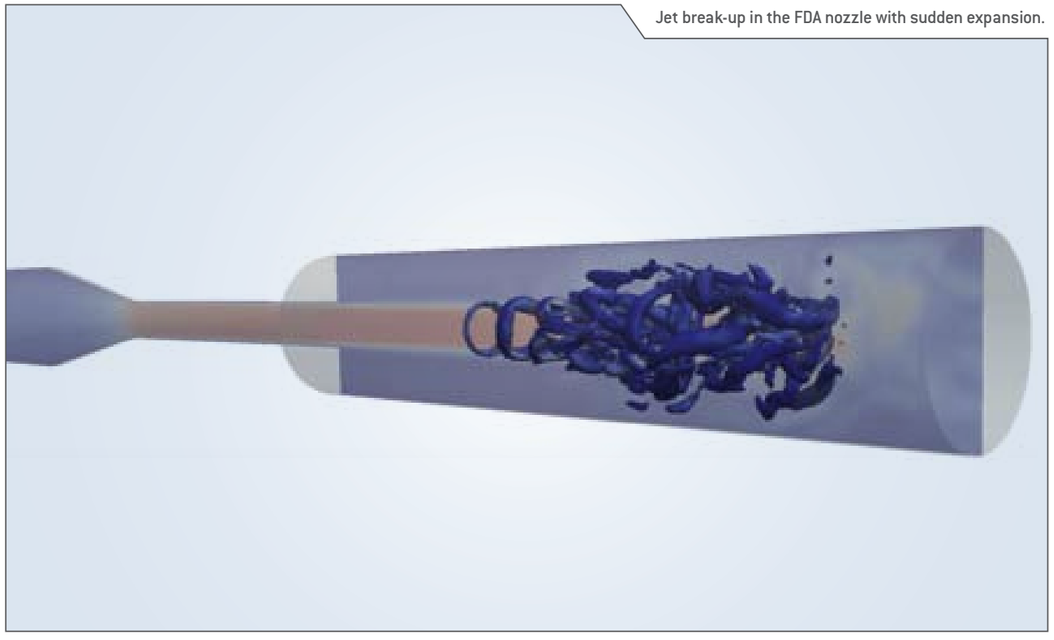


The objective is to develop efficient numerical methods for the unsteady incompressible viscoelastic flows of microstructured liquids; i.e. rigid rodlike polymers, with an emphasis on the Single-Walled Carbon Nanotube (SWNT) solutions.

SWNTs demonstrate unique properties in molecular scales, which makes them ideal candidate as building blocks for multifunctional nano-materials. Thus, this project aims to improve our understanding of nano-material assembly processes with the help of numerical methods. Our solution method is based on parallel, stabilized FEM for unstructured meshes.

The Galerkin/Least-Squares (GLS) formulation of stress-velocity-pressure with space-time elements are developed for the rigid rodlike polymeric liquids. The resulting nonlinear algebraic equations are then handled via Newton-Raphson (NR) iterative scheme. Within each NR iteration, linearized equation system is solved by the GMRES method.

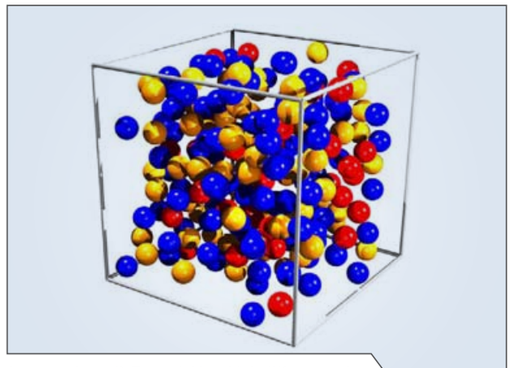
Jet break-up in the FDA nozzle with sudden expansion.



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

> Aging mechanisms of amorphous GeTe

Aging of materials refers to the slow structural evolution of important material properties with time. In glasses, aging is a particularly ubiquitous phenomenon because glasses are "frozen liquids" which have numerous metastable configurations. The atoms in glasses can hence rearrange to reach lower energy configurations without climbing over high barriers.



An amorphous GeTe model in which different colors indicate different Ge chemical environments

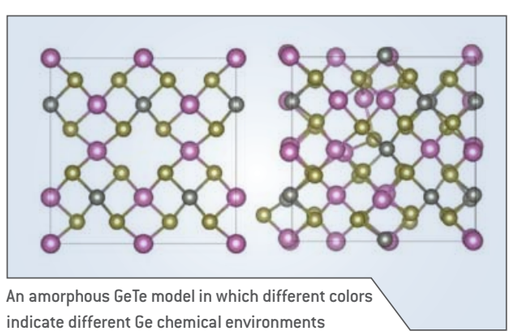
Aging becomes a very problematic issue in phase change memory devices because the electrical resistivity of the storage media will change upon time, known as "resistivity drift". This resistivity drift is believed to be linked with the evolution of local structure upon time. In this work, with ab initio simulations on a prototypical phase-change material, the amorphous GeTe, we could identify the underlying atomic rearrangement mechanism.

We could demonstrate that the local structure of the glass evolves towards a covalent amorphous network with increasing Peierls distortion, and the structural and electronic properties drift away from those of the resonantly bonded crystal. The behavior observed here is rather unique and differs from other glasses whose local structure resembles their crystalline phases. The resulting manuscript (J.Y. Raty et al., Nature Communications (2015)) has received widespread interest including several conference invitations.

> Tailoring the chemical bonds using disorder

Disorder exists in large number of compounds in which the enthalpy gained by the heteropolar bonds is overcompensated by the reduction in entropy.

For example, in a metallic alloy CuAu, the Cu-Au bonds are more stable than homopolar Cu-Cu and Au-Au bonds, and thus the system tends to order at low temperature. However, the high temperature enhances the entropic term (G=H-TS) and drives the alloy into disorder. We found in experiments that the properties of materials respond differently to disorder, e.g., disorder has a small effect on the properties of covalent and metallic alloys (such as SiGe, GaAlAs2, AgAu, etc), while it has a strong impact on resonantly bonded systems such as phase-change materials. To study the effect of disorder using first principles method, we constructed various crystalline models and introduced disorder. Our calculations provide crucial insights to guide experiments, since it is easier to change the degree of disorder in a controlled fashion in computations than in real experiments. The results of this study can help us tailor the properties of materials with different degrees of disorder. A publication about these exciting findings is presently under preparation.



An amorphous GeTe model in which different colors indicate different Ge chemical environments

> Disorder control using high pressure

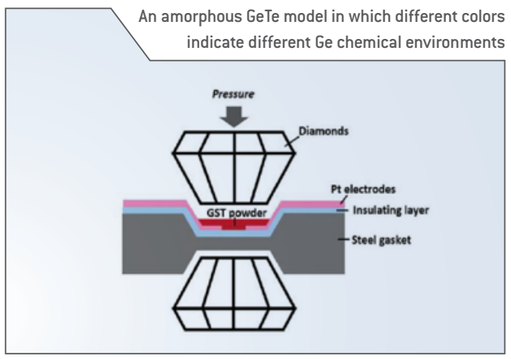
It is recently been discovered that the resistivity of crystalline phase change materials (PCMs) changes upon annealing temperature. This anomalous "annealing effect" is attributed to the disorder (random distribution of vacancies) in PCMs: temperature tunes the degree of disorder in the cation sites, which could localize/delocalize the electron wavefunctions (via "Anderson localization"), changing the mobility of charge carriers and eventually leading to the variation of resistivity. In this work, we explored the possibility of using pressure to tune the disorder.

Our large-scale ab initio molecular dynamics simulations demonstrate that pressure can lower the energy barrier for the anti- site migration in crystalline PCMs. The accumulation of these anti-site atoms largely increases the compositional disorder, adding localized electronic states near the conduction band. The disorder-induced electron localization triggered by pressure is a novel way to modulate the properties of materials. Furthermore, the random distortion of the lattice induced by the compositional disorder provides a new mechanism that contributes to the amorphization of crystalline PCMs at high pressure.

A disordered PCM under high pressure. The white regions denote the localized areas of electrons due to the anti-site pairs.

> Pressure reverses the electrical resistivity in $GeSe_2Te_4$

Pressure can tune the resistivity of amorphous Ge-Sb-Te (a-GST) by four orders of magnitude. We conducted similar experiments on the crystalline GST (c-GST) and demonstrated that the pronounced resistivity contrast between a-GST and c-GST is remarkably reduced and even reversed with increasing hydrostatic-like pressure. This anomalous resistivity reversal originates from the differences in the pressure induced atomic rearrangement of these two phases, as revealed by ab initio molecular dynamics simulations. Specifically, a low to medium pressure (<7 GPa) primarily compresses the bonds in crystalline GST without significantly displacing the atoms and vacancies off the lattice sites. As a result, only relatively small changes in the band structure are induced. In contrast, in amorphous GST, the fraction of voids changes drastically with pressure and the Peierls-like distortion is greatly reduced, yet the average bond length remains almost constant. These effects eventually turn the semiconducting glass into a metallic one. Our work reveals distinct behaviors of amorphous and crystalline phase-change materials under stress, shedding light on the mechanisms of electronic transport in different phases, and thus may have important implications on the design of phase-change memory devices.



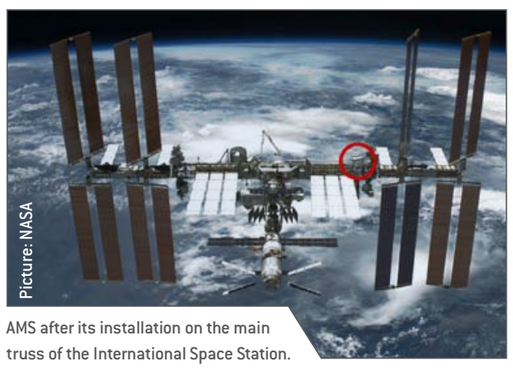
An amorphous GeTe model in which different colors indicate different Ge chemical environments

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 is a detector designed for precision spectroscopy of cosmic rays that was installed on the International Space Station in May 2011 (see picture). With dimensions of 5x4x3 m3 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. Physics Institute 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, Switzerland.



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

AMS so far has recorded more than 80 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 sub-detectors for particle identification (the TRD, an electromagnetic calorimeter and a ring-imaging Cherenkov counter) and two sub-detectors 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-HPC.

Two major papers have appeared in 2015. They deal with measurements of the cosmic- ray proton and helium spectra. Surprisingly, they reveal a progressive hardening of the spectral indices of both protons and helium at high energies, with high precision. Remarkably, the spectral index of the proton to helium flux ratio increases with rigidity up to 45 GV and then becomes constant. Both papers have been selected as Editor’s Suggestion by Physical Review Letters.

CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS / RWTH / Prof. Manfred Martin

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

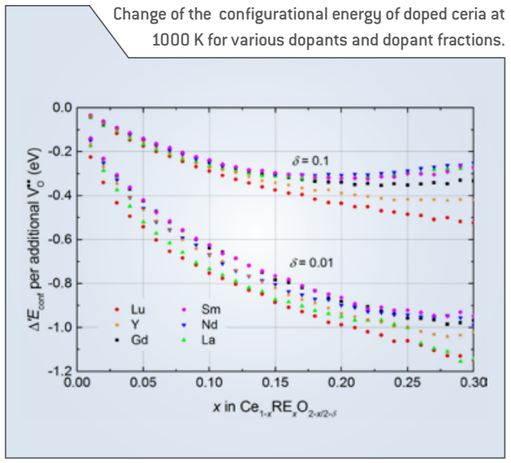
Doped ceria is known as promising candidate for the application as electrolyte in solid oxide fuel cells due to its high oxygen ion conductivity. Under reducing conditions ceria releases oxygen to the atmosphere leading to the formation of oxygen vacancies and electrons, which localize at cerium ions to form small polarons. In the last period we reported about the ab initio calculation of interaction energies between various defects in rare-earth doped ceria.

These energies were now used in Monte Carlo simulations to examine the defect distribution and the effect of defect interaction on the energy of reduction. The simulations reveal that the interaction between defects and their distribution in thermodynamic equilibrium leads to a decrease of the total energy compared to doped non-stoichiometric ceria with non-interacting defects.

The magnitude of this energy change increases with increasing non-stoichiometry as well as increasing dopant fraction in accordance with experimental results.

Furthermore, we extended this approach by calculating the interaction energies for ceria doped with zirconium and praseodymium. Subsequent Monte Carlo simulations are pending.

Change of the configurational energy of doped ceria at 1000 K for various dopants and dopant fractions.

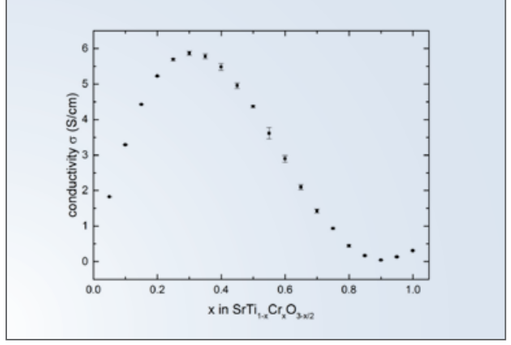


> Oxygen ion conductivity of doped $SrTiO_3$ and $CaTiO_3$: a DFT and Kinetic Monte Carlo study

$CaTiO_3$ is suggested as an electrolyte material for application in solid oxide fuel cells (SOFC) due to its high ionic conductivity which is comparable to that of yttria stabilized zirconia (YSZ).

Since $CaTiO_3$ crystallizes in a distorted orthorhombic perovskite structure between ambient and elevated temperatures, the computational demand for the calculation of migration energies is tremendous. Therefore, in this project $SrTiO_3$ with cubic perovskite structure was introduced as a model system with higher symmetry. This model system is utilized to prove the computational method as well as the model for the migration energy before calculating the more demanding $CaTiO_3$ system.

Simulated conductivity of the oxygen ions in $SrTi_{1-x}Cr_xO_{3-x/2}$ at 1000 K in a 16x16x16 simulation cell. The migration energies obtained from the 333 supercell were used.



In this period, migration energies in Cr-doped SrTiO3 have been calculated for three different supercells (2x2x2, 3x3x3 and 4x4x4) revealing a clear dependence on the supercell size which is attributed to covalent Cr-O-interactions. The resulting flat energy landscape with a large number of local minima increases the computational demand.

In addition, interaction energies between vacancies up to 7th nearest neighbor position and between vacancies and dopants up to 4 th nearest neighbor position were calculated. These interactions do not scale linearly with the number of defects on equivalent positions and consequently, the long range interactions in SrTiO3 cannot be represented by simple pair interactions.

With the so far obtained energies preliminary Kinetic Monte Carlo simulations have been performed to estimate the oxygen ionic conductivity of Cr-doped SrTiO3.

> Ab initio calculations of the defect energetics and dynamics at the ∑5(310) grain boundary in ceria

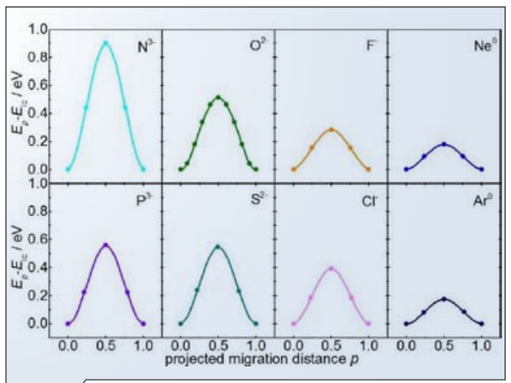
In preparation for our studies of oxygen-ion transport at the ∑5(310) grain boundary in ceria, we studied anion migration in the bulk. Employing DFT-NEB calculations, we determined the activation energies of migration for various anion moieties migrating by a vacancy mechanism. We obtained an oxygen migration energy of ΔEmig, O = 0.51 eV in very good agreement with the available data from experiments and theoretical studies.

The figure shows the energy profiles for the migration of N^{3-}, O^{2-}, F^{-}, Ne^{0}, P^{3-}, S^{2-}, Cl^{-} and Ar^{0}.

We compared our data with predictions from the standard model of anion migration in fluorite-structured oxides – Kilner and Brook's critical radius model – which is based on steric considerations. If one only compares ions of the same charge, surprisingly little influence of the ionic radius on the migration energy can be seen.

Instead, we see a clear correlation of the migration energies with the charge of the anions. As the migration energy increases with increasing negative charge, we suggest that repulsive Coulomb interactions between the migrating anion and the closest oxygen ions, form the main contribution to the energy barrier. A clear correlation between the migration energy and the difference in electrostatic energy between the initial and the saddle-point configuration further supports our new model of fast oxygen-ion conduction. Any optimization of the oxygen-ion conductivity must therefore be aimed at reducing the repulsive Coulomb interactions. The results of this project have already been published.[1]

[1] *A. R. Genreith-Schriever, P. Hebbeker, J. Hinterberg, T. Zacherle, R. A. De Souza, J. Phys. Chem. C 2015, 119, 28269-28275.*



Energy profiles of the migration of impurity anions along the <100> direction in CeO2. The lines are a guide to the eye and are natural cubic spline fits. For comparison the migration profile of oxygen is also depicted.

INSTITUTE FOR ADVANCED SIMULATION AND PETER GRÜNBERG INSTITUTE, THEORETICAL NANOELECTRONICS (PGI-2 / IAS-3) / FZ JÜLICH / Prof. Eva Pavarini

> Multiplet effects in strongly correlated material

Emergent phenomena are the hallmark of strong correlations and yet to unravel their nature remains one of the central challenges in condensed-matter physics.

The bottleneck is the description of electronic many-body effects in a realistic setting. Density-functional theory and its local- density approximation (LDA) was a major step forward. However, LDA and its generalizations fail even qualitatively for strongly correlated systems, predicting, e.g., a metallic ground state for Mott insulators.

