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High Performance Computing at RRZE

2018

HPC at RRZE

Regionales RechenZentrum Erlangen

Der IT-Dienstleister der FAU

HIGH PERFORMANCE COMPUTING@RRZE

HPC at RRZE

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Editorial

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Valued readers,

Scientific high performance computing (HPC) has gained quite some momentum in recent years, at FAU and elsewhere. As the demand of computational scientists for compute cycles grows, so does the need for infrastructure and user support at computing centers. Beyond the traditional application fields of engineering, physics, chemistry, bioinformatics, mathematics, and computer science, new kids have recently arrived on the block: Data analytics and machine learning are on the rise, with crosscutting applicability and disruptive consequences for old and new disciplines. Moreover, as if all this was not enough transformation for the day, Moore's Law is nearing its end, heralding an unsettling diversification of hardware architectures and software environments.

Looking at the reports collected in this booklet, I am satisfied to see how our HPC customers are embracing the winds of change. The stated aim of RRZE is to provide them with qualified advice and adequate and reliable compute resources. We can only rise to this formidable challenge by working closely with our customer base, the university administration, and the Bavarian State Ministry of Science, Research, and the Arts in order to build a sustainable service that reaches far beyond the next system procurement. Using these valuable resources effectively is of paramount importance to all those involved, and the results speak for themselves.

The great Thomas Edison once said: "Genius is one percent inspiration, ninety-nine percent perspiration." Despite all the hype around "artificial intelligence," we cannot do much about the inspiration part, and even the perspiration can only partially be substituted by the power of computers, be they super or not. In the end, it boils down to the hard work of the individual, following the painstaking scientific process that turns numbers into insight. That, however, holds so much ready for those who insist: discovery.

Dr. G. Hergenröder,
Technical Director, RRZE

HPC usage reports from our users

Dimerization of G protein-coupled receptors

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HPC resources used at RRZE
Large-scale project on Meggie

The biological activity of G protein-coupled receptors, transmembrane proteins targeted by 36% of drugs, is modulated by their dimerization. Unraveling the dimer interfaces enables us to understand the receptor molecular interactions and thus to modulate their pharmacological effects.

Motivation and problem definition

At first we have studied the heterodimerization of chemokine receptors CXCR4, CCR2, and CCR5 and the effect of cholesterol thereon. Dimers of chemokine receptors play important roles in the human immune systems but they are also involved in HIV infection and in cancer. Moreover, the activity of chemokine receptors is effected by membrane cholesterol. For the development of drugs, specifically targeting chemokine dimers, structural information about their dimerization patterns is required. Unfortunately, experimental data on the possible dimerization interfaces is strongly restricted.

In the second part of the project we have investigated the bivalent ligand binding to the heterodimers formed by the opioid receptors mu (MOR) and delta (DOR). Bivalent ligands consist of two linked ligands targeting two receptors. The common opinion is that the individual ligands are buried in the pockets of the receptors while the linker is located in the extracellular space. The crosslinking of the inactive DOR with the active MOR was shown to significantly reduce tolerance and dependence caused by MOR activators (e.g., morphium). Interestingly, the efficiency of the bivalent ligands depends on the length of the connector. Thereby, the most efficient linkers are too short to bridge the receptors through the extracellular space. Discovery of the binding poses of the bivalent ligand to the heterodimer and the path by which the connector connects the receptors is expected to enable design of pain killers with reduced side effects.

Methods and codes

GPCR dimerization is studied by performing multiscaling molecular dynamics simulations using the free GROMACS software. In the first step, ensembles (consisting typically of ~500 parallel independent runs) of molecular dynamics simulations at coarse-grained resolution are prepared, executed, and analysed by our methodology named DAFT [1]. The most significant dimers are then converted back to atomistic resolution using our program backward [2] and simulated atomistically to refine the interactions at atomistic detail and to enable ligand binding.

Therefore our computational needs are twofold. The ensembles of coarse-grained molecular dynamics simulations require few cores per a single run but many such runs, i.e., throughput computing. The atomistic simulations can only be tackled by highly parallel computing.

Results

Our MD simulations showed similar homodimerization patterns for the closely related CC chemokine receptors in cholesterol-free membranes. Interestingly, cholesterol appeared to specifically effect CC chemokine homodimerization, thus differentiating the closely related receptors from each other. Moreover, the heterodimerization patterns with CXCR4 and their cholesterol sensitivity differed. Therefore, apart from generating detailed structural information about chemokine homo- and heterodimers, our work sheds first light on the diversifying effects of heterodimerization and the influence of membrane surroundings on closely related receptors.

MOR and DOR form dimers exclusively by interfaces containing helices TM1 or TM5, thereby all possible interface combinations were observed. The different dimers display different linker lengths that would be required to connect the docked ligands. The shortest theoretical linker length is obtained for TM5/TM5 dimers. To these dimers it was possible to model the 19-atom long linker which passes between the helices TM5 and TM6 of the receptors and connects them directly through the lipid bilayer.

Outreach

A publication “Closely related yet unique: Distinct homo- and heterodimerization patterns of G protein coupled chemokine receptors and their fine-tuning by cholesterol” by S. Gahbauer, K. Pluhackova, and R. A. Böckmann, was submitted to PlosCB.

Both projects were presented by S. Gahbauer and K. Pluhackova at 19th IUPAB congress and 11th EBSA congress in Edinburgh in July 2017 and at the GLISTEN Symposium in Porto in March 2017.

The chemokine project is supported by the German Science Foundation (DFG) within the Research Training Group 1962 – Dynamic Interactions at Biological

Membranes and the emerging field initiative at the Friedrich-Alexander University Erlangen-Nürnberg (FAU) in Synthetic Biology.

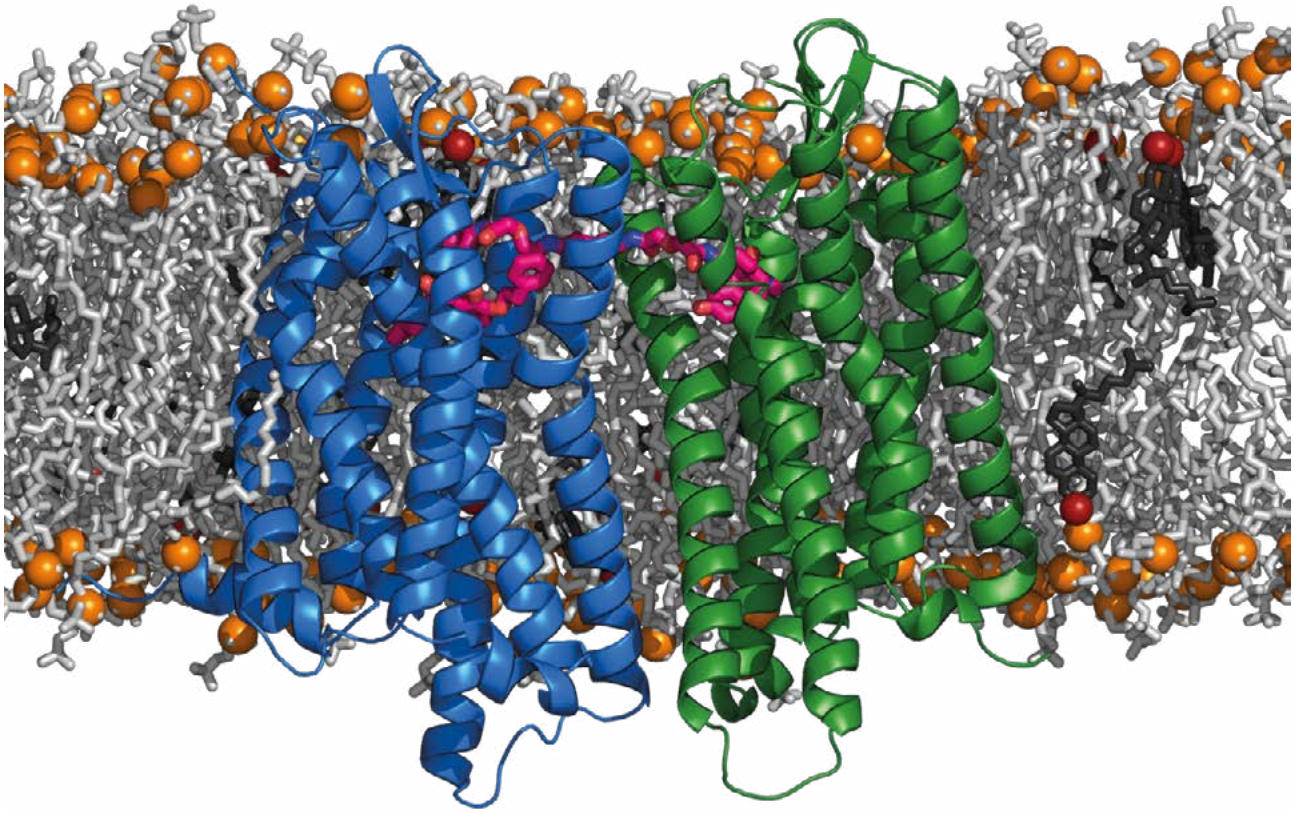
References

T.A. Wassenaar, K. Pluhackova, A. Moussatova, D. Sengupta, S.J. Marrink, D.P. Tieleman, R.A. Böckmann. “High-Throughput Simulations of Dimer and Trimer: Assembly of Membrane Proteins. The DAFT Approach.” J. Chem. Theory Comput. 11:2278-2291 (2015)

T.A. Wassenaar, K. Pluhackova, R.A. B\232ckmann, S.J. Marrink, D.P. Tieleman. “Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models.” J. Chem. Theory Comput. 10:676-690 (2014)

Researcher’s Bio and Affiliation

Kristyna Pluhackova graduated in Chemistry at the Charles University in Prague in 2009. She received her PhD degree in 2015 from FAU Erlangen-Nürnberg for developing methodologies and force fields for membrane-protein simulations in the Computational Biology group of Prof. Rainer A. Böckmann. She is currently a PostDoc in the same group. In the application of molecular dynamics she continues to see the biophysical and biological problems by the eyes of a chemist, interested mainly in the fascinating molecular details. K. Pluhackova has obtained in 2016 a junior investigator grant of the Biology Department at FAU and in fall 2017 she was awarded a research stipend from the German Science Foundation to join the experimental group of Prof. Müller at ETH Zürich for two years.



Heterodimer of two opioid receptors (DOR shown as blue and MOR shown as green cartoon) bridged by a bivalent ligand (pink sticks). The protein/ligand complex is embedded in a lipid bilayer (phospholipids are shown as grey sticks with headgroups highlighted as orange spheres) including cholesterol (shown as black sticks). Water and ions were omitted for clarity.

Allosteric modulation at G protein-coupled receptors

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HPC resources used at RRZE
Large-scale project on Meggie

The activation process of G protein-coupled receptors (GPCRs) is not fully understood yet. Allosteric modulators targeting GPCRs not only represent a group of novel drugs with the potential for increased drug safety but offer the chance to further unravel the process of receptor activation.

Motivation and problem definition

We studied the binding-mode of a negative allosteric modulator targeting the β_2 adrenergic receptor (β_2AR) as revealed by X-ray crystallography. The allosteric modulator was discovered by virtual screening in combination with SAR studies. Compared to conventional ligands targeting G protein-coupled receptors (36% of marketed drugs), allosteric modulators bind outside of the highly conserved orthosteric binding pocket. Therefore they have an increased potential for sub-type selectivity. Additionally, allosteric modulators mediate their effect by modulating the response to native hormones and neurotransmitters which can result in an improved drug tolerance. Besides the latter potential therapeutic advantages, allosteric modulators can also be useful tools to study the process of receptor activation. The X-ray structure of the β_2AR revealed a binding-site of the allosteric modulator at the membrane facing surface of the receptor in contact to a second antiparallel symmetry mate (Fig.). We wanted to use Molecular Dynamics (MD) simulations to investigate the stability of the proposed binding-mode without the additional crystal contacts.

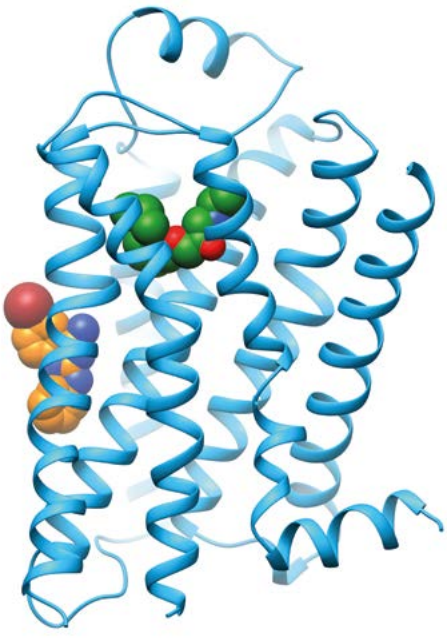
In other inactive state crystal structures of β_2AR a water molecule is located at this binding-site connecting E122 in transmembrane helix (TM) 3 and V206 and S207 in TM5. In the active state the water molecule is replaced and E122 directly interacts with TM5. As the modulator replaces this water molecule and stabilizes the interaction between TM3 and TM5 around a previously identified molecular switch for receptor activation formed by I121, P211 and F282 the X-ray crystal structure shows how the allosteric modulator can stabilize the inactive state of the receptor. Inspired by this pocket, mutagenesis studies were performed revealing a strong allosteric effect of this binding-site. The Arginine mutant was insensitive to agonist activation while the Glutamine mutant was more sensitive to receptor activation. To gain insight on the nature of the allosteric modulation on the molecular level we performed additional MD simulations of wild-type β_2AR (E122) and its mutants E112Q and E122R in the presence of the connecting water molecule.

Methods and codes

To test the stability of the binding-mode of the allosteric modulator revealed by X-ray crystallography we performed 12µs (3 x 4µs) atomistic MD simulations. The influence of the introduced mutations on interaction between TM3 and TM5 around the activation switch were analyzed with additional 4µs (2 x 2µs) MD Simulations, each. We applied the free open-source software GROMACS utilizing the general amber force filed (GAFF), the lipid14 force field and the ff14SB force field for small molecules, lipids and protein, respectively. The simulation systems contained about 70000 atoms. MD simulations of this scale are only feasible when utilizing highly parallel computing.

Results

The simulations of the described ligand receptor complex revealed a stable binding mode at the membrane facing surface of the receptor. The simulations confirmed that the ligand also binds to the receptor without a second protein stabilizing the binding mode like it is in the crystal structure. The simulations of the wild-type β_2AR (E122)



X-ray crystal structure of β_2AR in complex with the antagonist alprenolol and the negative allosteric modulator.

revealed a stable water mediated interaction of E122 of TM3 and V206 and S207 of TM5 as proposed by X-ray crystallography. While the Q122 forms less stable interactions to TM5 suggesting a higher sensitivity to receptor activation, R122 directly interacts with TM5 which may prevent the rearrangement necessary for receptor activation and therefore stabilizing the inactive state. The combination of Virtual screening, SAR studies, X-ray crystallography and MD simulations gave new insights in the activation process of the β2AR.

Outreach

A publication "Discovery of an allosteric modulator binding to a conformational hub" is in preparation.

The project was supported by the German Science Foundation (DFG) within the Research Training Group 1910 – Medicinal Chemistry of Selective GPRC Ligands.

Researcher's Bio and Affiliation

Jonas Kaindl graduated in Pharmacy at the FAU in 2014. Since then he has been pursuing his PhD in the Medicinal Chemistry group of Prof. P. Gmeiner. Jonas Kaindl is a member of the Research Training – Medicinal Chemistry of Selective GPCR Ligands (GRK1910) funded by the German Research Foundation (DFG).

Dynamics of Alzheimer-Peptide Aβ Aggregates

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HPC resources used at RRZE

Large scale project on Meggie; throughput on TinyGPU

Alzheimer's Disease (AD) is one of the most prevalent neurodegenerative diseases on earth, with alarming estimations of the evolution of patients' numbers. Using HPC resources, we intend to uncover some of the molecular details of one of the key players in AD, aggregates of the Aβ peptide.

Motivation and problem definition

It is already known from the original works of Alois Alzheimer from more than 100 years ago that one of the disease's hallmarks is the formation of deposits in the brain of patients. One type of those deposits, the plaques, is mainly composed of aggregates of the Aβ peptide, a small protein occurring in the body. The type of aggregate varies between short soluble forms and long, highly ordered fibrils. Understanding the molecular mechanism of aggregate formation may guide the development of interfering molecules, i.e. possible medications.

Since experimental techniques are limited in their ability to resolve the details of molecular motion, computer simulations have become a complement investigation method over the last decade. In this work, we apply molecular dynamics (MD) simulations to investigate the role of the first, so called 'N-terminal' amino acid residues, the protein building blocks, upon structure and stability of a certain experimentally determined Aβ fibril structure, since in the past most researchers considered those residues unstructured and not participating in fibril structure stabilization.

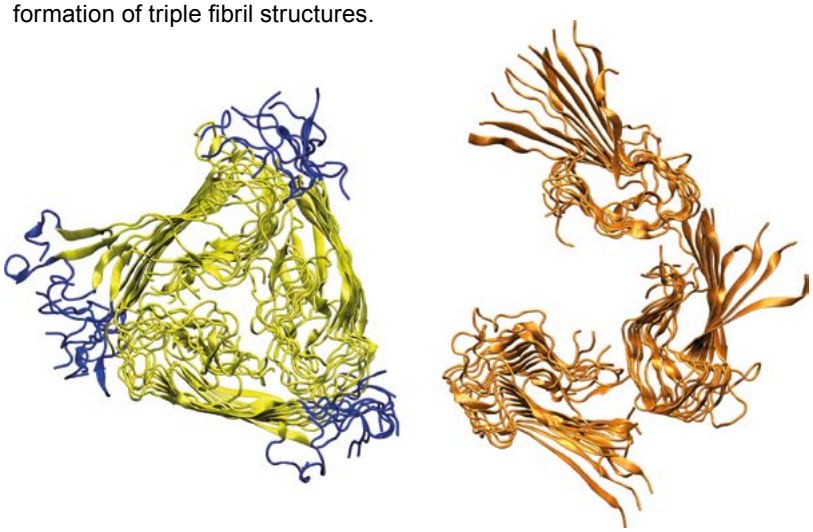
Methods and codes

We investigated two types of Aβ fibrillar structures, full-length and truncated species, which lack the first eight residues. For each species, four sizes of fibrillar aggregates were studied, with 6, 12, 24, and an infinite number of fibril layers.

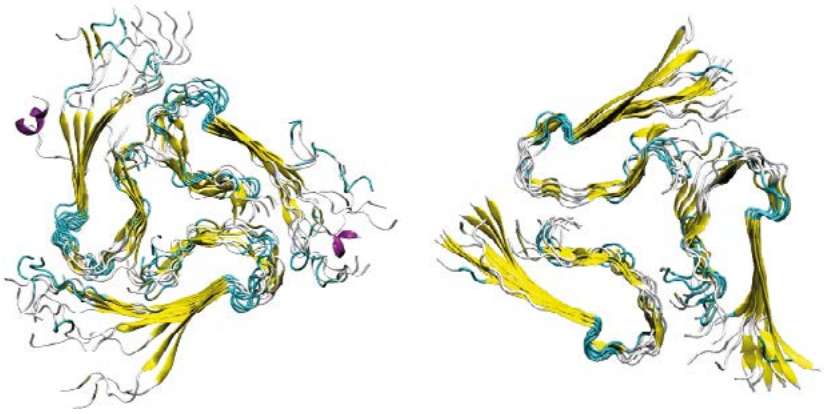
For our MD simulations we use the AMBER program suite. Calculations ran on both CPU and GPU clusters: the former are needed for the initial simulation stages to obtain a stable system and utilize MPI-parallel, optimized code; the latter are used for the MD production stage only and offer a good compromise between cost, accuracy, and speed. The HPC Services team at RRZE greatly supported the project by providing optimized executables for different RRZE clusters.

Results

Our MD simulations showed that the N-terminal residues play an important role in the stabilization of the Aβ fibrillar structure: Only with these residues present were the fibrillar aggregates structurally stable. We further identified key residues (Arg5, Glu7, Ser8) responsible for the interaction within the layers. Finally, we proposed a general mechanism involved in the formation of triple fibril structures.



Final structure of a fibrllar Aβ aggregate with 12 layers.
Left: full-length species (N-terminus in blue) with still intact super-structure.
Right: truncated species with lost super-structure



Left: Dynamics of the full-length Aβ fibril structure
Right: Dynamics of the truncated Aβ fibril structure.

Outreach

Christian A. Söldner, “Analyse der Stabilität verschiede-ner fibrillärer Oligomere von Amyloid-β40 durch Molekül-dynamik-Simulationen”, Master thesis, Erlangen 2016

Christian A. Söldner, Heinrich Sticht, Anselm H. C. Horn, “Role of the N-terminus for the stability of an amyloid-β fibril with three-fold symmetry”, PLoS ONE 2017, 12(12): e0189238 . DOI: 10.1371/journal.pone.0186347

Anselm H. C. Horn, “Role of Amyloid-β’s N-Terminus for the Stability of a Triple-Fibril Elucidated by Molecular Dynamics Simulations”, Talk chosen from the poster abstracts at the “2nd Düsseldorf-Jülich-Symposium on Neurodegenerative Diseases“, Düsseldorf 2017

The work was supported by the Alzheimer Forschung Initiative e.V. (AFI).

Researcher’s Bio and Affiliation

Anselm Horn obtained his degree in Chemistry at the FAU. After his diploma thesis in computational chemistry (Prof. Dr. Tim Clark) and some further project work at the computational chemistry center (CCC) he changed to the group of Prof. Dr. Heinrich Sticht (Bioinformatics), where he obtained his PhD for MD studies on the Aβ peptide, for which he was awarded the “CIC-Award for Computational Chemistry” from the Computers in Chemistry group of the German Chemical Society (GDCh). Currently, he is striving to finalize his habilitation in bioinformatics.

Ab-initio MD Simulations of Liquid Metals

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HPC resources used at RRZE

Large scale project on Meggie

Supported catalytically active liquid metal solutions (SCALMS) were developed at the FAU as a promising new concept in heterogeneous catalysis. Such catalysts are resistant to coke formation and therefore more stable and more economical than conventional dehydrogenation catalysts.

Motivation and problem definition

In chemical industry, most processes require the use of catalysts to efficiently obtain desired products. The investigation of the catalytic mechanism is thus of enormous economical and ecological importance. In a broad interdisciplinary cooperation at the Friedrich-Alexander University a complete new catalysis concept called “SCALMS” is explored. To understand the mechanism behind the catalytic reactions and improve their efficiency and stability, knowledge of the catalyst surface structure is required, which can be obtained in detail by electronic structure calculations to describe and complement experimental observations.

Methods and codes

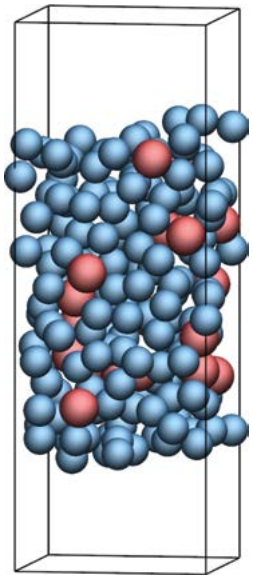
In this work, density-functional-based ab-initio Molecular Dynamics (MD) is used to study the behavior of mixtures consisting of gallium and a second metal such as palladium or rhodium. For these liquid systems, MD is the method of choice. The simulations are performed with the electronic structure code VASP using periodic boundary conditions. For the finite-temperature MD simulations a Nose-Hoover thermostat was used to sample a canonical ensemble. The equation of motion is solved by employing a Verlet algorithm. To obtain well-converged results with low statistical noise, several trajectories have to be simulated, each requiring several hundered thousand electronic structure calculations. Furthermore, these simulations can be parallelized over several nodes for each trajectory. This makes the project well-suited for the “Meggie” cluster.

Results

In combination with experimental results, in this project we were able to contribute to the clarification of the reaction mechanism in the dehydrogenation process of butane at the liquid metal surface and therefore the origin of the catalytic activity. It was found that these catalysts exhibit a layered surface structure with a depletion of the noble metal at the surface, which is in excellent agreement with experiments. Due to the high mobility of the liquid phase at temperatures of around 450° C, the noble metal atoms which are enriched in the subsurface, layer can occasionally reach the surface creating an isolated catalytically active site of one noble metal atom surrounded by a liquid Ga environment. This specific surface site can then catalyse the reaction at the surface.

Outreach

First work is published in two papers (Nat. Chem. 2017, 9, 862 DOI:10.1038/nchem.2822 and Chem. Eur. J., 2017, DOI:10.1002/chem.201703627), with two more papers being planned. The work was presented at the “Symposium on Theoretical Chemistry 2017” in Basel as a poster. The new catalyst concept SCALMS represents an important topic in the proposal for the new excellence cluster FUMIN at the FAU.



Periodic model used in ab-initio Molecular Dynamics simulations for the investigation of the SCALMS catalyst system. Ga atoms are depicted in blue, nobel metal atoms (e.g. Rh, Pd) are depicted in red.

Researcher’s Bio and Affiliation

Sven Maisel obtained his master’s degree in chemistry at the Friedrich-Alexander University in Erlangen in 2016 and is currently a Ph.D. student in the group of Prof. Dr. Andreas Görling at the chair of Theoretical Chemistry.

DFT investigation of CPP-fullerene and WF3/o-IDTBR

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HPC resources used at RRZE
Single-node throughout on Woody and LiMa

Structure, stability and fragmentation behavior of host-guest complexes of cycloparaphenyls with C_{60}, C_{70}, and C_{84} fullerenes have been analyzed by DFT.
The electron donor-acceptor system WF3/o-IDTBR was investigated to gain insight from DFT on a fast hole transfer between these molecules.

