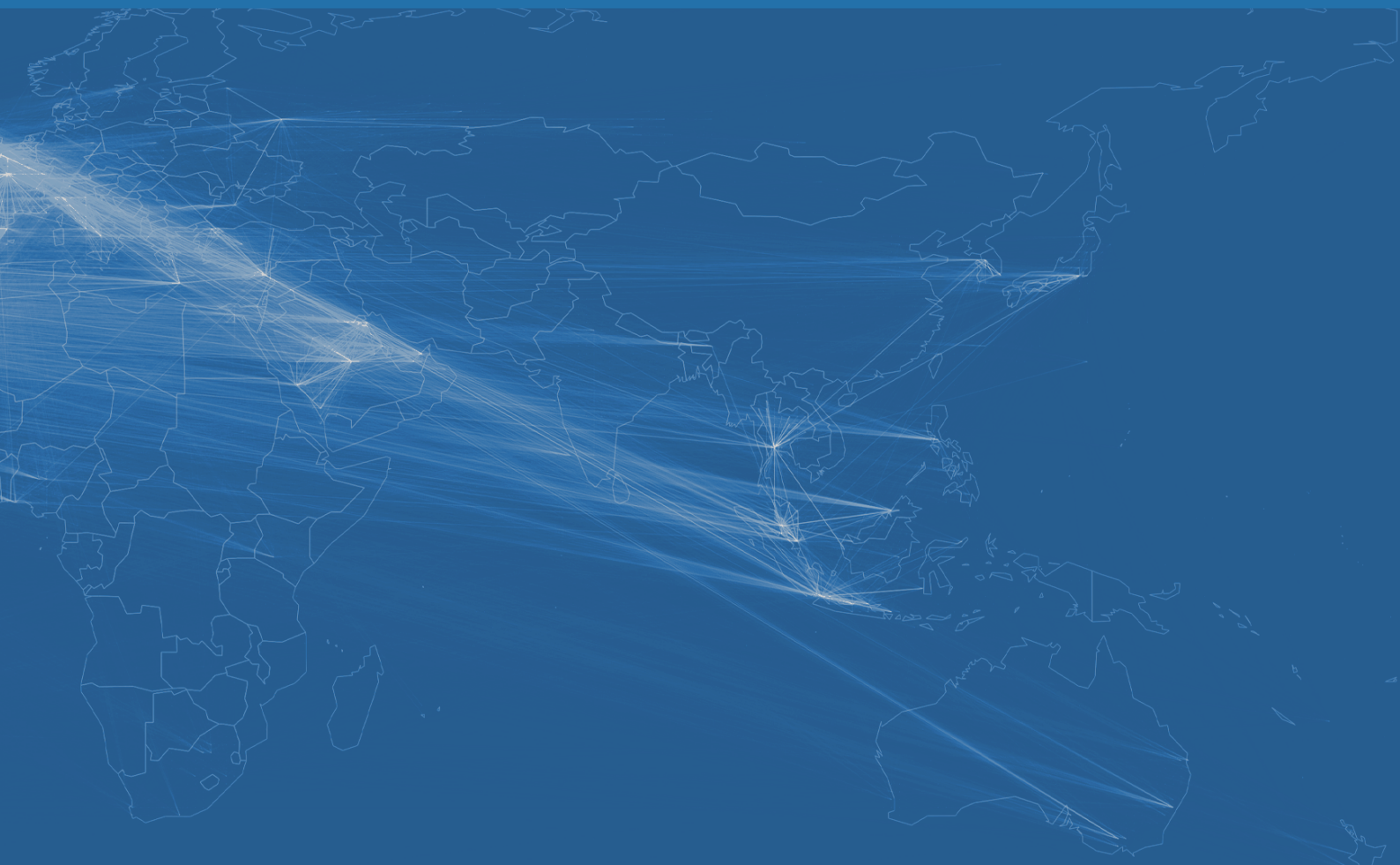
HGS MathComp

24/25 November 2014
Youth Hostel Speyer



Small World - Big Data

6th Annual Colloquium

of the Heidelberg Graduate School
of Mathematical and Computational
Methods for the Sciences

Organizing Committee

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We gratefully acknowledge The Boston Consulting Group for sponsoring.

Welcome to the *HGS MathComp* Annual Colloquium

Amongst us are people working in areas such as Mathematics, Informatics, Chemistry, Astronomy, Earth and Material Sciences, Medicine, Bio Sciences and Psychology. *Big Data*, the theme of this year's conference, is relevant to all these fields. We noticed that already our different groups have a different understanding about the meaning of Big Data. The importance of Big Data emerges from the ability to gather and process huge amounts of information produced by and about people, things, and their interactions. Complementary to theory-driven discovery, data-driven science may help to support the continuous assessment of theories or to even uncover new and surprising hypotheses, called the *unknown unknowns*. The identification of the complete human genome sequence for example cleared the way for the discovery of new drug therapies. This requires not only the collection of huge amounts of data but also scientists to understand and untangle the often very complex data sets. We have invited four speakers from different academic and industrial backgrounds to show us how people in their field typically work with Big Data.

Apart from the plenary speaker from IBM, the invited talks will take place on the second day. Every speaker in our oral sessions was explicitly asked to make his or her talk comprehensible to a general scientific audience and comprehensibility is also the measure we will apply in order to award the *best poster prize*. During the early evening, the poster session should provide a second opportunity for intellectual exchange, before we head on to the Christmas market here in Speyer to start with the social part of the conference.

The Annual Colloquium provides an excellent opportunity for insight into new fields and should act as a platform for the exchange of ideas and knowledge. We are all approaching related topics from different viewpoints with different ideas about problem solving. We would like to motivate every participant to benefit from this diversity.
As a final remark, the success of a conference depends most importantly on an open environment that encourages discussions amongst the fellows. We therefore hope that the nature of our conference will be open and informal and stimulate productive and interesting conversations.

Enjoy the conference.

The Organizing Committee.

Contents

Contents

HGS MathComp

The 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.

The Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences is the only graduate school in Germany to focus its research on scientific computing. The school is funded by the German Excellency 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...

Conference Location

This year's HGS annual colloquium will take place in one of the oldest cities in Germany, Speyer. Once founded by the Romans and it is now famous for its cathedral, its medieval west city gate (*Altpörtel*), its medieval jewish courtyard and much more.

This city is the ideal location for the annual colloquium, because it is very beautiful and offers nice possibilities for people interested in science such as the widely known Technikmuseum Speyer (technical museum), the big aquarium Sea Life Speyer, or the IMAX 3D cinema.

The event itself will be held in the DJH youth hostel Kurpfalz-Jugendherberge, which is approximately a 10 minutes foot walk outside of the old town. One option of the social program will be a small city tour with an extended stop at the local christmas market, which will be already open during our stay.

Youth Hostel Speyer

Geibstraße 5	speyer@diejugendherbergen.de
67346 Speyer	www.DieJugendherbergen.de
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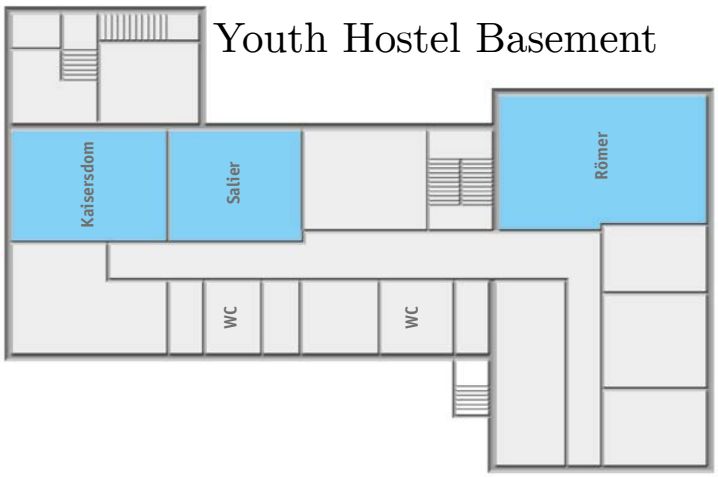
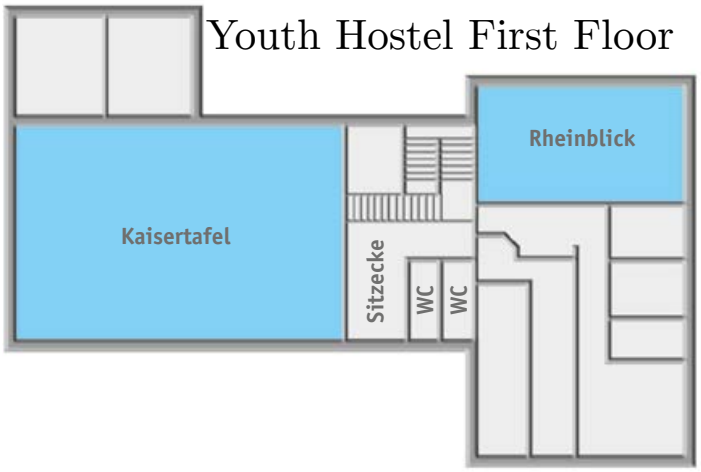
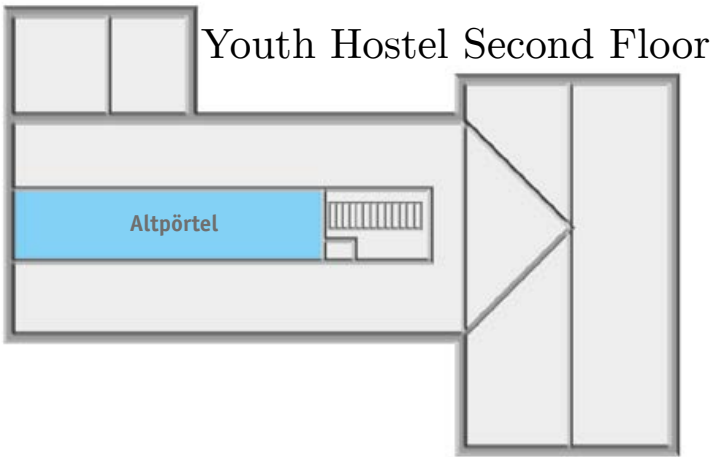
Youth Hostel Overview