The recent development of the LDA+DMFT approach which merges DFT with a powerful many-body approach, dynamical mean-field theory (DMFT) has strongly advanced the field. However, 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 develop and use general DMFT solvers based on the continuous-time quantum Monte Carlo technique.

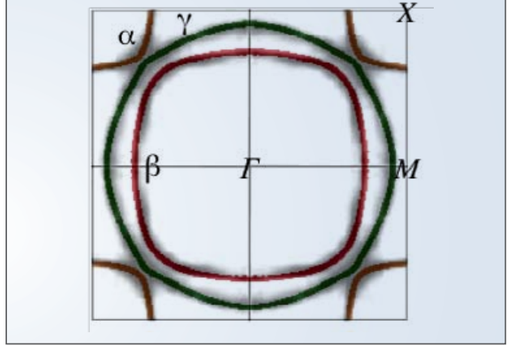
> Order-disorder transitions in strongly correlated systems

Cuprates and colossal magneto-resistance manganites are strongly correlated materials; thus electrons cannot be described individually, and standard ab initio or mean-field approaches typically fail.

Furthermore, these materials are characterized by disordered phases, the description of which requires large super-cells and configuration averaging, a remarkable challenge in the presence of strong correlations.

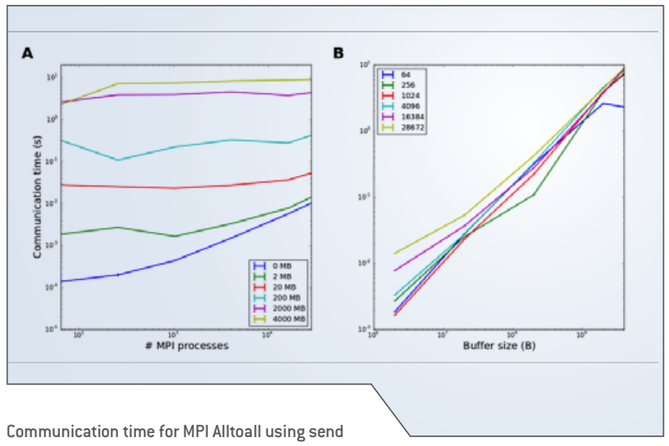
The main purpose of the present project is to understand the nature of the orbital order-to disorder transition in cuprates, manganites and similar transition- metal oxides in bulk and in the doped phases.

The Fermi surface of Sr_2RuO_4 calculated with LDA+SO+DMFT with anisotropic Coulomb interaction (Phys. Rev. Lett., in press). The grey map shows experimental data taken from A. Damascelli et al., Phys. Rev. Lett. 85, 5194 (2000).



INSTITUTE FOR ADVANCED SIMULATION, THEORETICAL NEUROSCIENCE (IAS-6) AND INSTITUTE OF NEUROSCIENCE AND MEDICINE, COMPUTATIONAL AND SYSTEMS NEUROSCIENCE (INM-6) / FZ JÜLICH / Prof. Markus Diesmann

> Brain-Scale Simulations (JINB33)



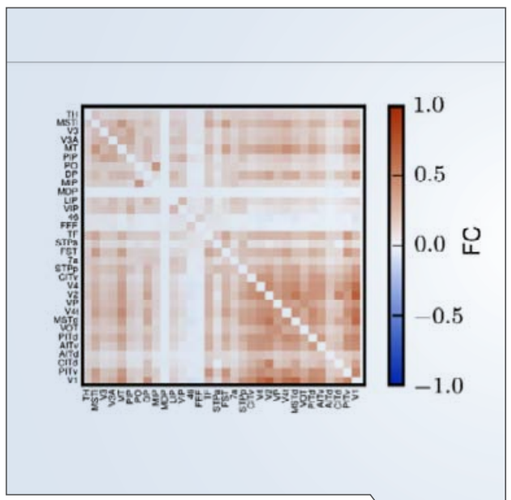
Communication time for MPI Alltoall using send buffers of varying size and varying numbers of MPI processes. Error bars denote SEM and are partly covered by markers. Data recorded in 10 × 20 trials. We used one MPI process/node. The plot shows that MPI Alltoall scales sufficiently well for numbers of processes typically used on supercomputers.

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 2015, we implemented the prototype for the next (5th) generation kernel of NEST with a new communication scheme and proved with benchmarks that its general principles work and show good scaling. Apart from that, we focused on the runtime performance of NEST and implemented a new network wiring scheme, exploiting the fact that connecting neurons local to one MPI rank leads to lower construction times for the network. Moreover, with the implementation of a communication infrastructure for time-continuous interactions, we added the possibility of simulating gap junctions to the NEST simulator.

On the neuroscientific side, we advanced the multi-area model of macaque visual cortex and found significant large-scale interactions resembling experimental fMRI data. This progress was enabled by a theoretical method to systematically modify the model connectivity to improve its network dynamics. Furthermore, we have implemented the 4x4 mm2 network model on JUQUEEN, which includes local topography, and found that the model exhibits a rich repertoire of network dynamics.



Functional connectivity (FC) in the model simulated for 50 s of biological time measured by the zero-time lag correlation coefficient of synaptic input currents.

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

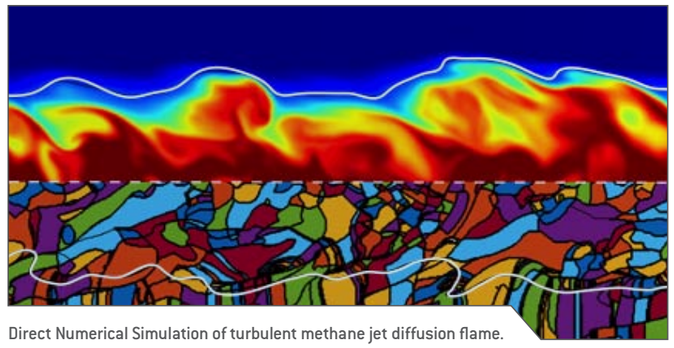
All JARA-HPC projects deal with the broad field of turbulent combustion. This includes turbulence, multiphase flows, engine and turbine simulations, combustion modeling and pollutant formation. Exemplary, details of three projects are given the following paragraphs.

> Regimes in turbulent non-premixed combustion

In this project, two highly resolved direct numerical simulations (DNS) of temporally evolving jet methane diffusion flames were conducted in order to find reliable models for the highly turbulent combustion regime. The starting conditions for the DNS were chosen to instigate both local extinction and re-ignition to provide a wide range of combustion phenomena for further investigation.

The data were analyzed by means of a Dissipation Element (DE) analysis, which is a method for measuring the local turbulent scales and allows to investigate the effect of small scale mixing. A DE analysis of the Mixture fraction field, representing the state of the chemistry, is shown in the picture.

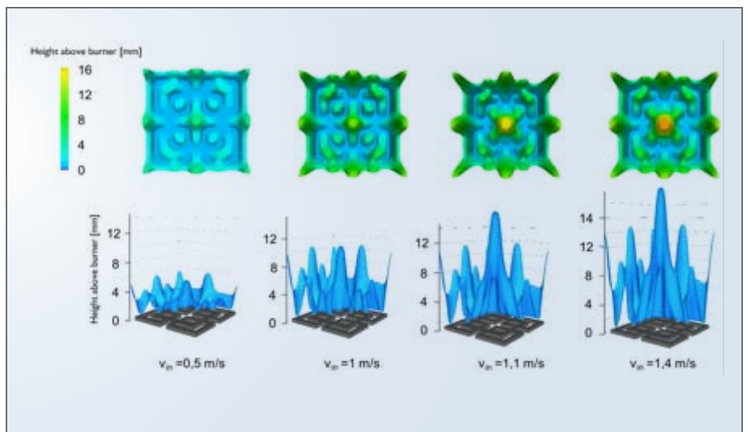
A key characteristic of the statistics obtained by the DE analysis is its strong invariance towards changes in the Reynolds number, making it predestined for future models for the small scale mixing regime.



Direct Numerical Simulation of turbulent methane jet diffusion flame. Upper part of the figure: Mixture fraction field in the cross section of the jet flame. The color red corresponds to regions of pure fuel while blue indicates regions of pure oxidizer. Lower part of the figure: Dissipation Element analysis of the mixture fraction field in the same plain. Individual elements are encompassed by a black contour.

> Investigation of Fractal Geometrie as Burner Designs

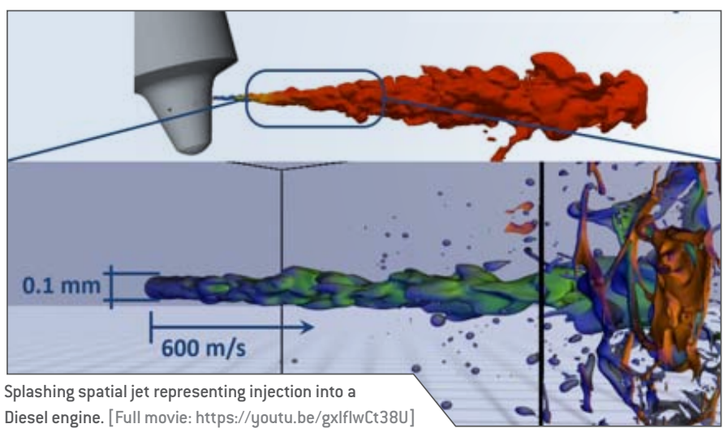
In this project, burners of domestic heating devices of modern low-energy houses are investigated. Particularly, a novel gas burner design with a larger range of operation than current designs at the current CO emissions level is developed. The burner design is derived from fractal geometries which are motivated as design basis by two things. First, fractal geometries can be uniquely defined easily which enables to use automated shape optimization algorithms. Second, fractal geometries are promising due to their multiscale nature which is likely to promote stable flames on a wide range of operation. Resulting flame structures with varying flow velocities are shown in the figure.



Simulated flame structures on fractal burner geometry with varying flow velocities

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

The figure shows a splashing multiphase jet representing the injection into a Diesel engine. This study was performed as part of the project "Detailed Investigation of Liquid Sheet Breakup Using Direct Numerical Simulation and In Situ Visualization", which addresses the understanding of the mechanism underlying the breakup of ligaments into multiple droplet. Therefore, simulations of multiphase jets are 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 and reduce the data size which has to be stored.

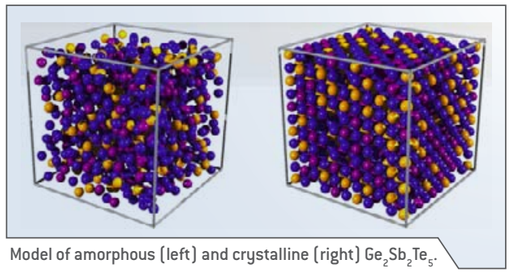


Splashing spatial jet representing injection into a Diesel engine. [Full movie: https://youtu.be/gxIfIwCt38U]

INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS, THEORETICAL NANOELECTRONICS / RWTH / Prof. Riccardo Mazzarello

> Ab initio study of crystallization of $Ge_2Sb_2Te_5$

We have investigated the crystallization properties of $Ge_2Sb_2Te_5$, a prototypical phase-change material (PCM), by ab initio molecular dynamics simulations [1, 2]. In the first work [1], we used the metadynamics method to accelerate the formation of post-critical crystalline nuclei. We also considered amorphous models inside a crystalline matrix. From the two sets of simulations, we obtained values of the growth velocity of the order of 1 m/s at 600 K.



Model of amorphous (left) and crystalline (right) $Ge_2Sb_2Te_5$.

More recently, we have considered a very large model containing 900 atoms to address finite size effects and to study the localization properties of the electronic states upon crystallization [2]. We have studied the growth of a nucleus generated with metadynamics and we have found a growth velocity of the order of 0.5 m/s (at 600 K), indicating that finite size effects do not play a dramatic role even for 500 atom models. The computed growth velocities are compatible with experimental data. Furthermore, our simulations show that the recrystallized model is very disordered and possesses electronic states localized around vacancy clusters and antisite defects, in agreement with our previous work about Anderson localization in crystalline GeSbTe compounds [3] (see also project "Metal-insulator transitions in crystalline GeSbTe compounds" below).

References [1] to [12] please see page 54

> Aging in amorphous phase-change materials

We have elucidated the microscopic mechanisms responsible for aging in GeTe, a prototypical amorphous PCM, by ab initio density functional theory (DFT) methods combined with photothermal deflection spectroscopy and impedance spectroscopy experiments [4]. To obtain relaxed models of the amorphous state, we have generated melt-quenched models of compounds similar to GeTe (namely, SiTe, GeSe and SnTe) and we have subsequently substituted selected types of atoms (Si « Ge, Se « Te, Sn « Ge). We have shown that aging brings about a progressive decrease in homopolar GeGe bonds and tetrahedral structures. Furthermore, amorphous GeTe evolves toward a covalent network with increasing Peierls distortion, whose structural and electronic properties become increasingly different from those of the resonantly bonded crystal [4]. This project has been done in close collaboration with Dr. J.-Y. Raty (Université de Liège, Belgium), Dr. C. Bichara (CINaM, CNRS and Aix-Marseille University, France) and the group of Prof. Wuttig.

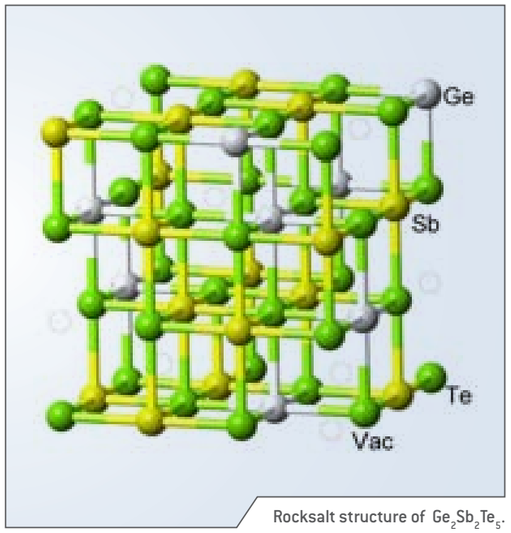
We are currently investigating the relaxation mechanisms in amorphous Ge2Sb2Te5 using similar methods. We are also studying the bonding properties of these models by the crystal orbital overlap population (COOP) method, which we have recently employed to investigate the PCM In3SbTe2 [5]. These projects are done in collaboration with Prof. Wei Zhang (Xi'an Jiaotong University, China), Prof. Wuttig and Prof. Dronskowski.

References [1] to [12] please see page 54

> Metal-insulator transitions in crystalline GeSbTe compounds

We are studying the localization properties of the electronic states and the metal-insulator transitions induced by annealing in crystalline GeSbTe compounds. In Ref. [6], we investigated (GeTe)x-(Sb2Te3)y PCMs with varying GeTe content by large-scale DFT simulations. We found that a stoichiometry-controlled metal-insulator transition occurs. More specifically, we showed that the models containing a high concentration of stoichiometric vacancies possess localized states at the Fermi energy. On the other hand, the GeTe-rich models exhibit metallic behavior.

Very recently, we have demonstrated the existence of atomic disorder on the Ge/Sb/vacancy sublattice in the rocksalt structure obtained upon fast crystallization of amorphous GeSbTe by combined direct atomic scale chemical identification experiments and ab initio simulations [7]. We have also identified the gradual vacancy ordering process upon annealing, which was predicted to trigger the transition to extended electronic states [5]. This work has been done in collaboration with Prof. Zhang and Prof. Evan Ma at Xi'an Jiaotong University.



Rocksalt structure of $Ge_2Sb_2Te_5$. One sublattice is occupied by Te atoms, whereas the other sublattice contains randomly arranged Ge, Sb and vacancies.

In collaboration with the experimental group of Dr. Raffaella Calarco (PDI Berlin), we have also investigated the structural properties of GeSbTe models with a high degree of structural perfection, obtained by engineering the complex stacking sequence of atoms and vacancies in the ternary alloy during epitaxial growth [8]. Our simulations have provided important information about the lattice symmetry and the distribution of vacancies. Interestingly, the samples have been employed in memory cells and have demonstrated a superior electrical switching as compared to metastable disordered GST [8].

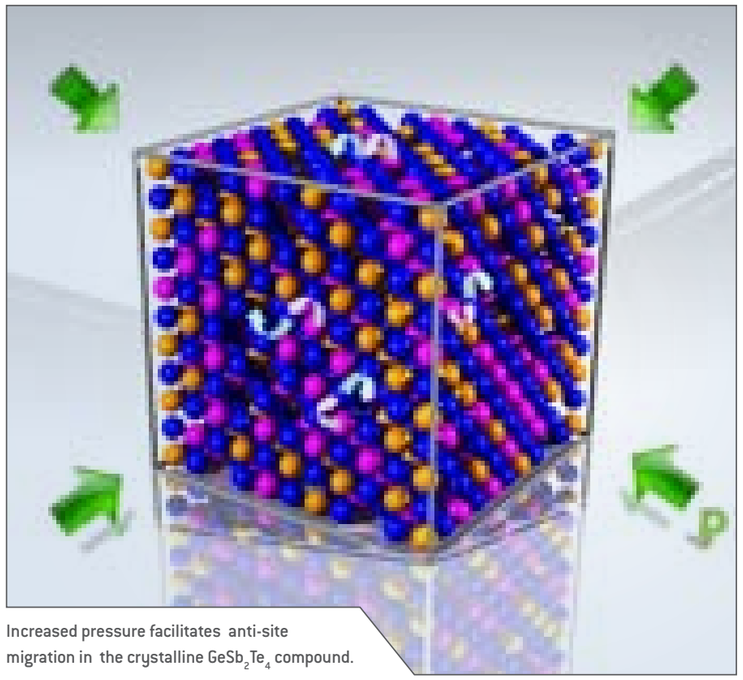
References [1] to [12] please see page 54

> Effects of pressure on crystalline and amorphous $GeSb_2Te_4$

We have investigated the effect of pressure on the structural and electronic properties of crystalline $GeSb_2Te_4$ [9].