Motivation and problem definition

[10]- and [12]Cycloparaphenyl fullerene monomers and oligomers were analyzed by mass spectrometry by T. Drewello et al. To improve the understanding of the stability of these complexes and their fragmentation behavior, DFT methods were applied.

In the WF3 / o-IDTBR system a fast hole transfer was measured by C. Brabec et al. As these systems are tested for application in solar technology, accurate insight on these processes is of special importance.

Methods and codes

We use Density Functional Theory (DFT), solving the Kohn-Sham equations self-consistently to gain insight on structure, energetics and excitation properties of the selected molecular systems.

TURBOMOLE 7.1-7.2 was used for single-node calculations on RRZE's Woodcrest and LiMa clusters.

Results

Structures for various CPP fullerene complexes have been determined. The fragmentation behavior from mass spectrometry could be confirmed, the positive charge is kept on the CPP as the HOMO of the complex is localized on the CPP and the negative charge is kept on the fullerene as it is the better electron acceptor.

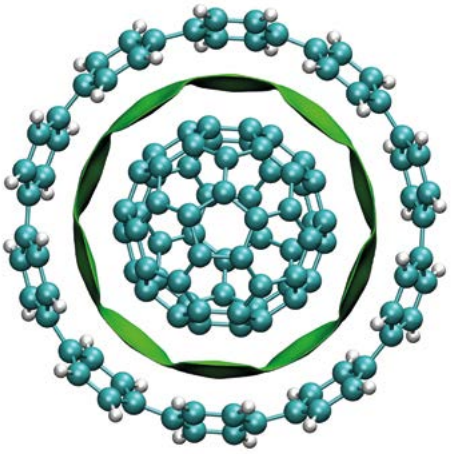
For the interacting WF3 / o-IDTBR system frontier molecular orbitals were obtained which are localized on both molecules. Because of similar HOMO energies of WF3 and o-IDTBR this interaction is possible. Excitations occur only from both interacting occupied orbitals, which further indicates the hole transfer between these orbitals.

Outreach

M.Minameyer, S.Frühwald, Y.Xu, M.von Delius, A.Görling, T.Drewello: Gas-phase Investigations of Cycloparaphenylenes and their Ring-in-Ring/Fullerene Complexes; in preparation.

S.Frühwald, N.Gasparini, C.Brabec, A.Görling: Density-functional investigation of the electron donor-acceptor systems WF3 / o-IDTBR and WF3 / PC70 BM; Poster at SolTech Conference Munich 4.10. – 5.10.2017.

Both projects are part of SFB 953: "Synthetic Carbon Allotropes".



Optimized geometry of neutral [10]CPP ⊃ C60 with visualized long-range interactions

Researcher's Bio and Affiliation

Stefan Frühwald is a PhD student in the group of Prof. Görling at the chair of Theoretical Chemistry. Research interests are Density-functional Theory investigations of molecules relevant for energy conversion and storage.

MD Simulations of Mesoporous Silica Formation

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HPC resources used at RRZE

Emmy cluster

The agglomeration of silica nanoparticles in aqueous solution is investigated upon association of SiO_2/$Si(OH)_4$ core/shell particles. Supplying multiple colloidal particles, our simulations rationalize the formation of hollow but stabile mesoporous silica structures hosting extended pores.

Motivation and problem definition

Mesoporous silica nanoparticles (MSNs) have gained significant attention since their large surface area make them ideal to host molecules, to be used as biocatalysts and drug/gene delivery vehicles, and also for various biomimetic processes. Despite broad interest, our in-depth understanding is rather limited. Understanding or controlling interfacial interactions, association and aggregation is vital for the goal-oriented use of colloidal silica particles. The aim of this work is to outline a molecular dynamics (MD) approach to colloidal silica association, ripening reactions and mesoporous precipitate formation. The inherent time-length scale was handled with a Kawska-Zahn approach originally developed for studying crystal nucleation from solutions.

Methods and codes

All MD simulations were performed with the LAMMPS software. The free energy for the interaction of two identical colloidal silica nanoparticles was calculated with the Collective Variable (colvar) module of LAMMPS. For necessary pre-/post-processing, WHAM code implementations on LAMMPS were employed. Due to the size of the simulation box and the requirements of carried calculations, parallel computing was absolutely required throughout the work.

Results

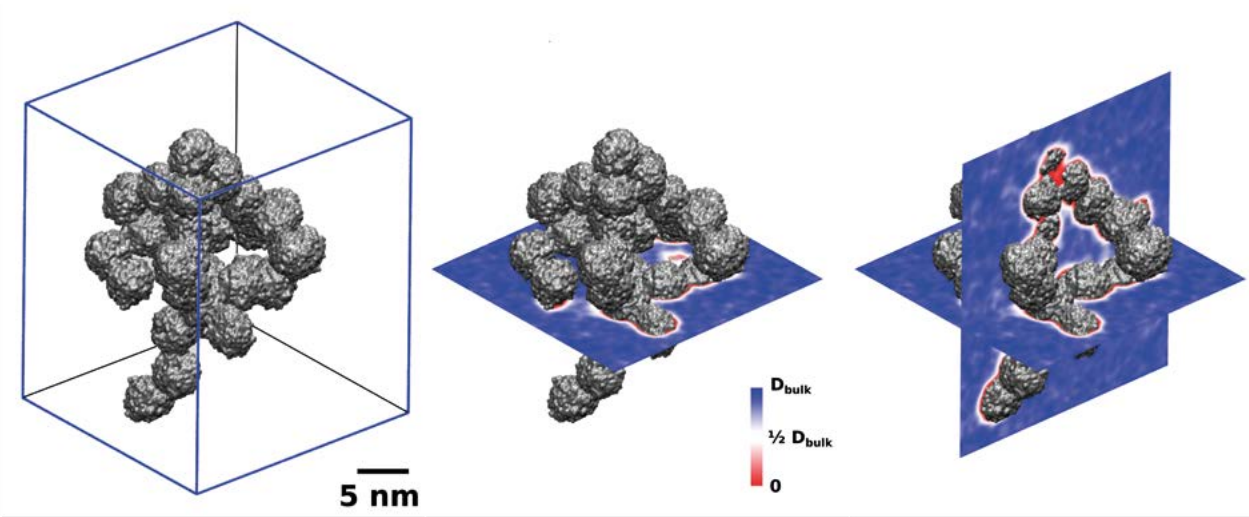
Using RRZE's Emmy cluster, we succesfully modelled the characterization of mesoporous silica. By modelling the mechanisms of the association of two colloid silica and the following ripening reactions, our simulations unravel atomic-scale details of the nature of cavities and pores formation and surface/interface properties.

Outreach

B. Becit, D. Zahn: Molecular Mechanisms of Mesoporous Silica Formation from Colloidal Silica; in preparation

Researcher's Bio and Affiliation

Bahanur Becit obtained her bachelor degree in Molecular Biology and Genetics at Bilkent University in Ankara/Turkey, and then her master's degree in Computational Biology and Bioinformatics at Kadir Has University in Istanbul/Turkey. She is currently a PhD student in the group of Prof. Zahn, who holds a professorship for theoretical chemistry at FAU.



Long scale characterization (6 ns) of water mobility next to the silica aggregate comprising 35 colloids. While the diffusions of water molecules at the immediate contact to silica are observed as 0.1-0.5 of the bulk value, the pore dimensions are found sufficiently large to permit nm-scale domains of bulk-like solvent mobility.

Molecular Dynamics Simulation of Metal Patch Formation on Silica Nanoparticles

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HPC resources used at RRZE
Meggie cluster

Nanoparticles covered with metal patches are of interest for their unique properties and potential applications in optics and catalytic reactions, through the creation of complex structures. The shape of the patch can greatly change when varying the experimental conditions. We investigate Ag^+ association and the growth of silver patches from solution by means of molecular dynamics simulations.

Motivation and problem definition

Colloidal nanoparticles have been of interest of the scientific community for many decades. The use of particles with functional groups opened a new world of possibilities enabling, for example, the creation of particles with mixed properties. In particular, patchy particles can be used to create new materials using the self-assembly of nanoparticles as building blocks. The shape of the metal patch is strongly dependent on the reaction condition. In order to have a reliable product we need to keep the shape of the patch as constant as possible. Thus the investigation of the growth of the patch over the nanoparticle is of great importance.

Methods and codes

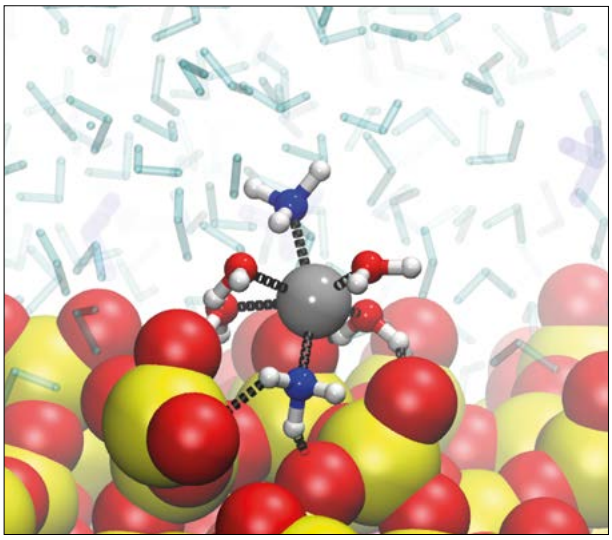
We use the molecular dynamics code LAMMPS. For the growth of metal patches the Kawska-Zahn method is adopted, while the Charge Equilibrium Method (qeq) is used for investigating of the metal patch shape. To check the validity and to extrapolate the parameters for the qeq method, DFT calculations using the software Quantum Espresso are performed. For the post processing the root libraries for C++ are employed.

Results

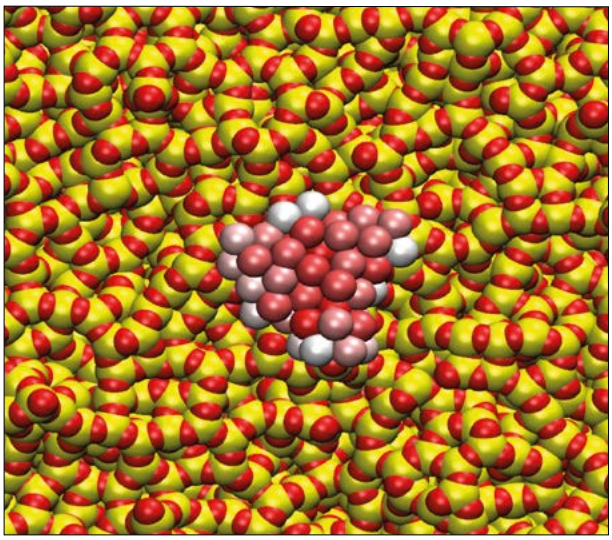
Using the RRZE's Meggie cluster we were able to create a model for the silica surface. We made a complete study on the diffusion of silver ions in solution and also investigated the diffusion and behavior of silver nanoparticles in solution.

Outreach

The first publication was on the diffusion of silver ions in water solution (The Journal of Chemical Physics 147, 114506 (2017); https://doi.org/10.1063/1.5003654).



Coordination of a Silver Ion on top of a Silicon oxide surface in contact with a water-ammonia solution at pH 10



Charge Distribution in a Silver Particle on top of a silicon oxide surface in Vacuum

Researcher's Bio and Affiliation

Sansotta Stefano obtained his Bachelor and Master degree in chemical engineering at "La Sapienza University of Rome" and is currently a Ph.D. student in the group of Prof. Dr. Dirk Zahn at the Computer Chemistry Centre.

Molecular Simulation studies on Magnetite Collagen Intergrowth

Tina Kollmann

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HPC resources used at RRZE

Emmy cluster

Biominerals are organic-inorganic hybrid materials abundant in nature. They are formed under highly controlled conditions, show complex morphologies and are very often hierarchically structured. An amazing biomineral is the chiton tooth: Magnetite coated teeth which are very hard, resistant and magnetic. To understand the mechanisms of intergrowing of magnetite with the elastic protein collagen MD simulations are performed.

Motivation and problem definition

Modelling biomimetic materials, such as composites of collagen and magnetite, hint at the suitability of the protein to bind iron and hydroxide ions, suggesting that collagen acts as a nucleation seed to magnetite nanoparticle formation, and enables the intergrowth of protein and nanoparticles already at the precursor stage of composite formation.

Methods and codes

The parallel molecular dynamics (MD) simulation software DL Poly is used. Ion Docking to collagen was modeled in aqueous solution using empirical force fields [1,2,3,4,5] and the Kawska-Zahn docking procedure [6].

Association complexes are then immersed in aqueous solution (periodic simulation cell comprising more than 15000 water molecules) and subjected to relaxation from 400 ps molecular dynamics runs at room temperature and ambient pressure. Proton transfer reactions are calculated by QM/MM approaches. Relaxation of the system for another 400 ps at room temperature and ambient pressure in aqueaos solution allows reorganization after switching potentials.

These simulations can be parallelized over several nodes for each trajectory. This makes the project well-suited for the Emmy cluster.

Results

We observed the iron clusters binding over salt bridges to the collagens surface without destroying the triple helical structure of the protein. Iron hydroxides themselves reorganize on the surface into tetrehedral and octahedral motifs trying to form the pursued magnetite crystal structure.

Outreach

This work is published in Adv. Funct. Mater. 2014, 24, 3187–3196 with two more papers being planned.

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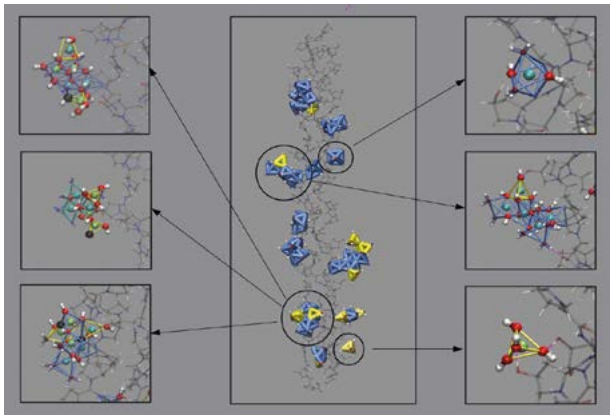

Researcher's Bio and Affiliation

Tina Kollmann obtained her master's degree in Molecular Nano Science at the Friedrich-Alexander-Universität Erlangen-Nürnberg in 2011 and is currently a Ph.D. candidate in the group of Prof. Dr. Dirk Zahn at the Computer Chemistry Centre.

Deactivation of Hazardous Chemicals at Oxide Surfaces

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HPC resources used at RRZE
Meggie cluster

The catalytic deactivation of hazardous chemicals at oxide surfaces is investigated using ab initio Car-Parrinello molecular dynamics simulations in order to explore the largely unknown chemistry of these compounds.

Motivation and problem definition

After World War II, large quantities of highly toxic chemical warfare agents, such as sulfur mustard, were disposed of in the Baltic Sea where they now constitute a major environmental hazard. New fast, secure, and non-destructive methods are required for the decontamination of highly corroded containers, which are nowadays frequently found in fishing nets or at beaches of the Baltic sea. A very promising approach is to use oxides as catalysts for the decomposition of the chemical warfare agents via hydrolysis reactions. In particular ZnO nanorods are promising candidates according to recent experimental work. However, a detailed understanding of the chemical process of defunctionalization at the solid/liquid interface is mostly lacking, as it is close to impossible to perform standard surface science experiments due to the high toxicity of the materials. Yet, basic insights into the reaction mechanisms at the surface are crucial for improving the catalyst performance. For such hazardous materials in silico research can greatly reduce the number of required experiments.

Methods and codes

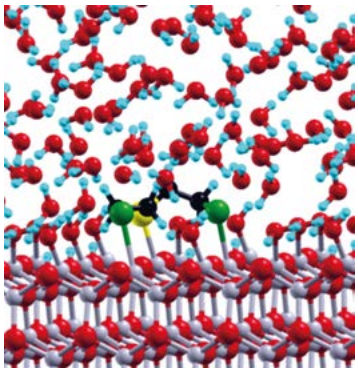
In the first stage of the project, high-throughput static DFT calculations employing the PWscf code (www.quantum-espresso.org) were performed to screen adsorption geometries of sulfur mustard molecules on ZnO surfaces in vacuum. In the second stage, the dynamics and first elementary decomposition steps of the sulfur mustard molecule in liquid water were studied using Car-Parrinello molecular dynamics (CPMD). Finally, the combined system consisting of a ZnO catalyst surface, a sulfur mustard molecule and an explicit water environment is considered. Ab initio CPMD simulations for such large systems (more than 600 atoms and 3300 electrons) became only possible after extensive improvement of the OpenMP and MPI parallelization of the CPMD code, which was done in close collaboration with Gerald Mathias from LRZ München in the framework of a KONWHIR project.

Results

The static DFT calculations provided a basic understanding of the molecule–substrate interactions. By using accelerated molecular dynamics techniques (well-tempered metadynamics), first decomposition steps of sulfur mustard molecules in water could be observed. Calculations of the reaction free energy barriers are in progress. The adsorption of sulfur mustard from liquid water onto the ZnO surfaces is currently investigated using umbrella sampling. Well-tempered metadynamics simulations already provided first insights into the decomposition of pre-adsorbed sulfur mustard molecules on the ZnO surface.

Outreach

This work is supported by the Cluster of Excellence EXC 315 “Engineering of Advanced Materials” (EAM). Additional computer time was provided by a “Summer of Simulation 2017” project of LRZ München. Results of the simulations were presented at the WATOC 2017 conference in München and the annual Spring Meeting of the Deutsche Physikalische Gesellschaft in Berlin. Two publications and a contribution for the Supercomputing Conference SC18 in Dallas, Texas (together with Gerald Mathias from LRZ) are currently in preparation. The simulations will form a major part of Tobias Klöffel’s PhD thesis.



Snapshot from an ab initio molecular dynamics simulation of a sulfur mustard molecule adsorbed at a water/ZnO interface.

Researcher’s Bio and Affiliation

Tobias Klöffel is a PhD student in the group of Prof. Bernd Meyer at the Interdisciplinary Center for Molecular Materials (ICMM) and the Computer-Chemistry-Center (CCC). He studied Chemistry at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) and received his Master’s degree in 2013.

Chemical Functionalization of Oxide Surfaces

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HPC resources used at RRZE

Emmy cluster

The chemical reaction of functional linker molecules with aluminum oxide surfaces in a liquid environment at finite temperatures is studied by ab initio molecular dynamics simulations. The simulations provide a detailed understanding of reaction mechanisms at the solid/liquid interface in which the solvent molecules are actively involved.

Motivation and problem definition

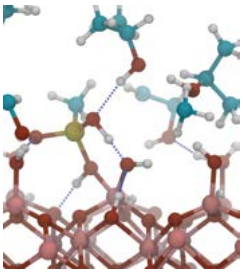
The functionalization of oxide surfaces by molecules plays an important role in many areas, such as nanoparticle synthesis, molecular electronics or in the fabrication of hybrid organic/inorganic solar cells. The attached molecules can protect the underlying surface from chemical attack, they can alter material's properties, e.g., the work function or electron injection barrier, or they can act as functional units themselves, e.g., as the conduction channel in a molecular field-effect transistor. Surface functionalization is mostly done by wet-chemical processes in which molecules are attached by condensation reactions, i.e., by elimination of water molecules. While adsorption of molecules from the gas phase has been studied extensively, mechanisms of chemical reactions at the solid/liquid interface are basically unexplored. Our simulations therefore aim at a first fundamental understanding of the important elementary reaction steps when a molecule from solution binds to a solid surface. In particular, we address the role of the solvent and the impact of the surface structure and composition. For our simulations we have chosen aluminum oxide as substrate, isopropanol as the liquid phase and methylsilanetriol as reactive molecule. This is a typical combination often utilized in experiment.

Methods and codes

For an unbiased description of the chemical processes we use ab initio molecular dynamics simulations, specifically the Car-Parrinello molecular dynamics (CPMD) method and code. CPMD is based on density functional theory (DFT) as the quantum-chemical electronic structure method. Wavefunctions are expanded in a plane-wave basis set and ionic cores are replaced by Vanderbilt ultrasoft pseudopotentials. Van-der-Waals interactions are included by Grimme's D2 correction scheme. A canonical NVT ensemble is established by Nose-Hoover thermostats and the equations of motion for the atoms and the wavefunctions are integrated with the Verlet algorithm. In order to be able to observe chemical reactions ("rare events"), we apply various accelerated sampling techniques, such as metadynamics, thermodynamic integration and umbrella sampling, which also give information on the free energy surface. Typical simulations (about 250 atoms per unit cell) require about 2.1 s for one MD step on ten Emmy nodes, which means that a 100 ps trajectory is obtained in about four weeks.

Results

The chemical binding of methylsilanetriol to the alumina surfaces can be divided into two steps: the coordination of the molecule to the surface and the final condensation reaction. While initial surface coordination is spontaneous in vacuum, it becomes hindered in the isopropanol liquid or in the presence of residual water on the alumina surface. For the condensation reaction we could identify two mechanisms, which differ in the relevant transition state: the reaction either proceeds via formation of a five-fold coordinated Si atom or via formation of an intermediate six-membered ring, involving the Si atom, a surface Al atom and the O atom of the leaving water molecule. The condensation reaction is found to be spontaneous under water-free conditions, but becomes activated in the presence of residual water.



Surface-coordination of methylsilanetriol shown in the six-ring transition state geometry.

Outreach

This work is supported by the Cluster of Excellence EXC 315 "Engineering of Advanced Materials" (EAM). The results were presented at the annual Spring Meeting of the Deutsche Physikalische Gesellschaft and at several EAM symposia. The PhD thesis of Paul Schwarz will be mainly based on the results of these simulations.

Researcher's Bio and Affiliation

Paul Schwarz received his Master's degree in Chemistry at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) in 2013. He is currently a PhD student in Prof. Bernd Meyer's group at the Interdisciplinary Center for Molecular Materials (ICMM) and the Computer-Chemistry-Center (CCC).

Molecular Friction in Graphite Intercalation Compounds

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HPC resources used at RRZE
Emmy cluster

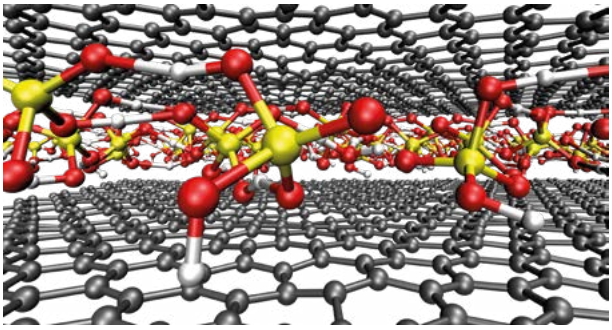
Oxidative wet-chemical graphite delamination is a promising method for large-scale graphene production. Ab initio molecular dynamics simulations show that ideal stacking and oxidation of the graphite layers reduce the friction of sulfuric acid molecules, thereby facilitating intercalation.

Motivation and problem definition

Over the past decade, graphene has attracted a lot of attention in physics, chemistry and materials science due to its outstanding electronic, mechanical and chemical properties. Chemical vapor deposition on a metal substrate is currently the method of choice for preparing large areas of high quality graphene. However, the overall amount of synthesized graphene remains rather small. An alternative process, which has the potential for large-scale graphene production for industrial applications, is the wet-chemical delamination of graphite. A widely used approach is based on the so-called Hummers' method, which comprises the following steps: first, graphite is intercalated by concentrated sulfuric acid. Then, the graphite intercalation compound (GIC) is oxidized. Finally, graphene oxide (GO) layers are separated in solution by hydrolysis and the post-processing of the GO with a reducing agent yields graphene. The overall process, however, is not well understood and is hampered by defect formation. Molecular dynamics (MD) simulations can provide new insights on the atomic scale about how oxidation and perturbations in the graphite lattice influence the overall intercalation process.

Methods and codes

To this end, we performed ab initio molecular dynamics simulations within the Car-Parrinello framework using the CPMD software package. In a recent KONWHIR project Tobias Klöffel, in collaboration with Gerald Mathias from LRZ, significantly improved the OpenMP and MPI parallelization of CPMD. These code modifications clearly boosted the performance, enabling us to treat quite large systems (unit cells with more than 500 atoms) in a reasonable amount of time. For typical simulations on 9 Emmy nodes (180 processes), the improved OpenMP parallelization saved up to 40 % of computer time. Energies and forces were determined from quantum-chemical density-functional theory calculations employing Vanderbilt ultrasoft pseudopotentials, the PBE exchange-correlation functional and Grimme D2 dispersion corrections. The simulations were done in the canonical ensemble close to room temperature conditions by using Nose-Hoover thermostats.



Snapshot from an ab initio molecular dynamics simulation of the sulfuric acid graphite intercalation compound.

A typical simulation for a trajectory of 70 ps requires 700.000 successive MD steps (each taking about 6 seconds on 9 Emmy nodes), resulting in a total simulation time of roughly 7 weeks. From the MD trajectory we determined equilibrium distributions of atoms (which can be converted into free energy profiles), diffusion coefficients, pair correlation functions or the friction coefficient, which describes the resistance for the sulfuric acid molecules to move between the carbon layers of the graphite crystal. It turned out that especially the computation of a converged friction coefficient requires well-equilibrated systems and quite long simulation times of several ten picoseconds.

