HGS MathComp

IWR Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Decoding Nature

9th Annual Colloquium
of the Heidelberg Graduate School of Mathematical
and Computational Methods for the Sciences

November 30 – December 1, 2017
DJH Jugendherberge Altleiningen

Organizing Committee

Adrian Dempwolff
Sonja Friman
Maximilian Herrmann
Manuel Hodecker
Julia Jäger
Chaiyod Kamthorncharoen
Aaron Pattee
Martin Zauser

HGS MathComp 9th Annual Colloquium

Book of Abstracts

Altleiningen 2017

Welcome to the HGS MathComp 9th Annual Colloquium

Welcome to the 2017 Annual Colloquium hosted by the Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences (HGS MathComp). This year's colloquium at Burg Altleiningen includes presentations and posters spanning a wide range of topics, accentuating the interdisciplinary, innovative, and international nature of the HGS. We hope that you will have the opportunity to establish networks with fellow doctoral candidates, take part in scientific discussions, and enjoy your time at Altleiningen!

Contents

1 HGS MathComp

The *Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences* (HGS MathComp) is located at Heidelberg University. Founded in 1386, it is Germany's oldest university, situated in one of the country's most beautiful cities. Ranked among Europe's top universities, Heidelberg offers a diverse and broad spectrum of subject combinations thus creating an optimal setting for individualized and interdisciplinary studies.

HGS MathComp is the only graduate school in Germany to focus its research on scientific computing. The school is funded by the German Excellence Initiative and is an integral part of the Interdisciplinary Center for Scientific Computing (IWR), which has shaped the discipline and achieved a high international visibility. Besides offering high quality education, HGS MathComp aims towards establishing scientific computing as a modern method in all fields of research. By launching pioneering projects the school is continuously exploring new fields of application for mathematical methods. All activities of the HGS MathComp follow the school's three guiding principles:

Scientific Excellence – Interdisciplinarity – Internationality

Scientific Methods

Students at the HGS MathComp become experts in a wide range of mathematical and computational methods:

- Simulation and Optimization
- Mathematical Modeling
- Image Processing
- Statistics and Data Analysis
- High Performance Computing
- Scientific Software Engineering

Application Fields

At the HGS MathComp students conduct research projects with a strong interdisciplinary and application oriented focus:

- Physics and Astronomy
- Quantitative Methods in Biology
- Theoretical Chemistry
- Environmental Sciences
- Humanities and Cultural Heritage
- Economics
- And many more...

2 Conference location

This year the annual colloquium of HGS MathComp will be held in the idyllically situated youth hostel *Burg-Jugendherberge Altleiningen*. Originally built in the first half of the 12th century, it was destroyed during the rebellion of farmers in 1525 and again in 1690 during the Palatinate war of succession. Nowadays the castle's vaults host the biggest population of free living bats in Germany.

Located at the northern end of the hilly area of the *Pfälzerwald*, visitors at castle Altleiningen can enjoy the stunning view over the Leininger Tal and the small village of Altleiningen. Taking a walk down to the village gives you the opportunity to visit the nice churches and the famous *20-Röhrenbrunnen* in the village center.

Burg-Jugendherberge Altleiningen

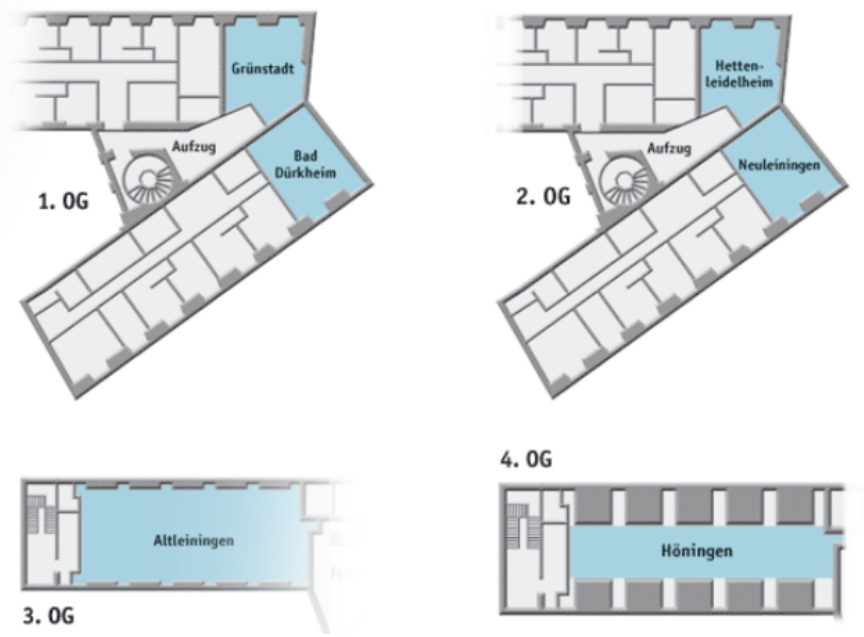
Burg 1
67317 Atleiningen
Telefon: 06356/1580

altleiningen@diejugendherbergen.de
www.diejugendherbergen.de
Telefax: 06356/6364

Youth hostel overview

Below is a floor plan of the hostel. Please note the following information:

- The opening and closing ceremonies as well as all talks will take place in Auditorium “Altleiningen” on the third floor.
- Breakfast, lunch and dinner will be served in the main dining hall.
- Coffee breaks will be held outside the Auditorium.



3 Registration and checkout

You will register at the registration desk where some of the organizers will welcome you. There you will get:

- The number of your room and possibly a key for your room.
- Your official HGS Annual Colloquium hoodie and name badge.
- Answers to (nearly) all of your questions.
- Coffee, cookies and the first possibility for socializing.

Due to the huge amount of fellows and limited resources of the youth hostel, please keep in mind that:

- The rooms are available first at **2:00 PM** on the first day.
- The rooms have to be left by **9:00 AM** on the second day.
- There are only one or two keys available per room.
- Please return the key if you are responsible for it.
- Your luggage will be stored in a separate room.
- WLAN is offered by the youth hostel. However, its availability is rather limited and users are required to pay for this service. The service costs €1.00 for 1 hour or €3.00 for 24 hours effective online time. This fee is not covered and will not be refunded by HGS.

4 Timetable

Time	Day 1 – Thursday, Nov 30	Day 2 – Friday, Dec 01
08:30		Breakfast
09:00	Bus Departure HD Main Station	
09:30		Invited Talk Ulrich Schwarz
10:00	Registration & Coffee Break	
10:30		Coffee Break
11:00	Opening Ceremony	Invited Talk Adrian Komainda
11:30	Introduction to Altleiningen Castle	
12:00	Fellows Talk Session 1	Lunch Break
12:30		
13:00	Lunch Break	Invited Talk Daniel Gerecht
13:30		
14:00	Fellows Talk Session 2	Closing Ceremony
14:30		Departure
15:00	Fellows Talk Session 3	
15:30		Arrival at HD Main Station
16:00		
16:30	Coffee Break	
17:00	Keynote Talk Björn Malte Schäfer	
17:30		
18:00	Dinner	
18:30		
19:00	Poster Session 1	
19:30	Poster Session 2	
20:00	Evening Activities	

5 Invited talks

I1 What's the thing with gravitational waves?

Prof. Dr. Björn Malte Schäfer

Centre for Astronomy of Heidelberg University (ZAH)

email: bjoern.malte.schaefer@uni-heidelberg.de DAY 1, 17h00–18h00

The detection of gravitational waves was **the** scientific sensation of 2016, and provided an incredible confirmation of relativity as the gravitational theory 101 years after its construction. I would like to take everybody through the fundamental concepts of gravity and show why one would exactly expect a wave propagation phenomenon in analogy to electrodynamics. Finally, I would like to discuss the working principles of gravitational wave interferometers and future developments in the field.

About the Speaker

Björn Malte Schäfer has been a professor for fundamental physics at the Centre for Astronomy of Heidelberg University since 2013. His scientific interests include cosmology, the formation and evolution of the cosmic large-scale structure, gravitational lensing and CMB-anisotropies as a probe of fundamental physics, and cosmostatistics.

I2 Keeping up with change in science

Prof. Dr. Ulrich Schwarz

Institute for Theoretical Physics, Heidelberg University.

email: schwarz@thphys.uni-heidelberg.de DAY 2, 09h30–10h30

Both scientific research and the organization of science are continuously changing, and the pace of this change has increased dramatically with the advent of the information age. It is both exciting and challenging to keep up with the dramatic changes currently taking place in science. I will discuss some of the most salient features of this change in the Heidelberg context: emergence of new research subjects at the interface between traditional disciplines (for example in quantitative biology), new ways to publish and disseminate scientific results (including preprint servers, open access journals and twitter), and new career pathways (like ERC-grants and tenure track professorships).