Registration and Check-Out

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 a key for your room.
- Your official HGS annual colloquium 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 the limited possibilities of a 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 until 9:00 AM on the second day.
- There are only 2 keys available per room.
- Please return the key if you are responsible for it.
- Your luggage will be stored in a separate room.
- There will be no W-Lan offered by the HGS.

Program

Time	Monday, Nov 24	Tuesday, Nov 25
8:00 – 9:00	Bus Departure	*Breakfast* & room cleaning
9:00 – 9:45	Registration	I2: Schick (HITS)
9:45 – 10:15		*coffee break*
10:15 – 11:00	*coffee break*	I3: Jung (KIT)
11:00 – 11:30	Opening Ceremony	
11:30 – 12:00	I1 **Keynote** Lang (IBM)	
12:00 – 12:30		*Lunch*
12:30 – 13:00	*Lunch*	
13:00 – 13:30		I4: Dietz (SAP)
13:30 – 14:00	O1.1 O1.2 O1.3	I5: Schmälzle (BCG)
14:00 – 14:30	O2.1 O2.2 O2.3	
14:30 – 15:00	O3.1 O3.2 O3.3	*coffee break*
15:00 – 15:30	*coffee break*	Closing Ceremony
15:30 – 16:00	O4.1 O4.2 O4.3	
16:00 – 16:30	O5.1 O5.2 O5.3	Departure
16:30 – 17:00	O6.1 O6.2 O6.3	
17:00 – 17:30		
17:30 – 18:00	Poster Session	
18:00 – 18:30		
18:30 – 19:00		
19:00 – 19:30	*Dinner*	
19:30 – 20:00		
20:00 – 20:30	Christmas Market	
20:30 – 21:00		

Invited talks

I1: Alexander Lang — Big Data - Little Impact? Raising the bar for "Data Science"
I2: Michael Schick — High-Performance Computing and Uncertainty Quantification
I3: Christopher Jung — Big Data in Scientific Practise
I4: Michael Dietz — Big Data in Enterprise Business Processes
I5: Michael Schmälzle — What a mathematician can do at Boston Consulting Group

Fellows talks

Time	**Room 1** (*Kaisertafel*)	**Room 2** (*Römer*)	**Room 3** (*Salier*)
SESSION I			
13:30	**O1.1**	**O1.2**	**O1.3**
	Katharina Beuke	Mareike Schmidtobreick	Marcel Mohr
14:00	**O2.1**	**O2.2**	**O2.3**
	Lutz Büch	Jürgen Gutekunst	Mohammed Ghanavati
14:30	**O3.1**	**O3.2**	**O3.3**
	Michael Herbst	Ghazal Jabbari	Hjalte Raun
SESSION II			
15:30	**O4.1**	**O4.2**	**O4.3**
	Jan Wenzel	Manuel Kudruss	Felix Lenders
16:00	**O5.1**	**O5.2**	**O5.3**
	Johannes Berger	Tsveta Miteva	Frederik Ziebell
16:30	**O6.1**	**O6.2**	**O6.3**
	La Huu Chuong	Yong Hu	Bartocz Bogacz

Abstracts of Talks

The talks are listed in session order.

Session I: *Time:* 13h30–15h00

O1.1 Modelling Inflammation in the liver – what is inflammation, how do we model it, and where are the challenges?

Katharina Beuke
Modelling of Biological Processes

Bacterial infection, or rather the invasion of bacteria in the liver is recognised by cells through protein molecules in the cell surface so called membrane receptors. These receptors can detect sugar molecules in the bacteria cell wall (lipopolysaccharides, or short LPS), which are only present in bacteria and not in human (or other animal) cells.
Once the receptors have bound and thereby recognised these sugar molecules, they initialise many internal steps, which eventually lead to the so called cell responses, either cell death (apoptosis), cell doubling (proliferation) or simply sending out new signals (paracrine or endocrine signalling). Such an intracellular information processing of an external stimulus is called a signalling cascade. Many of the molecules involved in signalling cascades are well studied. We know their size, their building blocks, sometimes we even have a 3D image available, we know many ways how they can be manipulated in their function (i.e. post-translational modifications). Biologists usually have a very specific idea of how these signalling cascades takes place, what happens first, second etc. Unfortunately, we usually know very little about the speed of these steps or the actual availability of the molecules in cells. On top of this lack of quantitative information, these signalling cascades usually remain incomplete. Here, modelling can help discover gaps and even point towards ways to fill them.
In this talk, based on my PhD project's work, I will explain how the available information still limits the model and why a model that does not represent the biological processes may still not be able to describe the available data, even though many of the model parameters may be non-identifiable. I will even try to motivate why, from a biological point of view, it can make perfect sense that these parameters are non-identifiable.

O1.2 Parallel Numerical Methods based on GASPI

Mareike Schmidtobreick
EMCL

Numerical simulations often play a key role in the analysis of complex physical and technical processes. Performing these simulations accurately often relies on computational resources only available on high performance computing (HPC) platforms. Depending on the complexity and size of these problems even with the use of parallel computers and commonly used parallel programming interfaces such as MPI (for distributed memory systems) or OpenMP (for shared memory systems) such applications reach limits, both in time and in memory space.

Another approach to parallel computing is the PGAS-modell which relies on a Partitioned but Global Address Space, designated for distributed memory systems. A rather new development within this field is GASPI, a Global Address Space Programming Interface. Here, from the outset, communication between processes is designed to be one-sided and together with fine-grained synchronization mechanisms, offers opportunities for an overlap of computation and communication.

Based on this new parallel programming interface numerical kernels, such as the multiplication of two quadratic dense matrices, or a dense solver, such as the LU decomposition, are implemented. The implementations aim at increasing the performance of the algorithms by making use of the one-sided communication so communication can proceed in the background whilst the processors itself are busy with ongoing computations.

O1.3 Plasma Cell Survival and Pathogenesis of *Multiple Myeloma*: The Niche matters

Marcel Mohr
Applied Analysis and Modelling in Biosciences

Multiple myeloma is a cancer that is caused by an accumulation of malignant plasma cells, so-called *myeloma cells* in the bone marrow. Plasma cells are antibody-secreting cells which differentiate via numerous intermediate stages of haematopoietic (blood-forming) stem cells, mostly settled in the bone marrow. They come into contact with other cells of the bone marrow which produce factors that allow their survival in the bone marrow. This specialised microenvironment, the *niche*, is necessary for long-term survival: Plasma cells may survive only for a few days if they are taken out of their milieu (e.g., as part of a bone marrow aspirate). In contrast, plasma cells may survive in the niche for more than 20 years.

New plasma cells are formed throughout the whole life and compete with resident plasma cells for niche space. Myeloma cells are also dependent on the interaction with the niche to survive in the bone marrow. However, in contrast to healthy plasma cells, they are able to proliferate and may partially become independent of the niche. Although the niche is physically restricted, it may be stretched due to a high cell accumulation, thus providing additional homing space for the cells.

To understand the complex processes impacting on accumulation of myeloma cells and their influence on pathogenesis, it is crucial to understand healthy plasma cell generation and their survival. We make use of mathematical models which describe the dynamics of healthy and malignant plasma cell populations, based on growth processes, cell-cell and cell-niche interactions. These models involve the current understanding of the disease and are being developed in close collaboration with Dirk Hose and Anja Seckinger (Multiple Myeloma Section, Heidelberg University Clinic) and Anna Marciniak-Czochra (Institute of Applied Mathematics, University of Heidelberg).