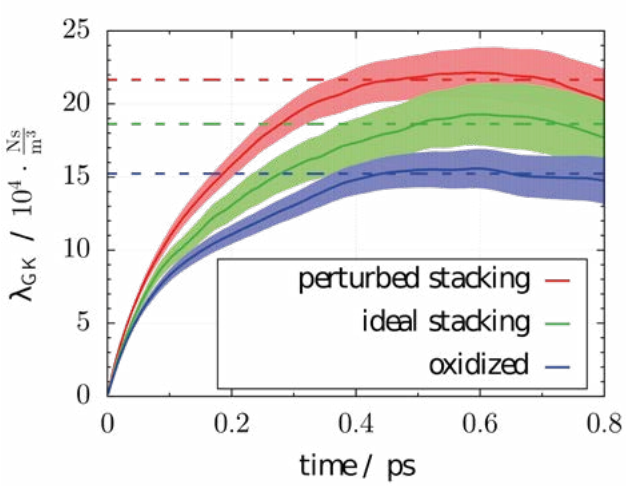
Results

Our main results were obtained from simulations of three model setups of the sulfuric acid graphite intercalation compound. Friction coefficients can be extracted from the plateau value of the Green-Kubo force autocorrelation function (see Figure). The plot shows that friction is significantly lowered in graphites with ideal AB stacking (see green line) and after oxidation (see blue line) as compared to the setup with perturbed stacking of the graphite layers (see red line). These observations are corroborated by the sulfur atom diffusion coefficient and the lateral distribution of the oxygen atoms in the simulation box and they are explained by a detailed analysis of free energy profiles and the electronic structure.

Altogether, we can conclude that the intercalation process strongly benefits from an initial oxidation and a high crystallinity of the graphite lattice. This explains experimental observations on the different behavior of different types of natural graphites.

Outreach

This work has been published in Nature Communications 9 (2018) 836 (DOI: 10.1038/s41467-018-03211-1) and it will be part of Steffen Seiler's PhD thesis. The project is financed by the Collaborative Research Center SFB 953 "Synthetic Carbon Allotropes".



Green-Kubo friction coefficient as function of simulation time for three different GIC model setups.

Researcher's Bio and Affiliation

Steffen Seiler obtained his Master's degree in Molecular Science at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) and he is currently a PhD student in the group of Prof. Bernd Meyer at the Interdisciplinary Center for Molecular Materials (ICMM) and the Computer-Chemistry-Center (CCC).

Quantum criticality of two-dimensional quantum magnets with long-range interactions

Sebastian Fey

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HPC resources used at RRZE

Emmy and LiMa cluster

We investigate the criticality and universality classes of the frustrated and unfrustrated Ising model with long-range interactions in a transverse field. Today, very little is known for these systems in two dimensions, so that we aim to close this gap with our studies.

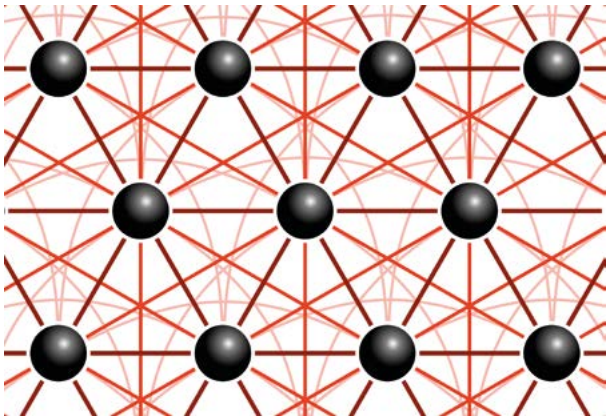
Motivation and problem definition

There are many areas in which long-range interactions become important, although in most studies they have been neglected so far. There are some results for the quantum critical points and universality classes of a one-dimensional quantum Ising chain. However, in two dimension almost nothing is known to date.

Our goal is to shed some light on the question where the phase transition between the polarized and the ordered Z2-symmetry-broken phase happens and what the corresponding universality class is – both for a square and triangular lattice in two dimensions.

Methods and codes

In a new approach we combine a inked cluster expansion method (PCUT) using “white graphs” with classical Monte Carlo calculations to obtain a high-order series of the one-quasiparticle gap. Afterwards Pade and DLog Pade extra-polations allow the extension of the sum’s convergence radius and an extraction of quantum-critical points and exponents.



Graphical illustration of long-range interacting spin-1/2 degrees of freedom.

The series expansion yields a large amount of high-dimensional infinite sums which need to be evaluated to obtain numerical data about the phase transition. These sums are evaluated using classical Markov-chain Monte Carlo integration where these sums can be computed for different seeds in parallel.

For all calculations in-house codes are used.

Results

For the ferromagnetic model on the square and triangular lattice there are three different regimes: The regime around the nearest-neighbor limit shows the nearest-neighbor universality class with the corresponding exponent. For very long-range interactions a mean-field exponent is obtained. In between those areas the critical exponent zv varies continuously when tuning the range of the interaction.

For an antiferromagnetic interaction we find a different behavior. For the complete parameter range the phase transition seems to stay in the nearest-neighbor universality class.

Outreach

Currently we are preparing a paper which we plan to submit to Physical Review Letters. The topic of the project is also a part of the application for an SFB.

Researcher’s Bio and Affiliation

Sebastian Fey is currently affiliated with Prof. Dr. Kai P. Schmidt at “Lehrstuhl für Theoretische Physik I” at the FAU Erlangen-Nürnberg. He studied physics at TU Dortmund and got his Master’s degree on the topic “Field-driven Instabilities of the Non-Abelian Topological Phase in the Kitaev Model”.

Porphyrins on Surfaces and their Electrophysical Properties

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HPC resources used at RRZE

Emmy cluster

Motivation and problem definition

Porphyrins are intensely coloured natural pigments to which we owe the green in our world, and the red in our blood to. Wherever and whenever there is life, some form of this “dye of life” is present. This is not surprising, as they are the key ingredients in a wide diversity of important biochemical reactions. Of particular interest are biological redox processes, such as the conversion of sunlight into chemically stored energy in chlorophyll. It is astonishing that only small variations on the basic structural theme translates into such diverse photophysical properties, while preserving the broad outline of their family.

An important cornerstone for mimicking the efficiency of nature in harvesting and using the energy is to understand the porphyrin interactions. Porphyrins interacting with surfaces are already used successfully in various applications such as surface catalysis, lighting and energy harvesting [1-5]. Research regarding porphyrin have a huge potential to further improve the efficiency of the devices they are used in, by exploiting the effects seen in biological systems. This will not only lead to biocompatible, environmentally friendly devices, but also the commercial production costs will also be drastically reduced using solution based manufacturing techniques.

Methods and codes

We use an ab initio software package, VASP. VASP is highly parallelized code that can also perform mixed GPU/CPU computations. We perform ab initio canonical ensemble molecular dynamics (MD) calculations in order to understand how the porphyrin interacts with the surface. The electronic structure is described within density functional theory, using various flavours such as hybrid functional HSE06. The long-range tail of the interaction potential is simulated with a variety of different correction schemes. In order to attain chemically meaningful simulation times using ab initio principles, we tune a mixed OpenMP/MPI parallelization scheme in order to minimize the communication between the nodes while attaining a maximum throughput between memory and the CPU. This type of calculation benefits greatly from the presence of GPU accelerator cards. For accessing the quasiparticle levels at a chemical precision comparable with the NIST database, we use GW approximation of Hedin, in particularly we use a variant of sc-GW originally suggested by van Schilfgaarde et al. and implemented in VASP. This is a calculation only possible on a cluster of shared-memory compute nodes with large loacal RAM. We require typically around 8-16 GB of memory per CPU, around 100-200 CPU, and naturally a very fast interconnect between the nodes for this kind of calculations.

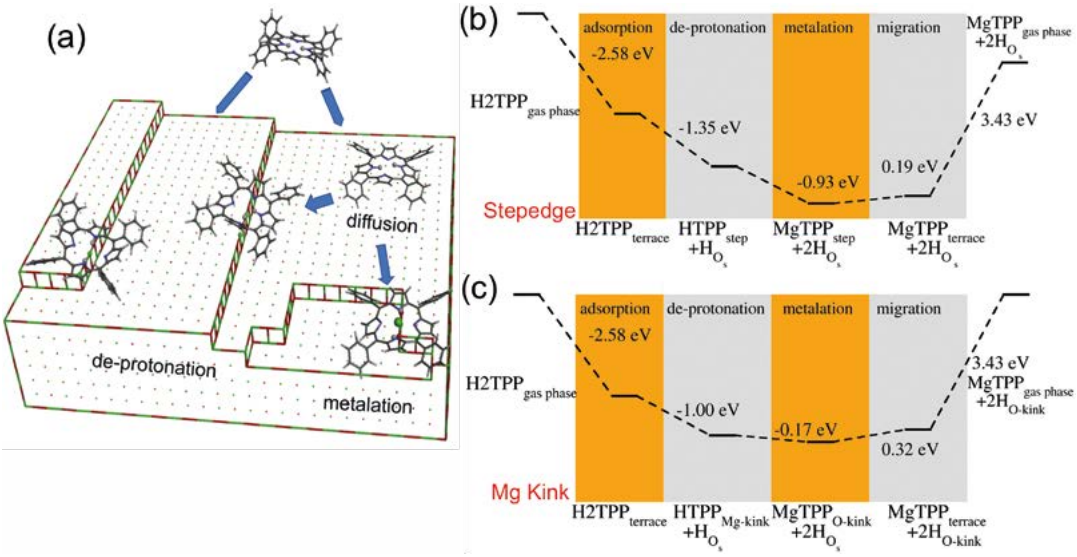


Figure 1: The ab initio molecular dynamics, unlike molecular dynamics using classical force field approximation, allows us to investigate the reactivity of the surface and its defects to porphyrin.

Results

The ab inito molecular dynamics simulations performed at RRZE revealed a pathway where H2TPP self metallates to MgTPP, shedding light to the experiment carried out by our collaborators [6]. In the proposed pathway, the H2TPP gets physisorbed to pristine MgO (100) terrace, migrates to step edges of (100) planes or Mg kink defects due to pedesis, metallates at the defect site, and moves back to MgO (100) terrace as MgTPP. Van der Waals dispersion (DFT-D3) corrections were used to address the free energy contribution. The dynamic hindrance due to phenyl rings explain experimentally observed mobility on the pristine surface [7, 8]. The common MgO (100) defects (the stepedge and the kink) provide the porphyrin with reactive anchor points. When porphyrin encounters such a defect, it rapidly deprotoniates, similar to what is observed in the TiO2 surface [9]. The metalation to MgTPP on these sites is energy driven, and once metallated, the barrier of MgTPP migrating back to the pristine (100) terrace is low.

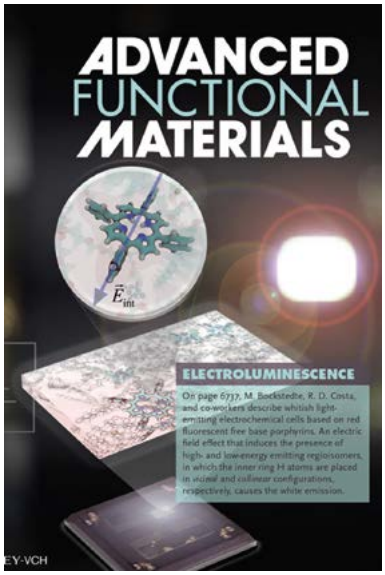
The scGW method is a many body perturbative method which is capable of producing chemically accurate (calibrated against NIST) quasiparticle levels. Our comparative analysis of the UPS experiment performed by the Funcos group [10] involved various isomers, conformers, and oligomers of H2TPP and MgTPP. We have found a possible supramolecular network which aligns perfectly with the features seen in the experiment. This supramolecular network exhibits various interesting effects that can easily be used in various commercial applications, most significantly dispersive bands. Such dispersive bands explain increased electroluminescence efficiency recently reported [11].

An all-organic, white light emitting device is an important goal in industry both due to economic and environmental reasons. Although H2TPP shows superior electrochemical and photophysical features compared to ZnTPP which has a Zinc atom core, ZnTPP performs better as a typical electroluminescent device. Our collaborators Ruben et al. found out that all organic H2TPP embedded in a matrix feature an unexpected yellowish white EL [12]. Since no degradation upon both charge injection and transport and/or difference in the device mechanism were noted, they postulated a change in the nature of the emitting excited state in H2TPP devices under electrical stimuli. We identified a tautomerization effect that explains the device data they measure. External electric fields have a profound impact on H2TPP while ZnTPP features no change as evidenced by device polarizability. We explain this by the induced local fields, creating a vicinal H2TPP tautomer, where hydrogens of the macrocycle align to counteract the induced local field.

Outreach

The results of these works are presented as oral contributions in APS march meeting 2017, DPG 2016, ECOSS 32 and as posters in PSI-K 2017, and in various departments. Furthermore, one of the publications was selected as the frontispiece of Advanced Functional Materials.

This project is part of the DFG-funded research group FOR 1878 (BO1851/4-1 till March 2017 and FWF I3385-N34 since June 2017 by FWF Austria, via D.A.CH). Publications that resulted so far from this project:



The paper was selected as frontispiece in Advanced Functional Materials.

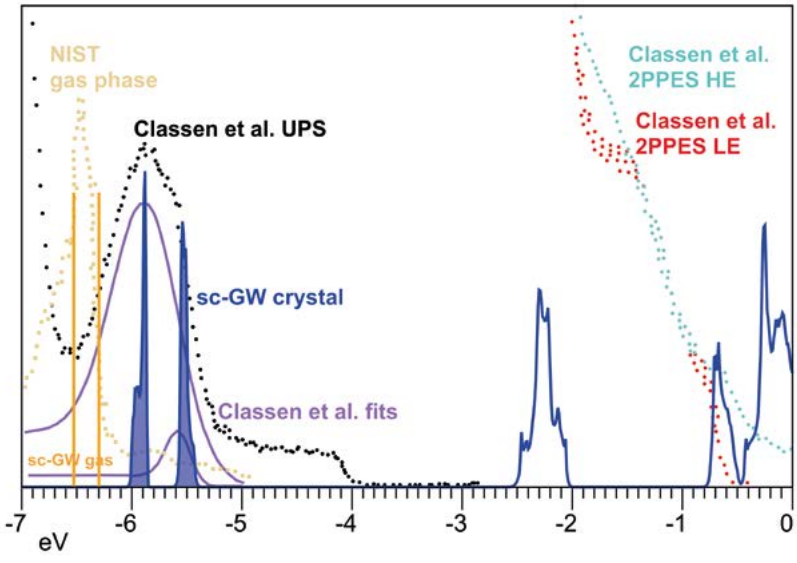


Figure 2: sc-GW calculated quasiparticle levels reproduce NIST calibration data. We have identified a possible supramolecular network on Ag using this method.

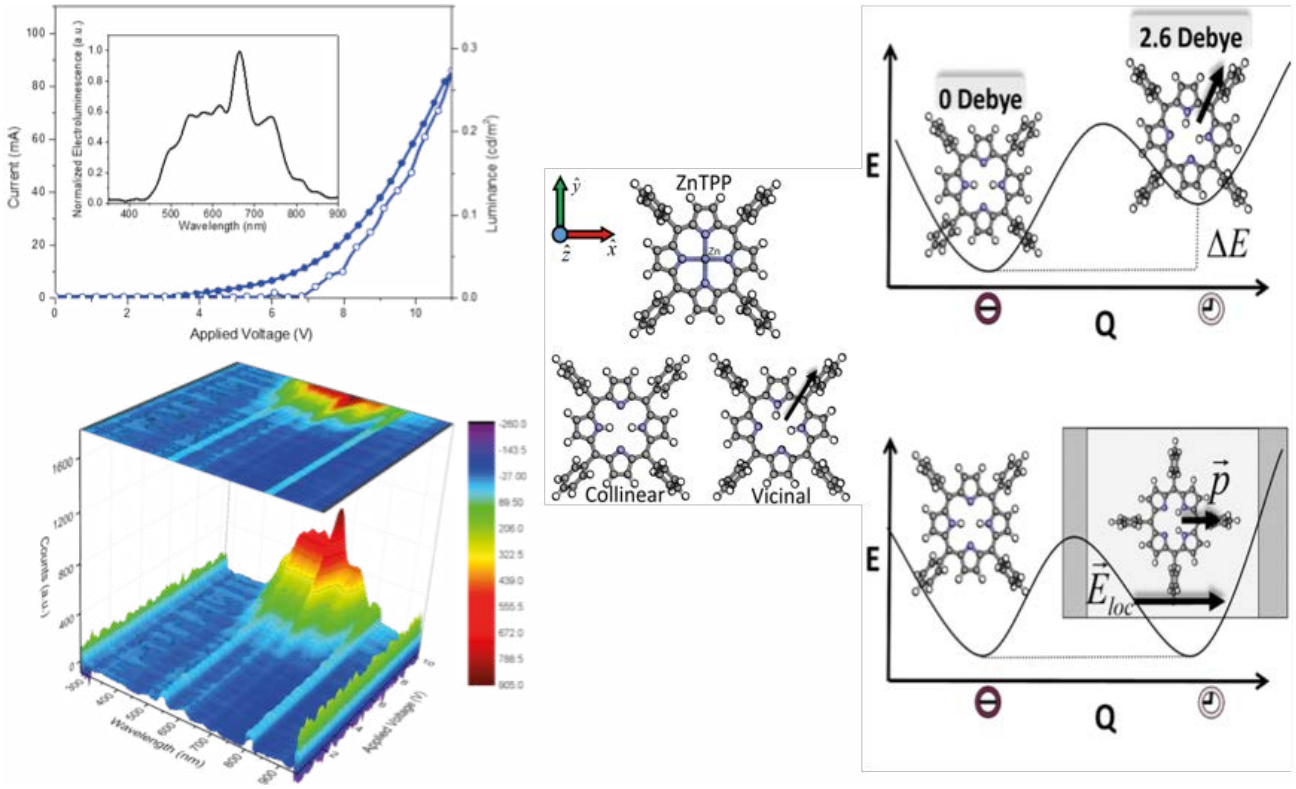


Figure 3: Local field effects cause tautomerization of the H2TPP, leading to electroluminescence above a certain voltage threshold.

Classen, A., et al., Electronic structure of tetraphenyl-porphyrin layers on Ag(100). Physical Review B, 2017. 95(11).

Weber, M.D., et al., From White to Red: Electric-Field Dependent Chromaticity of Light-Emitting Electrochemical Cells based on Archetypal Porphyrins. Advanced Functional Materials, 2016. 26(37): p. 6737-6750.

In preparation: O. B. Malcioglu, Ph. Auburger, M. Bockstedte, Energy driven self-metallation of H2TPP on MgO surface mediated by extended defects.

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Simulations of high energy particle showers

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HPC resources used at RRZE
Woody cluster

Working with Imaging Atmospheric Cherenkov Telescopes to detect very-high energy gamma-rays requires a good understanding of physical and instrumental effects. Therefore, simulations of particle showers, initiated by these gamma-rays, and the instrument response are needed.

Motivation and problem definition

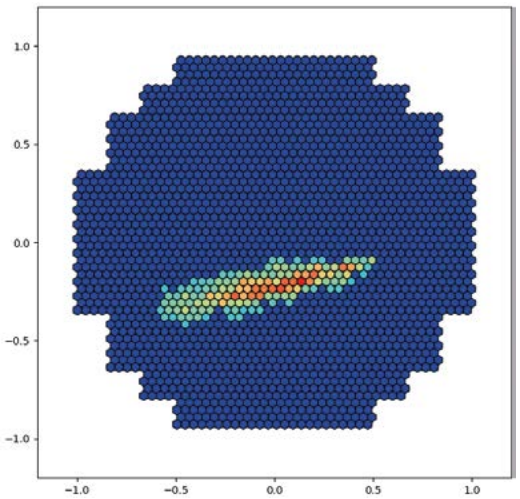
Advancing to the realm of very-high energy astrophysics, way beyond any thermal process, comes with many difficulties and the need of new detection techniques. One way to detect and analyze a special kind of particles, namely very-high energy gamma-rays, is to use so called Imaging Atmospheric Cherenkov Telescopes, like H.E.S.S., the experiment we are part of. The basic idea of a such telescope is to utilize the fact that high energetic gamma-rays do not penetrate the atmopshere but rather develop extensive air showers in it. These showers can be used to detect and investigate the primary gamma-rays and their origin. However, this approach struggles with some uncertainties, in physical effects as well as in instrumental effects. To overcome those uncertainties, simulations of such particle showers and also the corresponding response of the instrument are needed: on the one hand to understand the physics as well as the instrument and to develop and improve our advanced reconstruction techniques and on the other hand even to reconstruct the gamma-rays since any analysis is based on the results of these simulations.

Methods and codes

To simulate and analyze particle showers and our instrument, we basically use three different software packages. For the shower simulations the program “CORSIKA” (COsmic Ray SImulations for KAscade) is used, which is developed and maintained at the Karlsruhe Institute of Technology (KIT) and very well tested within many different experiments. For the response of our instrument H.E.S.S., we work with the software package “sim_telarray” which was developed by Konrad Bernlöhr especially to simulate Imaging Atmospheric Cherenkov Telescopes. Lastly, to analyze the simulated data (and also real data), we use software developed in our collaboration or by ourselves.

Results

The main results we obtained during the last months by using such simulations were energy spectra of other cosmic ray particles than gamma-rays, like electrons or protons which normally are background particles for the instrument. Furthermore, we develop a new analysis approach with neural networks to reconstruct gamma-rays.



Simulated camera image of an atmospheric particle shower induced by a gamma-ray with an energy of 5 TeV as it would be seen by one of the H.E.S.S. telescopes.

Outreach

Tim Lukas Holch, Idan Shilon, Matthias Büchele, Tobias Fischer, Stefan Funk, Nils Groeger, David Jankowsky, Thomas Lohse, Ullrich Schwanke, Philipp Wagner: “Probing Convolutional Neural Networks for Event Reconstruction in γ-Ray Astronomy with Cherenkov Telescopes”, Proceedings of Science – 35th International Cosmic Ray Conference

Additionally, further theses and papers about these simulations are in the pipeline.

Researcher’s Bio and Affiliation

David Jankowsky studied physics at the Friedrich-Alexander-Universität Erlangen-Nürnberg and received his masters’s degree in 2015. Currently he is working as a PhD student in the group of Prof. Dr. Stefan Funk in the field of high-energy astrophysics.

Simulation of the glassy dynamics of soft spheres and colloidal gels

HPC resources used at RRZE

LiMa cluster

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In many particulate systems a dramatic slowdown of the dynamics can be observed upon an increase of the packing fraction or a decrease of the temperature. The systems where such a slowdown of dynamics can be observed are manifold and usually the subject of very different research fields. For example, molecular liquids, colloidal suspensions, or emulsions might form glasses or gels at large densities, polymers during the folding process can end up in frustrated states, electrons in a metal might be almost localized, too many pedestrians can lead to dangerous congestions, and too many cars on a street cause a traffic jam. Though many of these phenomena are already known for a long time, the mechanism leading to the breakdown of dynamics still is the subject of ongoing research.

Motivation and problem definition

In our research project we consider a simple model system of soft spheres that repel each other if they overlap but otherwise do not interact at all. Our goal is to reveal the mechanisms that are associated with the slowdown of dynamics at high densities and low temperatures.

Methods and codes

We modify the protocol that is widely used to study jamming at zero temperature. In this approach the particles are initially placed at random positions. Then the potential energy is minimized by searching a local minimum without crossing any energy barriers. In case there are overlaps in the final configuration of this protocol, one calls the system “jammed” while if all overlaps have been removed, the system is termed “unjammed”.

In order to study glassy dynamics at non-zero temperature, we introduce some random steps in order to mimic the effects of random thermal motion. Therefore, in our approach we employ a protocol that is composed of minimization towards a local minimum as known from studies on athermal jamming and steps where energy barriers can be crossed.

Results

We find a transition packing fraction above which the system can no longer reach the ground states and therefore is effectively non-ergodic. Interestingly, for small but non-zero probabilities to cross energy barriers (corresponding to small but non-zero temperatures) this transition packing fraction does not depend on the probability and is much smaller than the transition density of athermal jamming. The state diagram of thermally jammed and unjammed states as a function of the packing fraction and the probability to cross energy barriers is shown in the figure.

Furthermore, we can analyze the critical behavior of the glass transition, which has turned out to be the same as for a random organization or a directed percolation transition. Note that this critical behavior of a system at small but non-zero temperature therefore is fundamentally different from a system at zero temperature.

Our interpretation of the glass transition as a function of density and at small temperatures is as follows: While at small densities rearrangements can occur locally and the subsequent relaxation is usually fast, above the glass transition density rearrangements may affect the whole system and may occur on a timescale that is (directed) percolated in time. To strengthen our interpretation, we also study the percolation in space as well as the relaxation of a system after an enforced rearrangement event.

Our main results are published in [1] and our protocol is based on the ideas stated in [2].

Related systems

While so far, we have mainly studied monodisperse spheres in 3D, we now also explore the glass transition of a bidisperse system in 2D, of ellipsoidal particles in 3D, as well as of active particles.