About the Speaker

Ulrich Schwarz is a professor at the Institute for Theoretical Physics (ITP) of Heidelberg University. His professional training is in statistical physics and soft matter physics, and his group works on a large range of subjects in cellular biophysics, including the structural organization, mechanics, adhesion and migration of biological cells. He has published more than 100 papers in scientific journals and in his work combines methods from continuum mechanics and stochastic dynamics. Since he moved to Heidelberg in 2005 as a junior research group leader, he has been a member of the Interdisciplinary Center for Scientific Computing (IWR) and the BioQuant-Center for Quantitative Biology. Currently he acts as managing director of the ITP, as member of the university senate and as editor for *New Journal of Physics* and *Physical Review E*. You find him on Twitter as @SchwarzUlrich.

I3 Computational Chemistry in Industry – Applications from Materials Sciences and Pharmaceutical Research

Dr. Adrian Komainda

Schrödinger, LLC, Mannheim.

email: adrian.komainda@schroedinger.com

DAY 2, 11h00–12h00

With increasing computational power available, simulations have become more and more important for the chemical industry in the last years. The presentation shall give an overview for which areas computational chemistry can have a major impact on the development of new products and processes. For the last decade atomistic-scale modeling based on laws of physics and numerical techniques have resulted in a speed-up of novel drug design. Simulations for new materials for various applications (polymers, composite materials, batteries, organic light emitting diodes, etc.) demand even more computational resources, but also in this field computational chemistry plays a crucial role and its importance is increasing with more and more technology approaching the molecular level (such as semiconductors). In addition to the scientific and business overview, this presentation will also give some ideas on how to get involved in the computational chemistry industry.

About the Speaker

Dr. Adrian Komainda has worked as a project manager for Schrödinger GmbH in Mannheim since January 2017. He is active in the Materials Science Business of Schrödinger, exploring and leading projects with industry partners. Prior to that, he studied chemistry at Heidelberg University and received a Ph.D. in Theoretical Chemistry in 2016, working on excited states dynamics of polyenic systems.

About Schrödinger

Schrödinger is a leading provider of advanced molecular simulations and enterprise software solutions and services for pharmaceutical, biotechnology, and materials science research. The predictive power of Schrödinger's software allows scientists to accelerate their research and development, reduce research costs, and make novel discoveries that might otherwise not be possible. Schrödinger also establishes deep partnerships and collaborations with companies in such fields as biotechnology, pharmaceuticals, chemicals, and electronics. Through significant long-term investments in basic research, Schrödinger has made scientific breakthroughs across many areas of drug discovery and materials science. Founded in 1990, Schrödinger has operations in the US, Europe, Japan, and India, with business partners in China and Korea.

I4 Career Opportunities and Working Life at SAP

Dr. Daniel Gerecht

SAP

email: daniel.gerecht@sap.com DAY 2, 13h00–14h00

SAP is a German software corporation that makes enterprise software to manage business operations and customer relations for its 365.000 customers. The world's third largest software company is headquartered in Walldorf and has more than 87.800 employees. Two years ago I finished my PhD at the HGS MathComp and started working for SAP. The aim of this talk is to offer an insights into the products and new technology trends of SAP. I will take you on a tour through my daily work life as well about career opportunities at SAP.

About the Speaker

Dr. Daniel Gerecht has been a developer at SAP since August 2015. He studied mathematics at Heidelberg University and did his graduate studies at the Heidelberg Numerical Analysis Group.

About SAP

SAP is a German software corporation that makes enterprise software to manage business operations and customer relations for its 365.000 customers. The world third largest software company is headquartered in Walldorf and has more than 87.800 employees.

6 Fellow talks

Session 1 – Aaron Pattee

T1 Mechanochemical Pattern Formation in Biological Tissues

Felix Brinkmann

Institute of applied mathematics, Heidelberg University.

email: f.brinkmann@stud.uni-heidelberg.de

DAY 1, 12h00–12h20

In this talk a finite element method for mechanochemical pattern formation will be presented. A biological application of this prototypical model is embryonic development of fertilized cells.
We model biological tissues using the simple, hyperelastic Saint Venant-Kirchhoff model. The growth processes are modeled by splitting the deformation gradient into an active part and an elastic response. The active part depends on the concentration of signaling molecules, which are modeled by an reaction-diffusion equation.
Evolving patterns are reinforced by a feedback mechanism which depends on mechanical cues, e.g. stress, compression or strain and which is robust to changes in the parameters or in the initial conditions.
Finally, implementation details such as parallelization will be addressed. All problems, in particular in 3D, are solved with the software library Gascoigne 3D.

T2 The simulation of the drug distribution in the human vitreous body

Simon Dörsam

Institute of Applied Mathematics, Heidelberg University.

email: simon.doersam@iwr.uni-heidelberg.de DAY 1, 12h20–12h40

The injection of a drug into the vitreous body of a human eye for the treatment of retinal diseases is the most common medical intervention worldwide. In the worst case the treatment prevents that the patient looses his eyesight. The aim of an optimal therapy is that the drug operates locally around the area of the macula as long as possible. We present numerical simulations of the drug distribution, which are generated by using the Finite Element method. Therefore, the mathematical model is a Darcy equation combined with a transport-anisotropic-diffusion equation. The numerical grid is constructed with the help of parameter estimation methods, which fit measurement data from different patients. The discretization is realized by using the Crank-Nicolson scheme in time, the Raviart-Thomas elements for the velocity, discontinous zero-order elements for the pressure and Lagrange elements for the concentration. Finally, we investigate the influence of the position of the injection on the drug distribution. That is realized by introducing specific output functionals, which measure the mean or relative amount of the drug in the vitreous and in the area of action. Our simulations show that the injections should be located in the center of the vitreous body for a more efficient therapy.

T3 From Protein to Organ: Modeling Brassinosteroid Response Across Different Scales

Ruth Grosseholz[1)], Nina Glockner[2)], Friederike Wanke[2)], Anna Feldman-Salit[1)], Sarina Schulze[2)], Stefan Scholl[3)], Karin Schumacher[3)], Birgit Kemmerling[2)], Klaus Harter[2)], Ursula Kummer[1)]

[1)] BioQuant, Center for Organismal Studies (COS), Heidelberg University; [2)] Center for Plant Molecular Biology (ZMBP), University Tübingen; [3)] Center for Organismal Studies (COS), Heidelberg University.

email: ruth.grosseholz@bioquant.uni-heidelberg.de DAY 1, 12h40–13h00

Plants are sessile organisms and, therefore, have to grow towards essential nutrients such as water or sunlight. However, since growth requires a lot of energy, it has to be tightly regulated. One class of hormones that is involved in the initiation and regulation of growth are brassinosteroids (BRs). The early response of plant cells to BR stimulation induces membrane hyperpolarization, cell wall acidification and elongation growth. In this work, we analyzed the BR response across different scales in *Arabidopsis thaliana* roots.

Starting at the level of the individual proteins, we specified the mode of interaction between the (co-) receptor, which is required for a proper downstream signalling, and a negative regulator of the BR-pathway. Specifically, the negative regulator blocks the (co-) receptor from interacting with the ligand-binding receptor to induce downstream signaling. Building on this knowledge we formulated a model consisting of ordinary differential equations (ODEs) that describes the early events of the BR-induced response. By fitting the model parameters to experimental dose-response data of the membrane potential, we generated an ensemble of 100 models. We further validated this model by making predictions regarding the signaling pathway's behavior in a different root zone and verifying them experimentally.

We expanded this work by including cell elongation growth making the volume of all compartments in the model variable. With this model we are able to describe the experimentally determined elongation behavior across the different root zones. Ultimately, we aim at establishing an agent-based model of the whole root that is linked to ODE models describing the intracellular processes of the early BR response.

Session 2 – Nikolas Schnellbächer

T4 Optimization-based Control and Estimation Help Saving Around 2% More Energy in Heavy Duty Trucks

Enrique Guerrero Merino[1)], Johannes P. Schlöder[1)], Christian Kirches[2)]

[1)] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University; [2)] Institute for Mathematical Optimization, TU Braunschweig.

email: enrique.guerrero@iwr.uni-heidelberg.de DAY 1, 14h00–14h20

Even state-of-the art Diesel engines reach thermal efficiency of only around 34%, which means that 76% of the energy contained in the fuel gets wasted. About the half of it (that is, around 30% of the total) gets wasted into the atmosphere as warm exhaust gas. As a counter-measure, waste heat recovery systems (WHRs) have been proposed. These devices are highly nonlinear, and some important components may suffer damage if certain nonlinear operational constraints are violated. In this talk, we analyse the results obtained after applying our nonlinear model-predictive control and moving-horizon estimation techniques to control a WHR. In comparison to the widespread PI and LQG control methods, our scheme not only satisfies the operational constraints, but is also able to regenerate around 2% more energy.