Our large-scale ab initio molecular dynamics simulations demonstrate that pressure can lower the energy barrier for the anti-site migration in this material. The accumulation of these anti-site atoms largely increases the compositional disorder, adding localized electronic states near the conduction band. The disorder-induced electron localization triggered by pressure may pave the way for the development of multi-state memory devices. Furthermore, the random distortion of the lattice induced by the compositional disorder provides a new mechanism that contributes to the amorphization of crystalline PCMs at high pressure.

In another work, we have demonstrated that the resistivity contrast between crystalline and amorphous GeSbTe is reduced and even reversed with increasing hydrostatic-like pressure, which eventually turns the semiconducting glass into a metallic one [10]. As revealed by ab initio molecular dynamics simulations, this anomalous resistivity reversal originates from the differences in the pressure-induced atomic rearrangement of these two phases.



Increased pressure facilitates anti-site migration in the crystalline $GeSb_2Te_4$ compound.

Our work reveals distinct behaviours of amorphous and crystalline phase-change materials under pressure, shedding light on the mechanisms of electronic transport in different phases, and thus may have important implications on the design of phase-change memory devices. These projects are done in collaboration with Prof. Wuttig and Dr. M. Xu.

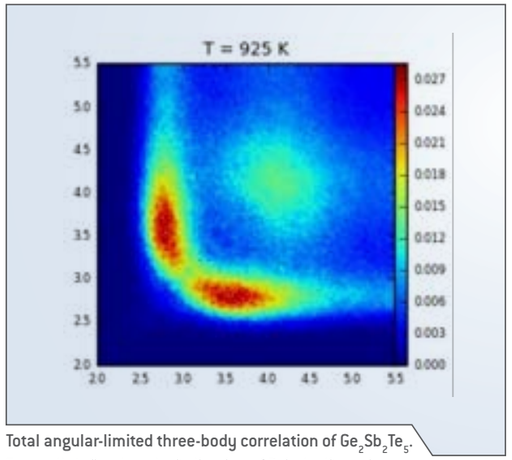
References [1] to [12] please see page54

> Structural and kinetic properties of liquid phase-change materials

We have investigated the structural and kinetic properties of liquid GeTe, $Ge_2Sb_2Te_5$ and Ag, In-doped Sb2Te by a combined experimental and computational approach [11].

Understanding the properties of this phase is important to clarify the amorphization and crystallization processes. We have found that the structural properties of the models obtained from ab initio and reverse Monte Carlo simulations agree well with neutron and x-ray diffraction experiments. The kinetic coefficients extracted from the molecular dynamics trajectories are also compatible with viscosity measurements. This project has been done in close collaboration with Dr. I. Kaban (IFF Dresden).

References [1] to [12] please see page 54



Total angular-limited three-body correlation of $Ge_2Sb_2Te_5$. Two well-defined peaks indicative of Peierls distortion are observed.

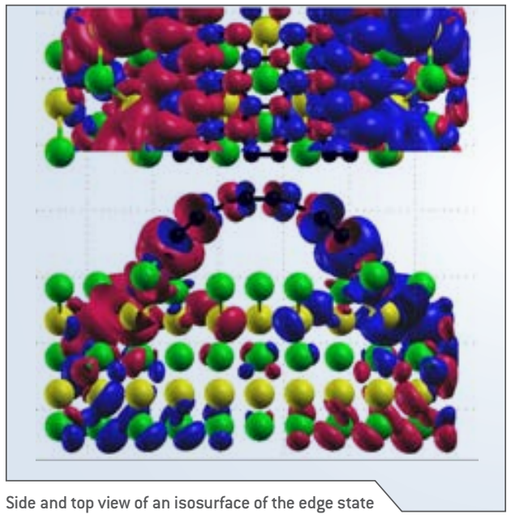
> Topological properties of crystalline phase-change materials

We have investigated zigzag graphene nanoribbons (GNRs) deposited on Sb_2Te_3, a 3-dimensional topological insulator, by density functional theory (DFT) [12]. The GNRs are expected to induce interesting effects on Sb_2Te_3. At the mean-field level, the magnetic edge states of zigzag GNRs exhibit ferromagnetic ordering along the edge and antiferromagnetic ordering across the nanoribbon. Hence, their effect on the surface states of a topological insulator could bear similarities with that of a domain wall, which is known to induce the formation of one-dimensional chiral states.

We have found that monohydrogenated GNRs interact weakly with Sb2Te3 and retain their edge magnetism when deposited on the TI. Furthermore, the GNR hardly affects the dispersion of the surface states, due to the large distance between the GNR and the substrate.

Interestingly, H-free GNRs on Sb2Te3 retain their magnetism as well, in spite of the strong chemical interaction with the substrate. Furthermore, the dispersion of the surface states is strongly affected by the presence of the GNR, due to the interplay between hybridization effects, warping effects and electron-electron interactions.

References [1] to [12] please see page 54



Side and top view of an isosurface of the edge state spin density of a H-free GNR on Sb2Te3. The system exhibits antiferromagnetic coupling between the two edges. The red (blue) surface indicates spin up (down) density.

> Properties of graphene nanoribbons deposited on topological insulators

We are studying the electronic and topological properties of interfacial phase-change materials (IPCMs) consisting of GeTe and Sb_2Te_3superlattices.

IPCMs are promising materials for faster and energetically less demanding non-volatile memory devices. It has been suggested that some of these superlattices may be topological insulators, whereas others may display three dimensional Dirac cones near the Fermi energy. Our results indicate that, in the energetically most stable structure, pressure can induce transitions between a standard insulating phase, a topological insulating state and a topological Dirac semimetal phase.

References [1] to [12] please see below

References (page 50-54)

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[12] *W. Zhang, F. Hajiheidari, Y. Li, and R. Mazzarello, Electronic and magnetic properties of H-terminated graphene nanoribbons deposited on the topological insulator Sb_2Te_3", submitted to Sci. Rep. One more paper about H-free nanoribbons is in preparation.*

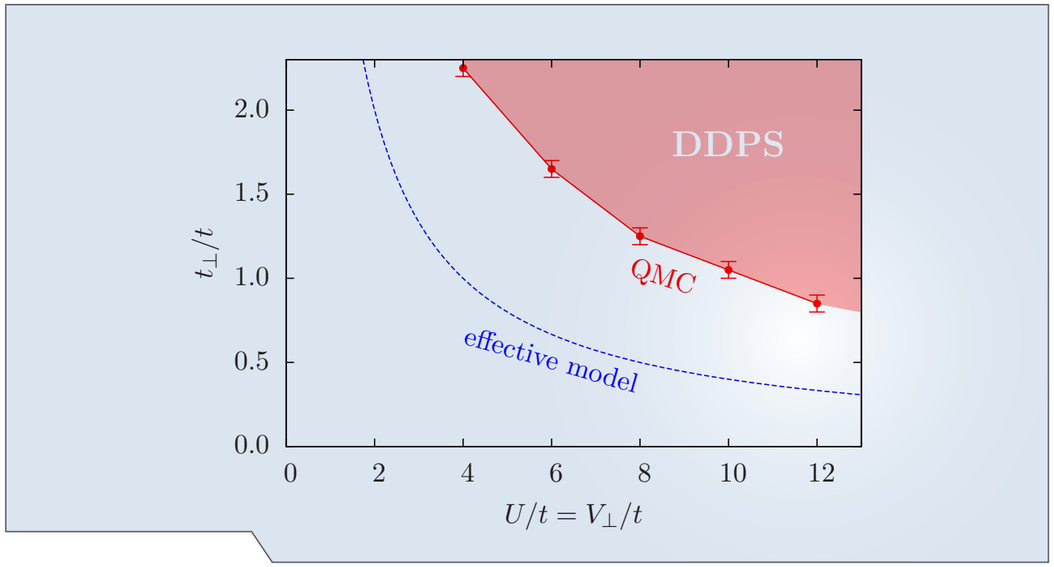
INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS, STRONGLY CORRELATED QUANTUM SYSTEMS / RWTH / Prof. Stefan Wessel, Ph.D.

> Numerical studies of Mott transitions and excitation spectra in strongly correlated quantum systems and
> Computational studies of competing interactions in strongly correlated electrons

In our project, we employed quantum Monte Carlo (QMC) methods to study the effects of competing interactions among strongly correlated electrons. Due to the notorious sign problem, only few studies thus far employed unbiased QMC simuations to analyze such systems.

We developed a local, bond-based decoupling scheme to access an extended region in parameter space to study non-local density-density interactions in extended Hubbard models on two-dimensional lattice structures. Our method can be readily integrated in codes that employ SU(2)-invariant decoupling schemes for local Hubbard interactions. In particular, we applied this approach to study the phase diagram of the square lattice bilayer with additional interlayer repulsion. For this model, we presented evidence for the presence of a direct dimer product state (DDPS) of a mixed S-Mott and D-Mott nature along the equal-coupling line of local Hubbard (U) and interlayer coupling, and in the region of strong interlayer hopping. The extend of the DDPS as obtained from the QMC simulations is shown in the figure, along with an estimate from a strong-coupling perturbative effective model.

We also applied our simulation scheme to the Hubbard model on the honeycomb lattice with next-nearest-neighbor interactions. In this model, previous mean-field studies suggested that an interaction-driven topological Mott-insulator phase can be realized. However, within the accessible parameter range, we do not observe evidence for this phase. Instead, we verified that the quantum phase transitions in the presence of the extended interaction belongs to the same universality class of the Gross-Neveu-Yukawa model as the purely local model, which has been intensively discussed recently.



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

> Simulation of Jet Engine and Axial Fan Noise

For the first project, the research is conducted within the European project Coupled Parallel Simulation of Gas Turbines (COPA-GT), in which a full turbine of a turbo-shaft engine is simulated. The major project goals are to analyze the flow for a complete non-generic nozzle geometry and to use hardly any modeling for the physical processes such that the results for the acoustic field are not contaminated by modeling errors and can be used to validate and/or calibrate simulation methods that describe turbulence noise sources.

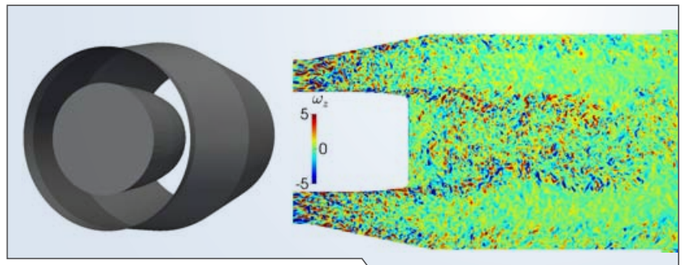


Figure 1: Nozzle geometry (left), instantaneous vorticity contours (right) of jet engine.

In this large scale computing project, the inside nozzle flow plus the jet flow are computed by a monotone implicit LES approach using a high mesh resolution of approx. 1.1 billion cells. The minimum number of processors for the flow simulation is 10,000. The statistical data requires approx. 120 TByte of disk space. The flow field is qualitatively illustrated in Fig. 1 by the instantaneous vorticity field in the rear part of the nozzle and the jet region. The mosaic- like structure of the vorticity distribution evidences the intricacy of the flow field and gives an idea of its multi-scale character.

In the second project, the prediction of the acoustic field of a low pressure axial fan using computational aeroacoustics (CAA) methods is tackled. The source distribution of the CAA analysis, however, requires highly resolved instantaneous flow field data. Since Reynolds averaged Navier-Stokes (RANS) computations strongly depend on the chosen turbulence model and are not always reliable due to, e.g., the strong streamline curvature dominating the flow structures inside the tip-gap region, the subsonic flow field is predicted by large-eddy simulation (LES). For this purpose, the unstructured flow solver ZFS (Zonal Flow Solver), which solves the Navier-Stokes equations for unsteady and compressible flows in the rotating frame of reference on Cartesian meshes, is used.

Simulations have been performed at a Reynolds number of Re=9.36×105 based on the outer casing diameter and the rotational velocity of the casing wall. The current mesh has approx. 1 billion cells, resolving only a 72° segment of the axial fan, i.e., one out of five blades, to reduce the high computational costs. This high resolution is necessary to accurately resolve the vortical flow structures and their development in the tip-gap region. The minimum number of cores required for a simulation using 1 billion cells is approx. 10,000, however, up to 92,000 cores have already been used. To obtain accurate statistical data from the turbulent flow field like, e.g., the Reynolds stress tensor and two-point correlations of the velocity components, a large number of samples of the instantaneous field is required. The statistical data alone requires about 80 TB of disk space.

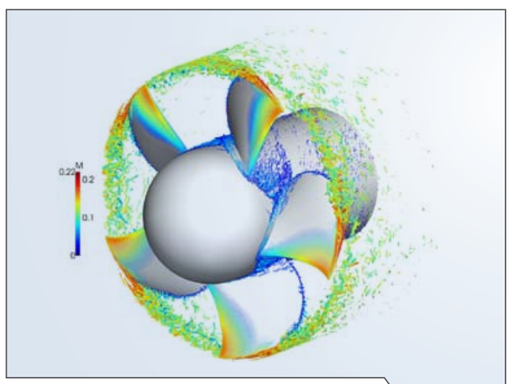


Figure 2: Instantaneous contours of the Q-criterion, coloured by the relative Mach number, show the vortical structures of the flow field of the axial fan.

> Noise Reduction through Chevron Nozzles via Multi-Point Optimization / Dipl.-Ing. Manuel Kosel

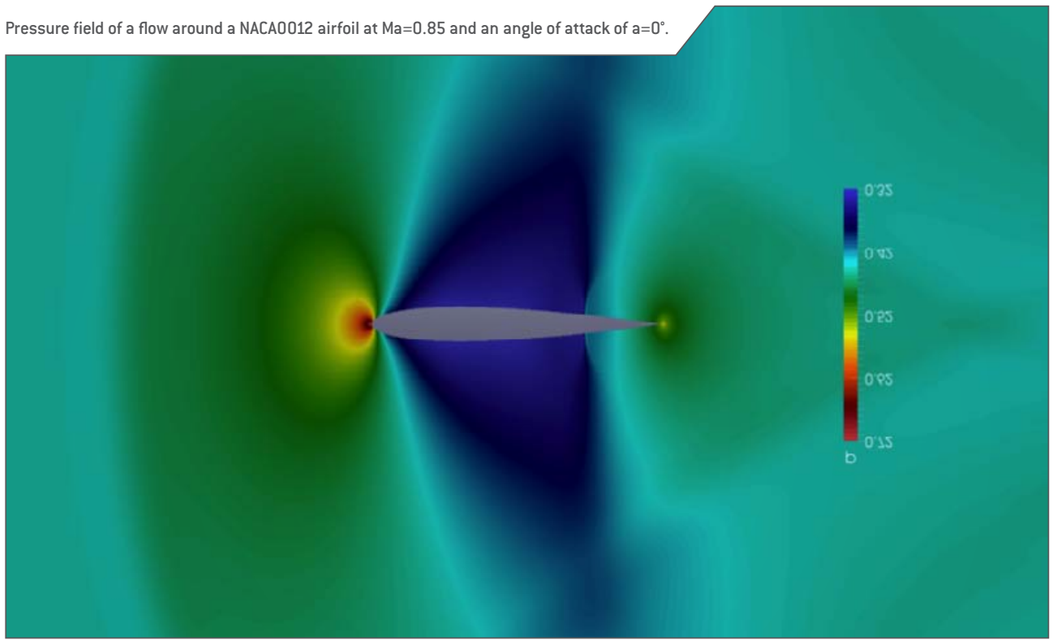
This project aims at reducing the noise of aircrafts during takeoff and landing by finding optimal designs for chevrons, i.e., for crown-like constructions mounted to the engine nozzle.

With this approach the demands of the "Flightpath 2050" initiative, which has been established by the Advisory Council for Aeronautical Research in Europe (ACARE) in 2011, is addressed. Therefore, the noise generation that is induced by the geometry and the jet flow is to be reduced to a minimum by adaptively reshaping the chevron geometry. The optimization process uses local, gradient-based algorithms to find an optimal shape and is constrained by the objective functions that are defined by the engine thrust and the produced noise.

The optimization process evaluates these objective functions based on flow solutions obtained by the Zonal Flow Solver (ZFS) of the Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH. The ongoing developments focus is on the direct integration of an optimizer into ZFS to allow for an online optimization during the simulation. To validate the algorithm, a benchmarking case provided by the Aerodynamics Design Optimization Discussion Group (ADODG) of the American Institute of Aeronautics and Astronautics (AIAA) is used. That is, the shape of a NACA 0012 airfoil profile at a Mach number Ma=0.85 and an angle of attack of a=0° in non-viscous Euler flow is subject to an optimization using a SLSQP optimizer.

The pressure field of a flow around the original shape is visualized in the picture. Preliminary results yield a reduction of the drag by about 8.6%.

Pressure field of a flow around a NACA0012 airfoil at Ma=0.85 and an angle of attack of a=0°.