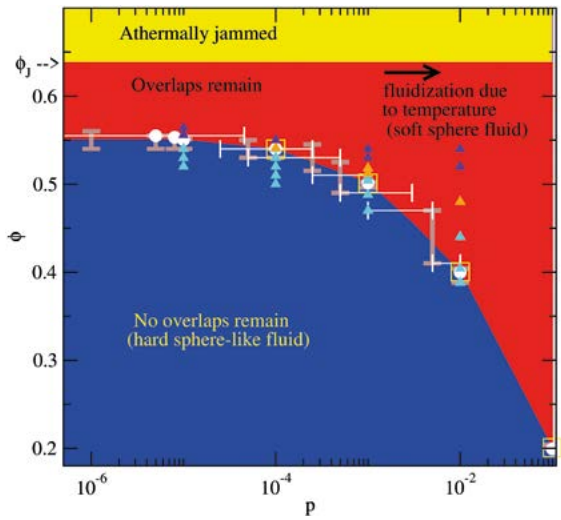
We are also interested in colloidal gels, where in an additional short-ranged attraction between the particles leads to the formation of network-like structures. By using Brownian dynamics simulations, we have discovered, that the solid properties of a gel are related to a directed percolated structure of the gel network [3,4] (cf. press release by the FAU: https://www.fau.eu/2016/06/23/news/research/fau-researchers-show-how-gels-develop-their-solid-properties/).

Conclusions

In our project we employ a new approach to study the glass transition as a function of density. We can analyze the critical behavior and can make predictions on how

the glass transition density depends on temperature. While many other approaches try to study glassy systems in quasi-equilibrium, it is possible with our approach to directly explore the glass transition in full non-equilibrium, i.e., in the way it usually occurs in nature.

We received financial support by the DFG (Grants SCHM 2657/2-1 and SCHM 2657/3-1).



State diagram of soft spheres as a function of the probability p of steps where energy barriers can be crossed and the packing fraction f. It is shown whether a ground state can be reached (blue) or not (red) or whether a jammed state occurs even at zero temperature (yellow). (Image: Moumita Maiti/Michael Schmiedeberg, published in [1])

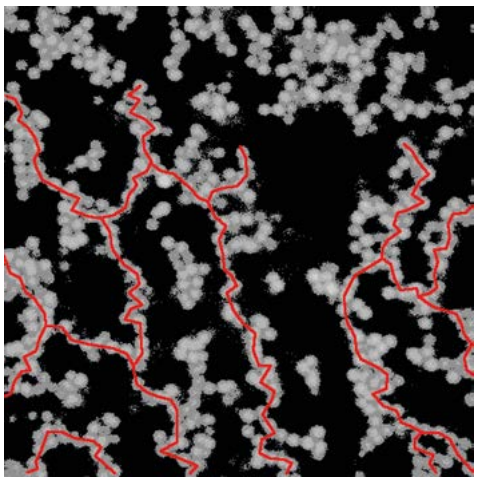


Image of a colloidal gel taken by confocal microsopy. Chains of the gel network are marked in red. (Image: Ronja Capellmann/ Michael Schmiedeberg, cf. results published in [3])

Outreach

[1] M. Maiti and M. Schmiedeberg, Ergodicity breaking transition in a glassy soft sphere system at small but non-zero temperatures, Scientific Reports 8, 1837 (2018).

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[3] M. Kohl, R.F. Capellmann, M. Laurati, S.U. Egelhaaf, and M. Schmiedeberg, Directed percolation identified as equilibrium pre-transition towards non-equilibrium arrested gel states, Nature Communications 7, 11817 (2016).

[4] M. Kohl and M. Schmiedeberg, Shear-induced slab-like domains in a directed percolated colloidal gel, Eur. Phys. J. E 40, 71 (2017).

Researcher's Bio and Affiliation

Michael Schmiedeberg studied physics in Konstanz, Kaiserslautern, and at the Yale University in New Haven (USA). For his PhD on the theory of soft colloidal quasicrystals he was in Konstanz, at the Max-Planck-Institute for Dynamics and Self-Organization in Göttingen, and at the TU Berlin where he finished his PhD in 2008. As a postdoc, he worked at the TU Berlin, the University of Pennsylvania in Philadelphia (USA), and at the Heinrich-Heine-Universität Düsseldorf where he was the principal investigator of an Emmy-Noether Junior Research Group. Besides soft colloidal quasicrystals, he is interested in colloidal structures on substrates, glassy dynamics, jamming, anomalous diffusion, and the motility of bacteria. Since fall 2015 Michael Schmiedeberg is professor of theoretical physics at the Friedrich Alexander University in Erlangen.

Moumita Maiti was a Postdoc in the group of Prof. Michael Schmiedeberg from 2015 to 2017. She completed her PhD in 2012 in India and has worked as a postdoc in Germany since 2013. At the moment she is a postdoc at the University of Münster.

Investigations on the electric field of the EXO-200 experiment

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HPC resources used at RRZE
Woody cluster

The EXO-200 detector is built to search for the neutrinoless beta decay in liquid xenon. Interactions in the liquid create free charges as well as scintillation light which are detected and used in a reconstruction process in order to find the energy as well as the position of an event. The electric field within the detector was investigated and modified to improve the agreement of events generated from Monte Carlo simulations and data.

Motivation and problem definition

The EXO-200 experiment searches for the neutrinoless double beta decay of ^{136}Xe. To do so, the detector utilizes a time projection chamber (TPC) filled with 200 kg of liquid xenon which is enriched to 80% in ^{136}Xe. An observation of an event would imply physics beyond the Standard Model of particle physics.

A decay event within the TPC deposits its energy in the liquid xenon and ionizes it. A fraction of the so created electrons recombines, which leads to the emission of scintillation light. The remaining charge carriers are able to escape. An electric field is applied to drift these electrons from the cathode at the center of the detector in direction of its end caps. Here, the charge as well as the light is detected, generating two signals which are combined to reconstruct the energy and the position of the event.

A Monte Carlo simulation of the whole detector system exists. The goal of the investigation is to improve the agreement of simulated Monte Carlo and data events, i.e., to change the electric field within the TPC in the simulation in order to better match the spatial distributions of these events. To do so, two approaches were carried out.

On one hand, the FEM model of the electric field was improved to also consider effects on the edges of the detector. On the other hand, data taken with the detector were used to gain information about the shape of the field within the detector. In the following, the focus is on the latter approach since it requires a large amount of computational resources which where provided by the LiMa cluster of the RRZE.

Methods and codes

An analytic function describing the shape of the electric field within the EXO-200 detector is defined. It depends on 20 parameters and is able to directly yield the path an electron at an arbitrary position within the TPC is traveling along. The parameter space is further reduced by setting 17 of them to constant values. The remaining three parameters have a strong influence on the final shape of the field lines and are object of optimization. For a given set of parameters, the simulation of the whole detector is carried out, generating 20 million events and yielding their reconstructed positions in the end. A comparison of the spatial distribution of them as well as of data events is made in order to evaluate how well the function of the electric field matches with the field present in the detector. Since the parameter space is nonlinear, the Nelder-Mead method (also known as downhill simplex method) was chosen for the optimization. A custom implementation in Python is used to provide a flexible code tailored to the needs of the problem.

Results

Due to the complexity of the parameter space, multiple local optima were found. All yielded parameter sets show a good agreement between MC simulations and data. In the end, this does not reveal the true shape of the electric field within the EXO-200 TPC but does provide details about it. The developed method therefore lays the foundations to successively reveal the electric field by performing optimizations on various sets of data.

Researcher's Bio and Affiliation

Sebastian Schmidt received his bachelor's and master's degrees in physics at the Erlangen Centre for Astroparticle Physics (ECAP) and is currently working on his PhD at the chair of Prof. Dr. Anton.

Simulation of flow-induced noise in cars

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HPC resources used at RRZE
large-scale project on Meggie

The complex flow field around a vehicle was analyzed and used in a hybrid fluid-structure-acoustic interaction workflow to determine the interior noise levels inside the passenger cabin.

Motivation and problem definition

The analysis of the acoustic behavior of flow fields has gained importance in recent years, especially in the automotive industry. The comfort of the driver is heavily influenced by the noise levels and characteristics, especially during long distance drives. With the help of numerical simulations, the acoustic properties of a car can be analyzed at an early stage of the development process. In this project, the flow-induced excitation of the structure and the radiation of sound into the passenger cabin is investigated on a simplified car geometry. This fluid-structure-acoustic interaction is solved using a hybrid approach, where a flow simulation is coupled to a separate structural and acoustic simulation.

Methods and codes

For the flow simulation, we use FASTEST-3D, an MPI-parallel finite volume solver that has been developed at the Friedrich-Alexander University Erlangen-Nürnberg since the early 1990s. It is used to solve the laminar and turbulent incompressible Navier-Stokes equations using either a Direct Numerical Simulation or Large-Eddy Simulation approach. It was optimized to increase performance, scalability and flexibility, making it suitable for current high-performance compute clusters.

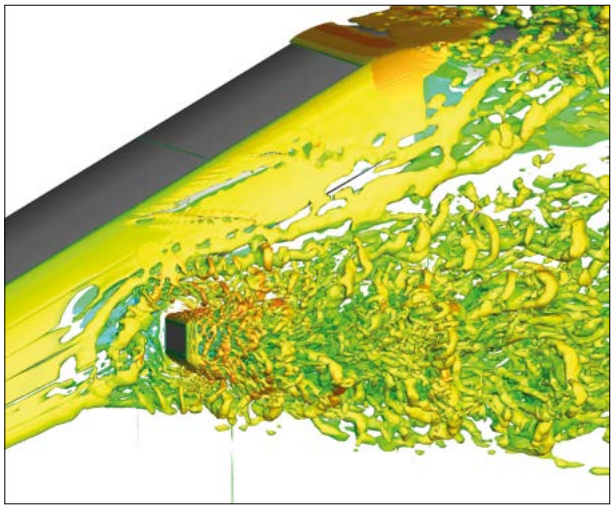
Results

The turbulent flow field around the car model was simulated. Acoustic source terms were computed using acoustic analogies and exported to the structural and acoustic solver together with the hydrodynamic excitation on the structure. With these coupled simulations, it is possible to model the sound radiation into the passenger cabin. Using this approach, we were able to analyze the different excitation mechanisms separately and to investigate the mechanism of sound generation further.

Outreach

Nusser K., Müller S., Scheit C., Oswald M., Becker S.: Large Eddy Simulation of the Flow Around a Simplified Car Model. Direct and Large-Eddy Simulation X, Springer, 2017, S. 243–249 (ERCOFTAC Series, Bd.24), DOI:10.1007/978-3-319-63212-4_30

Becker S., Nusser K., Oswald M.: Aero-Vibro-Acoustic Wind Noise-Simulation Based on the Flow around a Car. SAE Technical Papers (2016), DOI:10.4271/2016-01-1804.



Visualization of turbulent flow structures in the wake of the side mirror.

Researcher's Bio and Affiliation

Katrin Nusser studied Computational Engineering and is now a Ph.D. student in the group of Prof. Dr. Stefan Becker at the Institute of Process Machinery and Systems Engineering.

Axisymmetric Turbulent Boundary Layers

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HPC resources used at RRZE

Emmy & Meggie cluster

The convex transverse curvature effects in wall-bounded turbulent flows were analyzed along a streamwise orientated circular cylinder with a large length to diameter ratio. In such flows an axisymmetric turbulent boundary layer (TBL) develops that can deviate from the planar TBL.

Motivation and problem definition

Turbulent flows that evolve over surfaces with a strong curvature normal to the mean flow exhibit TBL that show different behavior than their well-known planar counterparts, like flat plate or channel flow. A classic research case with a strong transverse curvature is the flow along a streamwise orientated cylinder with a large length to diameter ratio. In flows along such geometries an axisymmetric TBL develops that has a thickness much larger than the cylinder radius. In this kind of flow curvature effects become important, leading to changes in TBL properties, especially on mean velocity profiles and turbulent fluctuations. These changes cause higher skin friction coefficients, different characteristics of wall pressure fluctuations and higher anisotropy in the near-wall flow.

Methods and codes

The open-source code OpenFOAM (5.0) was employed for the simulations. Several LES models were utilized to compare differences in the outcome. Among them are the Smagorinsky and One-Equation model with Van-Driest wall damping and the Wall-Adapting Local Eddy-Viscosity (WALE) model. A finite volume formulation was used with fully orthogonal O-type grid with up to $15 \cdot 10^6$ control volumes.

Results

Resulting mean velocity profiles, turbulent fluctuations, skin friction coefficient and TBL thickness are in good agreement with limited literature data. LES models show different results but none deviates significant from validation data. Gathered data can now be used as groundwork for further detailed investigations and the clarification of open research questions in connection with convex transverse curvature effects in wall-bounded turbulent flows.

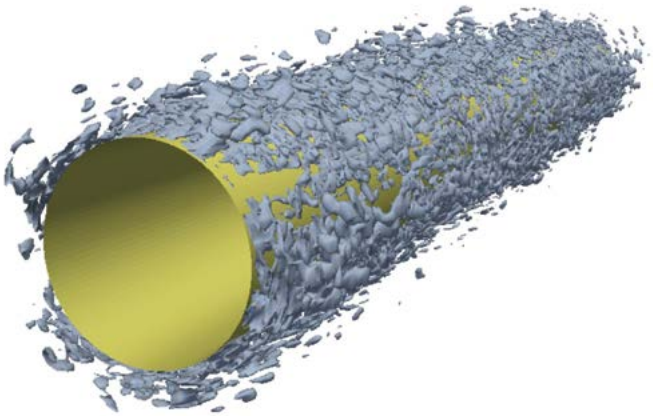
Outreach

Nusser K., Müller S., Scheit C., Oswald M., Becker S.: Large Eddy Simulation of the Flow Around a Simplified Car Model. Direct and Large-Eddy Simulation X, Springer, 2017, S. 243–249 (ERCOFTAC Series, Bd.24), DOI:10.1007/978-3-319-63212-4_30

Becker S., Nusser K., Oswald M.: Aero-Vibro-Acoustic Wind Noise-Simulation Based on the Flow around a Car. SAE Technical Papers (2016), DOI:10.4271/2016-01-1804

Researcher's Bio and Affiliation

Katrin Nusser studied Computational Engineering and is now a Ph.D. student in the group of Prof. Dr. Stefan Becker at the Institute of Process Machinery and Systems Engineering.



Visualization of turbulent flow structures around a streamwise oriented circular cylinder.

Direct numerical simulation of miscible flows

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HPC resources used at RRZE
large-scale project on Meggie

For the first time, direct numerical simulation of the mixing process underlying liquid anti-solvent precipitation in a T-mixer at operating condition is performed, which involves non-constant density and viscosity mixtures.

Motivation and problem definition

Liquid anti-solvent precipitation (LAP) is a basic and promising, but not well understood, pharmaceutical manufacturing process of drugs. The outcome in the form of drug nanoparticles is primarily controlled by mixing of solvent (e.g., ethanol) and anti-solvent (water). The industrial need for computational tools predicting in advance the yield dramatically increased in recent years. The first essential step to fulfill this demand includes the understanding of the mixing process in a micromixer under operating conditions. We do so by applying the most precise tool to prescribe turbulent flows, direct numerical simulation. We consider water-ethanol as one anti-solvent/solvent couple and study the mixing process in a T-mixer from Stokes flow up to operating conditions at which strong spatiotemporal turbulent motion is present.

Methods and codes

We employ a second order finite volume scheme in space (collocated arrangement) and an explicit low-storage Runge-Kutta scheme in time. The convective term in the convection-diffusion equation is discretized with a TVD scheme and flux limiter to preserve almost second order and a bounded solution for very high Peclet numbers.

We use the code FASTEST(a block-structured finite volume code) developed at the Institute of Fluid Mechanics at FAU (LSTM).. All missing routines to address this task have been implemented.

Spanning a Reynolds number range from 1 to 5000 in a T-mixer which demands between several thousands up to 250 million control volumes, highly parallel computing, in particular at high Reynolds numbers, is necessary to obtain statistics in an acceptable runtime.

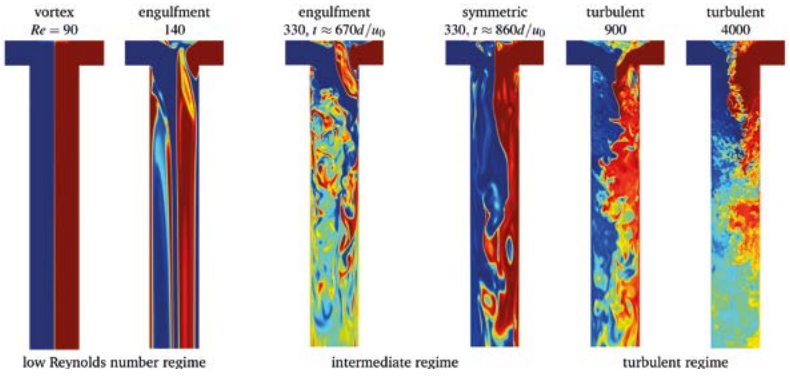
Results

We identified and understood the appearance of several new mixing regimes (hysteresis, the transitional regime, and asymptotic state) in a T-mixer for a water-water and water-ethanol mixture.

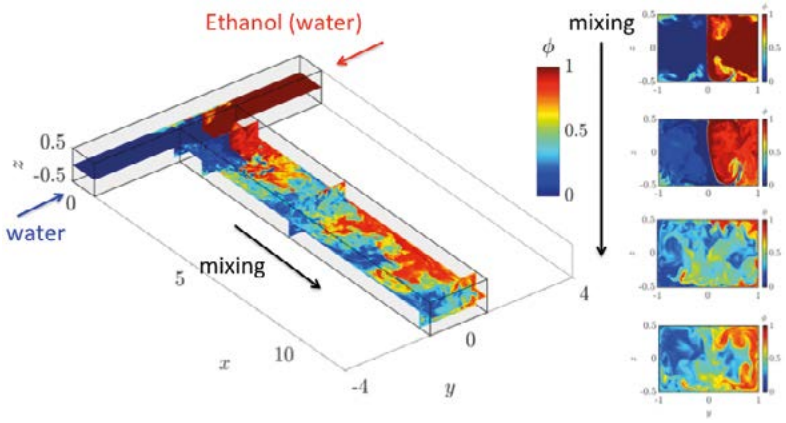
We highlighted the similarities and differences between mixtures having constant or concentration-dependent physical properties.

A comparative study between experiments and simulation showed good agreement, and we could give new insights into the experimental mixing characteristics.

The T-mixer appears to be a novel system to study decaying turbulence from a fundamental point of view, as the turbulence decay obeys power laws similar to other fundamental systems just as grid-generated turbulence.



Instantaneous snapshots of passive scalar φ at cross section z = −0.25 illustrating the mixing regimes occurring as the Reynolds number is increased (from left to right). In particular, a raise of the energy input (Reynolds number increase) doesn't necessarily imply an improvement in mixing as intuitively thought. More surprisingly, in a certain Reynolds number regime (intermediate) the flow switches continuously between good and bad mixing state as time evolves.



T-mixer geometry (grey-shaded) showing an instantaneous snapshot of passive scalar φ at Re = 2000, illustrated by four yz– cross sections and one xy–cross section. Two miscible fluids (red and blue color) collide in the junction and mix along the outlet channel (greenish color) due to the arising turbulence. The strong folding and stretching of the interface by turbulent motion is key to achieve fast mixing for mixtures with very small diffusion coefficients

Outreach

This project is a subproject of the EAM-BTS project "Bioavailability optimization for poorly soluble active pharmaceutical ingredients" funded by DFG and Bayer Technology Services.

Researcher's Bio and Affiliation

Tobias Schikarski is a Ph.D. student. From 01.12.2014 to 31.12.2017 he worked at the Chair of Fluid Mechanics (LSTM) under the supervision of Prof. Marc Avila. Since beginning of 2018 he is now at the Institute of Particle Technology (LFG) under the supervision of Prof. Wolfgang Peukert and cosupervisor Prof. Marc Avila.

Conference Poster

Schikarski, Peukert, Avila: Hydrodynamic mixing of miscible flows in a T-micromixer, Particle Simulations, Erlangen 2015.

Conference Talk

Schikarski, Peukert, Avila: Hydrodynamic mixing of turbulent miscible flows in a T-micromixer under real operating conditions, European Fluid Mechanics Conference, Sevilla 2016.

Schikarski, Peukert, Avila: T-mixer a novel system to investigate decaying turbulence in a wall bounded environment, GAMM, Weimar 2017.

Schikarski, Peukert, Avila: T-mixer a novel system to investigate decaying turbulence in a wall bounded environment, European Turbulence Conference, Stockholm 2017.

Schikarski, Trzenschiok, Peukert, Avila: Mixing characterization of a T-mixer: a full picture, International Congress EAM, Erlangen 2017.

Paper

Schikarski, Peukert, Avila: Direct numerical simulation of water-ethanol flows in a T-mixer, Chemical Engineering Journal 2017.

Schikarski, Peukert, Avila: T-mixer a novel system to investigate decaying turbulence in a wall bounded environment, to be submitted soon to Physical Review Fluids.

Schikarski, Trzenschiok, Peukert, Avila: Mixing characterization of a T-mixer: a full picture, to be submitted soon to Chemical Engineering Journal.

MD Simulation of Liquids with Dissolved Gases

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HPC resources used at RRZE
Emmy cluster

Molecular Dynamics (MD) simulations are used to access various thermophysical properties. Good agreement with corresponding experimental data is found. The predictive capabilities and the insight in microscopic structures make MD simulations a useful tool in thermophysical property research.

Motivation and problem definition

Mixtures containing liquids with dissolved gases are relevant in numerous applications of chemical and energy engineering such as catalytic reaction technologies [1] and separation processes [2]. Accurate knowledge of the thermophysical properties of such systems is necessary for an economical process design and for modelling purposes, but still scarcely available in literature. As an alternative to experiments requiring substantial ressources and effort, MD simulations can help to obtain thermophysical properties efficiently and for substances or thermodynamic conditions, where measurements are hard to realize. In a related research project funded by the German Research foundation (project number DFG FR 11-1), the benefits of MD simulations are applied to get a better understanding of how especially the molecular diffusion process is affected by the characteristics of the mixture components in liquids with dissolved gases.

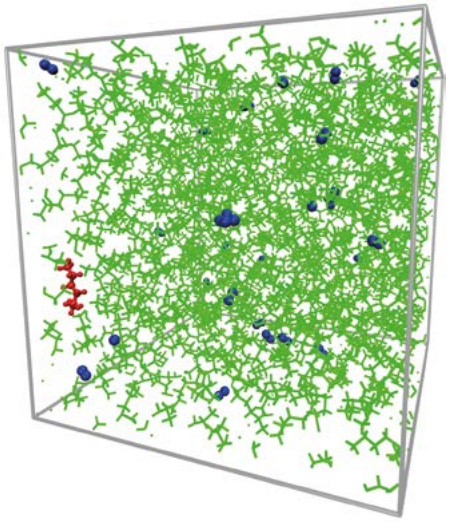

Fig. 1: Snapshot of a binary liquid mixture of n-hexane (green) with dissolved nitrogen (blue) in a simulation box with 525 molecules (i.e. 10,050 interaction sites) at a temperature of 363 K and a pressure of 2 MPa

Methods and codes

In this work, the GROMACS 5.1.2 [3] simulation software is used for performing equilibrium MD simulations of a large amount of interaction sites on the order of about 10,000, see Figure 1. To calculate, for example, densities and radial-distribution functions, corresponding tools included in the GROMACS package are used. On the other hand, for the computation of more sophisticated

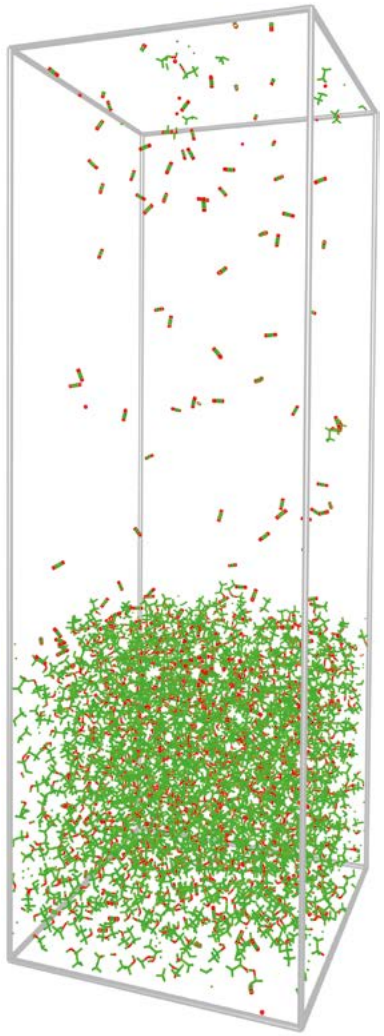

Fig. 2: Snapshot of a vapor-liquid equilibrium for the binary system consisting of ethanol and carbon dioxide (CO_2) at a temperature of 303 K. The partial pressure of CO_2 in the vapor phase was set to dissolve 10 mol-% CO_2 in the ethanol-rich liquid phase, which was reproduced well by our simulations using the chosen force field. Furthermore, good agreement of the simulated interfacial tension with experimental data was found.

properties such as the interfacial tension, dynamic viscosity, Maxwell-Stefan diffusivity, and thermodynamic factor, tailored post-processing tools were developed. Here, mainly FORTRAN codes are used to handle the large amounts of data necessary for calculating properties from statistical fluctuations. Python-based software is employed for fitting and uncertainty analysis. Especially for the performance of production runs and the post-processing, the HPC cluster “Emmy” is used to parallelize the tasks on up to 6 nodes.