T5 `Bohrium`: A framework for automatic parallelisation of array operations

Michael F. Herbst

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.

email: michael.herbst@iwr.uni-heidelberg.de

DAY 1, 14h20–14h40

Due to recent advances in the support of vectorisation instructions in CPUs, it has become very advantageous to design algorithms in such a way, that exactly the same operation is executed on all input data at once. This can be achieved rather elegantly by using so-called array programming, which essentially just uses a flat datastructure on top of linear arrays of data to view them as matrices or tensors. All typical tensor operations can then be written entirely as array operations, which just perform task after task on the full linear arrays, which represent the tensors. Parallelisation of an array operation in a shared-memory environment is of course trivial, since one only needs to divide the input array equally amongst all workers during the operation.
One drawback of array programming is, however, that some very common operations show an unfavourably large scaling with respect to memory. For example the multiplication of two square matrices of size $N \times N$ shows a cubic memory cost of $\mathcal{O}(N^3)$ in naive array programming compared to $\mathcal{O}(N^2)$ if the multiplication is carried out in the ordinary manner. Furthermore the most common package relying on array programming, the `python` library `numpy`, lacks parallelisation of most array operations.
Especially for the latter reason the group of Prof. Dr. Brian Vinter at the Niels Bohr Institute in Kopenhagen started the `Bohrium` project [0]. It offers a `numpy`-compatible interface to `python` users and under the hood performs so-called loop fusion [1] and a streamlined execution of the actual array operations to defeat the increased memory footprint [2]. By the means of a just-in-time compiled kernel of the actual operation both automatic parallelisation as well as an optimal execution for the running hardware is achieved. `Bohrium` includes a CUDA and an OpenCL backend, such that running the array operations on graphics cards takes no more than changing a operating system environment variable. Next to the `python` interface, `Bohrium` maintains entry points for C and C++ as well.
This talk will give a short introduction to `Bohrium` based on some live-coding in `python`.

[0] https://bh107.org

[1] M. R. B. Kristensen, S. A. F. Lund, T. Blum, and J. Avery, *Proceedings of the 2016 International Conference on Parallel Architectures and Compilation*, 2016.

[2] M. R. B. Kristensen, S. A. F. Lund, T. Blum, J. Avery, and B. Vinter, *Proceedings of the International Conference on High Performance Computing*, 2016.

T6 Collective behavior, anyone? The impact of promoter architecture on bacterial quorum sensing

Sarah Kaspar[1)], Valentina Rippa, Diana Wolf, Stephanie Trauth, Ilka Bischofs[1)], Jürgen Pahle[1)]

[1)] BioQuant, Heidelberg University.

email: sarah.kaspar@bioquant.uni-heidelberg.de

DAY 1, 14h40–15h00

Bacteria use quorum sensing (QS) to estimate their density and to trigger cooperative behaviour in response. In this process, the signals of various QS molecules are often fed into the same gene activation process. For example, in *B. subtilis* the species-specific and the strain-specific signals converge to regulate the master regulator ComA by independently regulating the overall abundance and the phosphorylation status of the transcription factor. Whether and how different QS signals are integrated at the level of gene expression is not well understood.

Here we provide experimental evidence suggesting that promoter architecture is a key factor for signal integration and the decoding of information encoded by different QS signals. We furthermore developed a mathematical model for QS-dependent gene expression composed out of two modules: (1) A DNA-binding and (2) a gene expression module. The model reveals promoter features that could be crucial with respect to the weighting between different QS signals. These features might therefore also play an important role in determining the extent of intra- and interstrain cooperative behaviour.

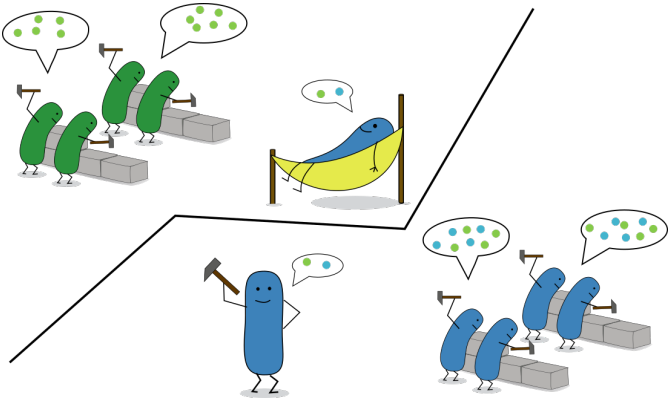


Figure 6.1: Bacteria cooperate, but with whom is signal-dependent.

Session 3 – Michael Herbst

T7 Parallel multiplicative Schwarz smoothers in particle transport problems

José Pablo Lucero Lorca, Guido Kanschat

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.

email: pablo.lucero@iwr.uni-heidelberg.de

DAY 1, 15h00–15h20

We implement a discontinuous Galerkin discretization to solve a non-linear particle transport problem in local thermodynamical equilibrium. The discretized is solved system using a Newton method with a GMRES solver for the linear systems, using a multigrid preconditioned with non-overlapping cell-wise Schwarz smoothers that solve the complete transport problem in each cell. We select the smoothers to be multiplicative or additive depending on the regime of the problem being solved, achieving robustness for the linear problem with respect its size and coefficients. In this presentation we show our results on a series of experiments selected to show robustness and general performance.

T8 Castles and Crossroads—Geo-referencing Three Centuries of Historical Maps

Aaron Pattee[1),2)], Bernhard Höfle[3)], Armin Volkmann[4)], Susanne Krömker[2)], Hubert Mara[2)]

[1)] Institute for European Art History, Heidelberg University; [2)] Interdisciplinary Center for Scientific Computing, Heidelberg University; [3)] Institute of Geography, Heidelberg University; [4)] Prussian Cultural Heritage Foundation Berlin.

email: aaron.pattee@iwr.uni-heidelberg.de DAY 1, 15h20–15h40

This study investigates the historical logistic infrastructure between six late medieval castle sites in the southwestern German region of the *Pfalz* by combining geo-referenced historical maps (1540–1840 A.D.) and trade information from medieval deeds and charters. Once the maps have been geo-referenced and combined with Aerial LiDAR data, information regarding waterways, roads and routes will be compared with *QGIS*-generated Watershed and *Least-Cost-Path* analyses (respectively) to determine where the historical water/land routes were located.

Currently, 18 maps have been geo-referenced using the *Thin-Plate-Spline* algorithm in conjunction with the *Nearest Neighbor* method to adjust for both local and global distortions within the maps. We chose key sites scattered throughout the former Holy Roman Empire and France as *Ground Control Points* (GCPs) for linking the historical maps to the modern map. These sites include the six case studies in addition to 200 other sites that repeatedly appear in the maps. To adjust for the changing built environment, the specific point for each GCP is a medieval structure—typically a cathedral or castle. Additionally, *Voronoi Diagrams* are being calculated for the geo-referenced assemblage to be compared with feudal regions marked within the historical maps.

Site locations and trade routes have been mapped for one of the six sites and will be augmented by QGIS-generated *Delaunay Triangulations* to develop a network analysis to be compared to historical roads and routes from the maps. The combination of geo-referenced maps and network analyses from medieval texts will develop a more accurate visualization of the past infrastructure.

Keywords: *GIS, Historical-Maps, Spatial-Analyses*

T9 Correlation of structural and magnetic properties in a series of mononuclear lanthanide complexes

A. E. Roberts[1),2)], L. J. Daumann[3)], D. I. Gorbunov[4)], R. Klingeler[5),6)], C. Koo[5)], M. J. Riley[7)], H. Wadepohl[1)], J. Werner[5)] and P. Comba[1),2)]

[1)] Institute of Inorganic Chemistry (ACI), Heidelberg University; [2)] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University; [3)] Faculty for Chemistry and Pharmacy, Ludwig-Maximilians-University (LMU) Munich; [4)] Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum, Dresden; [5)] Kirchhoff-Institute for Physics (KIP), Heidelberg University; [6)] Centre for Advanced Materials (CAM), Heidelberg University; [7)] School of Chemistry and Molecular Biosciences, University of Queensland, Australia.

email: asha.roberts@aci.uni-heidelberg.de DAY 1, 15h40-16h00

Single molecule magnets (SMMs) are a class of d- and f- block coordination compounds that, once magnetised by an external field, have the unique ability to retain this magnetisation even after the field is removed.[1] SMMs can be comprised of one or more magnetic centres, with unlimited combinations of 3d and 4f ions, both para and diamagnetic. Although magnetic coupling plays a big role in oligonuclear complexes, it is negligible in mononuclear complexes, meaning that the magnetic properties are dictated by the electronic structure of the single ion alone. As this is related to molecular structure, the magnetic properties are theoretically predictable and tuneable. In comparison to transition metals, ligand field effects upon lanthanides are quite small, however, they have been shown to be of central importance for molecular magnetism.