O2.1 Active Learning of Parameters for Record Matching

Lutz Büch
Parallele und Verteilte Systeme

Data analysis is an ubiquitous task in both academia and industry. The easy access to a wide range of data sources from within organizations or from the Internet advances every field. But it also creates the need for data integration tools. Integration tasks include record matching, which is the identification of equivalent records in different data bases, i.e. those that correspond to the same (real-world) entity. Systems that perform these tasks usually depend on data-specific parameters. That is, an expert has to specify some similarity measure and a threshold to define similarity for the data fields. Our Active Learning method can find the most appropriate similarity measure among a given set and adjusts the corresponding decision threshold. It converges to a high quality result with a small amount of human labeling.

O2.2 Leaping Horizon Model Predictive Control for Periodic and Switched Processes

Jürgen Gutekunst
Simulation and Optimization (IWR)

Real time optimal control of periodic and switched dynamical processes is a hard task, because it is not clear how to efficiently handle state discontinuities and switching events moving through the timehorizon.
In this talk we present leaping horizon model predictive control which is especially suited for processes with state discontinuities and switching events.
By adaptively choosing the timehorizon length, we are able to combine benefits of both the moving-horizon and shrinking-horizon scheme. First the ability of the moving horizon scheme to handle continuous processes, and second, the good initialization properties of the shrinking-horizon scheme, which helps us to keep the feedback delay of the controller sufficiently short.
With the leaping horizon scheme we are able to make a broader class of dynamical problems accessible to model predictive control. We analyse two possible real-world applications, namely the control of a simulated moving bed process from chemical engineering and the control of a power producing kite.

O2.3 Automated Memory Leak Diagnosis by Exploiting Functional Unit Tests

Mohammadreza Ghanavati
Parallel and distributed systems

Software systems are gradually becoming more complex due to growth in size and functionality. This increases the risk of latent defects which are difficult to be detected by traditional unit and integration testing. So-called memory leaks, i.e. defects causing memory depletion during execution are a prominent class of latent defects. Since they are frequently discovered only in a production scenario, they can have a significant economic impact. For example, a "latent memory leak bug" has caused a partial outage of Amazon's EC2 cloud service on 22 October 2012 [1], affecting operations of hundreds of EC2 customers. Most of current approaches for diagnosis of memory leaks follow a "symptom to root cause" algorithm to detect memory issues [2]. Despite of the advantages of these approaches in detection of memory leaks, they are hardly useful for automated testing for presence of memory leaks. We propose an approach for automated detection of memory leaks by exploiting existing unit tests. We also provide support for isolation of defect sites by offering to developers a ranked lists of suspicious allocation sites. To validate our approach, we evaluate it on Apache Hadoop, a large open-source project with over 2 million lines of code and about 800 unit tests. We inject 8 artificial memory leaks and try to detect and isolate them. Results show that our method has high accuracy in detection and isolation of injected leaks and imposes an acceptable instrumentation and execution overhead upon existing testing setups.

References

[1] Amazon AWS. Summary of the October 22,2012 AWS Service Event in the US-East Region. https://aws.amazon.com/de/message/680342, 2012.

[2] G. Xu, N. Mitchell, M. Arnold, A. Rountev, and G. Sevitsky. Software bloat analysis: Finding, removing, and preventing performance problems in modern large-scale object-oriented applications. In Proceedings of the FSE/SDP Workshop on Future of Software Engineering Research (FoSER), 2010.

O3.1 Everyday cryptography

Michael Herbst
AG Dreuw Computational Chemistry

The well-known revelations by Eduard Snowden and other whistle blowers in the recent past have shown the full extent of governmental surveillance. The leaked documents clearly draw a picture of a new kind of "selector-based" mass surveillance, which focuses on intercepting all communication at any time and on keeping this information for as long as possible. As a result each and every user of the Internet or the phone network not only has a constant responsibility for himself, but also anyone he communicates with. Whereas cryptography may not prevent surveillance from happening, it does, however, severely increase the computational cost required to obtain the transmitted data or to profile the communication partners.

In my talk I will try to give you an idea how commonly used cryptographic standards work and I will give some hints how to set these things up and use them yourself. We will briefly talk about why only open-source software (if any) should be trusted for cryptography. Further I will mention how even on proprietary operating systems like Windows or MacOS X open-source software can be used for encrypting your communication.

More specifically we will focus on common end-to-end encryption methods like off-the-record (OTM) messaging [1] to encrypt instant messaging (using Adium [2] or Pidgin [3]) or the GNU Privacy Guard (GPG) [4,5] to encrypt EMails in Thunderbird [6]. We will talk about an open-source alternative for videochat and if time permits a little bit about hard drive and file encryption.

References

[1] `https://otr.cypherpunks.ca/`

[2] `https://www.adium.im/`

[3] `https://pidgin.im/`

[4] `https://enigmail.net/`

[5] `https://www.gnupg.org/`

[6] `https://www.mozilla.org/thunderbird/`

O3.2 Quenching Molecular Photodissociation by Intermolecular Coulombic Decay

Ghazal Jabbari
Theoretical Chemistry

Dissociation of chemical bonds frequently accompanies electronic excitations and may take as short time as few tens of femtoseconds. If the electronically excited state is in an environment of other atoms and molecules another fast process - interatomic Coulombic decay (ICD) [1] - may happen as well. If ICD takes place alongside the dissociation the excited molecule de-excites by ionizing a neighbor and the dissociation is quenched.

It has been previously shown that the predissociation of electronically excited CO molecule is quenched by ICD in CO·Mg cluster [2]. In this report we present the study on a more complicated system where we investigate the effect of ICD on the dissociation of $Cl^-{\cdot}H_2O$ cluster following its photoexcitation to the lowest excited A'' electronic state of water molecule. In isolated water this excited state is known to dissociate within some femtoseconds. The dissociation remains the prominent pathway in cluster, although the cage effect of the neighboring chloride complicates the dynamics. We saw the ICD channel is open in the excited state close to the ground state equilibrium geometry. We computed the life time of ICD using Fano-Stieltjes-Lanczos method [3]. To see the quenching effect of ICD we run nuclear dynamics on a 2D cut of the full resonance potential surface. We assume that for the time scale of interest the dynamics will predominantly proceed along the stretching coordinates of the two H atoms. We showed that already in few femtoseconds following the photoexcitation more than 50 percent of the excited state decays via ICD terminating the dissociative dynamics. This results demonstrate that ICD should be taken into account when photochemistry in the environment is considered.

O3.3 LiDAR based semi-automatic pattern recognition within an archaeological landscape

Hjalte Raun
JRG, Digital Humanities

The utilization of airborne LiDAR data in the creation of Digital Elevation Models provides several novel approaches for locating, monitoring, and understanding cultural heritage monuments in our surrounding landscape.

The project, LiDAR based semi-automatic pattern recognition within an archaeological landscape, is focused on adapting and creating semi-automatic procedures for handling and processing LiDAR data within cultural heritage monument detection and large scale cultural heritage management. Particular emphasis is on the implementation of pattern recognition algorithms for semi-automatic detection within 3dimensional vector and 2dimensional raster data.

Further, in order to cope with the huge amount of generated 3dimensional LiDAR point clouds, systematic and semi-automated procedures needs to be defined and developed in order to control and handle the accumulated amounts of otherwise unrestrained point cloud data.

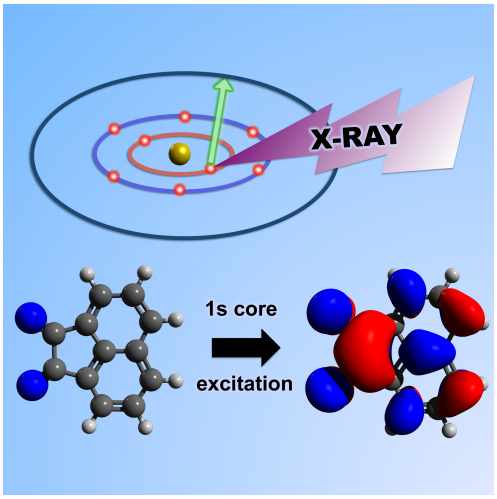
Session II: *Time:* 15h30–17h00

O4.1 How quantum chemical calculations help to understand the mechanisms of organic electronics

Jan Wenzel
Computational Chemistry

An important area of modern applied research is the study of materials used in organic electronics. For example, organic semiconductors are used as the active layer in organic solar cells or organic field-effect transistors (OFET). The annual global radiation power of the sun exceeds the world's required energy requests by several times, making solar cells a very promising alternative to today's fossil fuels. Photovoltaic devices based on organic materials are advantageous over established silica-based systems, since simple production processes are combined with low costs and fully recyclable materials.