Results

In the current DFG-funded project, we are focusing on the prediction of mass diffusion coefficients. For binary mixtures based on n-alkanes or n-alcohols and various dissolved gases at infinite dilution, in line with theory we obtained very good agreement between the self-diffusivities from MD simulations and own experimental data for the Fick mutual diffusivity obtained by dynamic light scattering. Furthermore, first investigation of the Fick mutual diffusivity, which can be accessed by MD simulations from independent calculations of the Maxwell-Stefan diffusivity and the thermodynamic factor, showed that also the concentration dependency of the mutual diffusivity can be described well by the simulations in comparison with the experimental data. The same statement is valid for further studied properties given by the viscosity and interfacial tension of binary mixtures of liquids with dissolved gases, see Figure 2. In all cases, the resources provided by the Emmy HPC cluster at RRZE helped to provide reliable data with low uncertainties, a fact which is necessary in order to judge about the capabilities of MD simulations.

Outreach

A first paper reporting about our aforementioned findings and entitled “Mutual and Self-Diffusivities in Binary Liquid Mixtures of n-Alkanes with Dissolved Gases at Infinite Dilution” was submitted on the 22th of January 2018 to The Journal of Physical Chemistry B and is currently under review. At least two further papers connected to the current research project are planned. Furthermore, we presented results at the Diffusion Fundamentals VII 2017 in Moscow, the 21st European Conference on Thermophysical Properties 2017 in Graz, and the Thermodynamik-Kolloquium 2017 in Dresden.

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Researcher’s Bio and Affiliation

Tobias Klein obtained his Master of Science (M.Sc.) degree in Energy Technology at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). Since April 2016, he is working a doctoral candidate in the Institute of Advanced Optical Technologies – Thermophysical Properties (AOT-TP) under supervision of Prof. Dr.-Ing. habil. Andreas P. Fröba.

DNS of Fluidized Beds with LBM

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HPC resources used at RRZE
Emmy cluster

A series of particulate flows at microscopic level were simulated to learn about their fluid dynamics. The results are compared to real life experiments and can ultimately be used to improve macroscopic models.

Motivation and problem definition

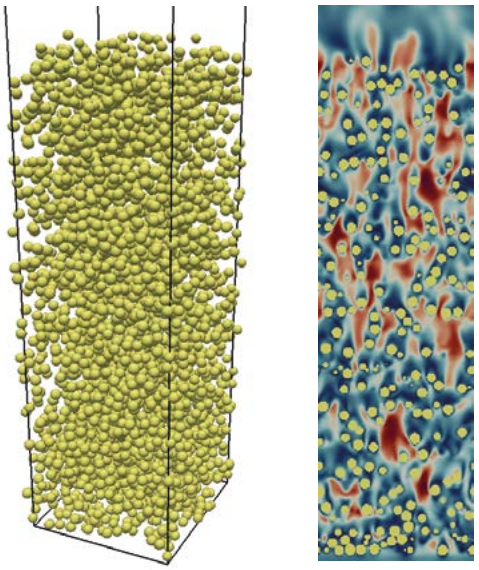
The fluidized bed reactor is a vertical particulate flow and a widespread tool in chemical engineering. Due to its strong intermixing, high contact surface area between solid and fluid phase and frequent collisions it is applicable to combustion, coating, catalytic cracking or drying processes. Coal combustion is still by far the largest power source in India. Improving the efficiency of fluidized bed reactors could save large amounts of natural resources.

Methods and codes

The fluid flow as well as the particle collisions are solved by the waLBerla code, which is developed at the Chair for System Simulation (Computer Science 10) at FAU. It is a strongly parallel, highly optimized framework for solving the Lattice Boltzmann method (LBM) and rigid body collisions. LBM computations are by nature memory-bound. In order to create simulation scenarios that can experimentally be rebuilt, it was necessary to apply several thousand particles and up to 100 million fluid cells.

Results

The simulation results made it possible to gain further insight into the dynamics of fluidized beds. We were able to analyze the effect of physical modelling approaches like the lubrication forces between particles or turbulence models. Furthermore we found a way to improve the numerical coupling at the solid-fluid interface.



Outreach

Master thesis: https://www10.cs.fau.de/publications/theses/2017/Schuster_MT_2017.pdf
Presentation at DSFD 2017 (together with Brajesh Singh)

Researcher's Bio and Affiliation

Dominik Schuster graduated in Computational Engineering at the FAU Erlangen-Nürnberg. After working in the team of Prof. Ulrich Rüde, he is now working on his PhD at CERFACS and IMFT in Toulouse, France.

Efficient Simulation of Nano Structures in Solar Cells

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HPC resources used at RRZE

Emmy cluster

We developed a multicore wavefront diamond blocking scheme with multi-dimensional cache block sharing for our hybrid-parallel (MPI+OpenMP) optical solar cell simulation code utilizing the Time Harmonic Inverse Iteration Method (THIIM) to discretize Maxwell's equations.

Motivation and problem definition

The goal of this project is to study and develop novel approaches to boost the performance of thin film solar cells. For this, 3D optical simulation of the photovoltaic devices is performed by discretizing Maxwell's equations. Efficient light management in solar cells is based on suitable nanostructures of the different layers and materials with optimized optical properties. The design, development and test of new solar cell prototypes with respect to an optimal light management are a time consuming processes. For this reason, suitable models and simulation techniques are required for the analysis of optical properties within thin-film solar cells. However, the introduction of nanostructures makes simulations computationally very intensive, since finer grids and smaller timesteps are required. To obtain simulation results in a feasible amount of time, efficient implementations are necessary.

Methods and codes

In our self developed simulation code we use the Time Harmonic Inverse Iteration Method (THIIM) to discretize Maxwell's equations. The result is a hybrid-parallel (MPI+OpenMP) finite-difference stencil code. The complex nature of the update algorithm (12 vector fields have to be updated per timestep) in combination with high memory requirements (640 Byte per grid cell) result in very high pressure on the main memory bandwidth. To tackle this problem, we developed a multicore wavefront diamond blocking scheme with multi-dimensional cache block sharing scheme (MWD) for our THIIM code [1,2]. By reusing data already loaded from memory the pressure on the main memory bandwidth is reduced and the performance of the simulation is enhanced.

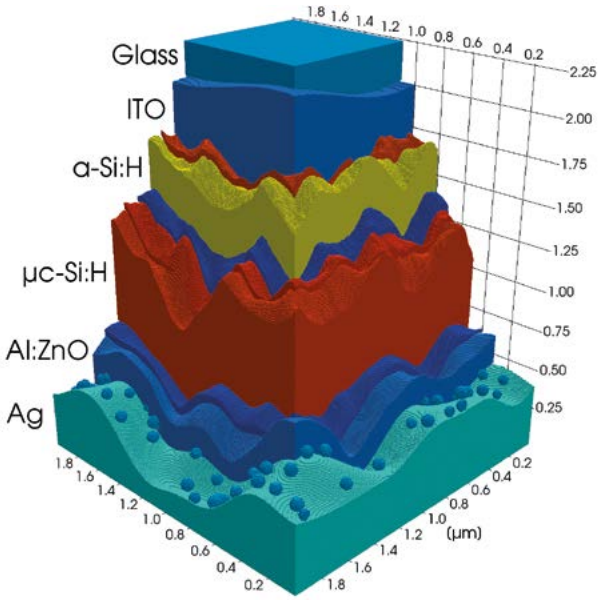
Results

With the implementation of the MWD approach we were able to achieve a single node speed-up of our simulation code of up to 4x on the Broadwell CPUs of the RRZE Meggie cluster, as well as a speed up of up to 2.5x on Skylake CPUs [1]. Furthermore, an efficient parallelization of the MWD approach was implemented, which allows to hide and overlap almost all of the boundary data communication behind the computation of the different MWD diamonds. This results in a very good parallel performance with a 2x parallel speedup on 64 nodes compared to the previous implementation.

Outreach

[1] Julian Hornich, Georg Hager, Christoph Pflaum, Efficient optical simulation of nano structures in thin-film solar cells, Proc. SPIE 10694, Computational Optics II, 106940R (28 May 2018); doi:10.1117/12.2312545

[2] Malas, T. M., Hornich, J., Hager, G., Ltaief, H., Pflaum, C., and Keyes, D. E., Optimization of an electro-magnetics code with multicore wavefront diamond blocking and multi-dimensional intra-tile parallelization, in [2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)], 142-151 (May 2016).



Sample simulation setup: Cross-section of a tandem thin-film solar cell. Textured surfaces are introduced in the solar cell to increase light trapping ability of the amorphous (a-Si:H) and microcrystalline silicon (µc-Si:H) layers. Additionally, SiO_2 nano particles are incorporated at the bottom electrode (Ag) to further increase light scattering.

The authors gratefully acknowledge funding of the German Federal Ministry for Education and Research (BMBF) in the frame of the SeASiTe project as well as the Erlangen Graduate School in Advanced Optical Technologies (SAOT) by the German Research Foundation (DFG) in the framework of the German excellence initiative. We are thankful for the support by the Bavarian Competence Network for Scientific High Performance Computing (KONWIHR).

Researcher's Bio and Affiliation

Julian Hornich graduated in Scientific Computing and Computational Engineering from KTH Stockholm and FAU Erlangen-Nürnberg. After working in the team of Prof. Pflaum at the chair for system simulation at FAU, he is now part of the HPC group of Prof. Wellein.

Topology Optimization of Phononic Band Gaps

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HPC resources used at RRZE

throughput on Woody

Within the Cluster of Excellence "Engineering of Advanced Materials" (EAM) we optimized phononic band gaps in a collaborative project with the Chair of Materials Science and Engineering for Metals (C. Körner), FAU.

Standard topology optimization fails to produce self carrying single phase structures. To this end we developed a shape optimization approach based on topology optimization code.

The obtained designs show relative band gaps up to a value of 6 (upper minus lower frequencies of the gap divided by lower frequency).

Motivation and problem definition

Phononic band gap structures suppress mechanical waves. They belong to meta-materials, which are designed materials with properties not found in nature.

A periodic base cell exhibiting a large phononic band gap is shown tiled 3x3.

Methods and codes

The structural optimization approach is gradient-based optimization based on complex-valued (Floquet-Bloch analysis) eigenvalue problems solved by the finite element method. The optimization solver is commercial (SNOPT), the structural optimization and FEM-Code is self developed (CFS++), the eigenvalue solver is open source (ARPACK).

Band gap problems are known to be non-smooth due to multiple and switching modes. Although we tried to compensate for these issues, the highly complex nonlinear problem formulation with approximately 72 non-smooth eigenvalue based constraints makes it difficult to solve the problems.

However, these problems could be overcome by a multiple-shot approach using RRZE's Woody cluster.

Results

New structures exhibiting phononic band gap behavior have been found.

Outreach

Wormser, M., Wein, F., Stingl, M., & Körner, C. (2017). Design and additive manufacturing of 3D phononic band gap structures based on gradient based optimization. Materials, 10(10), 1125. DOI:10.3390/ma10101125.

Researcher's Bio and Affiliation

Dr. Fabian Wein studied Electrical Engineering and Computation Engineering, his research interests are focused on structural engineering, e.g. optimization of meta-materials or optimization of multiphysic problems.

Recursive Algebraic Coloring Engine

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HPC resources used at RRZE

Emmy cluster

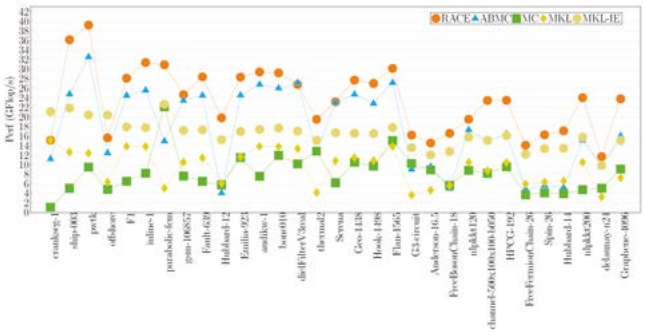
Many iterative numerical methods for sparse systems and important building blocks of sparse linear algebra feature strong data dependencies. The Recursive Algebraic Coloring Engine (RACE) is an algorithm and library that achieves high hardware efficiency for such problems on modern multi-core architectures

Motivation and problem definition

Many sparse linear algebra kernels, such as symmetric sparse matrix-vector multiplication (SymmSpMV) or the Gauss-Seidel iteration, are hard to parallelize due to write-after- write or read-after-write dependencies. We have developed a coloring method that can be seen as an alternative to the well-known multicoloring (MC) and algebraic block multicoloring (ABMC) algorithms, which have the problem that their matrix reordering can adversely affect data access locality. RACE aims at improving data locality, reducing synchronization, and generating sufficient parallelism while still retaining simple matrix storage formats such as compressed row storage (CRS).

Methods and codes

RACE implements a sequential, recursive, level-based algorithm that is applicable to general distance-k dependencies. It is currently limited to matrices with symmetric structure (undirected graph), but possibly nonsymmetric entries. The algorithm comprises four steps: level construction, permutation, distance-k coloring, and load balancing. If these steps do not lead to sufficient parallelism, recursion on sub-graphs can be applied. Using RACE implies a pre-processing and a processing phase. In pre-processing the user supplies the matrix, the kernel requirements (e.g., distance-1 or distance-2) and hardware settings (number of threads, affinity strategy). The library generates a permutation and stores the recursive coloring information in a level tree. It also creates a pool of pinned threads to be used later. In the processing phase, the user provides a sequential kernel function which the library executes in parallel as a callback, using the thread pool.



Performance of symmetric sparse matrix-vector multiplication using 31 matrices on an Intel Skylake Gold 6148 20-core processor, comparing RACE with multicoloring (MC), algebraic block multicoloring (ABMC), and two variants of calling the Intel Math Kernel Library (MKL)

Results

We benchmarked the performance of SymmSpMV for a range of matrices on different CPUs, including the Intel Ivy Bridge chips in Emmy and a Skylake SP in the RRZE test cluster. We compared RACE against ABMC, MC, and MKL implementations. RACE is faster than the alternatives (by up to a factor of 2.5) for almost all matrices, followed by ABMC, MKL, and MC. The advantage of RACE is especially pronounced with large matrices, where data traffic and locality of access is pivotal. One has to be aware that some algorithms may exhibit a change in convergence behavior due to the reordering. This has to be taken into account when benchmarking whole program performance instead of kernels.

Outreach

This work has been submitted as a poster [1] to the ACM Student Research Competition at the SC18 conference in Dallas, Texas, where it ranked #1. A journal publication is in preparation.

[1] https://sc18.supercomputing.org/proceedings/src_poster/src_poster_pages/spost109.html

Researcher's Bio and Affiliation

Christie Louis Alappat graduated with a master's degree in computational engineering from FAU. He is currently doing his Ph.D. here under the guidance of Prof. Dr. Gerhard Wellein. Research interests include performance modelling, sparse matrix algorithms, graph coloring, stencil algorithms and eigenvalue solvers.

Solving MINLPs using Adaptively Refined MIPS

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HPC resources used at RRZE
LiMa cluster

We propose a method for solving Mixed-Integer Non-Linear Programs (MINLPs) to global optimality by discretization of the nonlinearities. The main idea is based on using piecewise linear functions to construct MIP relaxations of the underlying MINLP. We show numerical results in the context of of gas network optimization.

Motivation and problem definition

Many real-world optimization problems can be modeled as an MINLP while both physically and combinatorial aspects are incorporated. Tackling these MINLPs, however, is in general a big challenge. Not only is it hard to find an optimal solution to the problem but also a solution at all. We focus on utilizing fast and robust MIP technology in order to solve these MINLP. Therefore, we develop a framework to solve MINLPs in which any MIP solver can be embedded in a black box fashion.

Methods and codes

We adaptively construct (easier to solve) MIP relaxations of the MINLP by piecewise linear approximations and solve these to global optimality. We proceed until the optimal solution of the MIP is an optimal solution of the MINLP within a given tolerance. Moreover, whenever a feasible solution of an MIP relaxation is found, we fix all discrete variables of the underlying MINLP problem according to the MIP solution obtaining an NLP problem, which we solve to local optimality. In this way, we are often able to find feasible solutions for the MINLP very rapidly. Our method is implemented within the C++ software framework LaMaTTO++ [1]. Furthermore, we use CONOPT3 as the local NLP solver within GAMS [2].

Results

We obtain promising computational results for compressor energy minimization problems based on the GasLib-582 [3] gas network. We model 200 of these problems as MINLPs and compare our results with state-of-the-art solvers like Baron and SCIP (within GAMS). In most cases the relative optimality gaps obtained by our approach are smaller than 0.10 and differ from the relative gaps computed by Baron and SCIP by almost an order of magnitude. Moreover, we obtain near-optimal solutions for instationary gas network optimization problems based on the GasLib-11 gas network.

Outreach

The results are part of the preprints [4] and [5] that are funded by the Sonderforschungsbereich/Transregio 154 “Mathematical Modelling, Simulation and Optimization using the Example of Gas Networks”.

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[2] G.D. Corporation, General Algebraic Modeling System (GAMS) Release 24.8.3, Washington, DC, USA (2017). Available at http://www.gams.com/.

[3] M. Schmidt, D. Aßmann, R. Burlacu, J. Humpola, I. Joormann, N. Kanelakis, T. Koch, D. Oucherif, M.E. Pfetsch, L. Schewe, R. Schwarz, and M. Sirvent, GasLib—A library of Gas Network Instances, Data 2 (2017).

[4] R. Burlacu, H. Egger, M. Groß, A. Martin, M. E. Pfetsch, L. Schewe, M. Sirvent, and M. Skutella. A Global Optimization Approach for Instationary Gas Transport in Pipeline Networks. Preprint, TRR 154, 2017. https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/221.

[5] R. Burlacu, B. Geißler, and L. Schewe. Solving Mixed-Integer Nonlinear Programs using Adaptively Refined Mixed-Integer Linear Programs. Preprint, TRR 154, 2017. https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/151.

Researcher’s Bio and Affiliation

Robert Burlacu studied Mathematics at the Friedrich-Alexander-Universität Erlangen-Nürnberg and received his diploma in 2013. Currently, he is a PhD student in the group of Prof. Dr. Alexander Martin in the field of discrete optimization.

Solo Voice Enhancement for Jazz Music Retrieval

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HPC resources used at RRZE

TinyGPU cluster

Retrieving short monophonic queries in music recordings is a challenging research problem in Music Information Retrieval (MIR). In this study, we present a data-driven approach based on Deep Neural Networks to learn a "salience" representation, which in turn improves the retrieval results.

Motivation and problem definition

In jazz music, given a solo transcription, one retrieval task is to find the corresponding (potentially polyphonic) recording in a music collection. Many conventional systems approach such retrieval tasks by first extracting the predominant F0-trajectory from the recording, then quantizing the extracted trajectory to musical pitches and finally comparing the resulting pitch sequence to the monophonic query. In this project, we introduce a data-driven method that avoids the hard decisions involved in conventional approaches: Given pairs of time-frequency (TF) representations of full music recordings and TF representations of solo transcriptions, we use a DNN-based approach to learn a mapping for transforming a "polyphonic" TF representation into a "monophonic" TF representation. This transform can be considered as a kind of solo voice enhancement. Besides retrieval applications, this TF representation can also serve as a preprocessing step in various other MIR-related tasks involving polyphonic music, such as music transcription or fundamental frequency estimation.

Methods and codes

In our approach, we model the solo voice enhancement step as a regression problem and use a DNN as a regressor. The input to the DNN is the "noisy" TF representation of jazz music recordings including the superposition of the soloist and accompanying musicians (e.g., drums, piano). The targeted output is a TF representation where the soloist is enhanced. As for the labeled data, we use annotated music recordings of famous jazz solos from the Weimar Jazz Database (http://jazzomat.hfm-weimar.de). The network is trained by using a combination of the open-source libraries Theano (http://deeplearning.net/software/theano/) and keras (https://keras.io) which we then run on the tinyGPU cluster.

Results

From the experiments we conclude that in the case of jazz recordings, solo voice enhancement improves the retrieval results. Furthermore, the DNN-based and current state-of-the-art approaches perform on par in this scenario of jazz music and can be seen as two alternative approaches. In future work, we would like to investigate if we can further improve the results by enhancing the current data-driven approach, e.g., by incorporating temporal context frames or testing different network architectures.

A web-based demo is available under the following address: https://www.audiolabs-erlangen.de/resources/MIR/2017-ICASSP-SoloVoiceEnhancement.

Outreach

The International Audio Laboratories Erlangen are a joint institution of the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) and the Fraunhofer-Institut für Integrierte Schaltungen IIS.

This work has been supported by the German Research Foundation (DFG MU 2686/6-1) and published in the following article:

Stefan Balke, Christian Dittmar, Jakob Abeßer, and Meinard Müller: Data-Driven Solo Voice Enhancement for Jazz Music Retrieval, In Proceedings of the IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP): 196-200, 2017. Web-Demo: https://www.audiolabs-erlangen.de/resources/MIR/2017-ICASSP-SoloVoiceEnhancement

In a follow-up work, we adapted a similar architecture to the task of transcribing walking bass lines in jazz music:

Jakob Abeßer, Stefan Balke, Klaus Frieler, Martin Pfleiderer, and Meinard Müller: Deep Learning for Jazz Walking Bass Transcription, In Proceedings of the AES International Conference on Semantic Audio: 202-209, 2017. Web-Demo: https://www.audiolabs-erlangen.de/resources/MIR/2017-AES-WalkingBassTranscription

Researcher's Bio and Affiliation

Stefan Balke studied electrical engineering at the Leibniz Universität Hannover. Since 2014, he is pursuing his PhD under the supervision of Prof. Dr. Meinard Müller (Lehrstuhl für Semantische Audiosignalverarbeitung) at the International Audio Laboratories Erlangen.

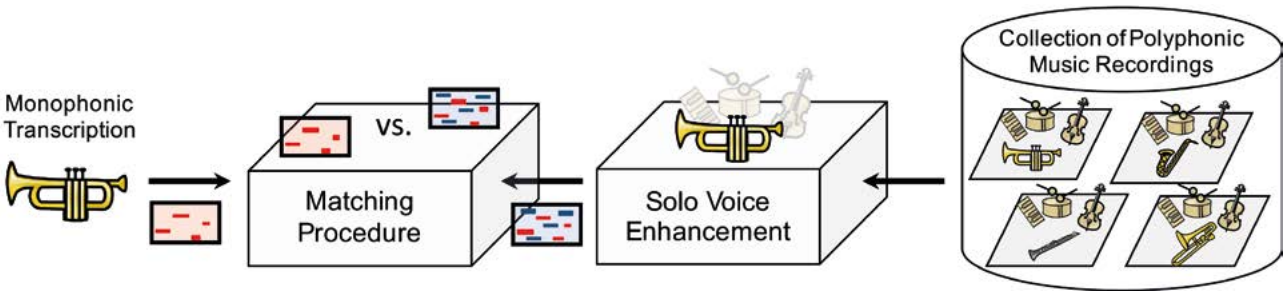

Illustration of the retrieval scenario. Given a jazz solo transcription used as a query, the task is to identify the music recording containing the solo. By enhancing the solo voice, we reduce the influence of the accompaniment in order to increase the retrieval results.

Assessing climate mode impacts on Kilimanjaro

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HPC resources used at RRZE

Emmy cluster

Using convection-permitting modelling and a long observational record, we show that humidity fluctuations above Kilimanjaro correlate more strongly with the Indian Ocean Zonal Mode than the El-Niño Southern Oscillation, with co-occurring in-phase events creating the strongest anomalies.

Motivation and problem definition

Accurate knowledge of the impact of internal atmospheric variability at high altitudes is required for the detection and attribution of climate change and for interpreting glacier records. However, current knowledge of such impacts in high-mountain regions is largely based on statistical methods, as the observational data required for process-based assessments are often spatially or temporally deficient. Understanding the impact of climate modes is required for unravelling the strong retreat of Kilimanjaro's glaciers observed over the 20th century into components due to internal and external (anthropogenic) variability.

Methods and codes

Using a case study of Kilimanjaro, we combined twelve years of convection-permitting atmospheric modelling with an eight-year observational record to evaluate the impact of climate modes on recent high-altitude atmospheric variability during the short rains (the secondary rain season in the region). The atmospheric modelling is done using the advanced research version of the atmospheric Weather Research & Forecasting (WRF) model. The code was developed by, and is maintained by, the National Centre for Atmospheric Research (NCAR; https://ncar.ucar.edu) but bug fixes, code development and physics improvements are contributed by the large community of users. The model is commonly configured with telescoping nested domains, from a large, coarser-resolution outer domain that is forced at its lateral boundaries by a global atmospheric reanalysis, to a finer-resolution innermost domain covering the study area. The model is designed for highly parallel computing.