This study investigates the subtle effects of small changes in geometry upon the electronic structure of rare earth metal centres. Theoretical and experimental methods have been utilised to analyse a series of mononuclear lanthanide complexes. The ligands employed are comprised of two bidentate donors (1-hydroxy-pyridine-2-one, 1,2-HOPO) with a linking chain of various lengths.[2] Depending on the identity and length of the chain, a different geometry can be enforced. The geometry of the complexes differs only slightly across the series, however, *ab initio* calculations of the complexes indicate that these geometrical changes have a significant impact on the magnetic properties. The ligand field effects are also experimentally evidenced by MCD and HF-EPR spectra as well as by magnetic measurements.

[1] R. Sessoli, D. Gatteschi, *Nature* 1993, *365* (6442), 141–143.

[2] L. J. Daumann, D. S. Tatum, *Inorg. Chem.* 2016, *55* (1), 114–124.

T10 Using Agent-Based Modeling for Exploration of the Influence of Working Memory Capacity in CPR Dilemmas

Nadia Said[1),2)], Debora Fieberg[2)], Helen Fischer[1)], Johannes Lohse[3)], Christian Kirches[4)]

[1)] Psychological Institute, Heidelberg University; [2)] Interdisciplinary Center for Scientific Computing, Heidelberg University; [3)] Department of Economics, University of Birmingham; [4)] Institute for Mathematical Optimization, TU Braunschweig.

email: nadia.said@psychologie.uni-heidelberg.de DAY 1, 16h00–16h15

Forests, water or international fisheries can be conceptualized as **common pool resources (CPR)**. As these resources are limited and can, in principle, be used by everyone, individual extraction decisions may lead to an overuse and cause a breakdown of the resource.

In our previous experiments participants' **working memory capacity (WMC)** turned out to be a key driver of their extraction behavior. In particular, when a group interacted with our CPR scenario, participants with a higher WMC were more likely to extract too much, which lead to a premature breakdown of the resource.

In this contribution we present first steps towards merging an **agent-based modeling (ABM)** approach with the declarative memory module of **ACT-R** in order to vary WMC in a controlled way for agents interacting with a common pool resource 6.2. ACT-R is a cognitive architecture which is widely used for modeling human cognition processes. Using the declarative memory module of ACT-R we can vary different cognitive parameters, like W (working memory) and τ (retrieval threshold), which represent the cognitive abilities of agents and therefore influence their extraction behavior. Thus, we can investigate the optimal level of WMC for sustainable resource use, and clarify whether a more limited human WMC might even prove beneficial for the use of common resources.

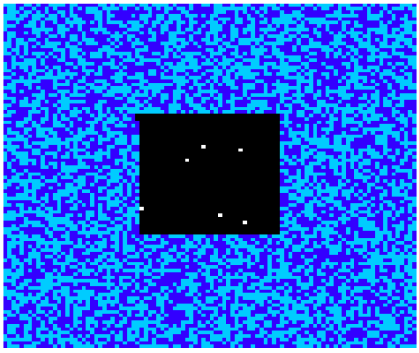


Figure 6.2: Simulation of agents n with different WMC (light blue & dark blue) interacting with a CPR (black square) in round j; random decision behavior.

T11 How do Macromolecules find their targets?

Fereydoon Taheri

Biophysics of Macromolecules (B040), German Cancer Research Center (dkfz.), Heidelberg.

email: f.taheri@dkfz.de

DAY1, 16h15–16h30

Molecules in living cells are primarily transported by random diffusion. Within individual compartments, such as the cell nucleus, mitochondria or the cytosol, biological macromolecules find their targets mostly by this thermally driven random motion which is fundamental to many intracellular processes such as proteins interaction, enzymatic reaction and signaling as well as pattern and domain formation. In the cellular interior, diffusion is obstructed by crowding and the dense packing of all cellular constituents and this viscoelastic nature has been shown to highly influence the type of transport observed in the cell. Here we investigated viscoelasticity in dynamic polymer network of cell nucleus by recording fast image series of two-dimensional sections of live cells and monitoring diffusion process in real time to gain a better understanding of the underlying physics. Our method of choice was light sheet fluorescence microscopy followed by cross correlation analysis between two distant pixels. This method allows us to perform Fluorescence (cross-) correlation spectroscopy on all image's pixels of the entire illuminated plane simultaneously. We studied the mobility of fluorescently labeled Histons inside the nucleus of Mouse Adult Fibroblasts in presence and absence of Lamin A, an intermediate filament protein, which provides stability to the nuclear envelope.
Our data clearly shows the existence of correlated movement both in cells and model systems. Our approach constitutes a framework to systematic and quantitative analysis of diffusion of macromolecules based on the viscoelastic properties of their surrounding environment.

7 Posters

P1 End-to-end learning of hierarchical clustering for image segmentation in connectomics

Alberto Bailoni

Image Analysis and Learning Group – Heidelberg Collaboratory for Image Processing, Heidelberg University.

email: alberto.bailoni@iwr.uni-heidelberg.de

In the recent years, image segmentation has been successfully applied to 3D electron microscopy (EM) images of neural tissue used in connectomics – a subfield of neuroscience devoted to reconstruct a map of an organism's nervous system. Most of the recent automated EM neuron segmentation methods consist of a pipeline with several steps. First, a convolutional neural network (CNN) predicts membrane boundary probabilities for every pixel. Second, these probabilities are used to find over-segmenting small segments, called superpixels. Third, superpixels are combined and merged into larger regions using graph-based algorithms. Agglomerative hierarchical clustering is an often used tool to perform the last step. This algorithm uses a merging policy that determines which merges are most likely and then starts agglomerating the segments with the highest merging probability.
Machine learning and neural networks have been successfully used for neuron image segmentation. Nevertheless, a common feature of these automated methods is that the three steps in the pipeline are trained separately, so that each module is isolated and cannot benefit from the knowledge learned in the other steps. Our proposed method uses a CNN that, for each iteration of the hierarchical clustering algorithm, is trained to predict which segments should be merged next and it bases its prediction both on the EM image and the additional shape clues given by the current segmentation. This allows us to train the model end-to-end and use a structured training approach based on the steps performed by the hierarchical agglomeration algorithm.

P2 Resonance Lifetimes of Large Molecules

Adrian L. Dempwolff, Andreas Dreuw

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: adrian.dempwolff@iwr.uni-heidelberg.de

Atoms or molecules can be electronically excited to states possessing an energy higher than the ionization potential of the respective species. Such so called resonance states are generally not stable and can undergo electronic decay processes as shown in figure 7.1, giving rise to possibly low-energetic free electrons, which are known to cause damage to tissues in living matter.
A characteristic number of resonance states is their *lifetime* or *decay width*, connected to each other via the Heisenberg uncertainty relation. Due to the unbound nature of the involved electronic states, the theoretical description of lifetimes is challenging, especially in the context of available electronic structure codes making use of square-integrable basis sets.
Different approaches to this problem have been proposed so far, one of which is constituted by the *Fano-ADC-Stieltjes* method, using the *Algebraic Diagrammatic Construction* (ADC) scheme for the polarization propagator for electronic state modeling. Here, we present an efficient implementation of this method, applicable up to mid-sized organic molecules. Example calculations for benzene and naphthalene are shown, being in good agreement with experimental findings.

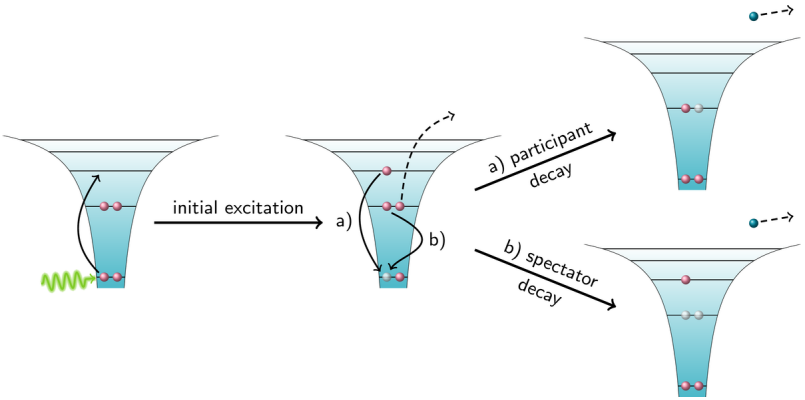


Figure 7.1: Schematic illustration of possible electronic decay processes of high-energetic excited electronic systems.