Quantum chemical methods aim at understanding the elementary processes and mechanisms of the photochemistry of such systems. Quantum chemical techniques can be used for calculating physical and chemical properties. For example, the photoreaction mechanism of a novel donor-acceptor-donor system that can be applied in photovoltaic devices has been successfully explained. Furthermore, the algebraic-diagrammatic construction scheme for the polarization propagator (ADC) up to third order in combination with the core-valence separation (CVS) for the calculation of X-ray absorption spectra has been implemented. This has provided a deep inside look at the electronic structure of a number of materials used for organic electronics. Results show that the extended variant CVS-ADC(2)-x, in particular, provides the most accurate results with errors of only 0.1% compared to experimental values.



O4.2 Nonlinear Model Predictive Control for Walking Control on Humanoid Robots

Manuel Kudruss
JRG Optimization of Uncertain Systems

In the KoroiBot project we investigate the core principles behind human walking motions and how methods of optimal control can be used to allow current humanoid robots to perform walking motions in the best and most human-like way. Applying optimization and nonlinear model predictive control to generate walking motions for humanoids modeled as systems of connected rigid bodies show that current state-of-the-art methods are not suitable for these problems. The intrinsic instability of bipedal locomotion needs fast and efficient control methods and the treatment of hybrid multi-body dynamics with implicit state dependent discontinuities needs for dedicated methods for optimal control.
In this talk, we present our first results of NMPC for hybrid dynamical system with discontinuities for a extended compass walker model in 2D.

O4.3 Sequential Linear Equality Constrained Programming Methods and Applications in Nonlinear Model Predictive Control

Felix Lenders
JRG Optimization of Uncertain Systems

In Mixed-Integer Nonlinear Model Predictive Control Applications a sequence of similar Mathematical Programs with Equilibrium Constraints (MPEC) has to be solved. MPECs do not satisfy Linear Independence Constraint Qualifications. As a consequence state of the art solution methods for Nonlinear Programs as Sequential Programming Methods typically are very inefficient when applied to these problems. Sequential Linear Equality Constrained Programming (SLEQP) Methods are Active Set Methods using a Trust Region Constrained Linear Program to determine the active set and subsequently solve a Trust Region Equality Constrained Quadratic Program to obtain a step. Replacing the Linear Program by a Linear Program with Equality Constraints (LPEC), this method can also be applied to MPECs. In this talk a preliminary SLEQP Algorithm will be presented and its performance on the CUTEst Problem Set and Example Problems arising in Nonlinear Model Predictive Control assessed. It turns out that the choice of the Trust Region plays a crucial role. A variant using Parametric Linear Programming (PALP) to choose the Trust Region will be discussed.

O5.1 A Geometric Minimum Energy Filter Approach for Camera Motion Estimation based on Nonlinear Observations of Optical Flow

Johannes Berger
Image and Pattern Analysis

In this talk I present a model for camera motion estimation and an approach on how to solve the corresponding filtering problem with the Geometric Minimum Energy Filter for Lie groups. Given some observations that are induced by the camera motion, such as optical flow, depth maps or focus of expansion, the task is to recover the unknown camera motion. This problem formulation is a typical filtering problem for which a range of methods have been developed in the past. However, to fully incorporate the geometry of this motion the corresponding evolution equations have to be formulated on the special euclidean group. As a result the proposed model together with the Geometric Minimum Energy Filter is superior against other approaches that do not take the special structure of the space of rigid motions into account.

O5.2 Resonant-Auger – ICD cascade in rare-gas dimers

Tsveta Miteva
Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg,

Interatomic (intermolecular) Coulombic decay (ICD) is an important source of reactive slow electrons and radicals in radiation chemistry. A mechanism for controlling both the generation site and the kinetic energies of the emitted slow electrons was recently proposed [1]. It utilizes core excitation of specific atoms in a cluster followed by the resonant-Auger – ICD cascade. This cascade has been experimentally investigated in a variety of systems such as molecular [2] and rare-gas dimers [3-5].

In this study we compute fully *ab initio* the ICD electron and kinetic energy release spectra produced following $2p_{3/2} \rightarrow 4s$, $2p_{1/2} \rightarrow 4s$, and $2p_{3/2} \rightarrow 3d$ core excitations of Ar in Ar_2 and ArKr. Our findings show that the manifold of ICD states populated in the resonant Auger process can be divided into fast and slow decaying states. ICD spectra in good agreement with the experiment can be obtained only if nuclear dynamics in the slow decaying states is taken into account. We also demonstrate that changing the neighboring atom to Kr has two consequences originating from the lower ionization potential of Kr. First, the total electron spectrum is shifted to higher energies compared to that of Ar_2, and second, new decay channels become open to ICD leading to an increase in the ICD efficiency.

References

[1] K. Gokhberg, P. Kolorenč, A. I. Kuleff, and L. S. Cederbaum, *Nature* **505**, 661 (2014)

[2] F. Trinter, et al., *Nature* **505**, 664 (2014)

[3] M. Kimura, et al., *Phys. Rev. A* **87**, 043414 (2013)

[4] P. O'Keeffe, et al., *J. Phys. Chem. Lett.* **4**, 1797 (2013)

[5] M. Kimura, et al., *J. Phys. Chem. Lett.* **4**, 1838 (2013)

O5.3 Mathematical Modeling of Neural Stem Cell Dynamics in the Adult Hippocampus

Frederik Ziebell
Anna Marciniak-Czochra

The dentate gyrus of the hippocampus harbours a niche of stem cells, capable of generating new neurons throughout adulthood. Although multiple studies have been conducted in the past to identify qualitative stem cell features such as multipotency or the age-related decline of the stem cell pool, a quantitative understanding of the dynamics of adult neurogenesis is still missing. This lack of quantification is mainly due to sparse data and diverse labelling approaches used by different studies in order to observe neural stem cells. Accordingly, different hypotheses about their dynamics have been formulated.

In the presented work, we examine the hypotheses of the two landmark papers on neural stem cell dynamcis of Bonaguidi et al. (2011) and Encinas et al. (2011). We formulate both models as a system of ordinary differential equations and perform a quantification of stem cell dynamics by estimating model parameters. Thus, we are able make experimentally testable predictions in order to differentiate between the two models.

O6.1 Dual control from an Optimal Experimental Design Point of View

Huu Chuong La
MOBOCON

When controlling uncertain processes, it is important to take into account the uncertainties of the current estimates as well as the possibility of gaining information to improve the future estimates. Dual control refers to strategies that attempt to balance the performance control and information gain. By quickly estimate unknown parameters without interfering much the original objective, we can have better control action in the future. This improves the overall performance. In this talk, a new approach to dual control is introduced. We treat the problem in the context of Nonlinear Model Predictive Control (NMPC) and make use of nonlinear Optimal Experimental Design (OED). Examples in vehicle control including the rocket car, moon lander, illustrate the efficiency of our approach as well as various aspects of controlling systems under uncertainties. Nominal control and some other approaches are also discussed and compared.

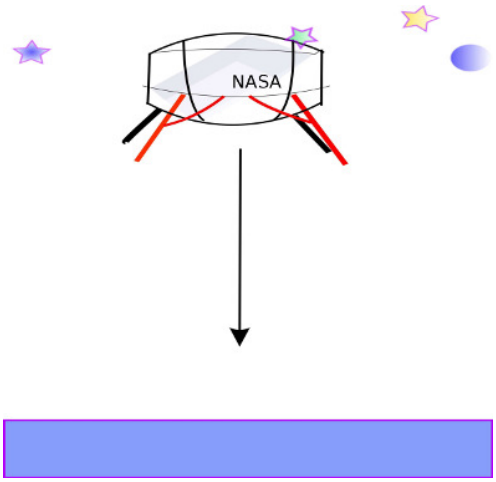


Figure 1: How to land a moon lander softly to the surface with minimum fuel consumption in case you do not know the rocket power beforehand?

O6.2 Transported Joint Probability Density Function Modeling of Turbulent Spray Flows

Yong Hu
Multiphase Flows and Combustion

Many industrial applications resort to the liquid fuel as the main energy source due to its convenience in transport and storage as well as the high energy content in liquids. In general, the chemical energy is converted into thermal energy through combustion of fuel in a turbulent flow. Combustion devices of practical interests include internal combustion engines, gas-turbines, and liquid-fueled rocket engines. In these applications, the liquid fuel is atomized to form a turbulent, evaporating spray before gas combustion of the air and vaporized fuel occurs.

The turbulent spray is characterized by a number of interacting processes including atomization, droplet dispersion, spray evaporation and turbulent mixing. The dynamics of dispersed droplets and mixing processes are crucial for the energy efficiency and pollutant formation in spray combustion. Therefore, It is worthwhile to study turbulent spray flows in order to evaluate suitable models for the turbulent mixing and its interaction with the evaporating spray.

Among many different turbulence models, the transported joint probability density function (PDF) method provides a suitable approach to couple the spray evaporation effect to the turbulent flow. In both non-reacting and reacting sprays, the momentum of the gas phase is strongly related to turbulent mixing, and this motivates the derivation and implementation of a joint PDF of the mixture fraction and gas velocity.