INSTITUTE OF BIO- AND GEOSCIENCES, AGROSPHERE (IBG-3) / FZ JÜLICH / Prof. Harry Vereecken

> Quasi-operational, real-time monitoring/forecasting of terrestrial systems

Prof. Stefan Kollet, FZ Jülich / IBG-3; Fabian Gasper, FZ Jülich / IBG-3; Klaus Görgen, FZ Jülich / JSC;
cooperation with: Jessica Keune; Prabhakar Shresta; Mauro Sulis (all MIUB, HPSC TerrSys);
Volker Küll, MIUB; Florian Pappenberger, ECMWF

The objective of this project in the framework of the Centre for High-Performance Scientific Computing in Terrestrial Systems (HPSC TerrSys) is to (i) produce and provide experimental, high-resolution daily monitoring simulations over North Rhine-Westphalia and Europe with the fully coupled Terrestrial Systems Modelling Platform (TerrSysMP) system in forecast-mode and thereby (ii) gain further insight in TerrSysMP physics features, feeding back to the technical model development of TerrSysMP, (iii) obtain information on the fully coupled terrestrial water budgets (from subsurface into the atmosphere), plant available water, discharge and mass fluxes between river catchments, etc. Model results are made publicly available daily as videos via the YouTube Channel of HPSC TerrSys [1].

The fully coupled TerrSysMP [2] (ParFlow+CLM+COSMO) is initialized daily in the early morning on the JSC/JURECA HPC system for a lead time of a day for the SFB/TR32 NRW domain at 1km/0.5km spatial resolution and about 3 days at 12km resolution for the EURO-CORDEX pan-European model domain. The deterministic simulations encompass different fluxes and states of the terrestrial hydrologic and energy cycles from aquifers across the land surface into the atmosphere. Despite the fully automatic modelling and processing chain (pre-processing, simulations, post-processing, diagnostics, analyses and visualisations, as well as movie generation and YouTube upload) are fully automatic, the system is not considered and meant in any way as an "operational forecast" but rather a "monitoring run". Aside from ongoing optimisations, upcoming developments focus on uncertainty assessments in ensemble simulations (different initial conditions and boundary forcing, configurations, parametrisations) and assimilation of near-real time observations via a parallel data assimilation scheme.

References [1] to [3] please see page 59

> TerrSysMP CORDEX

Jessica Keune, Bonn University/Meteorological Institute, HPSC TerrSys

The objective of this study is to present a high-resolution fully coupled aquifer-to-atmosphere modeling system over the European CORDEX domain. The integrated Terrestrial Systems Modeling Platform, TerrSysMP is used. The system is set up with a spatial resolution of 0.11° (12.5km) and closes the terrestrial water and energy cycles from aquifers into the atmosphere.

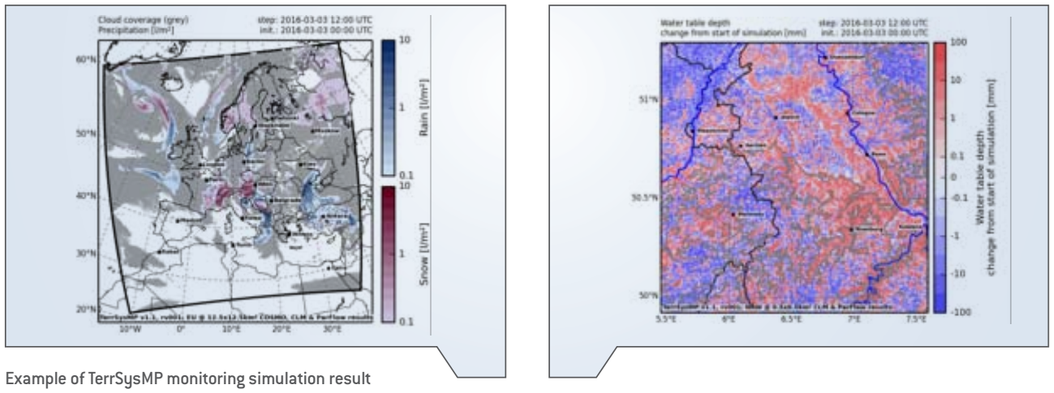
This system can be used to address the impact of soil moisture and groundwater dynamics at continental scales on climate. Such a physics-based system enables simulations of groundwater storage and enhanced representations of the terrestrial energy and hydrologic cycles over long time periods and in the context of climate change. On shorter timescales, the prediction of groundwater-related extremes, such as floods and droughts, are expected to improve. Simulations are performed over events, such as the 2013 flood in Central Europe and the 2003 European heat wave, and over extended time periods on the order of several years in an in part as an ensemble using spectral nudging. State and flux variables of the terrestrial hydrologic and energy cycle are analyzed and compared to both In Situ (e.g. stream and water level gauge networks, FLUXNET) and remotely sensed observations (e.g. GRACE, ESA ICC ECV soil moisture and SMOS).

> 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

Sebastian Knist, Bonn University/Meteorological Institute, FZ Jülich/JSC, HPSC TerrSys

The main focus of this project is on land-atmosphere (L-A) interactions in the context of regional climate change over Europe. L-A coupling is itself a complex feedback process and an integral component of processes, which e.g., influence the atmospheric boundary layer evolution, the development of extremes such as heavy precipitation, droughts or heat waves. Objectives are: (i) The production of transient regional climate simulations (all on JSC/JURECA) with the WRF RCM at two spatial resolutions (48km and 12km) for a pan-European model domain, downscaling the ERA-Interim reanalysis for validation purposes and the CMIP5 GCM control and projection simulations; this is the basis for further joint analysis within EURO-CORDEX and public global dissemination via the Earth System Grid Federation (ESGF) data nodes. The L-A coupling (strength) in EURO-CORDEX RCM ensemble members is evaluated against observations and RCMs are compared. An important aspect, also related to soil moisture temperature and precipitation feedback, is how this L-A coupling changes in a future climate. (ii) The production of 3km convection permitting WRF simulations for a central European domain for time slices of validation and projection time spans is another objective; the added value of increased resolution manifests itself e.g., in a more realistic reproduction of precipitation intensities and the diurnal cycle of convective precipitation [3]; in line with a change in surface heterogeneity in the high resolution model runs is also a modification of coupling processes. (iii) The impact of surface properties is investigated in specific sensitivity studies.

References [1] to [3] please see below



Example of TerrSysMP monitoring simulation result (2016-03-03 12:00 UTC) as staged on the HPSC TerrSys YouTube Channel [1] for public dissemination (Project 1). Left: European model domain, 12km resolution, precipitation (boundary forcing data provided by ECMWF); right: NRW model domain, 1km/0.5km resolution, water table depth change (boundary forcing data provided by DWD). Both simulations are initialized at 2016-03-03 00:00 UTC.

[1] https://www.youtube.com/channel/UCGio3ckQwasR5a_kJo1Gd0w

[2] Shrestha, P., M. Sulis, M. Masbou, S. Kollet, and C. Simmer (2014), A scale-consistent Terrestrial Systems Modeling Platform based on COSMO, CLM and ParFlow, Mon. Weather Rev., 142(9), 3466–3483, doi:10.1175/MWR-D-14-00029.1.

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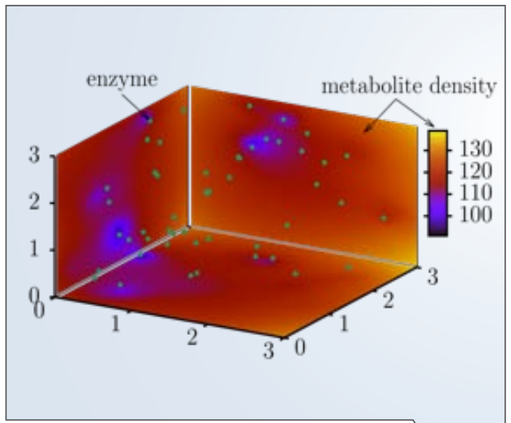
INSTITUTE OF BIO- AND GEOSCIENCES, BIOTECHNOLOGY (IBG-1) / FZ JÜLICH / Prof. Wolfgang Wiechert

> Multiscale simulation of inhomogeneities in cellular biochemistry and
> Scaling BD_BOX for simulation of intracellular environment

We have developed a multiscale approach for spatially resolved reaction-diffusion systems (RDS). This approach couples Brownian Dynamics simulations for macromolecules and the Finite Element Method (FEM) for the evolution of metabolite densities, and can be used to study the influence of structural heterogeneity (e.g. in the cytosol of a cell) on the performance of biochemical reactions. We have successfully applied this to understand the effects of stochasticity, heterogeneity and discreteness on enzyme catalyzed reactions. In particular we have demonstrated that discreetness plays a crucial role in RD systems for small number of enzymes, leading to a different quasi steady-state. Additionally, the response time of a system with a high number of less efficient enzymes is higher, as compared to a system with a lower amount of very efficient enzymes.

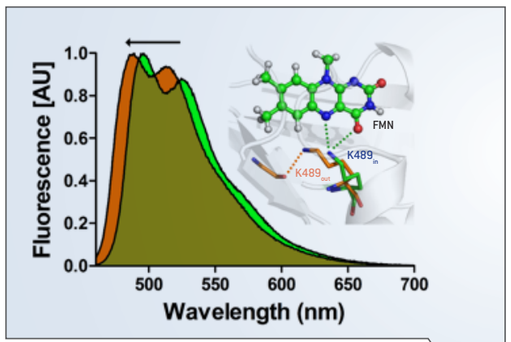


The snapshot from RDS simulations. The metabolites are represented as a continuous field, and enzymes, transforming these metabolites, as point-like sources/sinks (green circles).

INSTITUTE OF BIOTECHNOLOGY / RWTH / Prof. Ulrich Schwaneberg

> Toward an understanding of the spectral properties of flavin mononucleotide-based fluorescent proteins (FbFPs) by means of large scale hybrid quantum mechanics/ molecular mechanics (QM/MM) simulations)

Light, oxygen, voltage (LOV)-based fluorescent proteins (FPs) represent a promising alternative to fluorescent reporters of the green fluorescent protein family. For certain applications like multi-color imaging or the design of FRET-based biosensors, the generation of spectrally shifted LOV-based FPs would be required. In a recent theoretical study (Khrenova et al. J. Phys. Chem. B, 2015, 119 (16), 5176–5183) the photophysical properties of a variant of the LOV-based fluorescent protein iLOV were predicted using quantum mechanics/molecular mechanics (QM/MM) approaches.



Normalized fluorescence emission spectra of purified iLOV and iLOV-Q489K. Flipping the conformation of K489 from $K489_{in}$ to $K489_{out}$ conformations accounts for the change in direction of the predicted spectral shift from red to blue in the iLOV-Q489K variant. $K489_{out}$ conformation is the most populated conformation.

The variant contained a lysine residue at the position of a highly conserved glutamine residue (Q489K), which directly interacts with the O4 and N5 atom of the flavin mononucleotide (FMN) chromophore. Based on QM/MM calculations iLOV-Q489K was suggested to possess substantially red-shifted absorption and fluorescenceemission maxima with respect to parental iLOV.

Here, we describe the experimental characterization of this variant, which, surprisingly contrary to the theoretical prediction, shows blue-shifted absorption and fluorescenceemission maxima. Using molecular dynamics (MD) simulations and QM/MM calculations the molecular basis for the contradictory theoretical and experimental results is presented.

Essentially, our computational analysis suggests that in the Q489K variant two possible side-chain conformers exist (Shown in the figure): i) a least populated conformer $K489_{in}$ forming a hydrogen bond with the O4 atom of FMN chromophore and ii) a most populated conformer $K489_{out}$ with the side-chain amino group flipped away from the FMN chromophore forming a new hydrogen bond with the backbone oxygen of G487. QM/MM calculated spectra of the K489out conformer are blue-shifted compared to the calculated spectra of parental iLOV, which is in accordance with experimental data.

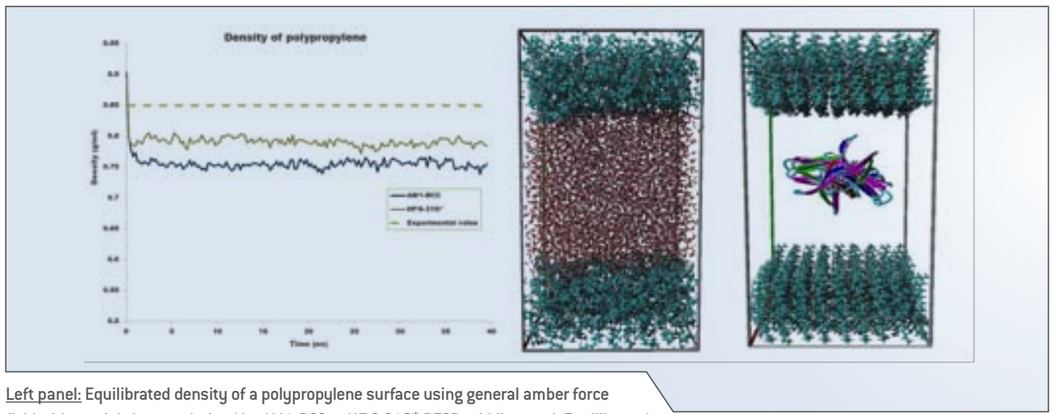
This suggests that the change in the conformation of K489 from $K489_{in}$ to $K489_{out}$ accounts for the change in the direction of the spectral shift from red to blue, thus reconciling theory and experiment.

> A systematic study of interactions of surface binding peptides (SBPs) and polymer surfaces

Anchoring of peptides is a new method for functionalization of polymer fibers. The immobilization of anchor peptide on polymer surfaces have various applications in biomedical devices or functionalizing textiles polymers.

Gaining deep knowledge about interaction between APs and polymers surfaces by using experimental techniques such as AFM, TEM and REM is extremely costly and needs enormous amount of tedious and repetitive experiments which in practice makes the investigation impossible or ineffective. Therefore, generation of a predictive model can be helpful to reduce experimental efforts. In addition considering the spatial and time scale of anchoring process and system size, molecular dynamics simulation is a method of choice.

This project uses molecular dynamics methods to understand the interactions between different anchor peptides (APs) and three chemically diverse polymer surfaces. This may ulti-



Left panel: Equilibrated density of a polypropylene surface using general amber force field with partial charges derived by AM1-BCC or HF 6-31G* RESP. middle panel: Equilibrated simulation box filled with water and polypropylene. Right panel: Simulation setup for a beta sheet containing surface binding peptide.

mately allow tailoring strength and specificity of APs binding on polymer surfaces. The final objective of our project is to estimate the binding affinity of different APs on three polymer surfaces and get atomistic information on adsorption, peptide folding and insertion mechanisms.

The binding process can be divided into a few kinetic regimes (diffusive and non-diffusive phase). In this project we focus on the non-diffusive phases but we may study diffusion regime as well. First we performed molecular dynamics simulation to identify binding conformations of AP to different polymer surfaces. like polypropylen (see figure). Intermediate results show that GAFF with HF-631G* derived RESP charges can reproduce the experimental polymer density best. Subsequently, we will estimate the relative binding strength of the interaction between APs and the polymer surfaces. Analysis of simulations will help us to identify the role of each amino acid in binding process of APs to polymer surfaces. Finally, with fundamental structural and binding mechanism understood, the knowledge gained can then be used to rationally design APs with tailored anchoring properties (e.g. strength, specificity) on polymer surfaces. This computational study in parallel with experimental studies in the group of Prof. Schwaneberg helps us to develop a predictive model for interactions/binding of APs on the polymer surfaces.

INSTITUTE OF COMPLEX SYSTEMS, STRUCTURAL BIOCHEMISTRY (ICS-6) / FZ JÜLICH /
Prof. Dieter Willbold, Jun.-Prof. Dr. Birgit Strodel

> Aggregation of Functional Amyloids

The aggregation of proteins into amyloid oligomers and fibrils is associated with diseases as well as functional roles. It is still unclear what differences exist between aberrant and functional amyloids. In this project, we performed molecular dynamics (MD) simulations to study the aggregation of a fragment of the amyloid-β peptide (Aβ), associated with Alzheimer's disease, and two functional amyloid-forming tachykinin peptides: kassinin and neuromedin K. Our simulations revealed that the charge of the C-terminus is essential to controlling the aggregation process. To the best of our knowledge, this is the first study that revealed atomistic insight into the determinants of toxic and non-toxic amyloid aggregation. During the study of monomeric Aβ we became aware that different force fields produce different conformational ensembles for this intrinsically disordered peptide. To this end, we benchmarked five modern force fields (OPLS, AMBER99SB, AMBER99SB*ILDN, AMBER99SBILDN-NMR and CHARMM22*) in their ability to model Aβ. We observed that all force fields except AMBER99SBILDN-NMR successfully reproduce experimental observables, with CHARMM22* being slightly better than other force fields. This is an important finding as it will guide the selectin of the proper force field in our future simulations of amyloid aggregation.

> Ligand binding studies for amyloid peptides

The extracellular deposition of Aβ fibrils is considered as a hallmark of Alzheimer's disease, and it has been shown that the presence of substoichiometric levels of Cu^{2+} ions doubles the rate of production of amyloid fibers and promotes cell death. Therefore, it is of upmost importance to understand the effect of Cu^{2+} binding on Aβ at the molecular level. To this end, we performed MD simulations in order to elucidate how Cu^{2+} modulates the dimerization of Aβ. A major finding from this study is that Cu^{2+} promotes β-sheet formation in the Aβ dimer and reduces the flexibility of the peptides. These conformational changes may promote further amyloid aggregation, which will be tested in our future simulations.

INSTITUTE OF ENERGY AND CLIMATE RESEARCH, ELECTROCHEMICAL PROCESS ENGINEERING (IEK-3) / FZ JÜLICH / Prof. Detlef Stolten, 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.

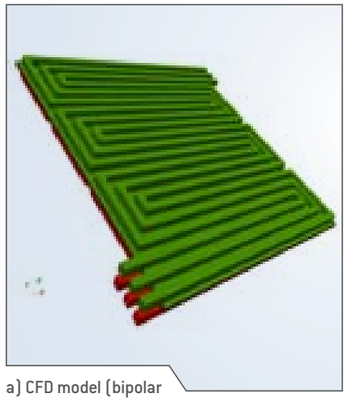
An existing SOFC model available at **http://openfuelcell.sourceforge.net/** was taken as a basis to develop a three-dimensional computational model to allow for calculations of conservation of mass, momentum, and energy transfer in both the liquid (phosphoric acid) and gas regions of a HT-PEFC.