P3 Theoretical investigations of biomimetic iron(IV)-oxo complexes

Dieter Faltermeier[1)], Peter Comba[1,2)]

[1)] Institute of Inorganic Chemistry, Heidelberg University; [2)] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.

email: dieter.faltermeier@aci.uni-heidelberg.de.

Mononuclear non-heme iron compounds play an important role in nature. They occur in many organisms and are indispensable. The chemical versatility of these enzymes is remarkable. Some examples of reactions with non-heme iron compounds include hydroxylation, halogenation and epoxidation. To understand enzymatic non-heme iron reactions, the study of biomimetic iron-oxo complexes is important [1–6]. Suitable biomimetic ligands for iron-oxo complexes are e.g. bispidines [7] or TMC ligands [8]. Due to the energetically close spin states ($S = 1$ and $S = 2$), it is very difficult to describe iron-oxo complexes without further theoretical investigations [7]. To attain a more accurate understanding of the chemical behavior of iron(IV)-oxo complexes, we use a broad variety of methods such as DFT (density functional theory) and multi-reference methods. One of the most popular approaches for the calculation of properties of transition metal complexes are correlated post-HF (Hartree-Fock) methods like CASSCF (Complete Active Space Self-Consistent Field). Due to the lack of dynamical correlation, we use the NEVPT2 (N-Electron Valence State Theory) or CASPT2 (Complete Active Space Perturbation Theory) theory to include dynamical correction. The focus will be on the calculation of the g- and D-values, which can then be compared with published values of experimentally measured compounds.

[1] W. Nam, *Acc. Chem. Res.* **48**, 2415–2423 (2015).

[2] W. Nam, Y-M. Lee, S. Fukuzumi, *Acc. Chem. Res.* **47**, 1146–1154 (2014).

[3] E. I. Solomon, T. C. Brunold, M. I. Davis, J. N. Kemsley, S.-K. Lee, N. Lehnert, F. Neese, A. J. Skulan, Y.-S. Yang, J. Zhou, *Chem. Rev.* **100**, 235–350 (2000).

[4] M. M. Abu-Omar, A. Loaiza, N. Hontzeas, *Chem. Rev.* **105**, 2227–2252 (2005).

[5] C. Krebs, D. G. Fujimori, C. T. Walsh, J. M. Jr. Bollinger, *Acc. Chem. Res.* **40**, 484–492 (2007).

[6] C. A. Grapperhaus, B. Mienert, E. Bill, T. Weyhermüller, K. Wieghardt, *Inorg. Chem.* **39**, 5306–5317 (2000).

[7] P. Comba, S. Fukuzumi, C. Koke, B. Martin, A.-M. Löhr, J. Straub, *Angew. Chem. Int. Ed.* **55**, 11129–11133 (2016).

[8] J.-U. Rohde, J.-H. In, M. H. Lim, W. W. Brennessel, M. R. Bukowski, A. Stubna, E. Münck, W. Nam, L. Que Jr., *Science*, **299**, 1037–1039 (2003).

P4 Imaging gas concentrations via Laser Induced Fluorescence for investigations of the mass boundary layer

Sonja Friman, Bernd Jähne

Heidelberg Collaboratory for Image Processing (HCI) and Institute of Environmental Physics (IUP), Heidelberg University.

email: sfriman@iup.uni-heidelberg.de

Exchange processes across the air-sea interface (e.g. momentum, mass and heat transfer) are limited by the diffusion in the mass boundary layers, which have a thickness of 100-1000 micrometers on the air-side and 20-200 micrometers on the water-side. Our approach to investigate the air-sided boundary layer is Laser Induced Fluorescence of sulfur dioxide. The gas concentration profiles can directly be deduced from the fluorescence intensities. The latest progress in the ongoing development of the experimental technique is presented.

P5 Theoretical Investigation of Singlet Fission on Acene Derivates

Jie Han, Andreas Dreuw

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.

email: jie.han@iwr.uni-heidelberg.de

Singlet fission is a process in which a singlet exciton shares its energy with a neighbor ground-state to produce two triplet excitons, whereas traditional solar cells only produce one exciton by one photon. Materials undergo singlet fission can dramatically increase solar cell efficiency and are promising candidates for next generation solar cells. Tetracene and pentacene are known to be attractive reference compounds for singlet fission, and the introduction of TIPS side groups make them soluble and serve here as starting points. Further modifications such as nitrogen to carbon substitution and halogen to hydrogen substitution have been made to enhance SF efficiency. In this work, the effects of the modifications on excited state dynamics of SF are theoretically investigated by quantum chemical methods. We employ time-dependent density functional theory and configuration interaction with constrained density functional theory to calculate excited state absorption spectra and transition rate, which are in good agreement with experiment. By combining information obtained from theoretical calculations with experiment, we identify the species involved in singlet fission, hence provide better understanding on how the triplet manifold is populated via the SF mechanism.

P6 Modeling of tropospheric ozone depletion events in one-dimensional and three-dimensional configurations.

Maximilian Herrmann, Eva Gutheil

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: maximilian.herrmann@iwr.uni-heidelberg.de

Ozone depletion events have been observed in the troposphere, the lowest part of the atmosphere, during spring and to a lesser extent fall in the Arctic and Antarctic. During an ozone depletion event, the mixing ratio of ozone in the atmospheric boundary layer drops from its background level of several 10 parts per billion (ppb) to small or even undetectable levels (less than 1 ppb) on a timescale of hours to days.
Today we know that the ozone depletion events are driven by halogen chemistry, which consists of gas phase reactions and heterogenous reactions occurring on the surface of substrates such as snow and ice and in aerosols. Halogens stored in substrates can be activated by HOBr and released into the gas phase as Br_2 or BrCl. Under sunlight, the photolysis of Br_2 forms two Br atoms, which consume ozone and form new HOBr. This autocatalytic process is referred to as "bromine explosion".
Often, several ozone depletions are measured at the same location, e.g. thirteen ozone depletion events were observed in Barrow, Alaska, in the spring 2009 . This recurrence of ozone depletion events was thought to be caused solely by horizontal transport of air masses from ozone-depleted regions to the measurement site. In order to demonstrate that the chemical system with vertical turbulent diffusion alone may lead to the recurrence of ozone depletion events, the chemical reactions in a one-dimensional configuration is studied where the vertical turbulent diffusion acts as the sole transport mechanism. In 7.2, an ozone depletion event with a recurrence after about 50 days is shown. Also, the Weather Research and Forecasting model coupled to Chemistry (WRF-Chem) is used to perform three-dimensional simulations of ozone depletion events. We extended the MOZART chemistry mechanism to include bromine species. We will model BrO clouds occurring north of Barrow, Alaska and compare the results to satellite data.

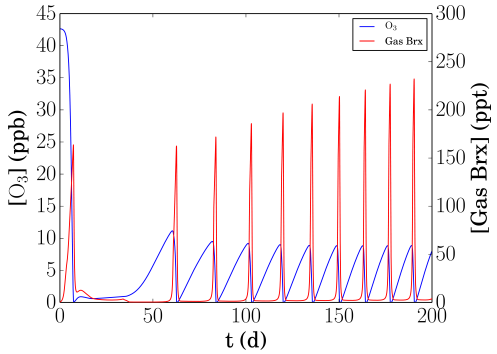


Figure 7.2: One-dimensional simulation of a recurring ozone depletion event, showing both the ozone and the total gas-phase bromine concentrations.

P7 Excitation Energies & Dipole Polarizabilities of Small to Medium-Sized Molecules

Manuel Hodecker[1)], Dirk Rehn[2)], Patrick Norman[2)], Andreas Dreuw[1)]

[1)] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University; [2)] KTH Royal Institute of Technology, Stockholms Universitet, Sweden.

email: manuel.hodecker@iwr.uni-heidelberg.de

The interaction of light and matter plays a crucial role in many chemical and biochemical processes. Understanding these processes is important for plenty of applications in all areas of science. For a theoretical description of these phenomena quantum-chemical methods are required. These methods can be divided into methods describing the electronic ground state of a molecular system, and the ones describing *excited* electronic states. One of the latter methods is the *algebraic-diagrammatic construction* (ADC) scheme, that has gained more popularity in recent years due to some of its advantageous features which include its reliability, accuracy and reasonable computational demand. A drawback of the method, however, is the description of the ground state which is based on Møller-Plesset (MP) perturbation theory. MP fails to describe the ground state correctly for example whenever a bond in a molecule is broken, as it happens in almost all chemical reactions. A method that is known to be more reliable in such and other cases is the so-called *coupled-cluster* (CC) model. In this work, a CC ground state is used within the ADC scheme of second order instead of an MP one and its influence on excitation energies and molecular properties is investigated.
It is shown that while for *excitation energies* the results are similar as for the stadard method, for molecular properties such as *dipole polarizabilities* a significant improvement is obtained when using CC amplitudes, especially for aromatic systems which had proven to be problematic cases for standard ADC approaches.