In this study, a Eulerian-Lagrangian numerical formulation is used to simulate the poly-dispersed turbulent dilute sprays experimentally studied at Sydney University. The solution of the joint PDF transport equation is achieved through a Monte-Carlo particle method, where spray dynamics is modeled using Lagrangian discrete parcel method with a point-particle approximation. The computational results of droplet size and liquid volume flux, mean and fluctuating droplet velocities are presented and discussed in comparison with the experimental data set B [1], where droplet size, droplet velocities and fluctuating velocities in both axial and radial directions of a turbulent free jet are studied. The comparison of experimental and computational results is very good.

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O6.3 Cuneiform Character Mining for Semantic Tablet Matching

Bartosz Bogacz
Forensic Computational Geometry Laboratory

More than 100.000 cuneiform tablets have been excavated in modern times. The tablets are important historical artifacts documenting the language, history and culture of the ancient Near East. Yet, most of the textual content is inaccessible to keyword search due to the lack of a robust method to match and retrieve cuneiform characters. This talk introduces the unique challenges posed by cuneiform character recognition and discusses methods we are currently developing to enable fast and robust recognition of characters.

We work with cuneiform characters represented as vectorized outlines traced by professional Assyriologists. Our goal is to develop a feature representation of cuneiform characters suitable for fast retrieval from a cuneiform database as well as search and character recognition in cuneiform tablets.

This talks presents and evaluates three methods we are currently developing to match cuneiform characters. First, converting the character traces to graphs and applying various graph kernel methods. Second, representing the traces as point-clouds and matching and fitting a prototype point-cloud to recognize characters. Finally, the talk presents a method that exploits the inherent structure of a character, the collection wedge-shaped impression it is made of, to model characters by the position and orientation of its wedges.

Abstracts of Posters

P1 Joint Segmentation and Tracking for Multiple Dividing Cells

Martin Schiegg
Multidimensional Image Processing Group (HCI)

Many biological questions can only be answered by tracking the fate of each and every cell in a sample. Tracking-by-assignment copes well with dividing targets / cells, but has hitherto always relied on a foregoing separate detection and segmentation step. Unfortunately, errors made in this first phase are then propagated to the tracking phase where they often cannot be discovered or compensated. It is therefore desirable to couple the two phases by modeling segmentation and tracking in a single holistic framework, allowing for a free flow of information between these subtasks. In response, we implement and evaluate the first probabilistic graphical model for the tracking of divisible cells across time. It jointly selects a subset from an overcomplete set of conflicting segmentation hypotheses, and combines these into consistent lineages. These decisions happen in unison, resulting in the overall most likely interpretation of the raw data, from the standpoint of this model. In an experimental evaluation on challenging 3D+t cell tracking data from embryogenesis, and on 2D+t data from a stem cell population, the model improves over the state of the art.

P2 Segmentation of Networks

Niko Krasowski
Multidimensional Image Processing Group (HCI)

Topological prior information is available in many tasks of image segmentation. The segmentation result can strongly benefit from the inclusion of this knowledge. We show how topological information based on abstract cell complexes can in general be used to constrain the shape of objects and show as an example the segmentation of network like structures. Since an unambiguously anchorage of a cell complex is possible only on an object's skeleton, we develop a deterministic skeletonization algorithm that allows to trace back the topological information from the skeleton to the original object and therefore allows the introduction of topological constraints on the object level.

P3 Modeling dependencies in probabilistic weather forecasting: Member-by-member postprocessing and ensemble copula coupling

Roman Schefzik
Applied Statistics

Contemporary weather forecasts are typically based on ensemble prediction systems, which comprise multiple runs of dynamic numerical models that differ in the initial conditions and/or the parameterized representation of the atmosphere. As they are subject to biases and dispersion errors, ensemble forecasts require statistical postprocessing. However, current postprocessing approaches, such as Bayesian model averaging (BMA) or ensemble model output statistics (EMOS), are mostly univariate and apply to a single weather quantity at a single location and for a single prediction horizon only, thereby failing to account for potentially crucial dependence structures.

In Gaussian settings, member-by-member postprocessing (MBMP) methods address this challenge, by retaining the rank dependence pattern from the unprocessed raw ensemble. Alternatively, such can be achieved by combining BMA or EMOS with the ensemble copula coupling (ECC) technique, in which the postprocessed forecast ensemble inherits the spatial, temporal and inter-variable dependence patterns of the unprocessed raw ensemble, by adopting its empirical copula.

We review the aforementioned approaches and elucidate the relationships between them. Their predictive performance is assessed and compared in an application to temperature forecasts over Germany, based on ensemble predictions from the European Centre for Medium-Range Weather Forecasts.

P4 Estimation of soil hydraulic properties on the basis of hydrogeophysical measurements

Stefan Jaumann
Terrestrial Physics

The Pedosphere is the thin boundary layer between the Lithosphere and the Atmosphere, that contains freshwater resources and nutrients, which are of major importance for plants, animals and human beings. The water content of soils can limit or amplify plant growth, groundwater regeneration and the distribution of pollutants and thus is a considerable variable in the climate system. In order to understand these vital processes, measurement methods and mathematical models have to be developed on a number of scales. Therefore, we recorded Ground Penetrating Radar (GPR) measurements during combined imbibition and drainage experiments in a well-known artificial lysimeter-scale soil architecture to develop methods that allow for both the reconstruction of the subsurface material distribution and the determination of the hydraulic properties of the respective materials simultaneously. Consequently, we couple the hydraulic model (Richards equation) with the electromagnetic model (Maxwells equations) and estimate the pertinent parameters of the implied heuristic material models on the basis of measurement data. Since heuristic models implicate systematic errors, the recorded data exhibit measurement errors, and the determination of the forcing suffers from limited accuracy, we will use Data Assimilation Methods to maximally exploit the information contained in the measurements during the parameter estimation procedure.

P5 Optimization of Mixed Traffic Model. A case study: Hanoi, Vietnam

Tuan Nam Nguyen
Discrete and Combinatorial Optimization

Mixed traffic systems in developing countries are basically different from those in developed countries. They are chaotic and very hard to control. One of the obstacles of traffic planning in these traffic systems is the lack of reliable traffic assignment models. In our research, we investigate a new User Equilibrium Model for a mixed traffic system dominated by motorcycles which is popular in developing countries like Vietnam, The Philippine, Taiwan and India. We also make a software named TranOpt to test our model with the data got from Openstreetmap website. The computational results doing for the traffic system in Hanoi, the capital city of Vietnam, is promising for traffic planners when they have to cope with such kind of traffic systems.

P6 Histone H4 lysine 16 acetylation influences the binding conformation of H4 tail: a simulation study

Ruihan Zhang
Biophysics of Macromolecules

The activation or repression of gene expression is regulated by the chemical modifications on chromatin. As the basic unit of chromatin fiber, nucleosome is composed of 147bp DNA wrapping around a histone protein core. It is well known that the modifications on the disordered histone tails induce chromatin remodelling, and correlate closely to the differentiation of stem cell, the development of organism and the occurrence of disease, but the molecular mechanism of how the histone modifications control the fate of gene still remains unclear. Here we focused on histone H4 lysine 16 acetylation(H4K16Ac), which induces gene activation by decompacting the chromatin structure as well as influencing the binding of transcriptional factors. Replica Exchange Molecular Dynamics simulation (REMD) was performed to investigate the influence of H4K16Ac on the binding conformation of histone H4 tail on the nucleosomal DNA. The non-standard acetylated lysine was parametrized by quantum mechanics approach. The parameters for REMD were tested to guarantee efficient sampling. As a preliminary result, we found the wild type K16 inserts into the DNA minor groove whereas the acetylated K16 stays on the DNA surface. The alteration reflects the effect of H4K16Ac on the single nucleosome, which influences the behaviour of H4 tail in context of chromatin. Further simulation with neighbouring nucleosomes is required to elucidate the role of H4K16Ac in chromatin remodelling.

P7 Computer-Aided Surgery: Soft Tissue Simulation in Cognition-Guided Surgical Operations

Nicolai Schoch
EMCL

In my PhD work, I am dealing with FEM-based soft tissue simulations in the context of surgery assistance systems. As part of my work in the context of the transregional collaborative research center (SFB TRR 125) "Cognition-Guided Surgery", I focus on simulations for Mitral Valve Reconstruction operations. In a mitral valve reconstruction (MVR) the functionality of incompetent mitral valves is re-established by applying surgical techniques. In addition to the biomechanical simulation of operation scenarios for an MVR itself, I concentrate on the simulation's integration into a knowledge-based surgery assistance system. Along with surgeons from the German Cancer Research Center (DKFZ), I defined an adequate framework (see Figure 1) for the surgical MVR workflow, which combines semantically stored surgical expert knowledge with the finite element-based simulation.Therefore, firstly, 'surgical rules', which ontologically represent assessment criteria for surgical decision-making, are transformed into boundary conditions for the simulation, and secondly, these are applied on patient-specific data, in order to yield patient-individual simulation results, to support surgeons during the operation.