Electrochemical reactions were taken into account by using a Tafel equation. The geometry of the fuel and air channels of the fuel cell used in this work is illustrated in figure 1 and corresponds to an in house testing cell. The active area of the cell is 16 cm2. Hydration and dehydration of the phosphoric acid as a function of local operating conditions lead to a change of the phosphoric acid concentration inside the membrane electrode assembly between gas inlet and gas outlet. Transport properties inside the phosphoric acid loaded polybenzimidazole membrane in combination with product water emerging on the cathode side results in different concentrations on anode and cathode side.

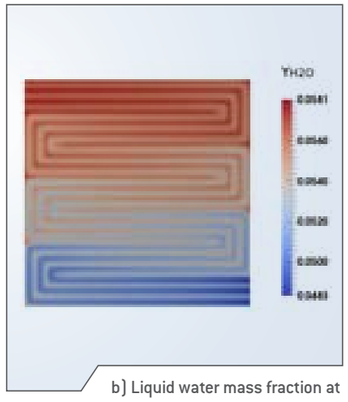
The picture shows the simulated liquid water mass fraction on the cathode and the anode sides of the membrane.

Initial comparisons of the results of the calculations and those from experimental data, in terms of (i) polarization curve and (ii) water collection at both anode and cathode outlets suggest the model is capable of being used predictively in the future [1].

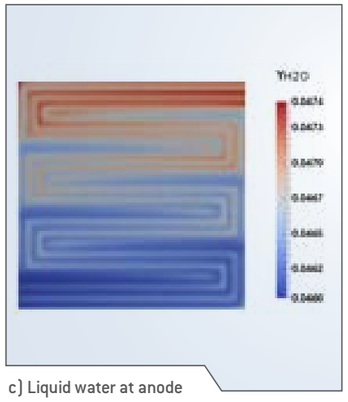
[1] Q. Cao, S. B. Beale, U. Reimer, D. Froning, W. Lehnert. The importance of diffusion mechanisms in high temperature polymer electrolyte fuel cells, ECS Transactions 69 (17) 1089-1103 (2015).



a) CFD model (bipolar plates not shown)



b) Liquid water mass fraction at cathode side of the membrane



c) Liquid water at anode side. (a) is taken from [1]

INSTITUTE OF ENERGY AND CLIMATE RESEARCH, NUCLEAR WASTE MANAGEMENT AND REACTOR SAFETY (IEK-6) / FZ JÜLICH / Prof. Dirk Bosbach

> Ab initio investigation of the new, actinide-bearing materials for safe management of high level nuclear waste,
> Simulation of radionuclides-bearing molecular complexes and solids,
> Improving the scientific basis of the safety case for deep geological disposal of high-level nuclear wastes: Understanding coupled reactive transport in fractured crystalline rocks at sub-millimetre scale and
> Computer simulation of the excess enthalpy in solid solutions: Application to nuclear waste corrosion studies

Dr. Piotr Kowalski, Dr. Guido Deissmann, Dr. Yan Li, Dr. Victor Vinograd, Prof. Dirk Bosbach

Understanding the behavior and safe management of radionuclide-bearing materials such as nuclear fuel and waste, building blocks of reactors and nuclear waste storage containers, and waste repositories under different technological and environmental conditions is a challenge for nuclear engineering. Spent fuel rods contain fission products, including long lived radionuclides, which can remain radioactive for thousands of years.

Because of that, these materials require deep geological disposal in chemically durable forms. Due to complexities in chemistry of actinide compounds, the thermodynamic and physical properties of many An-bearing materials are poorly understood. This limits our ability in finding the most suitable matrices for safe storage of nuclear waste. In our institute we synthesize different actinide-containing materials, such as actinide-bearing borates, phosphates, zirconates, barites and silicates, and perform systematic analysis of their structural, chemical, physical and thermodynamic properties.

The challenge is to understand changes in structural and thermodynamic properties of these materials due to incorporation of different cations, the corrosion behavior of waste forms in a deep geological repository, the migration of radionuclides in the repository near and far field and the thermodynamic properties of secondary minerals that form due to reactions between a corroded waste form, ground water and host rocks. This research benefits from HPC-aided simulations, which permit a unique atomic-scale insight into these processes, integration of hydrogeology and geochemistry to predict the long-term behavior of radionuclides in the repository environments, and provide important data which are difficult to measure due to radiotoxicity of the investigated materials. The aim of currently ongoing projects is to characterize the structural and thermodynamic properties of monazite- and pyrochlore- type ceramics that are considered as candidates for nuclear waste forms, to gain a more detailed insight into the coupled processes that impact the migration of safety relevant radionuclides, taking into account process flow and heterogeneities at the pore scale, and to understand the thermodynamics of mixing in the ternary $(Ba,Sr,Ra)SO_4$ solid solution, which is a secondary mineral capable to efficiently immobilize radium.

We succeeded in setting up an accurate and feasible ab initio computational methodology which gives results comparable to the experiments. This allowed us to explain the variation of heat capacities along lanthanide- and actinide-monazite series, derive the elastic moduli and the excess thermodynamic parameters of monazite-type $(La_{1-x}(Ln,An)_xPO_4)$ and barite-type solid solutions $((Ba,Sr,Ra)SO_4)$, and revise the defects formation energy diagrams for pyrochlore-type ceramics. The Reactive Transport Modelling have delivered crucial information on the redox buffering in physically and chemically heterogeneous rock systems.

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

> 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.

> 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.

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

The project “Steel ab initio” is concerned with first-principles calculations of iron-based materials. The focus in this period will be K-carbides in high-manganese steels.

> Quantum chemistry and structural exploration of crystalline molecular networks

The project “Exploration of Crystalline Molecular Networks” 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.

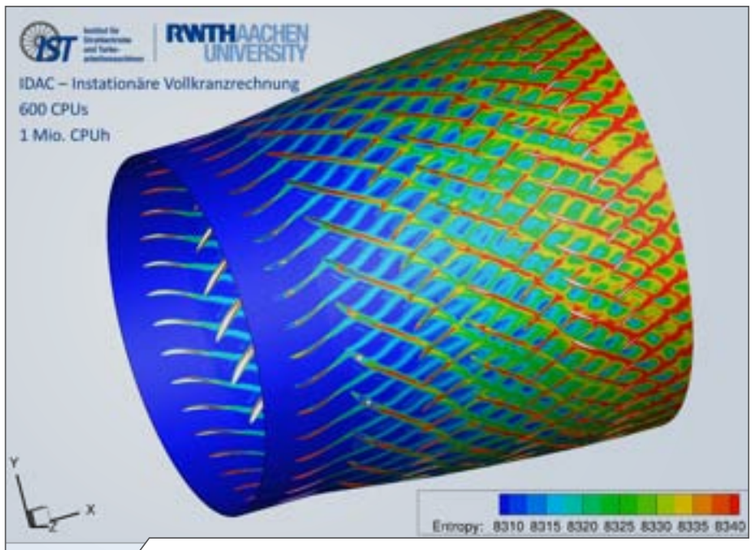
INSTITUTE OF JET PROPULSION AND TURBOMACHINERY (IST) / RWTH / Prof. Peter Jeschke

> Numerical investigation of circumferential flow distortion at the exit of multistage compressors

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.

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 the figure 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%.



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

> Analysis of Aerodynamic Noise Generation and Propagation in a Centrifugal Compressor

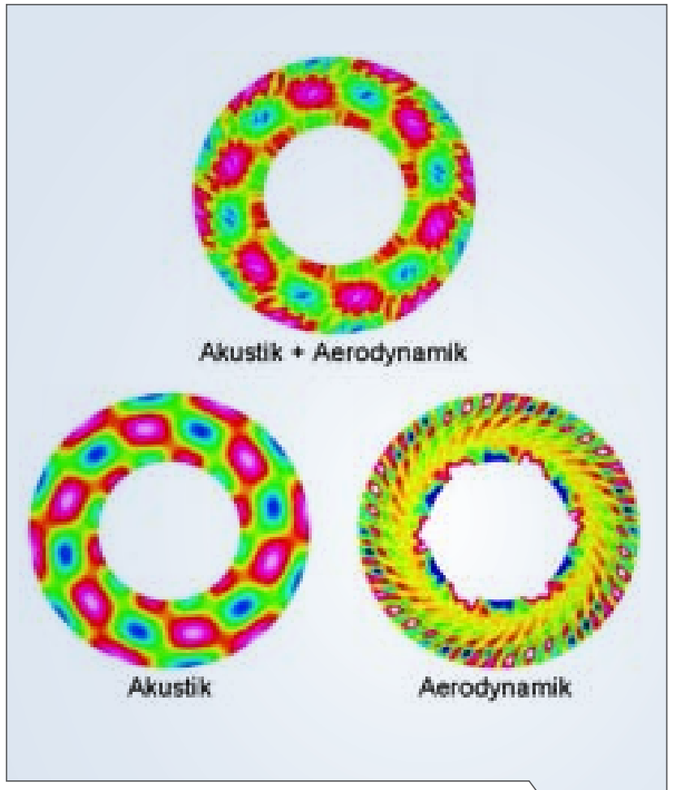
In this project aerodynamic noise generation mechanisms in a centrifugal compressor and the propagation of sound through the volute into the pressure pipe are investigated. The sound will consist of broadband components, where the sound pressure level is distributed over a band of frequencies, and tonal components with distinctive frequencies.

The acoustic spectrum in the pressure pipe is to be analysed and a modal analysis to be conducted in order to determine the dominant frequencies and modes as well as the existent sound pres-sure level. In the first sub-project numerical investigations are carried out, consisting of CFD- and CAA-simulations.

While numerical simulations provide a broad field of data and different modes can easily be distinguished from each other, the data obtained from measurements needs to be interpreted. Therefore, different measurement techniques to estimate the radiat-ed sound power are derived in the second sub-project. The third sub-project focuses on the measurement concept at the centrifugal compressor test rig and includes first experiments.

Thus far, all numerical and experimental publications on aerodynamic sound generation mechanisms focused on the pressure inlet domain. The high pressures and temperatures at the compressor outlet make measurements highly difficult and expensive. Moreover, the high temporal and spatial resolution needed for numerical simulations make the access to a high performance cluster inevitable.

As a result of the ambitious aims of the ongoing project, significant improvements in noise prediction are expected. With this knowledge, noise emissions can be reduced in future compressor designs and therefore the outcome of this project will have a major influence on the improvement of working conditions in the industrial sector. Furthermore, the results will help to understand the phenomena of acoustic resonance and hence improve the durability of radial compressors and in consequence reduce maintenance costs. First numerical results are plotted in the figure.



Numerical results of acoustically and aerodynamically pressure waves

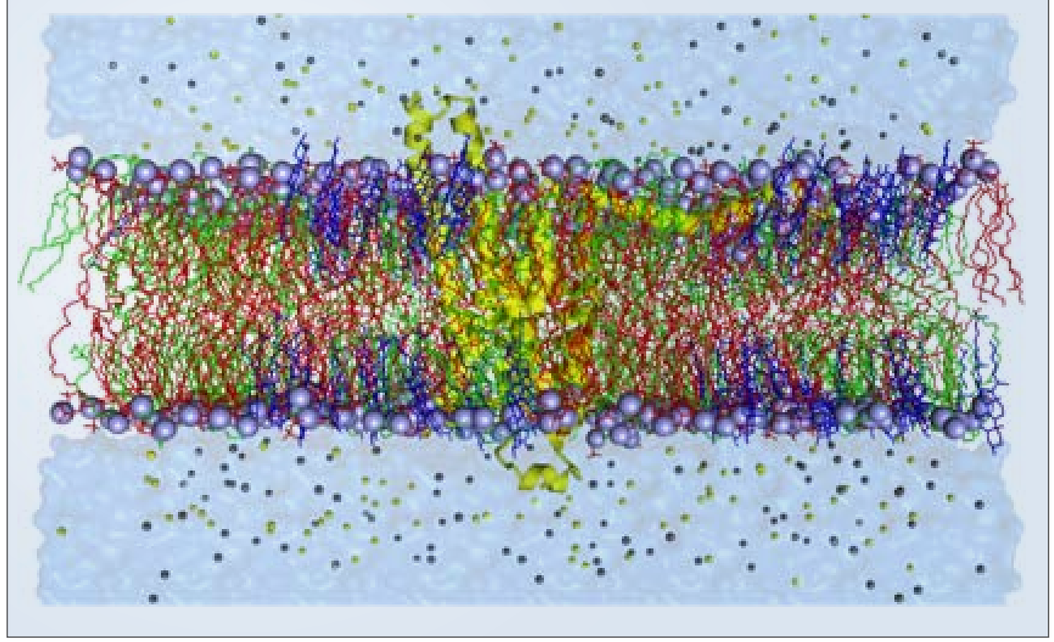
INSTITUTE OF NEUROSCIENCE AND MEDICINE, COMPUTATIONAL BIOMEDICINE (INM-9) / FZ JÜLICH / Prof. Paolo Carloni

> Molecular simulation and imaging of potent antagonists for stratal human adenosine receptor $hA_{2A}R$ (Extension)

Lipid composition may significantly affect membrane proteins function, yet its impact on the protein structural determinants is not well understood.

Here we present a comparative molecular dynamics (MD) study of the human adenosine receptor type 2A ($hA_{2A}R$) in complex with caffeine – a system of high neuro-pharmacological relevance – within different membrane types. These are POPC, mixed POPC/POPE and cholesterol-rich membranes. 0.8-μs MD simulations unambiguously show that the helical folding of the amphipathic helix 8 depends on membrane contents. Most importantly, the distinct cholesterol binding into the cleft between helix 1 and 2 stabilizes a specific caffeine-binding pose against others visited during the simulation. Hence, cholesterol presence (~33%-50% in synaptic membrane in central nervous system), often neglected in X-ray determination of membrane proteins, affects the population of the ligand binding poses.

We conclude that including a correct description of neuronal membranes may be very important for computer-aided design of ligands targeting $hA_{2A}R$ and possibly other GPCRs.

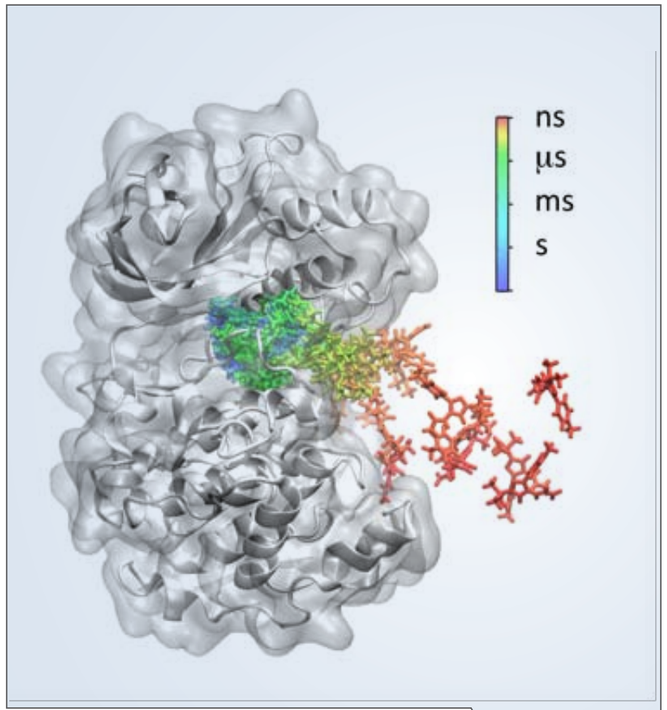


Human adenosine receptor $hA_{2A}R$ in native-like membrane environment formed by a mixed POPC/POPE and cholesterol-rich membranes.

> Predicting ligand-protein binding and unbinding kinetic data for neural signalling cascades (Extension)

Recent advances in metadynamics simulations developed in the Prof. Parrinello's group at ETHZ (Lugano, Switzerland) have led to a powerful approach that is able to provide quantitatively k_{on} and k_{off} of ligand binding to protein without the use of drastic simplifications or model calculations. In this project we apply this approach to predict kinetic constants of selected inhibitors of p38 MAP kinase.

These are derivatives of the so-called BIRB 796. This compound entered Phase II human clinical trials for the treatment of autoimmune disorders. The experimentally determined unbinding rate constants of these ligands differ by 6 orders of magnitude, allowing assessing the applicability of the method on a large spectrum of values. The calculations provide insights on the pathway of the drug from the binding site to the solvent in ligand design.



Unbinding of a type-II inhibitor (colored sticks) from p38 MAP kinase (white cartoon) obtained from a metadynamics trajectory. The inhibitor is colored according to the time required to unbind. The unbinding times are calculated from the metadynamics bias.

> Mechanism and Energetics of the Nucleotidyl-transfer Reaction Catalyzed by Human DNA Polymerase-η (Extension)

Human DNA Polymerase-η (Pol-η) – a member of Y-family polymerases – counteracts the damaging action of sunlight, life's energy source, which occasionally damages the DNA of living organisms via UV-induced covalent modifications of base pairs. One of these modifications, the cyclobutane pyrimidine dimer (CPDs), is particularly dreadful, as it impedes DNA replication leading cells to death. Recent X-ray structures have shown DNA Polymerase-η in complex with DNA double strand DNA (dsDNA) and the incoming nucleotidyl triphosphate (dNTP) coordinated by a bi-metal core. Given the key role of such enzyme within the genomic hindrance process, the detail understanding of the Pol-η enzymatic mechanism would therefore likely help the comprehension of genome expression and repair.