P8 Analyzing DNA Double-Strand Break Repair Processes with High-Resolution Localization Microscopy and Persistent Topology

Andreas Hofmann[1)], Matthias Krufczik[2)], Michael Hausmann[2)], and Dieter W. Heermann[1)]

[1)] Institute for Theoretical Physics, Heidelberg University; [2)] Kirchhoff-Institute for Physics, Heidelberg University.

email: andreas.hofmann@thphys.uni-heidelberg.de

In the past years, research in the field of genome dynamics has revealed that the genome and its underlying constituents are not randomly structured. Novel fluorescence light microscopic techniques enable optical resolutions down to the order of 10nm and open new insights into genome structure and organization. We irradiated cells of breast cancer cell lines with different doses. Specific fluorescently labeled antibodies were used to target histone modifications which are indicators for heterochromatin (H3K9me3). In addition γH2AX was tagged by antibodies. Localization microscopy uses two different spectral states of dye molecules to achieve optical separation and thus spatial isolation of single molecule positions. Spectral Position Determination Microscopy (SPDM) applied here works with conventional fluorophores in 3D conserved cell nuclei and does not require any additional staining or cumbersome sample preparation. With this super-resolution microscopy, we are able to determine the positions of specifically labeled molecules and to calculate density and distance distributions thereof. This data allows to quantify the complex changes of the chromatin which we find after irradiation caused by the damage and the arising repair mechanism. Our aim is to firstly identify regions of active repair processes and subsequently, to analyze both the heterochromatin density and its morphology around these clusters in order to gain new insights on the interplay of the repair mechanism and heterochromatin. To this end, we developed a new analytical methodology to also characterize the morphology of heterochromatin by means of persistence topology. The advantage of looking at topological properties of the heterochromatin structure is the intrinsic scale invariance that allows to compare structures without being restricted to a certain length scale.

P9 The Enemy Inside Me - How Malaria Parasites Remodel our Red Blood Cells

Julia Jäger, Ulrich Schwarz

Physics of Complex Biosystems, Heidelberg University.
email: julia.jaeger@bioquant.uni-heidelberg.de

Once inside the body, malaria parasites invade red blood cells in order to hide from the immune system and to digest hemoglobin. Over the course of 48 hours the parasite completely remodels the red blood cell, so that the cell becomes round and stiff and eventually breaks open to release about 20 new parasites. As part of this remodeling process the parasite induces adhesive protrusions called knobs on the surface of the red blood cell (see Figure 7.3), which keep the infected cells in the vasculature for a longer time, but these adhesive properties also cause the symptoms of the disease. The knobs change the elastic properties of the red blood cell membrane, but the relation to the underlying molecular processes is unclear.
We aim at a multiscale framework to simulate the relation between the parasite-induced molecular changes in the red blood cell and the resulting membrane properties. In addition to the usual interface Hamiltonian for the membrane, we take into account the connections between the outer lipid bilayer and the spectrin network underlying the plasma membrane, so that we can predict the effects of altering these connections. The results of the calculations can be compared with the data of membrane flickering experiments which can be used to measure quantities like the bending modulus and the confinement parameter of the membrane, which is proportional to the membrane's shear modulus.
As our main result we find how the confinement parameter scales with the number of connections and their strength. This implies that the malaria parasite either induces more connections between spectrin network and lipid bilayer or makes existing connections stronger. Therefore, we can explain how spectrin elongation leads to stronger connections and hence to a larger membrane shear modulus, by taking into account the strain hardening properties of spectrin molecules.

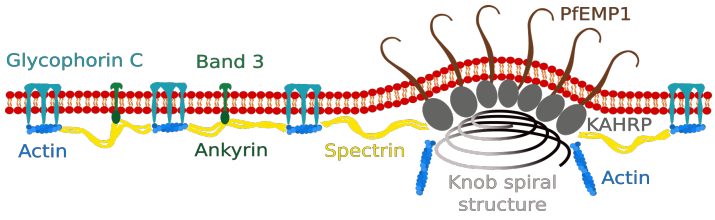


Figure 7.3: Alterations of red blood cell membrane structure as induces by the malaria parasite.

P10 How could Stiffness, Heterogeneity and Confinement Affect the Polymer Conformations?

Jiying Jia

Institute for Theoretical Physics, Heidelberg University.
email: jia@thphys.uni-heidelberg.de

The conformations of chromatin and many other polymers are influenced by many factors. Here we investigate the role of bending rigidity as well as its heterogeneity, confinement in the organization of linear polymers by exploring several properties such as the contact probability, persistence length, mean average crossing number and so on.
The bending rigidity influences the organization of free polymer in the length scale of persistence length, but won't change the properties in much larger scale. At the same time, the heterogeneity of bending rigidity, which exists in most real polymer systems, acts as a role of softener, i.e., flexibilizing the semiflexible chains compared to the homogeneous ones. This effect could be reflected via the contact probability together with other properties. Confinement could imposes drastic change on the conformations. In the cubic and rectangle boxes we study here, semiflexible chains have to spiral when the box size is small enough, leading to an oscillation in the contact probability and the orientational correlation function. Moreover, the symmetry of box also influence the packing of a semiflexible chain, which could be seen via the ordering of chain segments and the mean average crossing number.

P11 Visual Analysis of the Kalman Filter

Philipp Jung, Filip Sadlo

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: philipp.jung@iwr.uni-heidelberg.de

Vortical motion in flow fields is often visualized by extracting vortex core lines, i.e., the "centerlines" of vortices. In this paper, we focus on the extraction of vortex core lines from 3D vector fields containing tumble vortices, i.e., vortices with vanishing longitudinal velocity component. These types of vortices can appear in analytical vortex models, but also in simulated data, e.g., in flow close to boundaries. While there exist many different definitions for vortex core lines, these are typically formulated and extracted by means of the parallel vectors operator, i.e., as those points in space where two (derived) vector fields are parallel or antiparallel. However, in case of vanishing longitudinal component and other degeneracies which we investigate, the existing approaches to solve the parallel vectors problem tend to fail. We present a technique to solve these cases, based on subdivision and problem transformation, and examine and exemplify our technique by means of an analytical vortex model and data from computational fluid dynamics.

P12 Investigation of the mass boundary layer under small-scale air-sea interaction processes on a wavy water surface

Angelika Klein[1),2)]

[1)] Heidelberg Collaboratory for Image Processing (HCI), Heidelberg University; [2)] Institute of Environmental Physics (IUP), Heidelberg University.

email: angelika.klein@iup.uni-heidelberg.de

The gas transfer between air and water is mainly controlled by a small water sided mass boundary layer of a thickness of about 50 to 200 micrometers. We investigate the development of boundary layer streaks, microscale wave breaking and gas and heat transfer in dependence of different wind and fetch conditions. We present first results of two recent measurement campaigns, carried out at the annular wind-wave facility Aeolotron at the Institute of Environmental Physics, University Heidelberg.

P13 Machine Learning approaches for epigenetic network inference in T cells

Christoph Kommer[1),2)], Qin Zhang[1),2)], Ahmed Hegazy[3)], Max Löhning[3),4)], Thomas Höfer[1),2)]

[1)] German Cancer Research Center (DKFZ), Heidelberg; [2)] BioQuant Center, Heidelberg University; [3)] German Rheumatism Research Center, Berlin; [4)] Charité-Universitätsmedizin, Berlin.

email: c.kommer@dkfz-heidelberg.de

T-helper cells direct the cell- and antibody-based arms of the adaptive immune system via the secretion of signalling proteins. The classical view of naïve T-helper cells differentiating into a small number of stable steady states has recently been challenged by experimental findings that point towards multistable hybrid states away from a bistable fixed-point solution.
To interrogate the underlying regulatory mechanisms, we identified the epigenetic landscape in naïve and differentiated T-helper cells from histone modification patterns by applying different machine learning approaches and found distinct classes of enhancers and repressors according to their regulation by lineage-specifying transcription factors and/or extrinsic differentiation signals which are also cell-type specific. For mapping epigenetic states to target genes we furthermore developed a novel parametrized multivariable correlation measure model. With this approach, we recovered well-known cis-regulatory elements and predicted new ones with comparable confidence. Integrating these results with further experimental data we obtain a directed weighted multigraph from which we infer community clusters as well as cell-type specific networks that reveal underlying mechanisms of different steady states of T-helper cells.
We discuss the utility of these data to learn epigenetic regulatory network topologies in order to explain multistability.