Results

We examined two modes that have a well-established relationship with precipitation in East Africa, the El Niño Southern Oscillation (ENSO) and the Indian Ocean Zonal Mode (IOZM). Both modes correlate positively with humidity fluctuations, which are key drivers of glacier change, but the association is strongest with the IOZM in the air layers around the glaciers (see Figure), due to changes in zonal circulation and moisture transport, emphasizing the importance of the moisture signal from the Indian Ocean (IO). However, we found the most anomalous conditions during co-occurring positive events, due to the combined effects of extended positive sea-surface-temperature anomalies, enhanced

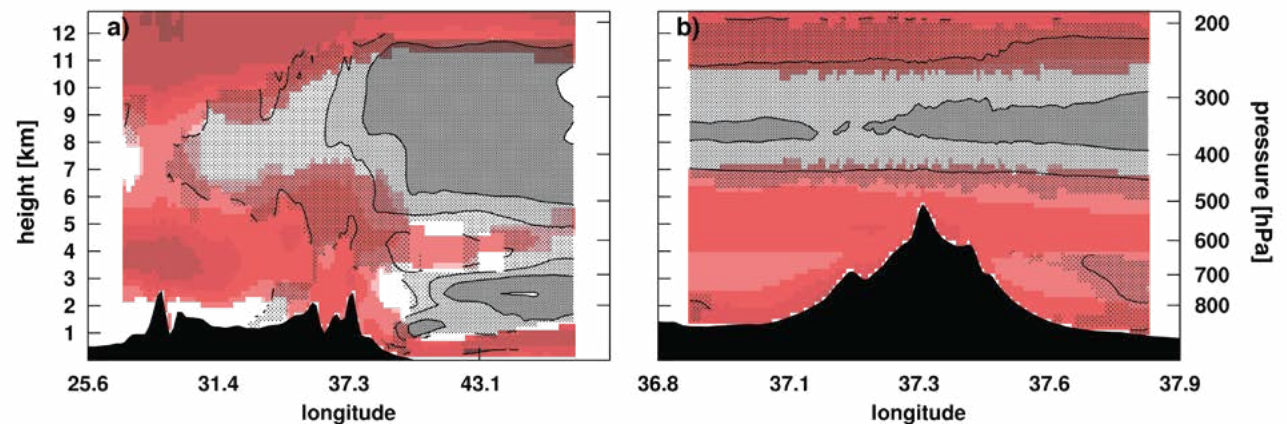
atmospheric moisture capacity from higher tropospheric temperatures, most pronounced weakening of the subsiding branch of the Walker circulation over East Africa, and stronger monsoonal moisture fluxes upstream.

Outreach

The results were presented at the European Geophysical Union (EGU) General Assembly (oral) and the American Geophysical Union (AGU) Fall Meeting (invited, oral) in 2016. The results have been described in a manuscript that is under revision for publication in the Journal of Climate. This research was funded by the DFG Grant No. MO 2869/1-1.

Researcher's Bio and Affiliation

Dr. Emily Collier completed a BSc and a PhD in atmospheric science at the University of Alberta in Edmonton, Canada. Her PhD research was developing an interactively coupled atmosphere-glacier modelling system that includes supraglacial debris for application in the Karakoram. As a postdoc, she has investigated the impact of atmospheric variability in the Nepalese Himalaya (University of Utrecht) and in East Africa (FAU Erlangen-Nürnberg) on mountain glaciers.



A longitudinal cross-section at the latitude of the automated weather station (installed on Kibo summit, Kilimanjaro, in February 2005) of the partial correlation between the Ocean Niño Index (ONI; a measure of ENSO events; shown in color shading) and the Dipole Mode Index (DMI; a measure of IOZM events; shown as pattern-fill shading) at a lag of 2 months for both indices with anomalies of specific humidity in (a) D1 and (b) D3, with 20-km and 800-m grid spacing, respectively, as a function of altitude and pressure.

Westerly circulation signature during High Asia monsoon

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HPC resources used at RRZE

Emmy cluster

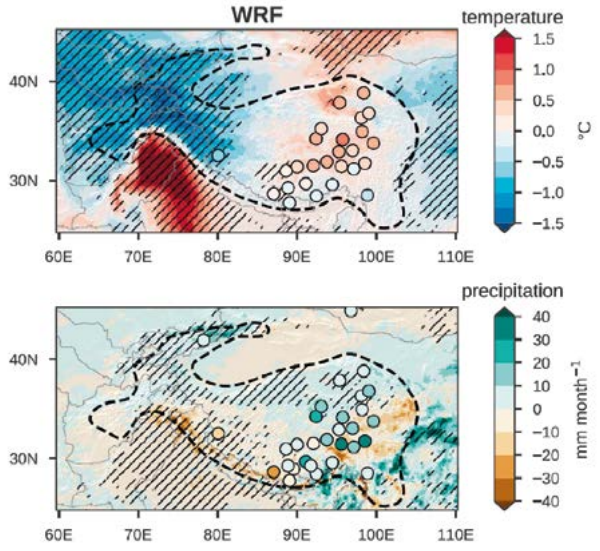
We assess the influence of the mid-latitude westerlies on local surface climates in the reach of the Indian Summer Monsoon and show that a southward shift of the upper-tropospheric westerlies produces two prominent surface dipole patterns in the core monsoon season (July-September).

Motivation and problem definition

High Asia has experienced strong environmental changes in recent decades, as evident in records of glaciers, lakes, tree rings, and vegetation. The multi-scale understanding of the climatic drivers, however, is still incomplete. In particular, few systematic assessments have evaluated to what degree, if at all, the mid-latitude westerly circulation modifies local surface climates in the reach of the Indian Summer Monsoon.

Methods and codes

Our methodology combined reanalysis (observation-based) datasets, station observations, and atmospheric modelling. The atmospheric modelling was done using the advanced research version of the atmospheric Weather Research & Forecasting (WRF) model. The code was developed by, and is maintained by, the National Centre for Atmospheric Research (NCAR; https://ncar.ucar.edu) but bug fixes, code development and physics improvements are contributed by the large community of users. The model is commonly configured with telescoping nested domains, from a large, coarser-resolution outer domain that is forced at its lateral boundaries by a global atmospheric reanalysis, to a finer-resolution innermost domain covering the study area. The model is designed for highly parallel computing.



Climatic anomalies in (top) 2-meter air temperature and (bottom) precipitation during July-September seasons when the westerly wave track is relatively far south, simulated with the WRF model for all relevant seasons between 1980 and 2014. Points indicate station data, stippled areas denote statistical significance (accounting for spatial autocorrelation), and the dashed bold line is the 2000-m elevation contour to delineate High Asia.

Results

We showed that a southward shift of the upper-tropospheric westerlies contributes significantly to climate variability in the core monsoon season (July-September) by two prominent dipole patterns at the surface: cooling in the west of High Asia contrasts with warming in the east, while moist anomalies in the east and northwest occur with drying along the southwestern margins. Circulation anomalies help to understand the dipoles and coincide with shifts in both the westerly wave train and the South Asian High, which imprint on air mass advection and local energy budgets.

Outreach

The results were presented at the European Geosciences Union (EGU) General Assembly (poster) in 2016. The research was supported by the DFG Grant No. MO 2869/1-1 and the results were published: Mölg, T., F. Maussion, E. Collier, J.C.H. Chiang, and D. Scherer (2017): Prominent Midlatitude Circulation Signature in High Asia's Surface Climate During Monsoon. Journal of Geophysical Research Atmospheres, vol. 122, pp. 12,702–12,712, doi:10.1002/2017JD027414

Researcher's Bio and Affiliation

Thomas Mölg received his diploma and doctoral degrees from the University of Innsbruck (Austria). His postdoctoral research took place at Innsbruck, at the University of California – Berkeley, and at TU Berlin. Since 2014, he is Professor of Climatology at FAU Erlangen-Nürnberg. Mölg's research is at the interface of atmospheric and cryospheric sciences and ranges from the weather time scale to the climate of the past 150 years.

MD Simulations of Cracks in Heterogeneous NiAl

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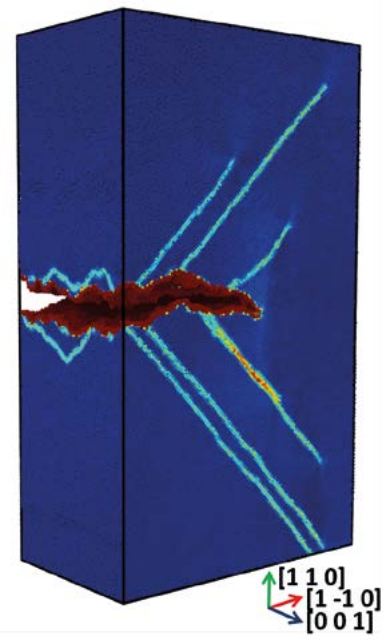
HPC resources used at RRZE

LiMa cluster

Molecular Dynamics simulations were performed to study the influence of heterogeneities on the fracture behavior of brittle intermetallics. Heterogeneities were created at both the atomistic and the mesoscale by varying the composition non-stoichiometric of B2 NiAl and by adding voids.

Motivation and problem definition

The fracture of (semi-)brittle solids is strongly influenced by material heterogeneities located directly at the crack front. Through their elastic interactions with the crack front, heterogeneities can accelerate, decelerate or deviate propagating cracks. In addition, the direct interaction of a propagating crack with heterogeneities can lead to (a) local crack front reorientations, which can lead to the activation of slip systems not available to the initial crack front; (b) changes of the crack front configuration, e.g. blunting, which can cause crack trapping or (c) dynamic perturbations of the crack front, e.g. crack front waves. So far, these effects have not been studied in detail. As fracture is ultimately the result of breaking of atomic bonds, atomistic simulations are ideally suited to study crack-obstacle interactions.



Atomistic simulation of the crack propagation in single crystalline NiAl in the presence of vacancies. Atoms are colored regarding their potential energy.

Methods and codes

We employ mostly molecular dynamics (MD) and statics with semi-empirical many body potentials of the embedded atom method (EAM) type. All simulations were performed with the massively-parallel MD software package IMD (ITAP Molecular Dynamics). Relatively large (8-15 million atoms) simulation boxes are required to minimize finite-size effects in the study of propagating cracks, thus making the use of high-performance clusters necessary.

Results

Using PRZE's Lima cluster, we could increase our sample size and were able to observe crack propagation through heterogeneous material over sufficient distances and time. At the atomistic scale, structural vacancies were shown to facilitate brittle fracture. At the mesoscale, crack propagation could be stopped by the presence of voids by two different mechanisms: the stimulated emission of dislocations and the variation of the local stress state. These results help to better understand and model the influence of microstructure on the fracture toughness of semi-brittle materials.

Outreach

The project contributed to the successful ERC CoG proposal "microKIc" – microscopic origins of fracture toughness and the proposal for a DFG research training group modeling fracture across the scales (FRASCAL). Parts of the project were featured in "Der Herr der Risse: Zerstören für die Wissenschaft", TV report in Franken-Fernsehen (https://www.frankenfernsehen.tv/mediathek/video/der-herr-der-risse-zerstoeren-fuer-die-wissenschaft-2/) and "Sinnvolle Zerstörung", Nürnberger Nachrichten, 17./18. Juni 2017. The results will be the basis for the author's PhD thesis and an according journal publication is in preparation.

Researcher's Bio and Affiliation

Polina Baranova received her Diploma of Specialist (Dipl.-Spec.) in Mechanics at Taras Shevchenko National University in Kyiv/Ukraine. Since May 2014, she is working as a doctoral candidate under the supervision of Prof. Erik Bitzek at the Department for Materials Science, Institute I.

2D study: Influence of the Powder in Additive Manufacturing

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HPC resources used at RRZE
LiMa cluster

The goal of our study is to examine the influence of the powder on a process window for powder fusion based additive manufacturing. The results show, for example, that higher powder bulk densities minimize the probability for binding faults and facilitate the usage of lower beam powers.

Motivation and problem definition

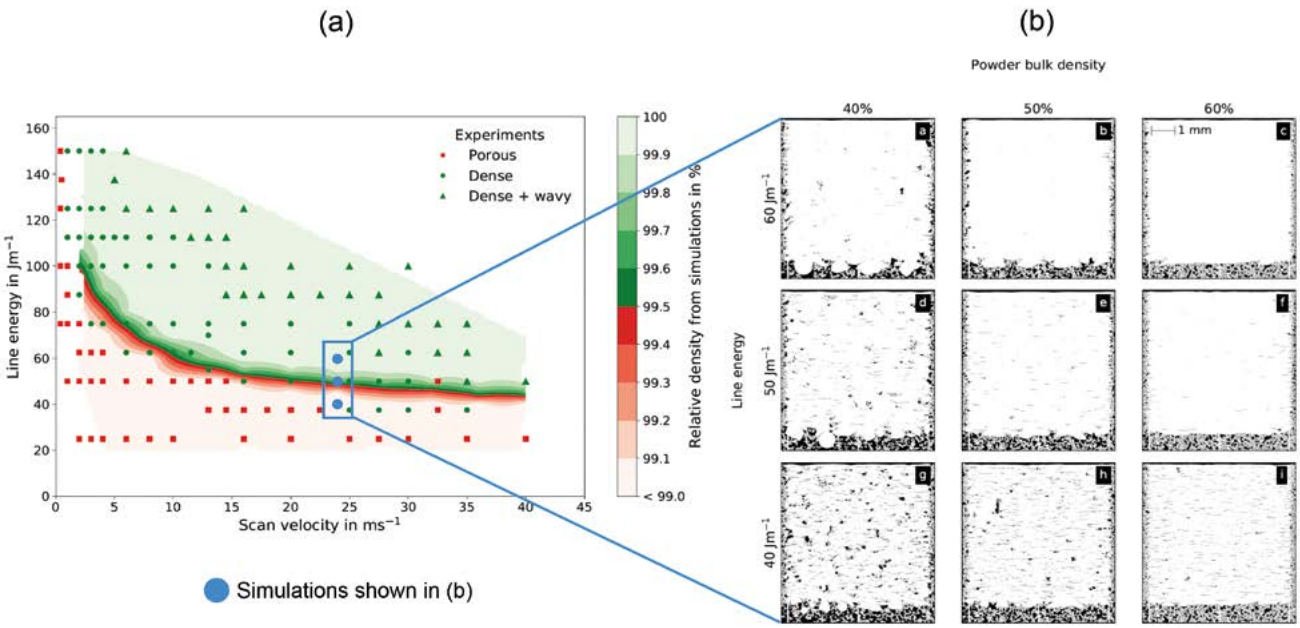
The porosity of parts is a crucial factor for parts that undergo mechanical loading. Especially, powder bed fusion based additive manufacturing techniques like Selective Laser Melting or Selective Electron Beam Melting suffer from residual porosity of built parts. Therefore, process windows can be determined that define the parameter ranges for dense parts. However, effects of the powder on such process windows are harder to quantify experimentally than for example the influence of the beam power. Here, numerical simulations can help to understand the underlying effects of different powder features. A major issue of simulating a whole process window for different additional parameters (as the powder bulk density) is the amount of numerical experiments that are required. A serial computation on one machine is not feasible because of the long simulation times. One simulation can last up to several days. Therefore, throughput-parallel computing using different parameters sets is inevitable to obtain results in an appropriate amount of time.

Methods and codes

The simulations are conducted with the OpenMP parallelized in-house software SAMPLE 2D written in C++. It is based on the Lattice Boltzmann Method and includes powder deposition, beam irradiation, heat transfer, melting, melt pool dynamics and resolidification.

Results

The results shown in the figure indicate that higher powder bulk densities are advantageous to obtain dense parts at lower beam powers.



Process window for Ti-6Al-4V manufactured with SEBM showing the experimental results (symbols) and the numerical results for the relative density (colormap) (a). Samples with a relative density higher than 99.5% are considered as dense. Additionally the influence of different energy inputs (line energies) are shown for different powder bulk densities (b-a – b-i). The parameters used therein are marked in (a) with blue dots. The figures are taken from [1].

Outreach

Rausch, A.M.; Küng, V.E.; Pobel, C.; Markl, M.; Körner, C. Predictive Simulation of Process Windows for Powder Bed Fusion Additive Manufacturing: Influence of the Powder Bulk Density. Materials 2017, 10, 1117. 10.3390/ma10101117.

A second paper for this topic is in progess.

Researcher's Bio and Affiliation

Alexander Rausch received his bachelor's and master's degree in materials science and engineering at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) in 2016. In the same year he started as a PhD student at the Chair of Materials Science and Engineering for Metals (FAU) under the supervision of Dr.-Ing. Matthias Markl and Prof. Dr.-Ing. habil. Carolin Körner.

Impact of parameters on additively built components

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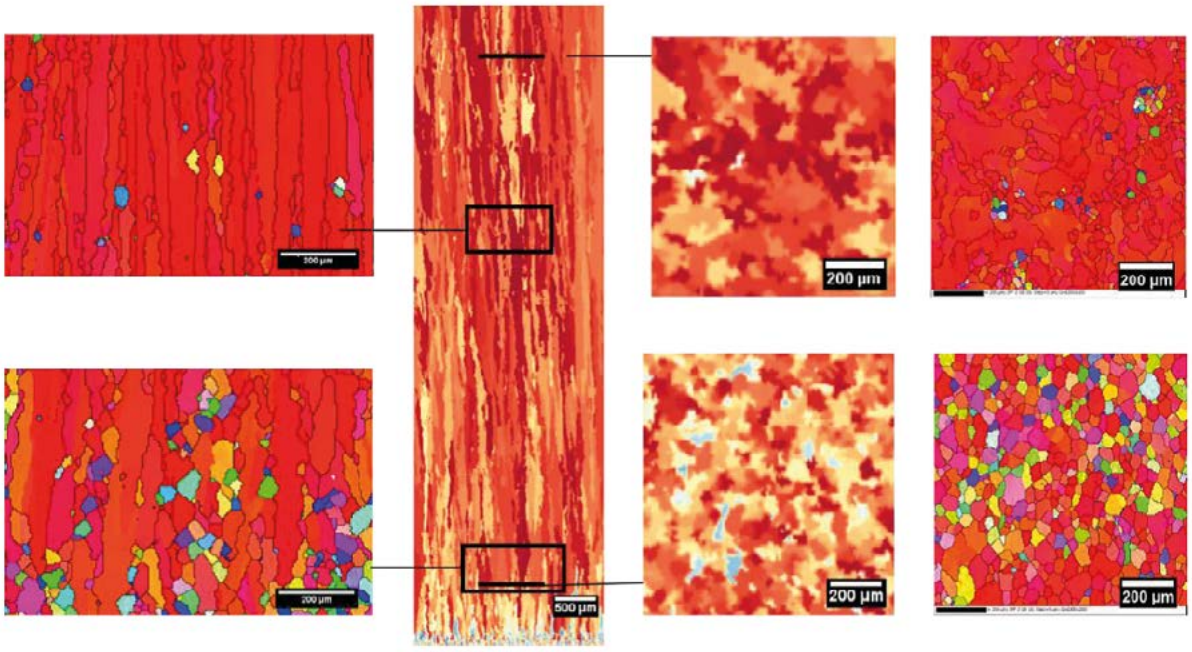
HPC resources used at RRZE

LiMa cluster

The impact of various build parameters on the resulting grain structure of additively built components is investigated numerically. The results enable the tailoring of the microstructure and thus the component properties for individual applications.

Motivation and problem definition

Beam-based additive manufacturing offers huge potential, but also great challenges. One of these challenges is the prediction of the resulting grain structure of the asbuilt part. The grain structure is of special interest because of its enormous influence on the resulting component properties. Fine-tuning grain structure in the manufactured part requires a detailed understanding of the influence of build parameters like power and velocity of the beam as well as different hatching strategies. Numerical simulations enable the prediction of the microstructure resulting from specific beam parameters, dispensing with the need for tedious calibration experiments. The underlying algorithms are extremely computationally intensive, resulting in computation times of several months on a single workstation. Utilization of massively parallel processing on a high-performance cluster computer allows the computation of the grain



Three-dimensional view of the simulated grain structure with a build height of 10mm (left) and comparison of a detailed two -dimensional view of the simulation results with EBSD-measurements taken from the first 5mm of the longitudinal section cut (right)

structure of a part consisting of a huge number of layers within several days.

Methods and codes

The simulations are conducted with the MPI parallelized in-house software SAMPLE3D_GS written in C++. It is based on a cellular automaton grain structure algorithm originally introduced by Gandin and Rappaz. The heat input is calculated using an analytical solution of the transient heat conduction equation.

Results

The figure shows the comparison of a simulated grain structure (center) with EBSD measurements (borders). Both longitudinal (left side) as well as traversal (right side) cross section cuts are in excellent agreement.

Outreach

The project part of the SFB 814 funded by the DFG.
Results of this work have been shown on the following conferences:

International Conference on Additive Technologies: iCAT (2016)

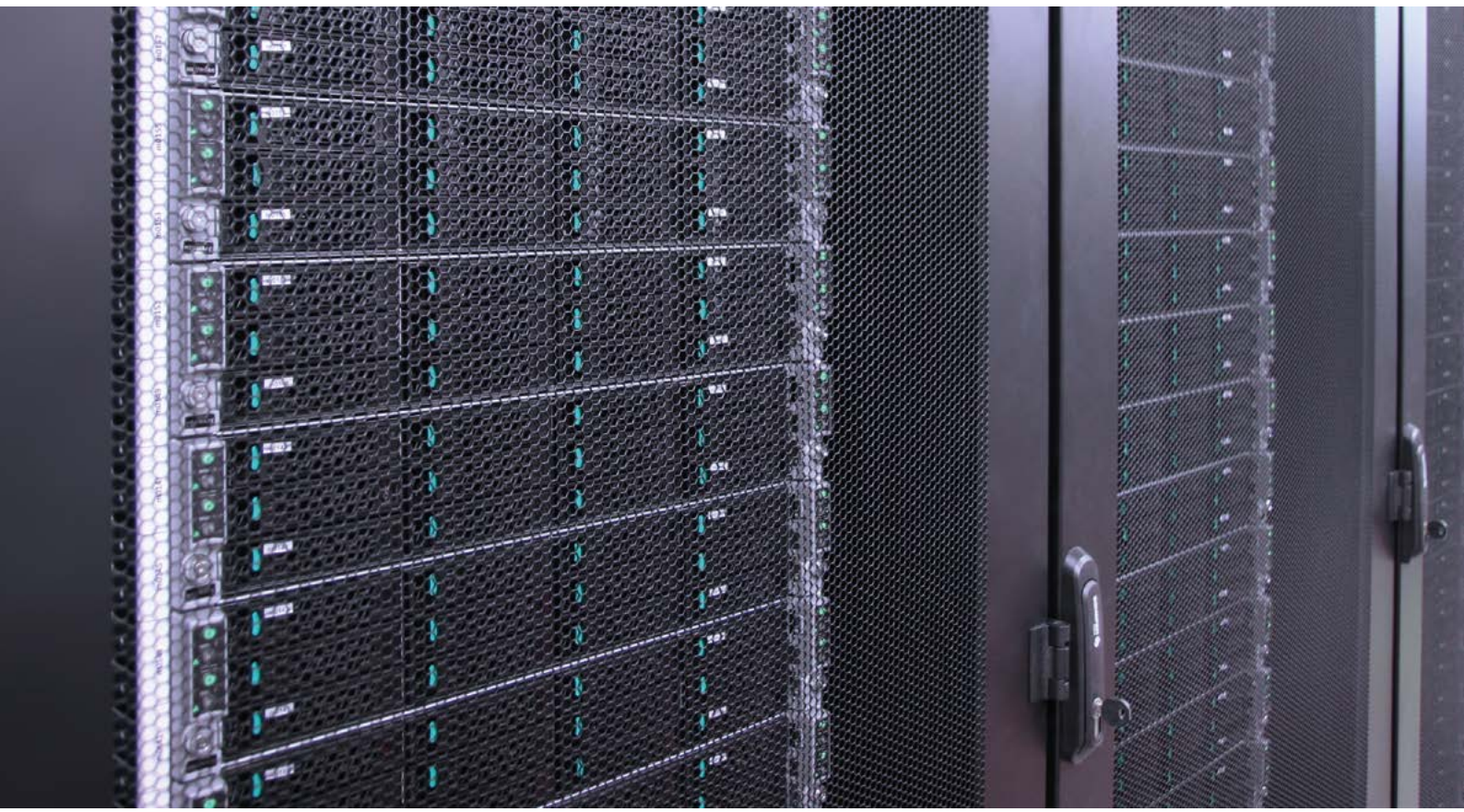
1st ECCOMAS Thematic Conference on Simulation for Additive Manufacturing SimAM (2017)

5. Industriekolloquium des Sonderforschungsbereichs 814 – Additive Fertigung (2017)

A couple of journal contributions on this work are in progress.

Researcher's Bio and Affiliation

Johannes Köpf studied materials science at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) and graduated in 2004. He worked as a project engineer at Neue Materialien Fürth Gmbh (NMF) until 2011 and as research associate at Zentralinstitut für Neue Materialien und Prozesstechnik (ZMP) until 2013. In 2014 he started as a PhD student at the Chair of Materials Science and Engineering for Metals (FAU) under the supervision of Dr.-Ing. Matthias Markl and Prof. Dr.-Ing. habil. Carolin Körner.



Numerical study of laryngeal aerodynamics

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HPC resources used at RRZE

Emmy cluster

Computational fluid dynamics (CFD) is used to simulate the laryngeal aerodynamics during the complicated process of human voice production. The aim of the study is to evaluate the clinical applicability of CFD tools to analyze the phonation process.

Motivation and problem definition

Human phonation process is a result of fluid-structure interaction between laryngeal airflow and the two elastic vocal folds. Owing to the restricted accessibility of the human larynx, experimental investigation of this process is difficult. Therefore, the clinical diagnostics are almost totally restricted to the visual inspection of the vocal fold motion and the acoustic voice signal. The basic purpose of our studies is to investigate the potentials of CFD models in the clinical applications. In addition, different aspects of this process such as various patterns of vocal fold motion and the effect of passive ventricular folds as the second constriction of the larynx are reproduced to analyze the aero-acoustic sound generation.