In the effort to investigate Pol-η enzymatic catalysis, and to clarify the role of a Arg61 for catalysis, we have used classical force field-based and first principles quantum mechanics/molecular mechanics (QM/MM) calculations for the modeling of the phosphoryl-transfer reaction in the ternary complex of Pol-η/dsDNA/dNTP.

We have considered different model systems to analyze the reaction catalyzed by Pol-η providing a consistent interpretation of available experiments and propose an elegant enzymatic strategy for bimetal-aided nucleotidyl-transfer catalysis in human DNA Pol-η.

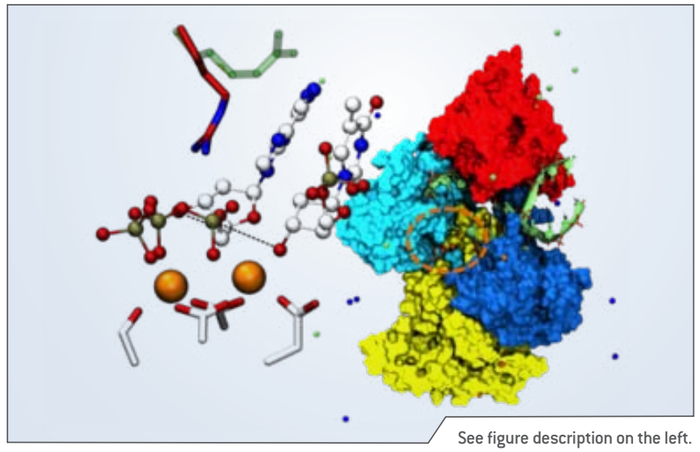
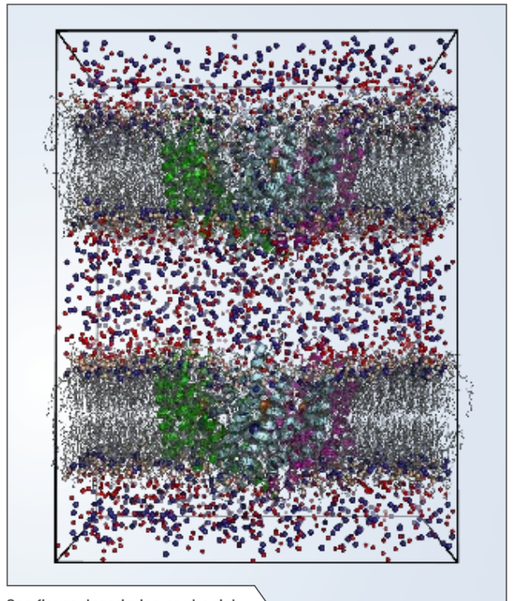


Figure: Global folded structure of the human Polymerase-η, in complex with the double strand DNA and the incoming dNTP. The orange dashed circle locates the active site of Pol-η. On the right, an atomistic-detailed view of the active site residues and metals of Pol-η in complex with substrates. In this figure, we report the canonical two-metal ion architecture. The orange spheres are the two magnesium ions. The surrounding amino acids are represented in stick while nucleic acid bases are in displayed CPK mode. The scissile phosphate is located in between the two Mg ions. The forming and breaking bonds are also indicated by yellow arrows.

See figure description on the left.

> Understanding the physics and chemistry of cation selectivity in biological ion channels - Phase II (Extension)



See figure description on the right.

Approaching the world of nanodevices from understanding how biology builds its devices is one route towards miniaturization. This project is in the framework of a European Research Area (ERA) initiative for the design biologically inspired nanopores using principles from ion channels of the cell membrane. In particular, we may identify the physicochemical parameters that govern cation selectivity to design artificial ion-selective nanopores.

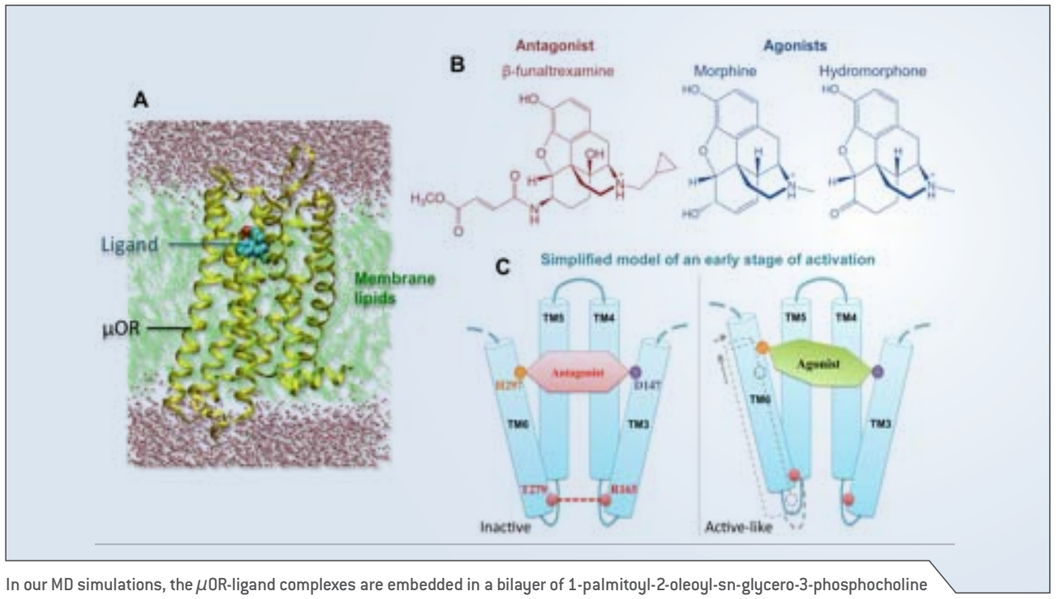
Biological ion channels have a narrow bottleneck region along the transmembrane pore that preferentially favors the permeation of a particular type of ions while hinders the permeation of the other types of ions. This region is known as selectivity filter and it is different for each type of ion channel. In this project we used atomistic molecular dynamics simulations to model the transport of Na+ and K+ across the bacterial sodium channel NavMs. Atomistic molecular dynamics simulations are performed to model the transport of Na+ and K+ across the bacterial sodium channel NavMs (Fig. 1). This also aimed to calculate the diffusion coefficients of the ions within the ion channel to be used as parameters in a reduced model describing ion conduction in confined volumes.

Figure: The simulation system used to efficiently calculate electrophysiological data in this project. The hydrophobic part of the lipid bilayer forming the membranes is colored in grey. The protein system where is located the selectivity filter is in the middle of the membranes. The use of a double membrane creates two separate compartments that allow the maintenance of a small charge imbalance (i.e. ion concentration, with negatively and positively charged ions represented by blue and red spheres, respectively) across the lipid bilayer.

> Biased and unbiased ligands binding the μ-opioid receptor (Extension)

Atomistic descriptions of the μ-opioid receptor (μOR) noncovalently binding with two of its prototypical morphinan agonists, morphine (MOP) and hydromorphone (HMP), are investigated using molecular dynamics (MD) simulations. Subtle differences between the binding modes and hydration properties of MOP and HMP emerge from the calculations.

Alchemical free energy perturbation calculations show qualitative agreement with in vitro experiments performed in this work: indeed, the binding free energy difference between MOP and HMP computed by forward and backward alchemical transformation is 1.2±1.1 and 0.8±0.8 kcal/mol, respectively, to be compared with 0.4±0.3 kcal/mol from experiment. Comparison with an MD simulation of μOR covalently bound with the antagonist β-funaltrexamine hints to agonist-induced conformational changes associated with an early event of the receptor's activation: a shift of the transmembrane helix 6 relative to the transmembrane helix 3 and a consequent loss of the key R165-T279 interhelical hydrogen bond. This finding is consistent with a previous proposal suggesting that the R165-T279 hydrogen bond between these two helices indicates an inactive receptor conformation.



In our MD simulations, the μOR-ligand complexes are embedded in a bilayer of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) lipid membrane in explicit aqueous solution (shown only partly for clarity) containing 0.15 M sodium chloride. (B) Molecular structures of the opioid ligands studied. (C) Our findings indicate that the agonists induce TM6 displacement relative to TM3 via their interactions with the anchoring residues H297 and D147, which disrupts the T279-R165 hydrogen bond at the intracellular side of μOR.

INSTITUTE OF PHYSICAL CHEMISTRY (IPC), THEORETICAL CHEMISTRY / RWTH / Prof. Arne Lüchow

> Investigation of chemical bonding with quantum Monte Carlo

Electron structure quantum Monte Carlo (QMC) is a technique for solving the electronic Schrödinger equation stochastically. Due to the strong coupling and the fermionic nature of the electrons the calculation of electron structure is notoriously difficult, and accurate methods scale steeply with the number of electrons. QMC is a method that scales like density functional theory (DFT) but allows for a higher accuracy because the electron interaction is treated explicitly rather than with an essentially unknown functional. While the cpu time is higher compared to DFT it is also easily and efficiently parallelizable due to the Monte Carlo nature. Benchmark calculations demonstrated excellent scaling up to more than 10,000 cores.

In two subprojects we investigate diatomic iron compounds, in particular the iron-sulfur system. The iron-sulfur bond is of great importance in many enzymes as well as in industrial processes. The importance is due to the many different spin states and orbital occupancies that arise from the partial occupancy of the iron atom d orbitals. The corresponding wave functions require several Slater determinants (strong correlation), and DFT results are often unreliable. With QMC we can now optimise the many-determinant wave function in the presence of a correlation factor describing the dynamical electron correlation. This is not possible in other wave function methods. We have shown that the correlated orbitals differ substantially from the standard orbitals. The optimisation of orbitals in the many-determinant wave function is demonstrated to be efficient due to update algorithms that allow to treat thousands of determinants with only a small factor in cpu time compared to single determinant calculations.

In another subproject we investigate the long range dynamical correlation effect, the London dispersion interaction (or van der Waals interaction). This interaction is responsible for the attraction in liquid noble gases but, more importantly, is often major contributor to the structure of large molecules such as proteins or polymers. With the DMC method, the London dispersion interaction is known to be accurately calculated due the stochastical projection. The actual wave functions employed in QMC describe the short-range electron correlation but not the long-range correlation. We investigate the long-range behaviour of several correlation functions for the model systems neon and argon dimer. New correlation that include the correct physics also for the long-range behaviour functions are suggested and tested.

INSTITUTE OF TECHNICAL AND MACROMOLECULAR CHEMISTRY (ITMC) / RWTH / Prof. Walter Leitner

> Investigations on the mechanisms of carbon dioxide hydrogenation to formate derivatives by iron and ruthenium catalysts

In this project the various mechanistic pathways for the hydrogenation of CO_2 to formate in aqueous basic medium was investigated by means of DFT computations with the aim to identify the active pathway(s) and to correlate the computed activation barrier with experimentally derived values.

Results: As expected the computations using contemporary dispersion corrected density functionals with large TZVPD basis sets in combination with continuum solvation models proved to be very time consuming which fully has justified the usage of the granted amount of computing time. The anticipated results finally could be obtained and are extremely encouraging. The mechanistic network could be fully explored unravelling the complex energy landscape of this seemingly simple reaction, which in fact turned out to be a quite complex one. Most satisfyingly it was possible to correlate computed and experimentally derived activation barriers quantitatively with good agreement. This is an important result as for future investigations DFT calculations can be used to evaluate catalyst perfomances in homogeneous transition metal catalysis even when “difficult” reactions are to be explored in “difficult” reaction media.

> Addition of metal coordinated N_2 to organic and inorganic substrates catalyzed by ruthenium complexes

In this project reactions between N_2 and and various organic and inorganic substrates are being explored with the aim of finding i) novel reaction products which are directly accessible through reactions of N_2 and the given substrate and ii) concomitant design of suitable catalyst structures to achieve such transformations.

Results: A huge variety of single reaction steps for various reactions were screened. The results have shown so far activation barriers which are way too high to envision any practical realization, which though disappointing in the first perception again show the importance of such computational based reaction screenings. According to these studies the transformation of N_2 will most likely not be possible by direct reaction, while, however, a bypass via (undesired) intermediates, which introduce an appropriate thermodynamic driving force should be feasible.

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

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

- Prof. Behr has been elected in 2015 by the International Association for Computational Mechanics to deliver a plenary lecture at the World Congress on Computational Mechanics in Seoul, Korea in July 2016 (one of three plenary speakers elected worldwide by IACM).

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

- Extension of SFB 917 Nanoswitches (Speaker M. Wuttig).
- Member of selection committee of Alexander von Humboldt foundation.

> CHAIR OF PHYSICAL CHEMISTRY I, PHYSICAL CHEMISTRY OF SOLIDS, RWTH
Prof. Manfred Martin

- Prof. M. Martin was invited as Adjunct Professor in the Department of Materials Science and Engineering of Seoul National University, Seoul, Korea.
- J. Köttgen received a Student Travel Award from the Materials Research Society (MRS) to present his results at the 20th International Conference on Solid State Ionics (SSI-20) in Keystone, Colorado, USA .
- J. Köttgen received a Scholarship of the German Chemical Society (GdCh) to present his results at the 114th General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung 2015) in Bochum, Germany.

> INSTITUTE FOR ADVANCED SIMULATION, THEORETICAL NEUROSCIENCE (IAS-6) AND INSTITUTE OF NEUROSCIENCE AND MEDICINE, COMPUTATIONAL AND SYSTEMS NEUROSCIENCE (INM-6), FZ JÜLICH
Prof. Markus Diesmann

- Moritz Helias, head of the Helmholtz young researcher group “VH-NG-1028: Theory of multi-scale neuronal networks”, was appointed junior professor at the RWTH, Faculty 1, Department of Physics, Aachen, Germany. https://www.physik.rwth-aachen.de/go/id/dwqp/gguid/0x330913105DB07B43A5C6F0F1313C7BA0/ikz/136930. In addition he was granted funding for a sixth year of his research group through the “Impuls- und Vernetzungsfond”.
- Markus Diesmann was appointed co-opted Professor at Department of Physics, Faculty I, RWTH, Aachen, Germany

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

- “Second Price” at “COMBURA 2015” (Oct 7th – 8th 2015) for poster presentation: “The effect of the perforation geometry of plate burners on flame stability – Experimental and numerical approach”

> INSTITUTE FOR THEORETICAL SOLID STATE PHYSICS, THEORETICAL NANOELECTRONICS, RWTH
Prof. Riccardo Mazzarello

- Visiting Professor, Xi’an Jiaotong University (China), 2015-2018.
- Editor for Scientific Reports within the field of Condensed Matter Physics (since June 2015).
- Also a member of the organizing committee of the symposium on phase-change materials that was held at the 2015 MRS Spring Meeting, San Francisco (USA), April 06-10, 2015.

> INSTITUTE OF BIOTECHNOLOGY, RWTH
Prof. Ulrich Schwaneberg

- Special appointed Professor at Graduate School of Engineering, Osaka University, Japan

> INSTITUTE OF COMPLEX SYSTEMS, STRUCTURAL BIOCHEMISTRY (ICS-6), FZ JÜLICH
Prof. Dieter Willbold

- Jürgen-Manchot fellowship awarded to Dusan Petrović.

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH, ELECTROCHEMICAL PROCESS ENGINEERING (IEK-3), FZ JÜLICH
Prof. Detlef Stolten, Prof. Werner Lehnert

- Andrei Kulikovsky, PhD, DSci received the Christian Friedrich Schönbein Medal of Honour at the 5th European PEFC & H2 Forum in Lucerne, Switzerland.
- Vitali Weißbecker and Andreas Schulze Lohoff won one of the main prizes of the NUK business plan competition with their planned spin-off for the production a novel carbon-based material for use in fuel cells. The prize from the association Neues Unternehmertum Rheinland e.V. (NUK) which supports new enterprises was awarded for “a very good business idea and an excellent idea outline with a high growth potential”.
- Michael Höh (IEK-3) won the Best Poster Award & Best Group Award at the International School on Energy Systems (ISES 2015).

> INSTITUTE OF ENERGY AND CLIMATE RESEARCH, NUCLEAR WASTE MANAGEMENT AND REACTOR SAFETY (IEK-6), FZ JÜLICH

Prof. Dirk Bosbach

- Cover page in Chemistry- A European Journal for studies of Xiao, B., Gesing, T. M., Robben, L., Blanca-Romero, A., Kowalski, P. M., Li, Y., Kegler, P., Klepov, V., Bosbach, D. and Alekseev, E. V. "Giant Volume Change and Topological Gaps in Temperature and Pressure Induced Phase Transitions: Experimental and Computational Study of ThMo2O8" (2015).

- Poster prize awarded to George Beridze by the European Mineralogical Union at Goldschmidt 2015 conference for a poster "Ab initio modeling of computationally challenging Earth (f-) materials" by Beridze, G., Li, Y. & Kowalski, P. (see EMU Poster Prizes at eurominunion.org). This poster was presented in "Crystal Chemistry of Earth and Planetary Materials" session (2015).