P14 The spin-flip algebraic diagrammatic construction scheme (SF-ADC) for the polarization propagator for molecular systems with few-reference ground-state wave functions

Daniel Lefrancois, Andreas Dreuw

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: daniel.lefrancois@iwr.uni-heidelberg.de

In general, for the theoretical description of systems with multi-reference ground-state wave functions as, for instance, in bond-breaking, singlet-triplet gaps, or at conical intersections, methods like complete active space self-consistent field (CASSCF) or multi-reference configuration interaction (MRCI) are required.
An alternative is offered by the so-called spin-flip (SF) methods. The key idea of SF is to choose the triplet ground-state as reference and to calculate a multi-reference singlet ground-state as "excitation", in which the spin of the excited electron is flipped, using standard single-reference methodologies. Indeed this only works as long as the triplet ground-state wave function is not spin-contaminated, which defines a few-reference system.
Here a spin-flip version of the algebraic diagrammatic construction (ADC) scheme for the polarization propagator up to third order perturbation theory (SF-ADC(3)) [1] is presented and benchmarked for systems with few-reference wave functions. The results show a qualitatively correct picture for the calculated bond-breaking situations and yields reasonable energies [1]. Furthermore SF-ADC happens to be very accurate for the calculation of adiabatic singlet-triplet gaps of various atoms and molecules with absolute mean errors of about 0.03 - 0.1 eV compared to experimental data [2].

[1] D. Lefrancois, M. Wormit, and A. Dreuw, *J. Chem. Phys.* **2015**, *143*, 124107.
[2] D. Lefrancois, D. R. Rehn, and A. Dreuw, *J. Chem. Phys.* **2016**, *145*, 084102.

P15 Development and Simulation of the Aqueous Humor flow in the Anterior Chamber for healthy and pathological eyes

Vladislav Olkhovskiy

Institute of Applied Mathematics, Heidelberg University.
email: vladislav.olkhovskiy@iwr.uni-heidelberg.de

One of the most common reasons for blindness is glaucoma. The primary risk factor for the development of the vision loss in glaucoma is an increased intraocular pressure (IOP) and lowering the IOP is currently the only therapeutic option with proven efficiency. To understand the behaviour of the aqueous humor flow and of the IOP in the anterior chamber of the human eye, a mathematical model is developed. This model is given by Stokes-Darcy equation with Beavers Joseph Saffman condition on the interface. The Stokes equation describes the flow in the anterior chamber and the Darcy equation describes the flow in the trabecular meshwork which is a porous medium. The characteristical physical properties are given by the inflow rate of the aqueous humor at the ciliary body, the pressure of the episcleral venes and it is assumed that the cornea, the lens, the iris and the zornules are impermeable. Geometries for healthy and pathological eyes are considered. First numerical simulations using the Finite Element method are performed in two dimensions. In the simulation, mixed finite elements are used and the solutions of the equations are generated with deal ii software and UMFPACK package. Comparison of simulation results in healthy and pathological cases are presented.

P16 Layamon's Brut – A Computational Approach to the Lexical Study of Medieval Manuscripts

Maria Rupprecht

Institute of English Studies, Heidelberg University and Interdiscriplinary Center for Scientific Compouting (IWR), Heidelberg University.

email: maria.rupprecht@iwr.uni-heidelberg.de

Following the great scribal tradition in the literary hubs of the monastic scriptoria in Anglo-Saxon England, Layamon's Brut represents the two first Middle English manuscripts since the Norman invasion. It is a captivating pseudo-history of England, beginning with the myth of Noah's Flood treating the Migration Period, and the legendary story of King Arthur. Fascinating scholars for centuries, there have been palaeographical, historical, philological, and linguistic studies on this monumental manuscript. Accordingly, there is a glossary of pivotal excerpts in existence, as well as there are various editions that are even digitized by now.

Unfortunately, we don't have a comprehensive glossary or dictionary for the manuscripts at our disposal that might serve as the foundation for an appropriate, contemporary linguistic investigation, like a thorough lexical or even literary study of Layamon's Brut. Making the manuscripts and the editions more accessible to scholars and students, we are planning with the support of the 'Dictionnaire Etymologique de l'Ancien Francais' (DEAF) and the Department of Computational Linguistics to create a digital and printed glossary. The DEAF is much more complex and extensive online dictionary, including any possible Old French source and functions that are not relevant for a rather simple glossary. Working tools from the IPD cooperation (Institut fuer Programmstrukturen und Datenorganisation), the electronical DEAF combines a My SQL data base, a WicketFrameWork surface, Hibernate, Databinder and the integration of XML structures for means of information management, process management and various context-bound functions. The greatest computational challenges of automatized processes like cataloguing, quantification, lemmatisation and contextualization have proved successful in the long lasting and extensive work of the DEAF and should be easy to transfer in the context of Middle English manuscript. Verifying and defining the lemmata will take the greatest effort but that is just another step.

P17 A Quantitative Approach to the Extraction of Lagrangian Coherent Structures

Toni Sagristà Sellés[1),2)], Stefan Jordan[2)], Thomas Müller[3)], Filip Sadlo[1)]

[1)] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University; [2)] Astronomisches Rechen-Institut (ARI), Heidelberg University; [3)] Max Planck Institute for Astronomy (MPIA), Heidelberg.

email: toni.sagrista@iwr.uni-heidelberg.de

The extraction of Lagrangian coherent structures by means of ridges in derived fields, such as the finite-time Lyapunov exponent, involves a multitude of parameters that have been difficult to determine and whose impact on the result has been hard to interpret. In this poster, we present a quantitative approach that helps choosing and interpreting these parameters, taking into account discretization, time scope, and separation properties. This not only eases the overall visualization process but also helps obtaining physically meaningful results. We exemplify and evaluate our approach using various synthetic and simulated examples from computational fluid dynamics.

P18 Deep Unsupervised Similarity Learning using Partially Ordered Sets

Artsiom Sanakoyeu

Heidelberg Collaboratory for Image Processing (HCI), Heidelberg University.

email: artsiom.sanakoyeu@iwr.uni-heidelberg.de

Unsupervised learning of visual similarities is of paramount importance to computer vision, particularly due to lacking training data for fine-grained similarities. Deep learning of similarities is often based on relationships be- tween pairs or triplets of samples. Many of these relations are unreliable and mutually contradicting, implying inconsistencies when trained without supervision information that relates different tuples or triplets to each other. To overcome this problem, we use local estimates of reliable (dis-)similarities to initially group samples into compact surrogate classes and use local partial orders of samples to classes to link classes to each other. Similarity learning is then formulated as a partial ordering task with soft correspondences of all samples to classes. Adopting a strategy of self-supervision, a CNN is trained to optimally represent samples in a mutually consistent manner while updating the classes. The similarity learning and grouping procedure are integrated in a single model and optimized jointly. The proposed unsupervised approach shows competitive performance on detailed pose estimation and object classification.

P19 Visual Analysis of the Kalman Filter

Kai Sdeo, Ole Klein, Filip Sadlo

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: kai.sdeo@iwr.uni-heidelberg.de

The ensemble Kalman filter is a commonly used data assimilation technique, i.e., a technique that feeds observations into running simulations to improve their predictive accuracy. Based on this filter, various enhanced and specialized variants have emerged. All these techniques, however, have in common that the interplay of observations and the underlying simulation models and their results is complex and thus hard to understand in detail. We present a novel visualization technique to analyze the processes involved in the Kalman filter, and outline its advantages at the example of the Lorenz system. This way, we aim at supporting the application and modeling of data assimilation techniques and help identify problems that may arise during their execution.

P20 An ILP Solver for Multi-label MRFS with Connectivity Constraints

Ruobing Shen

Institute of Computer Science, Heidelberg University.
email: ruobing.shen@informatik.uni-heidelberg.de

Integer Linear Programming (ILP) formulations of Markov random fields (MRFs) models with global connectivity priors were investigated previously in computer vision. In previous works, only Linear Programing (LP) relaxations or simplified versions of the problem were solved. This paper investigates the ILP of multi-label MRF with exact connectivity priors via a branch-and-cut method, which provably finds globally optimal solutions. The method enforces connectivity priors iteratively by a cutting plane method, and provides feasible solutions with a guarantee on sub-optimality even if we terminate it earlier. The proposed ILP can also be applied as a post-processing method on top of any existing multi-label segmentation approach. We demonstrate the power and usefulness of our model by several experiments in the BSDS500 image dataset, as well as medical images with trained probability maps.