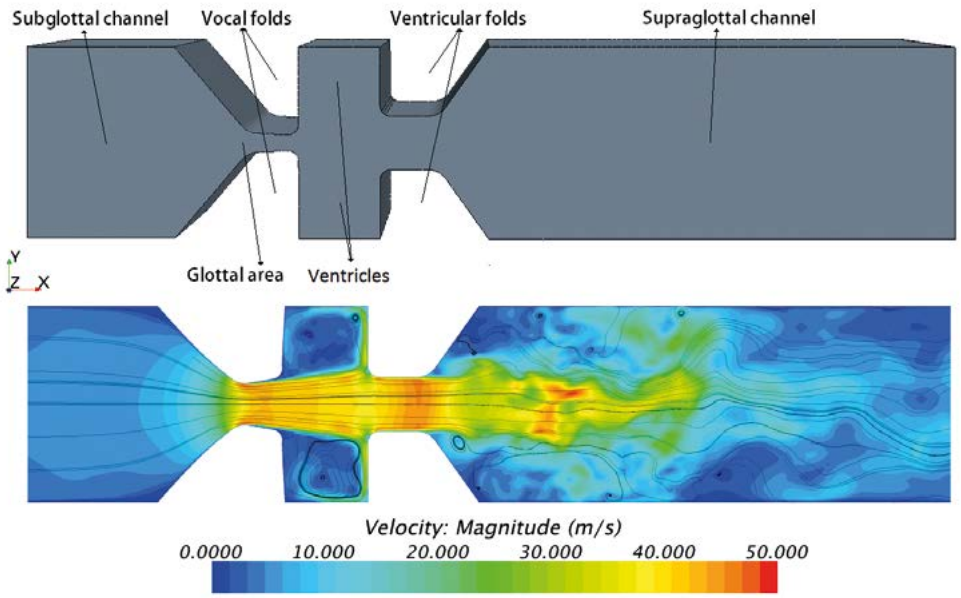
Methods and codes

The unsteady incompressible Navier-Stokes equations are the governing equations of flow motion in the larynx. Large eddy simulations were performed using the finite volume method fully integrated in the commercial software package STAR-CCM+ (Siemens). A simplified three dimensional larynx model with externally imposed oscillations of vocal folds based on an experimental synthetic larynx model is employed. Despite the simplification of the model, the complicated aerodynamics of phonation and consequently the high mesh resolution required in the larynx (between 1.58 and 2.39 million cells) make the use of high performance computing (HPC) systems inevitable. Therefore, five computer nodes of RRZE's Emmy cluster were used to perform the simulations in this study.

Results

Although none of the models simulated in our study, included a coupled fluid-structure interaction process, all of them reproduced characteristic features of laryngeal aerodynamics. These features include the glottal jet deflection in the cases without ventricular folds, intraglottal flow separation in the cases with convergent-divergent mucosal wave motion, fully three dimensional flow effects (such as the axis-switching effect) and finally straightening and elongation of the jet and increasing efficiency of phonation by inclusion of the ventricular folds.

It is worth mentioning that even with the mentioned use of HPC resources, the wall time of the simulations ranged up to more than 200 hours for ten cycles of vocal fold oscillation. Therefore, these models are not applicable in daily clinical routine at the moment, although they are very valuable in basic voice science. The reduction of computational time for these models is one of the goals in our studies.



Schematic of the larynx model and instantaneous velocity magnitude contours with streamlines in the mid-coronal plane.

Outreach

H. Sadeghi, S. Kniesburges, M. Kaltenbacher, A. Schützenberger, and M. Döllinger: Computational models of laryngeal aerodynamics: Potentials and numerical costs, Journal of Voice (Article in press).

The project is running since October 2015. Since February 2018, the study is supported by DFG (DO1247/10-1) and FWF (Prof. Kaltenbacher; TU-Wien) within a joint research project.

Researcher's Bio and Affiliation

Hossein Sadeghi obtained his Master degree in Computational Engineering at the Friedrich-Alexander University Erlangen-Nürnberg (FAU) and is currently a PhD student and scientific assistant under the supervision of Dr.-Ing. Stefan Kniesburges and Prof. Dr.-Ing Michael Döllinger (Head of research) at the division of Phoniatrics and Pediatric Audiology at the Department of Otorhinolaryngology, Head and Neck Surgery of University Hospital Erlangen and Medical Faculty of FAU.

Numerical study on four fin configurations for surfboards

Sebastian Falk

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HPC resources used at RRZE

LiMa cluster

Computational fluid dynamics (CFD) is used to simulate the governing fluid field around surfboard fins and to calculate their fluid dynamical characteristics. The aim of the project is to evaluate the lift and drag forces for different positions of the fins within the four fin configuration.

Motivation and problem definition

Until now, the surfboard shapers' experience highly dominates surfboard development in design and construction. Just recently, the shapers started to use milling machines for the board's fabrication. Nowadays plastics and epoxy compositions are the predominant materials for the fins. Using CFD can not only speed up the development of surfboard and fin design but can also improve the insight into the behavior of the complete surfboard system. The basic idea of our studies is to improve CFD models in order to acquire a knowledge base for the fluid dynamical characteristic of the surfboard system.

Methods and codes

The unsteady incompressible Navier-Stokes equations are the governing equations of flow motion around the surfboard fins. Unsteady Reynolds-averaged Navier-Stokes equations simulations were performed using the finite volume method fully integrated into the commercial software package STAR-CCM+ (Siemens). Four fins are inserted into a simplified three-dimensional rectangular fluid volume, with a defined velocity at the inflow. Despite the simplification of the model, the fluid behavior and consequently the high mesh resolution required around the fins (between 2.0 and 2.2 million cells) make the use of high-performance computing (HPC) systems inevitable. Therefore, eight nodes of RRZE's Lima cluster were used to perform the simulations in this study.

Results

The behavior of the lift and drag coefficients shows significant variations across the 24 different fin positions. Placing the fins closer to the outline curve of the surfboard generates higher maximum lift and drag forces. An increased angle of attack results in a decrease of the lift and drag forces, since the rear outside fin comes to lie further in the slipstream of the front outside fin. To get appraisal factors for the surfboards, stability and maneuverability the yaw and roll moments were established. Both moments arise simultaneously and are strongly dependent on lift and drag coefficients.

With the mentioned use of HPC resources, the wall time of the URANS simulations ranged up to 33 hours.

Outreach

Felix Böschen under the supervision of Dr.-Ing. Stefan Kniesburges, Prof. Dr.-Ing. Michael Döllinger and Prof. Dr.-Ing. Stefan Becker: Numerische Analyse der Hydrodynamik eines Drei-Finnen-Surfboard-Setups (Master Thesis).

Sebastian Falk under the supervision of Dr.-Ing. Stefan Kniesburges, Prof. Dr.-Ing. Michael Döllinger and Prof. Dr.-Ing. Stefan Becker: CFD simulation of four fin configurations and their impact on fluid dynamical characteristics (Master Thesis).

The project is running since August 2017.

Cooperation

Prof. Dr. med. Rolf Janka – Department of Radiology at the University Hospital Erlangen: Responsible for the CT Scans of the surfboard and the fins.

Dr. Roberto Grosso – Computer Graphics Group at the Friedrich-Alexander University Erlangen-Nürnberg (FAU): Responsible for the segmentation and post-processing of the CT data.

Researcher's Bio and Affiliation

Sebastian Falk obtained his master's degree in Mechanical Engineering at the Friedrich-Alexander University Erlangen-Nürnberg (FAU) from Prof. Dr.-Ing. Stefan Becker (Head of research) at the Institute of Process Machinery and Systems Engineering and is currently a PhD student and scientific assistant under the supervision of Dr.-Ing. Stefan Kniesburges and Prof. Dr.-Ing. Michael Döllinger (Head of research) at the division of Phoniatrics and Pediatric Audiology at the Department of Otorhinolaryngology, Head and Neck Surgery of University Hospital Erlangen and Medical Faculty of FAU.

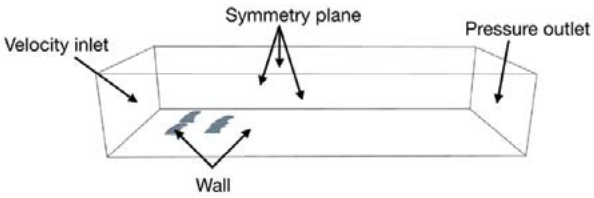


Figure 1: Three-dimensional rectangular fluid volume with the inserted fins.

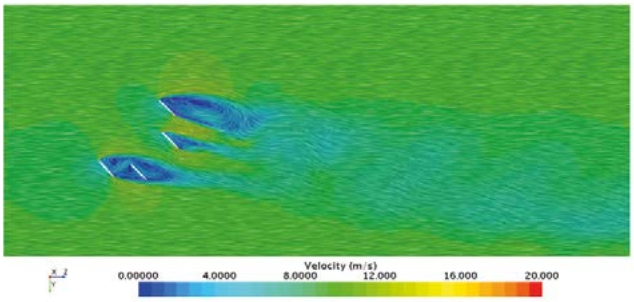
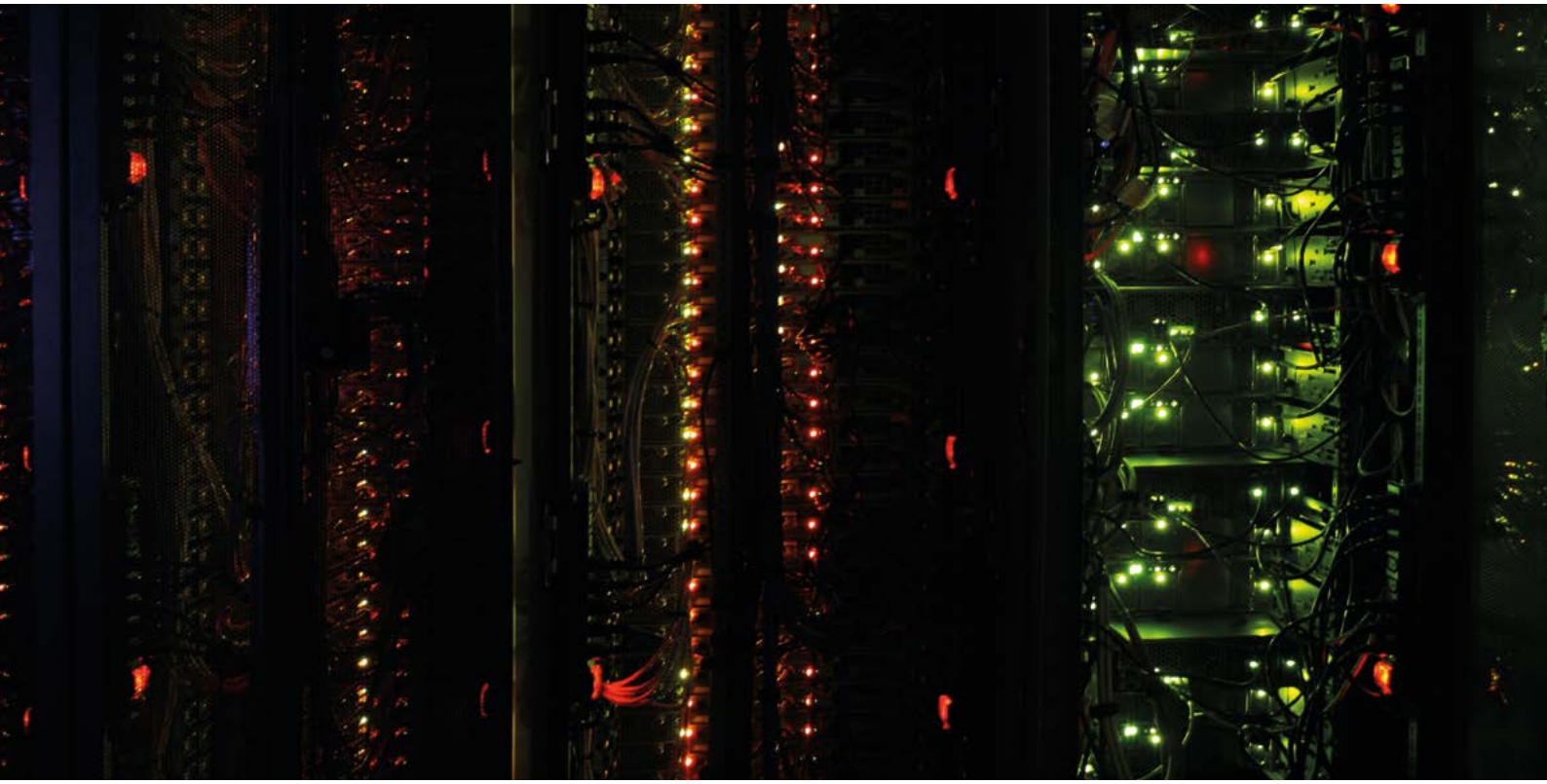


Figure 2: Velocity field which governs around the four fins at an angle of attack of 45°.



Nuclear Medicine Dosimetry by Monte Carlo Methods

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HPC resources used at RRZE
throughput on Woody cluster

The aim of the current project is to calculate energy-dose distributions for Nuclear Medicine radiotherapy, using Monte-Carlo simulations of radiation transport.

Motivation and problem definition

In Nuclear Medicine, radioactive substances are administered to patients in order to treat, e.g., cancer. The radiation damage to cancer and normal tissues is measured by dosimetry. Currently, dosimetry is carried out on organ level, which means that the average energy dose per organ (e.g. kidneys) is determined. In the future, dosimetry should be enabled on a voxel level, which means that the spatial distribution of energy dose inside an organ could be determined and dose-volume-histograms could be calculated. This is expected to allow for better estimates of organ damage due to radiation. Multiple methods are available for the voxel-wise dose calculation. One method which is regarded as "ground truth" is the Monte-Carlo simulation of radiation transport.

Methods and codes

A GEANT4 based Monte-Carlo simulation (GAMOS) was used simulate radiation transport (mainly beta and gamma particles) in order to determine voxel-wise energy-dose deposition in patients. GAMOS is publicly available. In order to obtain a dose-distribution with high statistical confidence, a large number of decays have to be simulated (about 10^{10}). This is very time consuming if only few CPU cores are available, but can be greatly accelerated via massive parallelism.

Results

So far, voxel-wise dose distributions of 20 radiotherapy patients were calculated with a statistical standard error smaller than 3%.

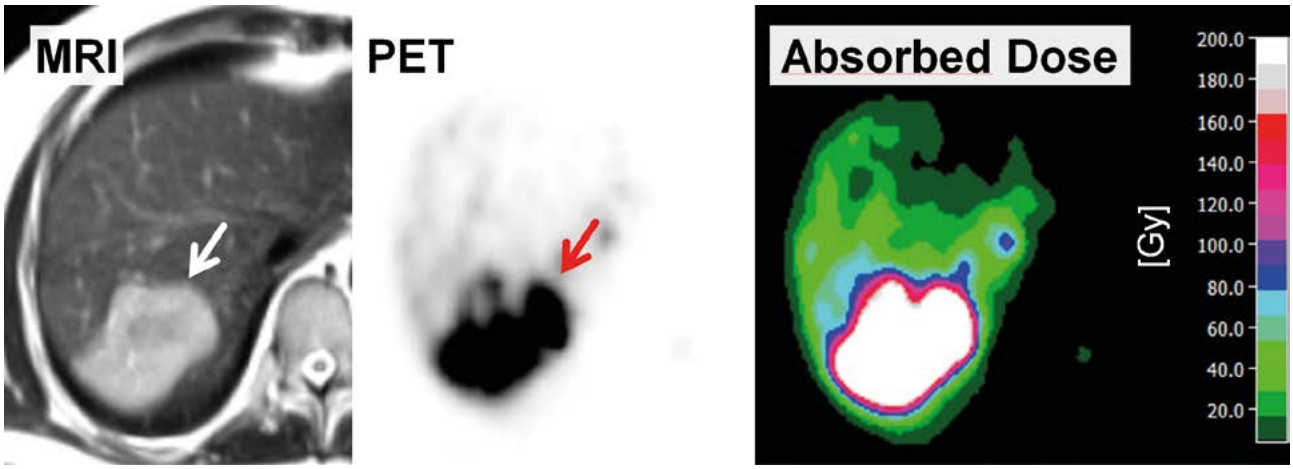
Outreach

Accepted: Presentation at the annual conference of the association of Nuclear Medicine Germany (DGN) April 2018.

In Preparation: Multiple conference and journal submissions.

Researcher's Bio and Affiliation

Philipp Ritt graduated in 2007 at the Particle and Astro-Particle Physics Lab, Department of Physics, FAU. He received his PhD (Dr.-Ing.) in 2012 from the FAU Erlangen-Nürnberg for his work at the Pattern Recognition Lab, Department of Computational Engineering. Since 2008, he works as medical physicist and researcher at the Clinic of Nuclear Medicine and currently is heading the research group for physics and imaging in Nuclear Medicine at the University Hospital Erlangen.



Left: Magnet Resonance Imaging (MRI) of a liver tumor (arrow) of a 57 yo male patient.
Center: Positron Emission Tomography (PET) image of the spatial distribution of a radioactive pharmaceutical injected for radiation treatment of the tumor.
Right: Distribution of absorbed dose in the liver due to treatment, calculated on basis of Monte-Carlo simulations.

Multimodal Corpus Linguistics

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HPC resources used at RRZE

throughput on all of RRZE's HPC clusters

While using linguistic annotation of textual data is mainstream in linguistic research, creating such datasets is expensive. For small collections, manual annotation ist still an option, but for large quantities of texts (i.e., billions of words) only automatic annotation is feasible. Even traditional textual analysis is computationally expensive enough to necessitate HPC resources. When audio-visual data comes into the picture, the required CPU time multiplies.

Motivation and problem definition

The aim of this research is to make collections of texts and audiovisual data searchable and to analyze it with automatic methods. In order to achieve this, forced alignment of transcripts and audio tracks are performed, followed by image analysis (currently mainly hand movement, head movement, facial expressions). Also, a full set of linguistic annotations is run on the data, e.g. PoS-tagging, lemmatization and dependency-parsing.

For monomodal text data, the linguistic annoatation and an analysis of co-occurrence frequencies is run on the HPC systems.

Methods and codes

The software used for Natural Language Processing (Stanford CoreNLP: https://stanfordnlp.github.io/CoreNLP/) ist mostly off-the-shelf, some features depend on our own code.

For the forced alignment, gentle (https://lowerquality.com/gentle/) is currently used for English.

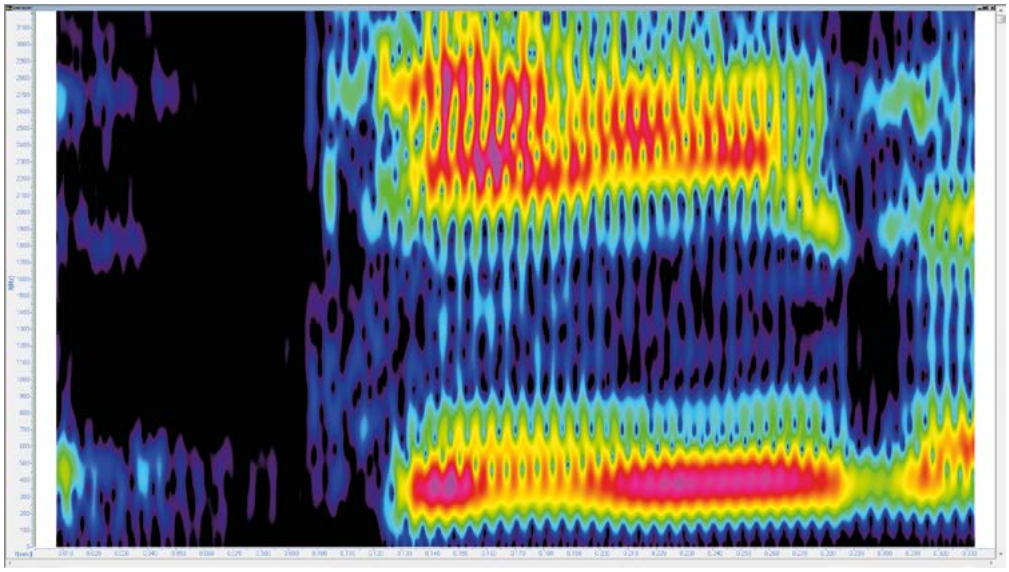
Gesture recognition is performed by a piece of software developed in the context of the Distributed Little Red Hen Lab (http://redhenlab.org) at Case Western Reserve University by Sergiy Turchyn, based on OpenCV (https://opencv.org).

Some of these tools can make use of multiple CPUs and/or GPUs, but the vast majority of the code is not parallel and thus relies only on throughput computing.

Results

The automatically annotated data enables users of our databases to find relevant data for their research projects, e.g., find abstract grammatical structures, find the exact locations of certain expressions in the video recordings, etc. The annotations are made available via a customized web-based search interface.

For instance, a study of clausal subjects in English, which are nearly impossible to find without syntactic annotation, was carried out on a much larger scale than otherwise possible. In multimodal research, the data is used to find gestures associated with certain constructions in a semi-automatic approach. To what extent a fullyautomatic approach can be used for different research questions is currently being investigated in an ongoing research project.



Spectrogram of the word „data" pronounced as [ˈdeɪʇə], automatically extracted from the NewsScape corpus.

Outreach

The following publications/talks report on the infrastructure or present results generated with RRZE's HPC facilities:

Book

Peter Uhrig (2018): Subjects in English [revised PhD thesis; will be published in spring 2018 in the series Trends in Linguistics. Studies and Monographs with De Gruyter Mouton]

Articles

Stefan Evert/Peter Uhrig/Sabine Bartsch/Thomas Proisl (2017): "E-VIEW-alation – a large-scale evaluation study of association measures for collocation identification." In Electronic lexicography in the 21st century. Proceedings of the eLex 2017 conference, Leiden, The Netherlands.

Peter Uhrig/Thomas Proisl (2012): "Less hay, more needles – using dependency-annotated corpora to provide lexicographers with more accurate lists of collocation candidates." Lexicographica 28.

Thomas Proisl/Peter Uhrig (2012): "Efficient Dependency Graph Matching with the IMS Open Corpus Workbench." LREC 2012, Istanbul.

Invited Talks

Peter Uhrig (2017): Texts – Sounds – Images: Multimodal Corpus Linguistics. LMU München.

Peter Uhrig (2017): Researching co-speech gesture in NewsScape – an integrated workflow for retrieval, annotation, and analysis. International Conference on Multimodal Communication: Developing New Theories and Methods, Osnabrück. [Plenary Workshop on Methods]

Peter Uhrig (2017): Demo on multimodal data extraction and annotation. Time concepts and their expression: creativity, cognition, communication: CREATIME workshop, Pamplona, Spain.

Peter Uhrig/Thomas Proisl (2012): Sprachstrukturen effizient speichern, verarbeiten und abfragen: Das Erlanger Treebank.info-Projekt. Vortragsreihe Digital Humanities Erlangen. [Repeated for the general public: Lange Nacht der Wissenschaften 2013, Erlangen.]

Peter Uhrig (2012): A fast and user-friendly interface for large treebanks. Universität Trier.

Peter Uhrig/Thomas Proisl (2011): Treebank.info – Ein System zur Abfrage syntaktisch annotierter Korpora. Otto-Friedrich-Universität Bamberg.

Further Talks and Conference Papers

Stefan Evert/Peter Uhrig/Sabine Bartsch/Thomas Proisl: E-VIEW-alation – a large-scale evaluation study of association measures for collocation identification. Electronic Lexicography in the 21st century: Lexicography from scratch. Leiden (Niederlande).

Peter Uhrig (2017): NewsScape and the Distributed Little Red Hen Lab – A digital infrastructure for the large-scale analysis of TV broadcasts. Anglistentag 2017, Regensburg.

Peter Uhrig (2017): Gesture and Argument Structure – gesture as evidence for item-specific and general knowledge. 14th International Cognitive Linguistics Conference, Tartu (Estonia).

Peter Uhrig (2017): A corpus infrastructure for accessing multimodal data: NewsScape and the Distributed Little Red Hen Lab. ICAME 38, Prag.

Sabine Bartsch/Stefan Evert/Thomas Proisl/Peter Uhrig (2015): (Association) measure for measure: Comparing collocation dictionaries with co-occurrence data for a better understanding of the notion of collocation. ICAME 36, Trier.

Thomas Proisl/Peter Uhrig (2012): Using Dependency-Annotated Corpora to Improve Collocation Extraction. ICAME 33, Leuven.

Peter Uhrig/Thomas Proisl (2012): Geparste Korpora für alle! Pre-Conference Workshop auf dem GAL-Kongress 2012, Erlangen.

Peter Uhrig/Thomas Proisl (2011): A fast and user-friendly interface for large treebanks. Corpus Linguistics 2011, Birmingham.

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Researcher's Bio and Affiliation

Dr. Peter Uhrig is a researcher at the chair of English Linguistics. He is currently working on a post-doctoral project on large-scale multimodal corpus linguistics, for which HPC resources are essential.

Receptor design using molecular dynamics (MD)

Dr. Noelia Ferruz

Birte Hoecker's Protein Desing Group
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HPC resources used at RRZE

TinyGPU

The design of ligand-binding proteins has proven to be a difficult task [1]. We aim to analyze and redesign the binding landscape of two periplasmic binding proteins (PotF/PotD) by a combinatorial approach using MD and experiments.

Motivation and problem definition

PotF and PotD undergo large conformational rearrangements upon binding of their cognate ligands, PUT and SPD, respectively. Recently, PotF's selectivity was swapped to SPD by grafting the first shell of residues in the pocket [2]. Further research suggested that the concrete protein closure might depend on the bound-ligand or/and specific mutant form. In this work we aim to (i) understand PotF/D intricate modulation by ligands and mutations and (ii) redesign new PotF variants selective for new ligands.

Methods and codes

The different systems of study in this work were produced with the MD software ACEMD [3]. The simulations ran using an unsupervised adaptive sampling protocol that allows for a more efficient exploration of the landscape without biasing the dynamics of the system [4]. The simulation ensembles were analyzed with Markov state models (MSMs), a probabilistic method that allows to estimate thermodynamics and kinetics of binding in equilibrium [5].