> 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

- Distinguished Professorship, RWTH, to Prof. Dr. R. Dronskowski

6. SELECTED CONFERENCE PARTICIPATIONS

> Chair of Experimental Physics, I. Institute of Physics (IA), RWTH

Prof. Matthias Wuttig

- **The Impact of Disorder on Transport in crystalline Phase Change Materials** (invited talk), April 08, 2015, MRS San Francisco, USA
- Discussion Workshop on **"Electron Transport and Correlation Effects in Oxides and Higher Chalcogenides"**, The Metal – Insulator Transition: Origins and Pathways (invited talk), May 21, 2015, Sorrento (Italy)
- **The role of structure and bonding for aging and crystallization in Phase Change Materials** (invited talk), July 20, 2015 , Cecam Workshop Mainz, Germany
- **Designing new Phase Change Materials via Disorder and Stoichiometry** (invited talk), September 07, 2015, European Phase Change Symposium in Amsterdam, Netherlands
- **Designing new Phase Change Materials via Disorder and Stoichiometry** (invited talk), October 10, 2015 , NVMTS Symposium in Beijing, China

> Chair of Experimental Physics, I. Physics Institute B, RWTH

Prof. Stefan Schael

- **The e— Spectrum and e+ Spectrum from AMS"**, AMS Days at CERN, April 15, 2015, Switzerland
- **"Precision Measurement of the (e++e—) Flux in Primary Cosmic Rays from 0.5 GeV to 1 TeV with the Alpha Magnetic Spectrometer on the International Space Station"**, 34th International Cosmic Ray Conference (ICRC), July 31, 2015, Den Haag, The Netherlands

> Chair of Physical Chemistry I, Physical Chemistry of Solids, RWTH

Prof. Manfred Martin

- 39th ICACC, Daytona Beach, Florida, USA, January 25-30, 2015
- 20th International Conference on Solid State Ionics Keystone, Colorado, USA, June 14-19, 2015
- PACRIM 11, Jeju, Korea, August 30-September 04, 2015
- MS&T 2015, Columbus, USA, October 04-08, 2015

> Institute for Advanced Simulation and Peter Grünberg Institute, Theoretical Nanoelectronics (PGI-2 / IAS-3), FZ Jülich

Prof. Eva Pavarini

Several invited talks at international conferences and schools among which

- **Building models for molecular nanomagnets**, Molecular Electron Spin Qubits, January 12-15, 2015, Manchester, UK
- **Many-body models for molecular nanomagnets**, 17th Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, January 15-17, 2015, Trieste, Italy
- **Understanding strongly-correlated transition-metal compounds**, 1st International Conference on Computational Design and Simulation of Materials, August 17-19, 2015, Shenyang, China
- **Origin of orbital-ordering and orbital-order melting transitions in strongly correlated systems**, Ψ-k-2015 Conference, September 06-10, 2015, San Sebastian-Donostia, Spain
- **Building many-body models for molecular nanomagnets**, International Conference on Single Molecules Electronics, September 15-17, 2015, Regensburg, Germany

> Institute for Advanced Simulation, Theoretical Neuroscience (IAS-6) and Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), FZ Jülich

Prof. Markus Diesmann

Talks by Markus Diesmann:

- **Towards multi-layered multi-area models of cortical networks**, BIRS Workshop, December 2015, Banff Centre, Calgary, Canada
- **Computational Neuroscience: interplay of structure and dynamics**, Conversations in Neuromedicine, BNI Seminar Series, November 2015, University of Chile, Santiago, Chile
- Role of biophysical modelling, Workshop **"Challenges in Linking Statistical and Mathematical Neuroscience"**, October 2015, SAMSI, Boston, USA
- **Brain-Scale simulations at cellular and synaptic resolution: necessity and feasibility**, CCNS Opening Workshop, August 2015, SAMSI Hamner Conference Center Auditorium, Durham, USA
- **Simulation of networks or My brain is finite**, 2nd HBP School – Future Computing, August 2015, Obergurgl, Austria
- **Simulation of brain-scale neuronal networks at cellular and synaptic resolution**, Workshop "Unraveling Mesoscopic Coding Principles Using Ultra-High Magnetic Field MRI and Neural Network Modelling", July 2015, Salerno, Italy
- **Deterministic neural networks as sources of uncorrelated noise for probabilistic computations**, HBP SP9, Fürberg workshop 2015, June 2015, Fürberg, Austria
- **Are we building the right thing? – Requirements from theory for simulation environments and neuromorphic computing**, 1st community workshop HBP network simulator, March 2015, Paris, France
- **Computational neuroscience emerging from the dark ages**, Workshop on "Media for Simulating the brain", January 2015, Lüneburg, Germany

> Institute for Combustion Engines (VKA), RWTH

Prof. Stefan Pischinger

- 2015 JSAE / SAE International Powertrains, Fuels & Lubricants September 01-04, 2015, Kyoto, Japan
- Combura, October 07-08, 2015, Soesterberg, The Netherlands

> Institute for Combustion Technology (ITV), RWTH

Prof. Heinz Pitsch

- Bode, M., Göbbert, J.H., Pitsch, H., **Novel multiphase simulations investigating cavitation by use of In Situ visualization and Euler/Lagrange coupling**, PRACEdays15, May 26-28, 2015, Dublin, Ireland.
- Boschung, J., Gauding, M., Hennig, F., Peters, N., Pitsch, H., **An alternative definition of order dependent dissipation scales**, European Turbulence Conference, August 25-28, 2015, Delft, The Netherlands.
- Hennig, F., Boschung, J., Peters, N., **Statistics of Streamline Segments in a Turbulent Channel Flow with a Wavy Wall,** European Turbulence Conference, August 25-28, 2015, Delft, The Netherlands.
- Gauding, M., Boschung, J., Hasse, C., Peters, N., **Dissipative Range Scaling of Higher Order Structure Functions for Velocity and Passive Scalars**, European Turbulence Conference, August 25-28, 2015, Delft, The Netherlands.
- Mayer, D., Beishuizen, N., Pitsch, H., **Detailed simulation and flamelet modeling of laminar premixed flames interacting with cold walls**, COMURA, October 07-08, 2015, Soesterberg, The Netherlands.

> Institute for Theoretical Solid State Physics, Strongly Correlated Quantum Systems, RWTH

Prof. Stefan Wessel, Ph.D.

- Recent Advances in Monte Carlo Methods, October 2015, Trento, Italy

> Institute for Theoretical Solid State Physics, Theoretical Nanoelectronics, RWTH

Prof. Riccardo Mazzarello

- **"Edge magnetism in graphene nanoribbons on metal and semiconductor substrates"**, invited talk given at the 8th International Workshop on Materials Behavior at the Micro- and Nano- Scale, June 01-03, 2015, Xi'an, China
- **"Edge states in graphene nanostructures on metal surfaces"**, 17th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, January 15-17, 2015, Trieste, Italy

> Institute of Aerodynamics and Chair of Fluid Mechanics (AIA), RWTH

Prof. Wolfgang Schröder

- Wolfgang Schröder et al., **"Cartesian Mesh Simulation of Tip-Leakage Flow of a Ducted Axial Fan"**, International Supercomputing Conference, July 2015, Frankfurt am Main, Germany
- FOR 1779 Symposium Active Drag Reduction, November 09-10, 2015
- Pauz, V., Meinke, M., Schröder, W.: **"Large-eddy simulations of jet flows of chevron nozzles"**, 17. STAB-Workshop, November 10-11, 2015

> Institute of Bio- and Geosciences Biotechnology (IBG-1), FZ Jülich

Prof. Wolfgang Wiechert

- Leweke, S.; von Lieres, E.: **Chromatography Analysis and Design Toolkit (CADET)**, ACHEMA, June 15-19, 2015, Frankfurt am Main, Germany

> Institute of Biotechnology, RWTH

Prof. Ulrich Schwaneberg

- **Tailor-made proteins for interactive materials**, Leibniz Institute of Polymer Research, Max Bergmann Center of Biomaterials, Dresden, Germany
- **Protein Engineering for Material Science**, Bayer CropScience, Lyon, France
- **Engineering for Industrial Biotechnology**, Tianjin Institute of Industrial Biotechnology, CAS, Tianjing, China
- **Directed Enzyme Evolution: Concepts and Lessons**, Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Japan
- **Steering Directed Enzyme Evolution: Concepts and Lessons**, Qingdao Institute of Bionergy and Bioprocess Technology (QIBEBT), Qingdao, China
- **Steering Directed Enzyme Evolution: Concepts and Lessons**, East China University of Science and Technology, Shanghai, China
- **Protein Engineering** Henkel Laundry & Home Care Technology, Advisory Board Meeting, Düsseldorf
- **Kolloquimsvortrag zu aktuellen Themen des Proteinengineerings**, Fraunhofer Institut Angewandte Polymerforschung, Potsdam, Germany
- **Protein engineering for biocatalysis**, TU Graz, Austria
- **Eine durchflusszytometriebasierte Durchmusterungstechnologieplattform für die Gelenkte Enzymevolution**, Deutsche Biotechnologietage 2015, Cologne, Germany
- **Protein engineering for biocatalysis**, 2nd International NanoBioTechnology Symposium, Köycegiz, Turkey
- **Engineering for Industrial Biotechnology applications**, Amano Enzyme Inc, Gifu, Japan

> Institute of Complex Systems, Structural Biochemistry (ICS-6), FZ Jülich

Prof. Dieter Willbold

- XXVII IUPAP Conference on Computational Physics, Guwahati, India (December 2015). Invited talk: **Thermodynamics and kinetics of amyloid aggregation from atomistic simulations** (Birgit Strodel)
- 249th ACS Meeting, Boston, USA (March 2015). Invited talk: **Revealing the interplay between amyloid-beta and membranes through molecular simulations** (Birgit Strodel)
- Conference on "Physical Biology of Proteins and Peptides: Theory, Experiment and Simulation" in Mexico City, Mexico (February 2015). Invited talk: **Thermodynamics and kinetics of amyloid aggregation from atomistic simulations** (Birgit Strodel)

> Institute of Energy and Climate Research, Electrochemical Process Engineering (IEK-3), FZ Jülich

Prof. Werner Lehnert

- Q. Cao, S. B. Beale, D. Froning, U. Reimer, D. Froning, W. Lehnert. **The importance of diffusion mechanisms in high temperature polymer electrolyte fuel cells**, 288th ECS Meeting, October 11-16, 2015, Phoenix, USA
- Beale, S. B., Reimer, U., Froning, D., Lehnert, W., Stolten, D. **The openFuelCell project: recent progress and future development**, European Fuel Cell Technology & Applications Conference - Piero Lunghi Conference, December 16-18, 2015, Naples, Italy

> Institute of Energy and Climate Research, Nuclear Waste Management and Reactor Safety (IEK-6), FZ Jülich

Prof. Dirk Bosbach

- Kowalski, P.: Goldschmidt2015 Conference, **"Ab Initio Modeling of Excess Mixing Parameters of Solid Solutions Relevant for Nuclear Waste Management"**, 2015, Prague, Czech Republic (invited)
- Kowalski, P./Neumeier, S.: Materials Science & Technology Conference (MS&T 2015), Materials Issues in Nuclear Waste Management in the 21st Century, **"Feasible and Reliable Atomistic Simulations Approach to Modeling Materials Relevant for Nuclear Waste Management"**, 2015, Columbus, OH, USA (invited)
- Molinero, J./Deismann, G.: Materials Science & Technology Conference (MS&T 2015), **"Multiphysics and geochemical couplings in the subsurface environment"**, 2015, Columbus, USA (invited)
- Kowalski, P.: ThUL School 2015, **"How challenging is it to compute actinides?: Atomistic modeling of nuclear materials relevant for nuclear waste management"**, 2015, Karlsruhe, Germany (invited)
- Kowalski, P.: 11th International Conference on Ceramic Materials and Components for Energy and Environmental Applications, **"Feasible and reliable ab initio approach to computation of materials relevant for nuclear waste management"**, 2015, Vancouver, Canada
- Kowalski, P.: 9th International Conference on f-elements, **"Atomistic modelling of materials relevant for nuclear waste management"** 2015, Oxford, UK

> Institute of Inorganic Chemistry (IAC), Chair of Solid-State and Quantum Chemistry, RWTH

Prof. Richard Dronskowski

- **"A Chemical (Bonding) Perspective on Phase-change and Related Materials"**, R. Dronskowski, American Ceramic Society, Miami, USA (May 2015)
- **" A Chemical (Bonding) Perspective on Phase-change and Related Materials"**, R. Dronskowski, 15th V. A. Fock Meeting on Quantum and Computational Chemistry, Vladivostok (June 2015)
- **"Chemical Bonding (in Solids) from Local Orbitals and Plane Waves"**, R. Dronskowski, 3rd International Conference on Chemical Bonding, Kauai, USA (July 2015)

> Institute of Jet Propulsion and Turbomachinery (IST), RWTH

Prof. Peter Jeschke

- Jeschke, P., Penkner, A.:
  "A Novel Gas Generator Concept for Jet Engines Using a Rotating Combustion Chamber"
  In: ASME J. Turbomach.: Vol. 137, Nr. 7 (2015), doi: 10.1115/1.4029201, S. 071010-1-8
- Rossbach, T., Rube, C., Wedeking, W. , Franz, H., Jeschke, P.:
  "Performance measurements of a full-stage centrifugal process gas compressor test rig"
  In: 11th European Conference on Turbomachinery: March 23-27, 2015, Madrid, Spain, ETC2015-084
- Henninger, S., Jeschke, P., Ashcroft, G., Kügeler, E.:
  "Time-domain implementation of higher-order non-reflecting boundary conditions for turbomachinery applications"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42362

- Stummann, S., Jeschke, P., Metzler, T.:
  "Circumferentially non-uniform flow in the rear stage of a multistage compressor"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42935
- Speak, T., Sellick, R., Kloos, V., Jeschke, P.:
  "Dual drive booster for a two-spool turbofan - Performance effects and mechanical feasibility"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42360
- Penkner, A., Jeschke, P.:
  "Advanced rayleigh pressure loss model for high-swirl combustion in a rotating combustion chamber"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42277
- Bartsch, C., Hölle, M., Jeschke, P., Metzler, T.:
  "1D adaptive measurement grid for improved pneumatic probe measurements"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42352
- Rube, C., Rossbach, T., Wedeking, M., Grates, D., Jeschke, P.:
  "Experimental and numerical investigation of the flow inside the return channel of a centrifugal process compressor"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42600
- Franz, H., Wedeking, M., Rube, C., Jeschke, P.:
  "Numerical investigation of the return channel of a high-flow centrifugal compressor stage"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-43640
- Junge, L., Jeschke, P., Ashcroft, G., Frey, C.:
  "On the application of frequency-domain methods to multistage turbomachinery"
  In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-42936
- Schmidt, J., Schwarz, P., Wilkosz, B., Jeschke, P., Smythe, C.:
  "Detailed performance analysis of a centrifugal compressor stage with pipe diffuser and immerged tandem deswirler"
- In: Proceedings of ASME Turbo Expo 2015: June 15-19, 2015, Montréal, Canada, GT2015-43484
- Behre, S., Kluxen, R., Jeschke, P., Guendogdu, Y.:
  "Development of turbulence intensity and integral lenght-scale in a 1.5 stage axial flow turbine"
  In: Proceedings of International Gas Turbine Congress: November 15-20, 2015, Tokyo, Japan
- Gand, O., Hoffmann, I., Jeschke, P., Brignole, G.:
  "Numerical sensitivity analysis of the stator clearance on the functionality of axial-skewed slot hub treatments"
  In: Proceedings of International Gas Turbine Congress: November 15-20, 2015, Tokyo, Japan
- Hölle, M., Bartsch, C., Hönen, H., Jeschke, P., Fröbel, T., Metzler, T.:
  "Measurement uncertainty analysis for multi-hole pressure probes combined with a temperature sensor"
  In: Proceedings of International Gas Turbine Congress: November 15-20, 2015, Tokyo, Japan

> Institute of Neuroscience and Medicine, Computational Biomedicine (INM-9), FZ Jülich

Prof. Paolo Carloni

Invited talks to:

- International Conference on Computational Physics (ICCP9), January, 2015, University of Singapur, Singapur
- Workshop in honour of Wanda, February, EPFL, Lausanne, Switzerland
- Modeling of Chemical and Biological Reactivity (MCBR4), February, 2015, Heidelberg, Germany
- Workshop "Nanopores: Experiments and mathematical modelling", March, 2015, Darmstadt, Germany
- Telluride, Workshop Ion Channels, July, Telluride, USA
- II WBioTEI, August, 2015, Sao Paulo, Brazil
- Fismat, Palermo, Italy

> Jülich Supercomputing Centre (JSC), FZ Jülich

Prof. Erik Koch

- 20th Mardi Gras Conference on Petascale Many Body Methods for Complex Correlated Systems
  February 12-14, 2015, Louisiana State University, Baton Rouge, Louisiana, USA
  Stochastic sampling for the analytic continuation of imaginary-time data
- Workshop on Theoretical Chemistry: Quantum Monte Carlo
  February 24-27. 2015, Mariapfarr: **Quantum Monte Carlo and Dynamical Mean-Field Theory**
- International Conference on Computational Design and Simulation of Materials
  June 17-20, 2015, Shenyang, China: **Stochastic sampling for the analytic continuation of imaginary-time data**

> Software and Tools for Computational Engineering (STCE), LufG Informatik, RWTH

Prof. Uwe Naumann

- Invited talk and one-day seminar at ICBI Global Derivatives Trading and Risk Management, April 2015, Amsterdam, Netherlands

7. SELECTED NATIONAL AND INTERNATIONAL COOPERATIONS

> Chair and Institute for Power Plant Technology, Steam and Gas Turbines (IKDG), RWTH

Prof. Manfred Wirsum

- ALSTOM Mannheim, Germany
- ALSTOM Rugby, UK

> Chair for Applied Geophysics and Geothermal Energy (GGE), E.ON - Energy Research Center, RWTH

Prof. Christoph Clauser

- Professor Thomas R. Rüde, Lehr- und Forschungsgebiet Hydrogeologie, RWTH, Germany
- 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
- FZ Jülich, Jülich, Germany (within EU project EoCoE)
- Maison de la Simulation, Paris, France (within EU project EoCoE)

> Chair for Computational Analysis of Technical Systems (CATS), RWTH

Prof. Marek Behr, Ph.D.