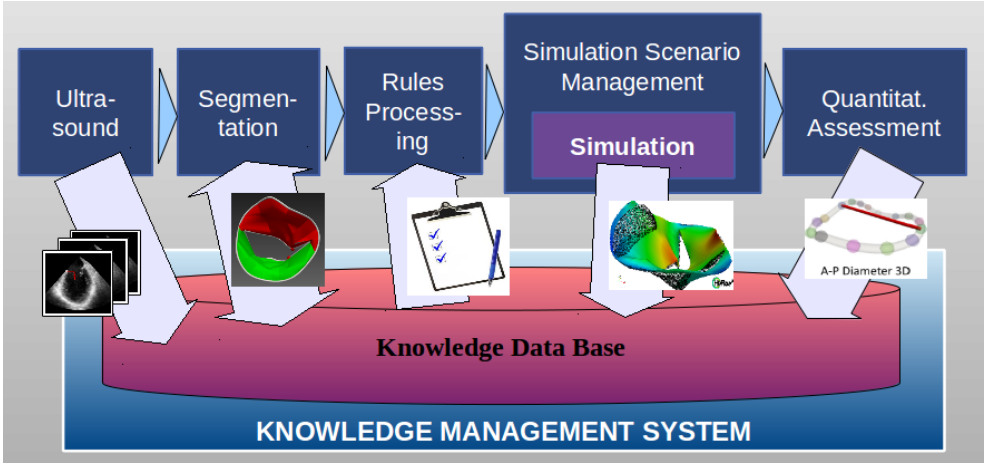

Figure 1: Framework for knowledge-based simulation-supported MVR surgery assistance system

P8 Stochastic Dynamics of Interferon Type I Signaling

Nikolas Schnellbächer
Physics of Complex Biosystems

Interferons (IFN) of Type I are a class of homologous signaling molecules that play a pivotal role in the innate immune response against viral infectious disease. They are secreted by many nucleated cells to indicate the presence of an intracellular viral infection to their environment and inhibit viral replication. They bind to a shared, heterodimeric cell surface receptor (IFNAR = Interferon Alpha Receptor) to form an active ternary signaling complex, which triggers an intracellular response. The most prominent pathway engaged by interferons is the canonical JAK/STAT signaling pathway, where STAT molecules dock at the receptor associated Janus kinases (JAKs) at their cytoplasmic domains. This work looks at the assembly dynamics in the plasma membrane and its role for downstream processes. A central question of this system is to explain the differential information processing of different interferons through the same transmembrane receptor system. Notoriously low copy numbers of the receptors on the cell surface are a typical cause for a high degree of intrinsic stochasticity. Therefore stochastic and spatial simulation methods are applied to analyse the activation dynamics, which allow to quantify the fluctuations in the system. By investigating dose responses under different conditions such as varying surface concentrations of the receptors and an explicit treatment of the diffusivity of the involved components we try to investigate the role of the spatial organization for interferon mediated signal transduction.

P9 Computational studies on the relation between macromolecular dynamics and protein binding and function

Antonia Stank
Molecular and Cellular Modeling Group, Heidelberg Institute for Theoretical Studies

We describe computational tools developed to characterise the interaction properties and dynamics of proteins as well as an application to predict protein-protein interactions:
Firstly, the ProSAT+ web server is presented, which is an extension of the ProSAT and ProSAT2 [1] web servers. It allows visualisation of a 3D protein structure with highlighted functional regions together with residue specific annotations. These annotations from different data sources include sequence variability and the influence of mutations on the protein functionality. ProSAT+ provides the new possibility to add sequence annotations from evolutionarily related proteins and to display the sequence conservation with other annotations on the 3D structure simultaneously.
To study protein interactions with small molecules a protein binding site superposition tool based on the existing ProBiS [2] algorithm is presented. It is included in the LigDig web server and enables the analysis of protein binding sites. One benefit of the tool is that it identifies similarities of binding sites even if the overall protein structures are different.
For detailed studies on the dynamics of protein binding sites the TRAPP [3] web server is introduced. TRAPP already analysis transient binding pockets in proteins and we plan new features, for example, a score calculation that helps to predict the ability to bind drugs.
Further, an application of protein-protein interaction analysis using Brownian dynamics simulations is presented. The simulations with chaperone proteins provide a structural interpretation of experimental data and new insights into the specificity of the chaperone interactions.

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P10 Numerical Modeling of Coil Embolization in Cerebral Aneurysms

Augusto Sanches
Multiphase Flows and Combustion

Cerebral aneurysm is a vascular disease characterized by the local dilatation of arterial walls in the intracranial space. The aneurysm may rupture and cause subarachnoid hemorrhage, which is associated with high mortality and morbidity. Computational techniques offer new capabilities in the healthcare provision for cerebral aneurysms. Due to improved and widely used imaging methods in clinical surgery practice, detection of cerebral aneurysms that are not ruptured becomes more and more frequent. To reduce the risk of rupture and hemorrhage in cerebral aneurysms and to identify highly effective treatment options, the understanding of the involved hemodynamic mechanisms is of great importance. The availability of a simulation tool for virtual coil embolization is extremely useful to support the decisions of treatment options by medical experts and to develop and optimize new implant designs. In this project, the development of a computational tool for the modeling and simulation of the hemodynamic effects of endovascular coil embolization before and after the intervention is performed. An attempt is made to shed light on the above issues from the point of the hemodynamics changes induced in the system after the deployment of the first coil, during the intermediate coiling process, as well as after the completed procedure. An idealized geometry based on computational fluid dynamics is employed as an efficient tool to model the blood flow and wall shear stress in cerebral aneurysm, providing a realistic insight into the pathological vessel parameters and better evaluation to predict the risk of rupture for a given patient.

P11 Model predictive control for walking and sit-to-stand motions

Davide Corradi
ORB

The average age of the population is increasing due to the higher life expectancy and falling birth rate. As a consequence, mobility disabilities caused by old age are becoming more and more common, creating obstacles to everyday activities and reducing the fitness and vitality of those affected. Proper assistance is important to counter the problem, and the demand for professional nursing staff is constantly rising and cannot be entirely fulfilled. Robotic assistive devices may represent a solution, since they can provide features which are now exclusive to human carers such as adaptive posture support, sit-to-stand assistance, navigation aid and health monitoring. The MOBOT European project is designing such a device, a walker equipped with various sensors (depth sensors, force sensors, kinect cameras, microphones) to perceive the current state of the user and understand his commands, and with actuated wheels and handles to provide him with the necessary optimal mobility support.

The present work is part of the MOBOT project. Its specific goal is to develop methods that allow an online adaption of the shape and the actuation of the mobility assistant in a way that optimally supports the motion of the subject during walking and sit-to-stand motions. The device should be able to mimic a human carer, compensating lack of balance and strength while promoting fitness and independence by avoiding excessive support. The employed methodology consists in computing optimal sit-to-stand trajectories with offline optimal control techniques, while using online nonlinear model predictive control (NMPC) for balance control when standing and walking, trying to detect when the patient is about to fall and executing a proper maneuver with the handles to reestablish balance. The main challenge lies in the interaction between a controllable sub-system, the walker, with a non controllable and partially unknown sub-system, the user, whose behavior can only be predicted in an approximate way. Other essential questions are how to model the user's dynamic and cognitive behavior, also including the effects of old age, and how to measure his balance and distinguish safe situations from potentially dangerous ones that might lead to a fall.

P12 The force is strong in this one – The JEDI analysis

Tim Stauch
Theoretical and Computational Chemistry

The force is strong in this one – The JEDI analysis

On the microscopic level, our life is determined by the interactions of molecules and by the forces acting between them. For example, the vital folding and unfolding of proteins (the essential building units of living tissue) as well as the activity of muscles is a consequence of mechanical forces acting on molecules. Furthermore, in our everyday life we experience the wear and tear of synthetic material when it is subject to mechanical stress.

Strangely, however, theory can neither explain nor predict satisfactorily how a molecule changes under the influence of mechanical force. In particular, up to the present day we cannot answer the questions why a certain material breaks under a given force while another one stays intact, where the rupture point is localized and how mechanical stress is distributed in the molecule.

As a first step to answering these questions, we have developed the JEDI (**J**udgement of **E**nergy **DI**stribution) analysis[1], which is the first theoretical tool that allows a quantitative understanding of the distribution of mechanical force in molecules. This tool has been applied to a number of illustrative problems in the field of mechanochemistry, thus shedding light on some fundamental processes governing the behavior of molecules under mechanical stress.

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P13 A fully Eulerian approach for fluid-structure interaction problems

Stefan Frei
Numerical Analysis (Rannacher/Richter)

Fluid-structure interaction problems play an important role in a variety of applications in biology, medicine or the engineering sciences. In many cases, the Arbitrary Lagrangian Eulerian (ALE) method provides an elegant and robust technique to deal with moving interfaces and subdomains. The ALE method shows problems for large deformations or movements of the structure, however, as the underlying grid may degenerate.