P21 Motion of the vitreous humour in a deforming eye

Elfriede Friedmann[1)], Vít Průša[2)], Judith Stein[1)], Karel Tůma[2)]

[1)] Institute for Applied Mathematics, Interdisciplinary Center for Scientific Computing, Heidelberg University; [2)] Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic.

email: judith.stein@iwr.uni-heidelberg.de

Although linked to several vitreoretinal pathologies the material behavior of the vitreous body in response to mechanical loads is not well understood. In this study, we analyze the motion of vitreous humour in a deforming eyeball which shows a viscoelastic behavior due to a network of collagen fibers.
According to the literature this behavior can be described by the viscoelastic Burgers fluid model and it interacts with the deforming sclera and the lens, nonlinear elastic solids. In order to compare a healthy versus a pathological vitreous with liquefaction or complete vitrectomy, we compare the viscoelastic versus the viscous Navier-Stokes model.
Our simulations show that due to the very elastic sclera the choice of the rheological model has nearly no influence on the force and flow fields, but it has significant impact on the mechanical stress distribution in the domain of interest.

P22 Numerical Modelling of Facade Degradation

Michal Tóth[1)], Peter Bastian[2)]

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.

email: [1)] mtoth@iwr.uni-heidelberg.de, [2)] peter.bastian@iwr.uni-heidelberg.de

The most common material used for facades is a concrete. Although it is durable, after longer periods of time every material shows the signs of wearing down. The key to maintenance is to have reliable information about material condition, and to know the appropriate time for the remediation.
Our numerical method aims to answer both these questions. It models water, air and contaminant transport inside the porous medium (facade), chemical reactions of contaminants, and porosity change. We focus on chemical reactions causing degradation -carbonation, and leaching. Each process is described by a differential equation, which is often nonlinear or degenerate. Various weather conditions can be modeled by a suitable modification of boundary conditions. We use DUNE toolbox to carry out the computation.
Since the project exists for 2 months now, we have no publishable results yet. Main workload will be calibrating and adjusting the model to the problem. Data for water and air flows are provided by Comenius University in Bratislava.

Keywords: *numerical model, porous medium, contaminant transport, porosity change*

P23 The restricted virtual space (RVS) approach in algebraic diagrammatic construction scheme (ADC) for calculations of excited state properties

Chong Yang, Andreas Dreuw

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: chong.yang@iwr.uni-heidelberg.de

The accuracy and efficiency of the restricted virtual space (RVS) approach calculations of excitation energies employing the algebraic diagrammatic construction (ADC) scheme has been evaluated [1]. The calculations of excited state properties, such as oscillator strength, dipole moments and transition properties between excited states are performed on octatetraene, indole, and pyridine using the RVS-ADC(2) method with the triple-zeta basis set (TZVP) based on systematic restrication of the virtual orbital space. The results show that the accuracy of the excited state properties is not affect sinificantly by restrication of a fraction of high-lying virtual orbitals. A comparison of the RVS approach calculation with the full virtual orbital space calculation indicates that the loss of accuracy for the oscillator strength, dipole moments, transition dipole moments is negligible when freezing core and less than 30% of high-lying virtual orbitals. The effect of the transition character of low-lying excited states on the accuracy of excited state properties calculations with the RVS-ADC approach is discussed. Calculations on various excited state properties demonstrate the reliability and applicability of the RVS-ADC approach.

[1] C. Yang, and A. Dreuw. *J. Comput. Chem.* **2017**, *38*, 1528.

[2] C. Yang, and A. Dreuw, The calculations of excited state properties with the restricted virtual space (RVS) approach in algebraic diagrammatic construction scheme (ADC), *in preparation.*

P24 Automated image analysis of calcium waves in roots of Arabidopsis thaliana

Martin Zauser[1)], Rik Brugman[2)], Janos Löffler[2)], Guido Grossmann[2)], Jürgen Pahle[1)],

[1)] Biological Information Processing Group/BIOMS/BioQuant, Heidelberg University, Heidelberg, Germany; [2)] Centre for Organismal Studies, Heidelberg University, Heidelberg, Germany.

email: martin.zauser@bioquant.uni-heidelberg.de

Plants respond to a sudden change of environmental conditions and bacterial challenges by increased activity of intracellular signaling by calcium ions. For the model plant textitArabidopsis thaliana it could be shown that calcium signals propagate in waves through the root and show stimulus-specific signatures, if the plant is stimulated by salt or bacterial peptides. We investigate the propagation of waves through the root by quantifying intracellular calcium signaling.
For this purpose, we developed a computational approach for calcium wave visualization and quantification which is capable of processing time-lapse image stacks of fluorescence microscopy images of plant roots and analyzing the intensity changes caused by increased concentrations of intracellular calcium. This work is composed of three key steps. The first is the automated generation of a time-space diagram (kymograph) by detecting the outline of the root and calculating the mean intensity at each position perpendicular to the axis of the root. The second is a position-related scaling of the kymograph resulting in a distinct representation of the calcium wave called the "Crestline Plot". The kymograph as well as the crestline plot can easily visualized as a 3D-like surface plot. The third contribution is an algorithm for analyzing the crestline plot by identifying key points of the calcium wave. The starting position and starting time of the wave are calculated as well as the speed into both directions along the axis of the root (Fig 7.4). The analysis is augmented by a quality check of the image data including a detection of artifacts or defective datasets. The algorithm was applied to different datasets of high-resolution microscope images of genetically modified *Arabidopsis thaliana* plants stably expressing a calcium sensor.

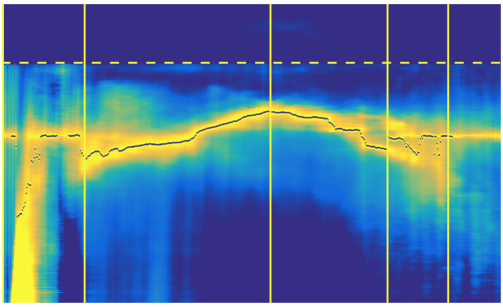


Figure 7.4: Automated image analysis of calcium wave propagation in plant roots in response to a stimulation with the bacterial peptide flg22.

P25 Visualization of Field Similarity

Boyan Zheng, Bastian Rieck, Heike Leitte, Filip Sadlo

Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University.
email: boyan.zheng@iwr.uni-heidelberg.de

In this project, we present a novel approach to the analysis of vector fields. A vector field assigns to each point of its domain a respective vector value. In other words, it maps from the domain to the data range. In our approach, we investigate the opposite mapping, i.e., how domain points relate to the range, or in other words, we investigate the mapping from the range to the domain. The resulting visualization technique, which consists of a static overview component augmented with interactive exploration methods, not only supports the analysis of similar regions within a given dataset, but also provides a means for comparative visualization of different vector fields. We demonstrate and evaluate our approach with synthetic fields, measured fields, and data from computational fluid dynamics.

8 List of presenters

Invited Speakers

I4 Dr. Daniel Gerecht
I3 Dr. Adrian Komainda
I1 Prof. Dr. Björn Malte Schäfer
I2 Prof. Dr. Ulrich Schwarz

Fellow Speakers

T1 Felix Brinkmann
T2 Simon Dörsam
T3 Ruth Großeholz
T4 Enrique Guerrero Merino
T5 Michael Herbst
T6 Sarah Kaspar
T7 José Pablo Lucero Lorca
T8 Aaron Pattee
T9 Asha Roberts
T10 Nadia Said
T11 Fereydoon Taheri

Fellow Poster Presenters

P1 Alberto Bailoni
P2 Adrian Dempwolff
P3 Dieter Faltermeier
P4 Sonja Friman
P5 Jie Han
P6 Maximilian Herrmann
P7 Manuel Hodecker
P8 Andreas Hofmann
P9 Julia Jäger
P10 Jiying Jia
P11 Philipp Jung
P12 Angelika Klein
P13 Christoph Kommer
P14 Daniel Lefrancois
P15 Vladislav Olkhovskiy
P16 Maria Rupprecht
P17 Toni Sagristà Sellés
P18 Artsiom Sanakoyeu
P19 Kai Sdeo
P20 Ruobing Shen
P21 Judith Stein
P22 Michal Tóth
P23 Chong Yang
P24 Martin Zauser
P25 Boyan Zheng

9 Notes

HGS MathComp

Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences

Chairman

Prof. Dr. Peter Bastian
Interdisciplinary Center for Scientific Computing (IWR)
Mathematikon
Im Neuenheimer Feld 205
69120 Heidelberg

Administrative Director

Dr. Michael J. Winckler
Interdisciplinary Center for Scientific Computing (IWR)
Mathematikon
Im Neuenheimer Feld 205
69120 Heidelberg

Phone: +49 (0) 6221 54 -14 430
Email: michael.winckler@iwr.uni-heidelberg.de

Office

HGS MathComp
Mathematikon • Room 5/214
Im Neuenheimer Feld 205
69120 Heidelberg

Phone: +49 (0) 6221 54 -14 410
Email: hgs@iwr.uni-heidelberg.de

Opening Hours
Monday & Thursday: 09:00 –12:00 • 14:00 –16:00
Wednesday: 10:00 –12:00 • 14:00 –16:00
Tuesday & Friday: closed

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

www.mathcomp.uni-heidelberg.de