Results

We have performed large-scale molecular dynamics on the PotF:PUT and PotF:SPD systems comprising more than 100 µs. We projected our ensembles onto a dihedral subspace defined by the protein opening and twisting angles, which we used to produce a 3-state MSM for each ensemble. The analysis revealed that the one of the systems explores a wider conformational landscape than the other as was suggested by previous experiments. The basic understanding of the wild-type systems is very useful for the setting and analysis of the next simulation batches containing protein mutants.

Outreach

The results summarized here will take part in a manuscript that is currently being drafted. The global idea and proposal might be used as a proposal for the DFG grant.

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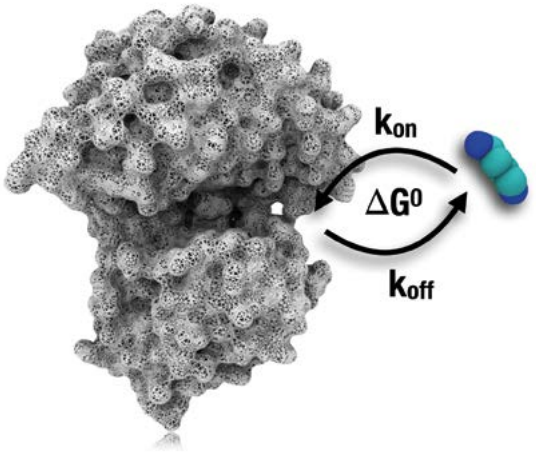

Protein-ligand interactions play a critical role in many biological processes, yet our understanding of these processes remains incomplete. High-throughput molecular dynamics enable the simultaneous characterization of kinetics, thermodynamics and poses. This work focuses on the periplasmic binding protein PotF, an interesting scaffold for the design of biosensors.

Researcher's Bio and Affiliation

Noelia Ferruz received her B.Sc. and M.Sc. in Chemistry in Zaragoza, Spain (2011). After a year as a M.Sc. student in Cambridge, UK, she undertook a M.Sc. in Bioinformatics for Health Sciences in Barcelona, Spain (2013), where she also received her PhD (2016). The she did a short stay in Boston, MA as a postdoctoral researcher in a pharma company. She is currently working as a postdoctoral researcher at Birte Hoecker's Protein Desing Group at the University of Bayreuth.

Spillway design for small dams

Max Heß

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HPC resources used at RRZE

LiMa cluster

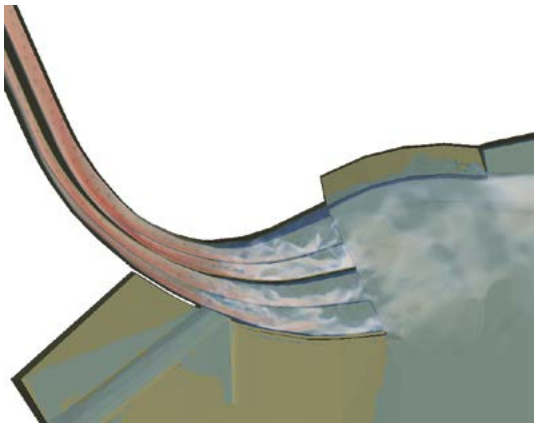
Flood retention reservoirs need to be adapted to take into account the magnitude of the flood peak. For this purpose CFD simulations have been conducted to estimate the hydraulic conditions for an existing spillway and to work out solutions to guarantee its flood safety.

Motivation and problem definition

Due to the latest scientific findings, reported by the Intergovernmental Panel on Climate Change (IPCC), it can be expected, that flooding in summers and winters as well as in transitional periods will become more intense. This depends, e.g., on the geographical location and demonstrates even more clearly the negative impacts of climate change. Updated statistics based on recent flood events increase the design discharges for spillways and cause the need to recover the flood safety for those structures. In order to regain the hydraulic effectiveness of the flood retention reservoir Friedrichswalde Ottendorf in the Free State of Saxony (Germany) investigations on three-dimensional hydrodynamic-numerical simulations have been performed.

Methods and codes

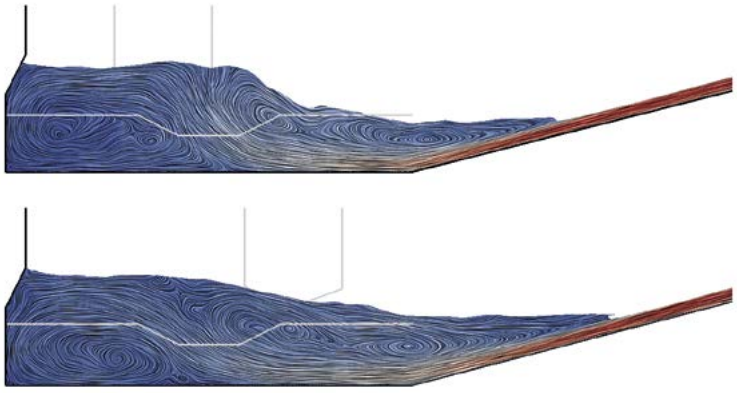
With the usage of the open source CFD-code OpenFOAM® on the LiMa cluster of the Erlangen Regional Computing Center (RRZE), numerical models have been developed to be investigated in terms of hydraulic functionality of the structural variations. Based on the highly turbulent flow conditions in the stilling basin we had to use the Large-Eddy-Simulation (LES) method. With this method the large turbulent eddies are calculated directly and only the smallest turbulent fluctuations are simplified by a modelling procedure. Therefore the mesh quality must be very high and the calculations require huge compute resources.



3d volume rendering of velocity in the spillway

Results

After the calibration and validation of the numerical models using measured values gained at a physical model at the laboratory for hydraulic engineering at the Technische Hochschule Nürnberg, the numerical simulations were conducted. With the highly appreciated compute recourses and support provided by the RRZE the numerical simulations could be accomplished within a tight time schedule. As a result of the investigations a design has been worked out which improves the hydraulic functionality of the spillway and therefore the flood safety of the flood retention reservoir.



comparison of water level and velocity at stilling basin

Outreach

The described method as well as the results of the investigations will be presented at the Wasserbausymposium in Graz 2018.

Researcher's Bio and Affiliation

Max Heß received his master degree in civil engineering at the Technische Hochschule Nürnberg Georg Simon Ohm and is currently working at a scientific assistant at the Institute for Hydraulic Engineering and Water Resources Management of the Technische Hochschule Nürnberg.

3d-hydronumeric simulations as part of a Bachelor thesis

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HPC resources used at RRZE

LiMa cluster

CFD simulations are used to perform three-dimensional simulations by students in connection with Bachelor/Master thesis and other research papers. In this particular case the main focuses were the simulation of dyke overflow and the implementation of measures to prevent damages to the dyke.

Motivation and problem definition

Due to flooding of a one percent annual probability river flood event, a breach of a dyke occurred near the village Nepperwitz in 2002 and 2013 and the infrastructure within the area was damaged. As a result a new dyke was built behind the damaged dyke to guarantee more safety in case of flooding. The main focus of the Bachelor thesis was the investigation of probable damage of the embankment base of the new dyke due to overflow of the old dyke. For that purpose different flood events were simulated and the effect of overflowing water and the resulting hydronumeric properties were investigated. The aim of the study was the implementation of constructive measures based on the results of the thesis.

Methods and codes

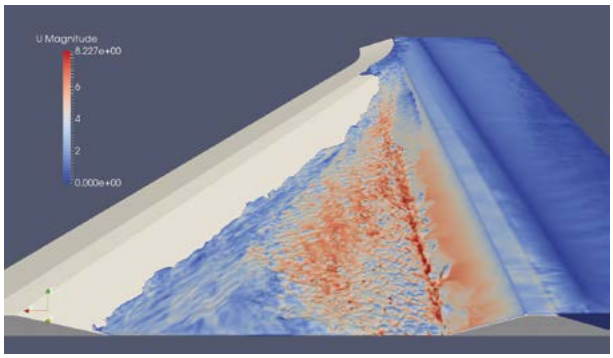
Using the open source CFD-code OpenFOAM at the LiMa cluster of the Erlangen Regional Computing Center (RRZE), numerical models have been developed and investigated in terms of hydraulic functionality of the structural variations. Due to the highly turbulent flow conditions in the area of the embankment foot the simulations needed to employ the Large-Eddy-Simulation (LES) method. With this method the large turbulent eddies are calculated directly and only the smallest turbulent fluctuations are simplified by a modelling procedure. Therefore the claims to the mesh quality are very high and the calculations require huge compute resources.

Results

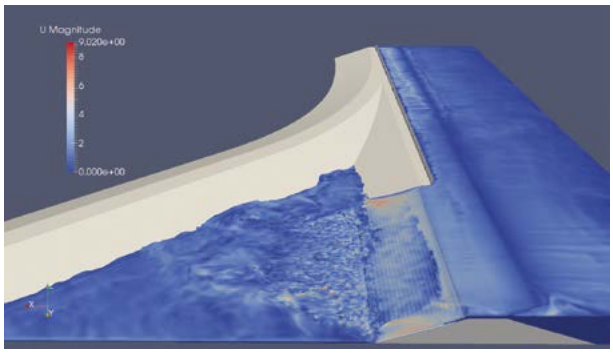
Due to the investigations executed in the context of the Bachelor thesis, different proposals were made to ensure reasonable assurance in case of flooding and to prevent damaging of the new dyke. Resulting from the short schedule of a Bachelor thesis and the high quality meshes of the flow simulations, powerful computer resources were necessary to conclude the research in time. This could only be accomplished by the support provided by the RRZE and the LiMa-Cluster.

Outreach

The execution and the results of the investigations were part of a Bachelor thesis.



Dyke overflow due to flooding of an adjacent river



Impact of constructive measures on the dyke overflow

Researcher's Bio and Affiliation

Michael Kögel received his master's degree in civil engineering at the Technische Hochschule Nürnberg Georg Simon Ohm and is currently working as a scientific assistant at the Institute for Hydraulic Engineering and Water Resources Management of the Technische Hochschule Nürnberg.

Computational Cardiology

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HPC resources used at RRZE
LiMa cluster

Computational Fluid Dynamics simulations of blood flow and contrast agent transport are performed on authentic cardiovascular 3D-geometries. Our aim is the analysis of systematic errors in quantitative perfusion measurements [1-4] with the help of contrast-enhanced magnetic resonance imaging.

Motivation and problem definition

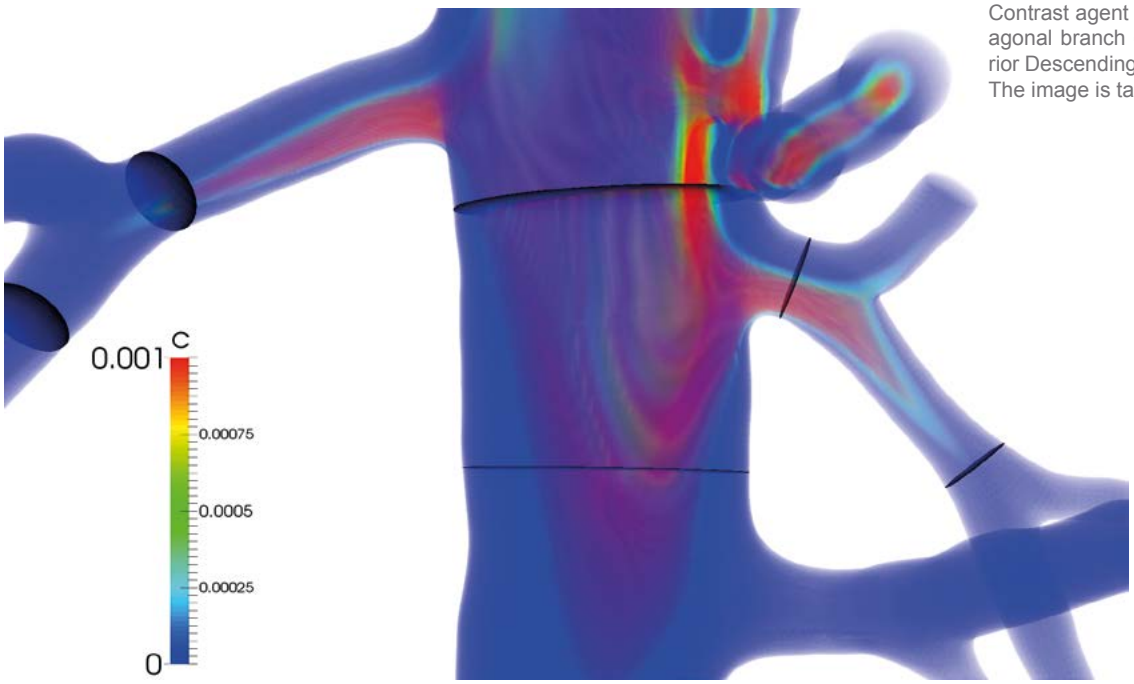
In dynamic contrast-enhanced MRI perfusion measurements, passage of intravenously injected contrast agent (CA) through tissue is monitored to quantify myocardial blood flow (MBF). This requires knowledge of the shape of CA wash-in through upstream coronary vessels, the arterial input function (AIF). For technical reasons this is measured in the left ventricle, which introduces risks of systematic errors in MBF quantification due to bolus dispersion in coronary vessels. To analyze and quantify this effect Computational Fluid Dynamics (CFD) simulations of blood flow and CA transport are performed. To guarantee physiological relevance, boundary conditions must be defined carefully [5].

Methods and codes

With dedicated software (SimVascular, www.simvascular.org) 3D-models of coronary arteries are extracted from medical imaging data. After discretization with a computational grid (cfMesh, creativeFields), consecutive simulations of blood flow and CA transport are performed with the CFD software OpenFOAM (www.openfoam.org). Analogous to electrical circuits, an alternate boundary condition (BC), which comprehends tissue as an electrical capacitor [6], integrates myocardial pressure acting on cardiac vessels into the simulations. The computation jobs are performed on LiMa with on 24 processors. Simulations of both blood flow and CA transport take ~4 days altogether.

Results

We have devised and optimized an alternate BC, which yields qualitatively improved blood flow behavior with increased blood flow in diastole compared to systole compared to previously used BC [5]. It allows CFD simulations of blood flow with application of realistic pressure time-curves at the model inlet. Subsequent CA transport simulations show MBF underestimation of 7-21% due to CA bolus dispersion within the model. These results are in agreement with previous findings [1-5]. However, the range of the results as well as their sensitivity to the choice of BC parameters show that fine-tuning is still necessary. Nonetheless, a detailed analysis of particle



Contrast agent transport in a diagonal branch of the Left Anterior Descending coronary artery. The image is taken from [3].

transport in general (medication, CA, vasodilators etc.) within coronary vessels to different regions of interest remains of high interest.

Outreach

The obtained results are part of a manuscript in preparation. The performed analyses are part of the BMBF grants 01EO1004, 01E1O1504 and the optimization of the new BC may be part of a following DFG-proposal.

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Researcher's Bio and Affiliation

Johannes Martens received his "Diploma" in Physics in Bonn, Germany (2011). After 3 years as a technical assessor at the "Gesellschaft für Anlagen und Reaktorsicherheit" (GRS) in Cologne, Germany, he started work at the Comprehensive Heart Failure Center (CHFC) in Würzburg, Germany, in 2015 as a PhD student at Prof. Laura Schreiber's Chair for Cellular and Molecular Imaging.

CFD simulation for the optimization of fans

Manuel Fritsche

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HPC resources used at RRZE

LiMa cluster

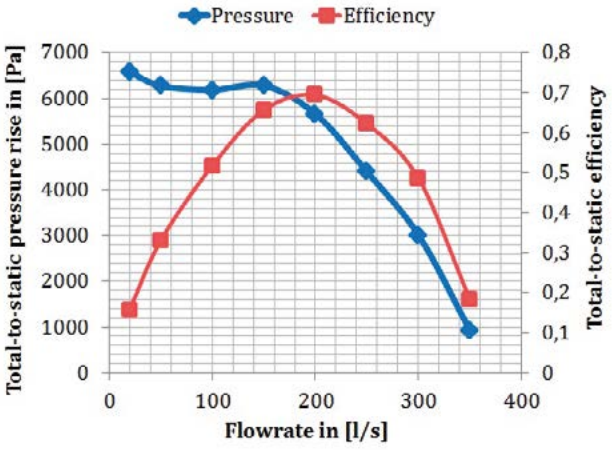
Professional CFD simulations provide a detailed insight into the flow field within fans. The impact of geometry changes can quickly contribute to optimizing the machine and thus increasing energy efficiency of the fan.

Motivation and problem definition

Industrial turbomachines, such as fans and blowers for drying, venting, cooling or conveying tasks, are often used in industrial applications and frequently are a large energy consumer. Thus there is a need for their further optimization and efficiency increase. For large fans and blowers, gaps between moving parts are unavoidable due to manufacturing tolerances and possible thermal expansion. In this study, the radial and axial gap between stationary inlet nozzle and rotating impeller and its impact on the performance characteristics are investigated by CFD simulations.

Methods and codes

The turbulent flow field in a turbomachinery is typically three-dimensional, diffusive, dissipative and chaotic. Therefore, the CFD simulations were performed with Reynolds Averaged Navier Stokes equations (RANS) utilizing the commercial code ANSYS CFX. In order to



Evaluated characteristics of the fan

resolve the fluid flow in the gap as well as possible, a very fine mesh is required. These simulations are solved in parallel with 24 partitions on the LiMa cluster of the Erlangen Regional Computing Center (RRZE) and afterwards evaluated automatically. This makes it possible to generate more result data in a shorter time compared to conventional desktop computers.

Results

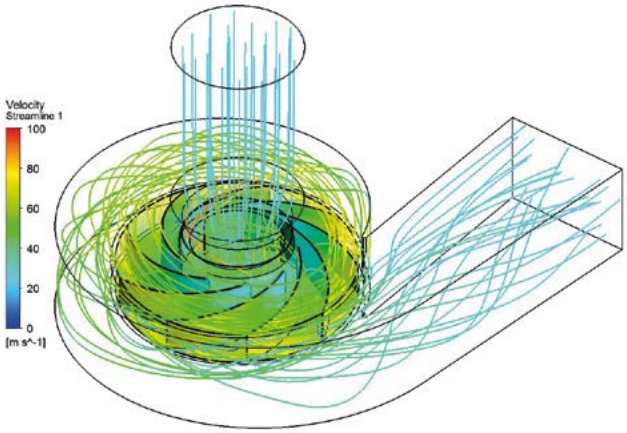
After evaluation of the simulation results it can be stated that the axial and radial gap between the stationary inlet nozzle and the rotating impeller has a significant impact on the expected fan characteristics. The smaller the gaps the lower the leakage flow rate and correspondingly the better the achievable characteristics. Due to the powerful computer resources of the LiMa cluster a variety of geometry variations could be performed to obtain an optimal design of the inlet nozzle.

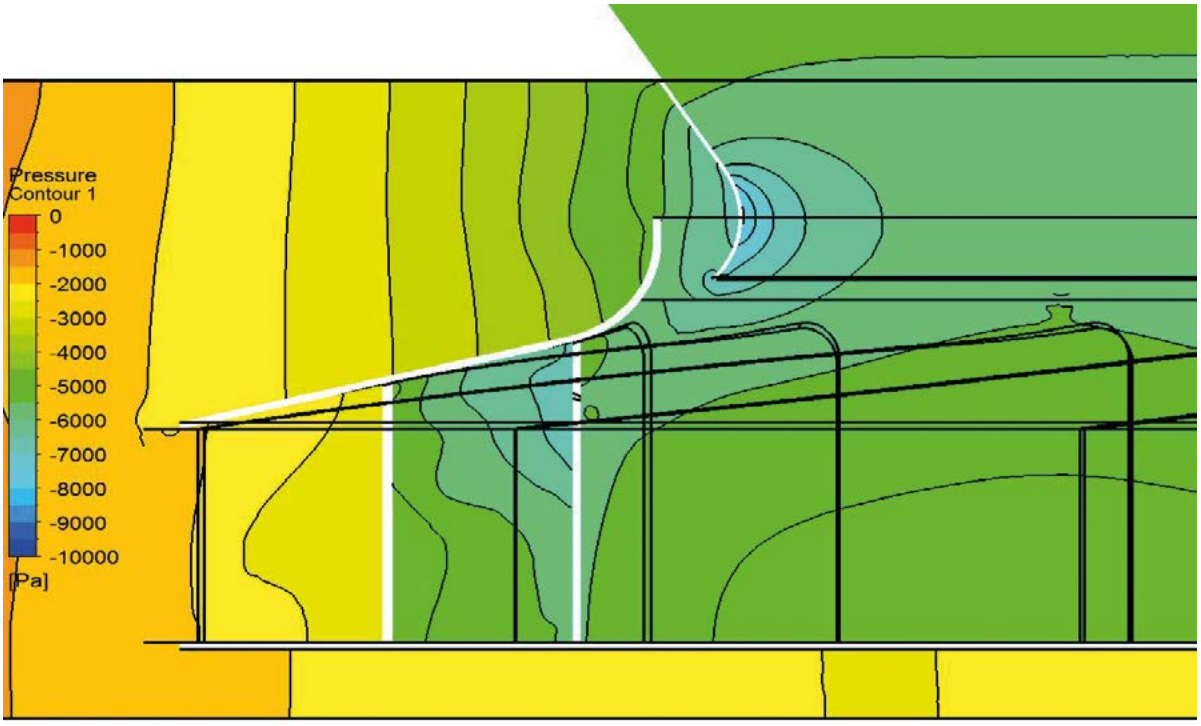
Outreach

The detailed results are currently being prepared for an ASME journal publication.

Researcher's Bio and Affiliation

Manuel Fritsche received his master's degree in development and management in mechanical engineering and automotive at Coburg University. He is currently working there as a research assistant in the team of Prof. Dr.-Ing. Philipp Epple in the field of fan optimization. He is also PhD student of Prof. Dr.-Ing. habil. Antonio Delgado at the Institute of Fluid Mechanics (LSTM) at the Friedrich-Alexander-Universität Erlangen-Nürnberg.





Fluid flow within the gap

Interfacing science and high performance computing

www.hpc.fau.de

RRZE runs high-performance systems, provides expertise on their effective use, and conducts research in the field of high performance computing (HPC).

Modern supercomputers

Parallelism is the key to achieving high computational performance on supercomputers: Many networked compute nodes work together to solve a problem that would be too complex for a single PC. In order to push performance levels even higher, more and more systems comprise additional accelerator hardware.

Efficient use

- Parallelization: How can I orchestrate 1000 processors to solve my problem effectively?
- Optimization: What can I do to make best use of the expensive hardware?
- Computer architecture: Which kind of supercomputer is best suited for my problem?

Research focus

- Performance engineering
- Sparse linear algebra
- Fault tolerance
- Performance tools
- Evaluation of computer architectures

User support

- Project support for scientists with challenging numerical problems
- Parallelization and program optimization
- Assistance with access to and use of supercomputers

Teaching

- Lectures and seminars at FAU
- International courses and tutorials

Scientific collaborators, projects, and supporters:

Bundesministerium für Bildung und Forschung

DFG

KONWIHR III

lrz

SPPEXA

ProPE

PRACE

Los Alamos NATIONAL LABORATORY EST. 1943

HPC Resources

Supercomputers at RRZE

	↑ Emmy	↑ Meggie
Cores	11.200	14.560
Cores per node	20	20
Peak performance (TFlop/s)	233	512
Processor	Intel „Ivy Bridge" 2,2 GHz	Intel „Broadwell" 2,2 GHz
Memory per node	64 GByte	64 GByte
Network	QDR InfiniBand	Omni-Path
Parallel file system	437 TByte	850 TByte
Operating system	CentOS	CentOS
Installation	September 2013	September 2016
Main users	Bioinformatics, Chemistry, Computational Biology, Geography / Climate Science, Fluid Mechanics , Materials Science	

HPC Team at RRZE

As the group leader, **Prof. Dr. Gerhard Wellein** is responsible for coordination of all HPC activities at RRZE. His HPC interests cover modelling and optimization of application performance, evaluating the potentials of new HPC architectures and parallel programming. He has obtained his PhD in theoretical physics at the University of Bayreuth where he started his work in the field of exact diagonalization methods for strongly correlated quantum many-body problems – which is still one of his major research interests.

Dr. Georg Hager holds a PhD in computational physics from the University of Greifswald. He is mainly interested in understanding the interaction of software and hardware in the context of high performance computing using advanced modeling techniques. He has also developed considerable experience in teaching HPC concepts to students and practitioners.

Dr. Thomas Zeiser obtained his PhD in computational fluid mechanics at FAU with a focus on large-scale lattice Boltzmann simulations. At the same time he has great expertise in HPC programming, the application of special tools for program analysis and profiling, and the performance monitoring of HPC clusters. Since joining the HPC group in 2004, he has been a main point of contact for many users of RRZE's HPC systems. Behind the scene he also takes care of the procurement processes and infrastructure aspects.

Having joined the group in August of 2006, **Dipl.-Inf. Michael Meier** is responsible for administration and orchestration of all high performance systems at RRZE, including coordination with standard services. Through his efforts, all aspects of HPC systems management have become much easier to cope with.

Selected Papers

G. Hager and *G. Wellein*: Performance Engineering. Informatik Spektrum, ISSN 1432-122X, Online first, DOI: 10.1007/s00287-018-1122-1. (in German)

F. Shahzad, J. Thies, *M. Kreutzer, T. Zeiser, G. Hager*, and *G. Wellein*: "CRAFT: A library for easier application-level checkpoint/restart and automatic fault tolerance". Accepted for publication in IEEE Transactions on Parallel and Distributed Systems. DOI: 10.1109/TPDS.2018.2866794, Preprint: arXiv:1708.02030

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