In a Fully Eulerian ansatz, in contrast, domains and interface move over a fixed background mesh. This ansatz is thus capable of dealing with arbitrary movements up to contact of e.g. a solid structure with a wall. The difficulty in the Eulerian ansatz lies in the correct treatment of cells that are split by the interface. Applying standard discretization methods leads to a reduced order of convergence and stability issues.

In this poster, we present modified discretization schemes in both space and time in order to avoid these issues. The proposed finite element discretization in space corresponds to a fitted finite element method that uses a fixed patch mesh. Instead of moving mesh nodes, we resolve the interface locally by an adapted parametric approach. For time discretization, we use a modified time-stepping scheme that is based on the fixed-mesh ALE method proposed by Codina et al (2009). For both discretization in space and time we can show second-order convergence. Finally, we illustrate the capability of our approach by means of benchmark problems and prototypical applications.

P14 Calculating Absorption Spectra of Molecules in Complex Environments - The FMO-ADC-Method

Stefan Prager
Theoretical and Computational Chemistry

Usually, chemical reactions do not occur in the gas phase, but in solution. Molecules are surrounded by the solvent molecules, e.g. water. In most cases, however, the solvent is not inert. Instead, it interacts with the dissolved molecules leading to a change in the observable properties and even to different reaction mechanisms. Thus, it is obvious that in theoretical investigations, the environment has to be considered as well. In quantum chemistry, the maximum size of a system which can be investigated is limited by computer power. Using high-level methods, a maximum system size of 100 atoms can be computed. Considering the environment as well would require a system size that is 10 to 50 times larger than this, which is not feasible on a reasonable timescale. The fragment molecular orbital (FMO) approach allows to include the solvent molecules explicitly but with a linear scaling in terms of computational cost for every extra solvent molecule.

In the FMO approach, the total system (e.g. a chromophore surrounded by 20 water molecules) is divided into smaller subsystems, called fragments. Each fragment is calculated individually, but the electrostatic interaction with the electron density and the nuclei of all other fragments is included. One fragment, the chromophore, is treated at a high level of theory, while all other fragments, the water molecules, are calculated at a low level of theory. This allows the calculation of the chemical properties of the chromophore including the effects of the water on the chromophore. Combining this FMO approach with the method developed in our group, the algebraic-diagrammatic construction (ADC) method, which is capable of calculating electronically excited states, allows the calculation of UV-Vis absorption and fluorescence spectra, as well as the simulation of photochemical reactions in solution.

P15 Social Network Extraction and Exploration of Historic Correspondences

Hui Li
Database System Research

Driven by the continuously increasing number of digitized and transcribed historic documents, natural language processing (NLP) and text analysis tasks are now frequently applied to historic texts to extract useful information and thus to enrich this cultural heritage. These tasks face several challenges, such as dealing with spelling variations, lack of orthography, and, oftentimes, missing reference language corpora.

In this paper, we present our approach to information extraction from a large corpus of correspondences written in the first half of the 16th century. For around 9,700 letters written in Early New High German by the German reformer Philipp Melanchthon, we develop and extend approaches to named entity recognition to extract information about geographic places, persons and organizations, and time. The extracted information serves as the basis for creating a social network structure that includes information about senders and addressees of letters as well as people mentioned in letters. This correspondence network structure is to be exploited in terms of analyzing the evolution of the correspondences, key persons and communities, and eventually topics covered by the letters over time, thus resembling key analysis tasks applied to today's typical social networks.

P16 Approximate Inference for Tracking Dividing Cells

Carsten Haubold
Multidimensional Image Processing Group (HCI)

Tracking cells in 3D+t Selective Plane Imaging Microscopy (SPIM) data is a crucial task in developmental biology. Most recent research on tracking multiple objects does not take the possibility of dividing objects into account. State of the art tracking-by-assignment approaches coping with divisible objects rely on holistic probabilistic graphical model (PGM) formulations. An integer linear program (ILP) is formulated from this PGM, incorporating constraints similar to flow conservation, but allowing for divisions. This ILP is then optimized by commercial solvers. Unfortunately the memory requirements of such ILPs easily become impracticable for large datasets. To circumvent this, I analyzed the LP relaxation and explored dual decomposition, but the tractability could not yet be improved. The next step is to develop methods to decompose this constrained graphical model and to solve it approximately, such that cell tracking scales better to large data while having reasonable hardware requirements. Additionally to improving the optimization method, we apply structured learning to refine our model.

P17 Excited state proton transfer and the fluorescence quenching of benzaldehyde in water

Katharyn Fletcher
Theoretical and Computational Chemistry

Excited state proton transfer and the fluorescence quenching of benzaldehyde in water

Katharyn Fletcher and Andreas Dreuw Amines are a class of organic (i.e. containing carbon) molecules that feature a nitrogen atom with a lone pair of electrons. They are important analytes in a wide variety of areas and are used for studying food spoiling, bacterial infection, and cancer signatures. In fact, amines may even facilitate the monitoring of disease states. To date, many approaches are available for detecting amines. Amine indicators work, for example, by changing color upon reaction with an amine. Colorimetric and fluorimetric amine recognition generally occurs in the presence of an organic solvent. Recently, in the group of Prof. Dr. U. H. F. Bunz in Heidelberg, water-soluble aldehyde-substituted distyrylbenzenes and cruciform dialdehyde fluorophores were observed to good detectors for primary, secondary, and 1,n-diamines [1]. However, the dialdehydes exhibited either no or barely any fluorescence in water [2]. In this work, we propose and confirm the mechanism of fluorescence quenching of benzaldehyde, a basic structural unit of the dialdehydes, in water. In aqueous solution, the carbonyl groups of benzaldehyde molecules are bound by hydrogen bonding to water molecules. It is thus feasible that excited-state proton transfer could occur from water, a protic solvent and the Brønsted acid, to the aldehyde as the Brønsted base. Benzaldehyde thus acts as an excited state base in water and, after intermolecular electron transfer, nonradiative decay to back-transfer of the hydrogen atom to the OH radical is possible. With an understanding of this mechanism, a more finely tuned synthesis of new amine indicators is possible.

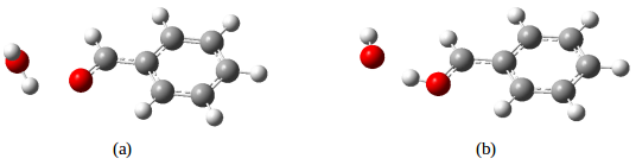

Figure 1: Excited state proton transfer going from (a) neutral benzaldehyde - water to (b) protonated benzaldehyde- hydroxide anion is crucial to fluorescence quenching.

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P18 Nickel(II) Bispidine complexes as catalysts for C-H activation

Johannes Straub
Prof. Comba

The selective oxidation of hydrocarbons to the corresponding alcohols is a demanding reaction as the substrate can easily be over-oxidized to carbonyl compounds. There are numerous non-heme enzymes containing e.g. iron as the active metal center catalyzing this reaction using molecular oxygen as oxidant. For a detailed investigation of these enzymes many biomimetic model complexes of e.g. iron(II) or nickel(II) have been synthesized and characterized. A typical model reaction involves a metal complex as catalyst, a substrate (e.g. cyclohexane, adamantane) and an oxidant (e.g. meta-chloroperbenzoic acid mCPBA or hydrogen peroxide) and is tested for the formation of the corresponding alcohol and over-oxidized products like carbonyls.

In this project, the activity and mechanistic aspects of the catalysis using nickel(II) bispidine (3,7-substituted-9-oxo-2,4-bis(2-pyridyl)-3,7-diazabicyclo[3.3.1]-nonane-1,5-dicarboxylate methyl ester) complexes are investigated experimentally and theoretically. On the one hand, the influences of different reaction conditions (e.g. different substrates, oxidants, solvents etc.) are analyzed spectroscopically (UV-Vis) and chromatographically (GC, GC-MS). On the other hand, these experimental results are supported by investigation of the characteristics of nickel(II) and nickel(III/IV)-oxo complexes as well as the reaction mechanism using density functional theory DFT. This involves geometry optimizations, transition state searches and subsequent e.g. MO, charge and structure analysis. The computational studies are carried out using the hybrid-functional B3LYP and a triple-zeta basis set (def2-TZVP).

P19 Ancient Khmer Characters Recognition

Chamroeun Khim
Analysis Group

Ancient Khmer script is one of the oldest scripts in Asia. In the past, ancient Khmer characters were widely used to record the culture, architecture, and literature of Khmer. Regarding its importance, this poster introduces mathematical concepts using the geometric structures to recognize ancient Khmer characters. Our experiment results show that geometric structure analysis of characters stroke can significantly distinguish ancient Khmer characters and preserve invariant translation, rotation and scaling.