- Prof. Matteo Pasquali, Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, USA
- Prof. Nikos Chrisochoides, Department of Computer Science, Old Dominion University, Norfolk, Virginia, USA
- Prof. Kazuo Kashiyama, Department of Civil Engineering, Chuo University, Tokyo, Japan
- Prof. Dominik Schillinger, Department of Civil Engineering, University of Minnesota, Minneapolis, USA
- Prof. Antonio Huerta, Department of Applied Mathematics, UPC BarcelonaTech, Barcelona, Spain

> 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
- Prof. A. Kapitulnik, Stanford University, USA
- Prof. T. Siegrist, University of Florida at Tallahassee, USA
- Prof. Wei Zhang, Xian, China

> Chair of Experimental Physics, I. Physics Institute B, RWTH

Prof. Stefan Schael

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

> Chair of Physical Chemistry I, Physical Chemistry of Solids, RWTH

Prof. Manfred Martin

- Prof. P.C. Schmidt, Technical University of Darmstadt, Germany
- Prof. H.-I. Yoo, Seoul National University, Korea
- Prof. Y. Aoki, Hokkaido University, Japan
- Prof. J. Janek, Giessen University, Germany
- Prof. S. Ebbinghaus, Halle University, Germany

> Institute for Advanced Simulation and Peter Grünberg Institute, Theoretical Nanoelectronics (PGI-2 / IAS-3) / FZ Jülich

Prof. Eva Pavarini

- 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, Theoretical Neuroscience (IAS-6) and Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), FZ Jülich

Prof. Markus Diesmann

- **Human Brain Project**
  http://www.humanbrainproject.eu
  - > Markus Diesmann is leader of task 6.2.1 - Brain simulation engines: The Network Simulator
  - > Sonja Grün is leader of work package 5.3 - Tools for the analysis of functional data
  - > Abigail Morrison is leader of task 4.3.3 - Models of human cognitive function: Models of biologically realistic network states; wakefulness & sleep
- **Helmholtz Portfolio Theme - Supercomputing and Modeling for the Human Brain (SMHB):**
  - > Task 3.4 Application-side interfaces for visualization and interactivity.
    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, Lehrstuhl für Motorentechnik, Spain
- Technische Universität München, Germany
- Universität Kassel, Germany
- TU Hamburg-Harburg, Germany
- Tsinghua University, China

> Institute for Combustion Technology (ITV), RWTH

Prof. Heinz Pitsch

- Venkat Raman, University of Michigan, USA
- Seongwon Kang, Sogang University, South Korea
- Michael Mueller, Princeton University, USA
- Gus Nathan, University of Adelaide, Australia
- Vincent LeChenadec, University of Illinois at Urbana-Champaign, USA

> Institute for Theoretical Solid State Physics, Strongly Correlated Quantum Systems, RWTH

Prof. Stefan Wessel, Ph.D.

- Assaad, F.F., Uni Würzburg, Germany
- Vojta, M., TU Dresden, Germany
- Mila, F., EPFL Lausanne, Switzerland
- Honecker, A., Université de Cergy-Pontoise, France

> Institute of Aerodynamics and Chair of Fluid Mechanics (AIA), RWTH

Prof. Wolfgang Schröder

- Professor Dr. Nicolas R. Gauger, Technische Universität Kaiserslautern, Chair for Scientific Computing (SciComp)
- 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

> Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZ Jülich

Prof. Wolfgang Wiechert

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

> Institute of Bio- and Geosciences, Agrosphere (IBG-3), FZ Jülich

Prof. Harry Vereecken

- Reed Maxwell, Colorado School of Mines: International Groundwater Modeling Center
- Eric Wood, Princeton University and Marc Bierkens: Hyperresolution global Hydrological Modeling Project
- FOR 2131, DFG: Data Assimilation for Improved Characterization of Fluxes across Compartmental Interfaces
- MilKip, BMBF: Decadal Climate Predictions
- SFB/TR32: Patterns in soil-vegetation-atmosphere systems: monitoring, modeling and data assimilation
- Research and Development collaboration with the German Federal Institute of Hydrology, (BfG) Koblenz
- 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.
- DFG, Gradiertenkolleg GRK 1628/1, Selectivity in Chemo-and Biocatalysis, Prof. Takashi Hayashi, Department of Applied Chemistry, Graduate School of Engineering, Osaka University
- Cooperation for a sustainable bioeconomy with several instititutes from Heinrich Heine University (Düsseldorf), Friedrich Wilhelms University (Bonn) & Jülich Research Center in the frame of Bioeconomy Science Center, www.biosc.de
- 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

> Institute of Complex Systems, Structural Biochemistry (ICS-6), FZ Jülich

Prof. Dieter Willbold, Jun.-Prof. Dr. Birgit Strodel

- Prof. Dr. Victor Batista, Yale University, USA (Birgit Strodel)
- Prof. Dr. Lynn Kamerlin, Uppsala Univerity, Sweden (Birgit Strodel)
- Prof. Dr. David Wales, University of Cambridge, UK (Birgit Strodel)

> Institute of Energy and Climate Research, Electrochemical Process Engineering (IEK-3), FZ Jülich

Prof. Detlef Stolten, Prof. Werner Lehnert

- Prof. V. Schmidt, Ulm University, Germany
- Dr. I. Manke, Helmholtz-Zentrum Berlin GmbH, Germany
- Prof. J. Pharoah, Queens University, Canada

> Institute of Energy and Climate Research, Nuclear Waste Management and Reactor Safety (IEK-6), FZ Jülich

Prof. Dirk Bosbach

- Modeling of irradiated graphite (and other materials), collaboration with EDF and CEA, France (Dr. Philippe Baranek (EDF) , Dr. Alein Chartier (CEA) & Dr. Laurent Van Brutzel (CEA).
- Modeling of pyrochlore-type ceramics, collaboration with Curtin U., Australia (Prof. Nigel Marks and Prof. Julian Gale).
- Improving the massively parallel reactive transport code PFLOTRAN, collaboration with Sandia National Laboratory, USA, and Amphos21, Spain (Dr. Glen Hammond and Dr. Jorge Molinero).

> Institute of Inorganic Chemistry (IAC), Chair of Solid-State and Quantum Chemistry, RWTH

Prof. Richard Dronskowski

- With all corresponding colleagues of RWTH and MPI for Iron Research (Düsseldorf) within Sonderforschungsbereich 761, "Steel ab initio"
- With all corresponding colleagues of RWTH and FZ Jülich within Sonderforschungsbereich 917, "Nanoswitches"
- With Prof. Reinhard Conradt, RWTH, within Priority Programme 1594, "Topological Engineering of Ultrastrong Glasses"
- With Prof. Shinichi Kikkawa, Hokkaido University, Sapporo, on the characterization of complex oxides and oxide nitrides
- With Prof. Andrei Tchougréeff, Lomonosov State University, Moscow, on the many-body theory of nitrogen-based pseudo-oxides

> Institute of Jet Propulsion and Turbomachinery (IST), RWTH
Prof. Peter Jeschke

- MTU Aero Engines, Germany
- MAN Diesel & Turbo, Germany
- GE Aviation, USA
- Deutsches Zentrum für Luft- und Raumfahrt (DLR), Germany
- Forschungsvereinigung Verbrennungskraftmaschinen (FVV), Germany

> Institute of Neuroscience and Medicine, Computational Biomedicine (INM-9), FZ Jülich
Prof. Paolo Carloni

- The Ernesto Illy Foundation, Trieste, Italy
- Dr. Achim Kless, Grünenthal, Aachen, Germany
- Prof. Modesto Orozco, IRB, Barcelona, Spain
- Prof. Gabriele Varani, University of Washington, USA
- Dr. Rachel NechushtaiThe Hebrew University of Jerusalem, Israel

> Institute of Physical Chemistry (IPC), Theoretical Chemistry, RWTH
Prof. Arne Lüchow

- Andreas Savin and Benoît Braïda, Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Paris, France

> Jülich Supercomputing Centre (JSC), Computational Science, FZ Jülich
Prof. Erik Koch

- DFG Forschergruppe 1346/2: Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials
- DFG Graduiertenkolleg 1995/1: Quantenmechanische Vielteilchenmethoden in der kondensierten Materie

> Software and Tools for Computational Engineering (STCE), LufG Informatik, RWTH
Prof. Uwe Naumann

- P. Korn, Max-Planck Inst. for Meteorology, Hamburg, Germany
- N. Bellas, Univ. of Thessaly, Volos, Greece
- J.-D. Müller, Queen Mary Univ., London, UK
- R. Kopmann, Bundesanstalt für Wasserbau, Karlsruhe, Germany
- J. Holden, The Numerical Algorithms Group Ltd., Oxford, UK

8. VISITING SCIENTISTS

> Chair for Computational Analysis of Technical Systems (CATS), RWTH
Prof. Marek Behr, Ph.D.

- Prof. Kenjiro Terada, Department of Civil Engineering, Tohoku University, Sendai, Japan
- Prof. Karol Miller, University of Western Australia, Perth, Australia

> Chair of Experimental Physics, I. Institute of Physics (IA), RWTH
Prof. Matthias Wuttig

- Dr. Christophe Bichara, Marseille, France
- Dr. Nicholas Breznay, Berkeley, USA
- Prof. Dr. Teresa Puig, Barcelona, Spain
- Prof. Dr. Austen Angell, Phoenix, USA
- Prof. Dr. Eun Soo Park, Seoul, Korea
- Prof. Dr. Junji Tominaga, Tsukaba, Japan
- Dr. Yuta Saito, Tsukaba, Japan

> Chair of Physical Chemistry I, Physical Chemistry of Solids, RWTH
Prof. Manfred Martin

- Dr. Bo Wei, Department of Physics, Harbin Institute of Technology (HIT), Harbin, P. R. China
- Hyung-Jong Choi, School of Mechanical Engineering, Korea University, Seoul 136-713, Korea
- Yu Hashimoto, Department of Materials Science and Engineering, Nagoya Institute of Technology, Japan

> Institute for Advanced Simulation and Peter Grünberg Institute, Theoretical Nanoelectronics (PGI-2 / IAS-3), FZ Jülich
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 FZ Jülich, highly increasing the visibility of the FZ Jülich in the field of strongly correlated materials.

> Institute for Advanced Simulation, Theoretical Neuroscience (IAS-6) and Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), FZ Jülich

Prof. Markus Diesmann

- Mikael Djurfeldt, International Neuroinformatics Coordinating Facility (INCF), PDC Center for High Performance Computing at KTH Royal Institute of Technology, Sweden (since 2013)
- George Gerstein, University of Pennsylvania, Philadelphia, USA (March-April 2012)
- John Hertz, Niels Bohr Institute, Copenhagen, Denmark and Nordita, Royal Institute of Technology and Stockholm University, Stockholm, Sweden (April 2011 and Dec 2013)
- Pedro E Maldonado, Programa Disciplinario de Fisiología y Biofísica, Instituto de Ciencias Biomédicas Facultad de Medicina, Universidad de Chile. Santiago, Chile (since 2013)
- Hans Ekkehard Plesser, Department of Mathematical Sciences and Technology, Norwegian University of Life Sciences, Norway (since 2013)
- Alexa Riehle, Institut de Neurosciences de la Timone (INT), CNRS-AMU, Marseille, France (since March 2013)

> Institute for Combustion Engines (VKA), RWTH

Prof. Stefan Pischinger

- Ricardo Carreño, CMT-Motores Térmicos, Universitat Politècnica de València, Spain

> Institute for Combustion Technology (ITV), RWTH

Prof. Heinz Pitsch

- Venkat Raman, University of Michigan, USA
- Seongwon Kang, Sogang University, South Korea
- Gus Nathan, University of Adelaide, Australia
- Vincent LeChenadec, University of Illinois at Urbana-Champaign, USA
- Nicolas Eaves, University of Toronto, Canada

> Institute of Aerodynamics and Chair of Fluid Mechanics (AIA), RWTH

Prof. Wolfgang Schröder

- Young June Moon, Korea University, Korea
- Ellen K. Longmire, University of Minnesota, USA - Petros Koumoutsakos, ETH Zürich, Switzerland
- Makoto Tsubokura, Kobe University, Japan
- Kazuhiro Nakahashi, JAXA, Japan

> Institute of Bio- and Geosciences, Agrosphere (IBG-3), FZ Jülich

Prof. Harry Vereecken

- Chris Duffy, Civil & Environmental Engineering Department, Pennsylvania State University

> Institute of Biotechnology, RWTH

Prof. Ulrich Schwaneberg

- Dr. Cheng Zhou, Institute of Microbiology, Chinese Academy of Sciences, Beijing, China
- Hao Cao, Beijing University of Chemical Technology, China

> Institute of Energy and Climate Research, Electrochemical Process Engineering (IEK-3), FZ Jülich

Prof. Detlef Stolten, Prof. Werner Lehnert

- Prof. Yongfeng Liu, Beijing University of Civil Engineering and Architecture, China
- 2) Prof. Liangfei Xu, Tsinghua University, China
- Prof. Martin Andersson, Lund University, Sweden
- Prof. Dirk Henkensmeier, KIST, 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. Sachin Nanavati, University of Pune, India

> Institute of Neuroscience and Medicine, Computational Biomedicine (INM-9), FZ Jülich

Prof. Paolo Carloni

- Vito Genna, IIT, Genoa, Italy
- Diniz Maciel de Sena, Universidade Regional do Cariri, Brasil
- Mateusz Jasik, Silesian University of Technology, Poland
- May Huang, International School for Advanced Studies, Italy

9. YOUNG RESEARCHER GROUPS ESTABLISHED IN JARA-HPC INSTITUTES

> Computational Nanoferronics Laboratory

Prof. Dr. Marjana Lezaic

Helmholtz Young Investigators Group

Peter Grünberg Institute, Quantum Theory of Materials (PGI-1 / IAS-1), FZ Jülich

> Complex Ordering Phenomena in Multifunctional Oxides

Prof. Dr. Manuel Angst

Helmholtz Young Investigators Group

Peter Grünberg Institute, Scattering Methods (PGI-4 / JCNS-2)

> Topological Nanoelectronics Group

Prof. Dr. Yuriy Mokrousov

Helmholtz Young Investigators Group

Institute for Advanced Simulation, Quantum Theory of Materials (IAS-1), FZ Jülich

> Functional Nanoscale Structure Probe and Simulation Laboratory

Prof. Dr. Samir Lounis

Helmholtz Young Investigators Group

Institute for Advanced Simulation, Quantum Theory of Materials (IAS-1), FZ Jülich

> Modular Synthetic Enzyme Cascades

Dr. Dörte Rother

Helmholtz Young Investigators Group

Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZ Jülich

> Actinide Solid State Chemistry - A direct Link from fundamental Science to the safe Management of high-level nuclear waste

Dr. Evgeny Alekseev

Helmholtz Young Investigators Group

Institute of Energy and Climate Research, Nuclear Waste Management and Reactor Safety (IEK-6), FZ Jülich

> Boderline Magnetism

Dr. Carolin Schmitz-Antoniak

Helmholtz Young Investigators Group

Peter Grünberg Institute (PGI-6), FZ Jülich

> E3-NET. Effciency, Emergence and Economics of future supply networks

Dr. Dirk Witthaut

Helmholtz Young Investigators Group

Institute of Energy and Climate Research, Systems Analysis and Technology Evaluation (IEK-STE), FZ Jülich

> Microscale Bioengineering

Prof. Dr. Dietrich Kohlheyer

Helmholtz Young Investigators Group

Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZ Jülich

> Theory of Multi-scale neuronal networks

Dr. Moritz Helias

Helmholtz Young Investigators Group

Institute of Neuroscience and Medicine, Computational and Systems Neuroscience (INM-6), FZ Jülich

> Computational modeling of materials for nuclear Technology

Dr. Piotr Kowalski

Helmholtz Young Investigators Group

Institute of Energy and Climate Research, Nuclear Waste Management and Reactor Safety (IEK-6), FZ Jülich

> Ab initio description of double and charge transfer excitations: from solvable models to complex systems

Dr. Nicole Helbig

Helmholtz Young Investigators Group

Institute for Advanced Simulation, Quantum Theory of Materials (IAS-1), FZ Jülich

> Active-Materials: Cell tissues in silico

Dr. Jens Elgeti

Helmholtz Young Investigators Group

Institute of Complex Systems, Theoretical Soft Matter and Biophysics (ICS-2 / IAS-2), FZ Jülich

> Instrumental and Data-driven Approaches to Source-Partitioning of Greenhouse Gas Fluxes: Comparison, Combination, Advancement (IDAS-GHG)

Dr. Alexander Graf

Helmholtz Young Investigators Group

Institute of Bio- and Geosciences, Agrosphere (IBG-3), FZ Jülich

10. APPOINTMENTS DURING 2015

Univ.-Prof. Torsten Wolfgang Kuhlen (Steering Board CSG ImmVis)

Dr. rer. nat. Torsten W. Kuhlen has been university professor of virtual reality and immersive visualization at the Faculty of Mathematics, Computer Science, and Natural Sciences at RWTH since October 2015. He is head of the Department of Computational Science and Engineering at the RWTH IT Center. He and his team research three dimensional, multimodal human-computer interfaces and their application in science and tec

11. GENERAL INFORMATION

> 11.1. JARA-HPC members

On December 31, 2015, 43 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. Wolfgang Dahmen	Institute for Geometry and Practical Mathematics (IGPM), 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 Kuhlen	CSG ImmVis 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 ParEff 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. Detlev Reiter	Institute of Energy and Climate Research, Plasma Physics (IEK-4), FZ Jülich
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

> 11.2. Involved institutes

> 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, CO2-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 simulation quality, 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 Jülich Supercomputing Centre 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 Jülich Supercomputing Centre 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 calibration, 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. Wolfgang Dahmen, 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
Plasma Physics (IEK-4) – Prof. Detlev Reiter
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 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

12. JOINT PUBLICATIONS

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