P20 Walking, Tripping, Falling: Analysis of human push recovery using inverse optimal control

Malin Schemschat
ORB

As the human gait is a very complex movement, it is hardly surprising that people go through different stages of abilities during their life. Not knowing how to manage a stable gait, young children often fall. Once adult, humans normally learned to perform an efficient and versatile gait. While they are able to react on disturbances in a suitable way to avoid falling for most of their lifetime, humans become more likely to fall again reaching a certain age. But the injuries they sustain are worse than in their childhood.
The focus of this project lies in the analysis of the reaction on perturbations and fall avoidance strategies. For a selection of different perturbations and recover strategies motion capture experiments are going to be performed to gain reference data. For the mathematical analysis these different situations have to be translated to a mathematical formulation and applied to a human model that implies the relevant joints and senses. An objective function for an optimal control problem can be formulated as a linear combination of different criteria based on known aspects from undisturbed movement. The weights of this function can be determined by solving an inverse optimal control problem. This two-stage-optimal control system can be formulated as mathematical program with equilibrium constraints (MPEC). To find a regularization of the resulting MPEC a suitable relaxation or lifting scheme is going to be developed. Finally the results can be used to determine a mathematical formulation for decision rules to switch between recover strategies.
The improved understanding of human movement can be used to support medical diagnoses and treatment planning as well as to develop devices that prevent eldery people from falling. Another application of the results is the development of new control strategies for humanoid robots.

P21 Combining Computational and Spectroscopic Methods to Determine Molecular Structure

Markus Rössler
Peter Comba Group

Classifying a set of elements based on a common characteristic and deducing further common properties of this class can be considered a way of understanding the properties: they are due to the initial characteristic. Similarly in chemistry molecules may be classed according to structural patterns they show and measurable properties, e.g. reactivity or their interaction with electromagnetic radiation, can be ascribed to the substructure. This readily provides an approach to understand biological active species and immediately suggests the requirements for a synthesized compound to mimic the biological behaviour.
Obviously, a prerequisite for this approach is both structural insight and the availability of measured properties. While the latter often is available, the former proves to be not trivially obtained, especially in solution, the common environment of biological species. Therefore, we aim at generalizing and automatizing a literature known combination of computational chemistry and experimentally obtained data to gain knowledge of solution structures. Computationally one obtains structural proposals for an unknown molecular geometry by minimization of the energy in a given model. Subsequently, calculating properties of possibly a plethora of computed structures and comparing them to experimental results validates or invalidates a structural proposal and in the simplest case allows for sorting out the 'true' structure.

P22 Developing methods: Ionization Potential and Electron Attachment

Matthias Schneider
Theoretical and Computational Chemistry

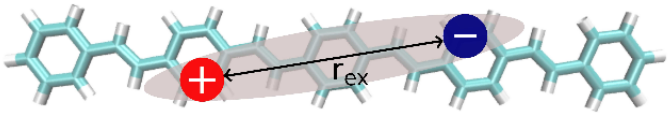
The field of theoretical and computational chemistry are of increasing importance in modern chemistry. The ability to simulate, understand, and predict chemical processes without doing experiments is a huge advantage in chemical research. A main topic in simulation and computational chemistry are quantum chemistry programs like Q-Chem. Our group is developing and implementing the so-called algebraic-diagrammatic construction (ADC) in Q-Chem. The ADC scheme presents a way to construct matrix representations of the Hamiltonian for electronic excitation, ionization, and attachments based on regular perturbation theory. The code is built in a modular way, so that the environment and general algorithms or routines can be used for different ADC methods. For example, the module for ionization potential is similar to the earlier implemented excitation energy module.
Ionization and electron attachment are fundamental common process in nature, which can be induced by light. With our code, it is possible to compute vertical ionization potentials and electron affinities in a black-box way. This means no large knowledge of quantum chemistry and the underlying theory is required to compute ionization potential or electron affinities of molecules. IP-ADC and EA-ADC are implemented for close and open shell medium sized molecules in second (2) and third (3) order.
We present here for the first time IP-(U)ADC(2), IP-(U)ADC(3), EA-(U)ADC(2) and EA-(U)ADC(3) results of small and medium-sized molecules.

P23 Analysis of Excitons in Conjugated Organic Polymers

Stefanie A. Bäppler
Theoretical and Computational Chemistry

My work is concerned with the understanding of a new generation of electronics, which is based on organic compounds. Devices like OLED displays, organic solar cells and many more have been introduced successfully and convince with new designs, low cost production and broad applicability. Albeit a lot of knowledge about the materials could be gained, some methodological challenges still remain concerning the study of their electronic structure.

As quantum chemical calculations were extended to ever larger systems in the past decades, the tools for systematic analysis also need to be adopted to access information that is crucial for these systems, while in earlier work with smaller systems it was usually sufficient to use less elaborate strategies. A lot of progress has been made, in particular to link concepts from quantum chemistry with solid-state physical approaches that were originally set up to describe electronic properties of inorganic semiconductors. Recently, we developed an approach which allows to compute electronic properties in such a way that the results are easily comparable to the solid-state picture and furthermore to experimental data. The poster will show the method developed and an application to poly(*para* phenylene vinylene) which is a prominent molecule in the development of organic solar cells.



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[2] F. Plasser, S. A. Bäppler, M. Wormit, A. Dreuw, *J. Chem. Phys.* **2014**, DOI:10.1063/1.4885820

[3] S. A. Bäppler, F. Plasser, M. Wormit, A. Dreuw, **2014** (*submitted for publication*)

P24 Enhancing 4D PC-MRI in an aortic phantom considering numerical simulation

Jonas Kratzke
EMCL

Anatomical aspects of aortic disease have been thoroughly investigated in the last decades by means of CT, MRI and ultrasound. To date, morphologic variations can be determined individually and with high sensitivity. However, with respect to the coherence between biomechanical behavior and aortic disease, various open questions exist, such as for a more extensive acquisition of risk factors for atherosclerosis, aneurysm formation or aortic dissection. Within the scope of increasing understanding of vascular pathology, development of functional imaging of the aorta becomes more and more important. An innovative method to investigate the biomechanical behavior of blood vessels is given by aortic silicon phantoms and 4D phase contrast (PC)-MRI measurement. Entirely made of non-metallic components, blood-like fluids can be flown through aortic phantoms and the time-resolved velocity field can be measured by PC-MRI technology. In this work we propose a mathematical model of an aortic silicon phantom and a framework that allows to enhance 4D PC-MRI imaging by means of combining numerical simulation with MRI data. As the elasticity of the silicon phantom wall plays a significant role and is reflected in the Windkessel effect in the case of the aortic bow, we model the wall as elastic structure. The resulting fluid-structure interaction problem is solved numerically in a monolithic finite element based approach using the HiFlow^3 software framework. The proposed setup is calibrated by means of 4D PC-MRI imaging of the considered silicon phantom. It is evaluated by comparing experimental and numerical data in the framework of the aortic phantom. In addition to the measured velocity field it provides information about wall shear stress and stress distribution in the phantom's wall.

P25 Development of a novel spray flamelet model

Hernán Olguín Astudillo
Multiphase Flows and Combustion

The simulation of turbulent spray flames is of vital importance for the development of more efficient combustion devices with reduced pollutant emission. In order to properly predict the characteristics of these flames, the consideration of detailed chemical reaction mechanisms in numerical simulations is essential.

Flamelet models represent a very promising way for including detailed chemistry in an effective way. However, classical flamelet models are mono-regime and turbulent spray flames are inherently multi-regime, since various combustion regimes can take place simultaneously. Thus, non-premixed, premixed, partially premixed and evaporation-controlled combustion have to be taken into account if spray flames are to be studied. For this reason, the formulation of a comprehensive spray flamelet model is a very challenging task.

Recently, attempts have been made to extend classical single regime flamelet models to more complex situations, where at least two combustion regime coexist. The objective of this work is to develop a framework in which two-regime flamelet models can be described and combined in order to advance in the development of a comprehensive flamelet model for turbulent spray flames. For this, a set of multi-regime spray flamet equations is derived takes into account all combustion regimes found in spray flames. The derived set of spray flamelet equations is then used to evaluate structures of laminar ethanol/air spray flames in the counterflow configuration in order to determine the significance of different combustion regimes. The present study concerns spray flames with no pre-vaporized liquid in the oxidizing gas phase, and it is found that only non-premixed and evaporation-controlled combustion regimes exist, so that premixed effects may be neglected.

P26 Improving functional electrical stimulation patterns for drop foot correction in hemiplegic patients by nonlinear model predictive control

Maedeh Aram
Optimization in Robotics and Biomechanics

Drop foot syndrome is one of the common impairments, experienced by about 20% of the stroke survivors. It makes the patients unable to lift the foot tip (dorsiflexion) during the swing phase of walking. This impairment is due to a partial or total paresis of the muscle involved in dorsiflexion of the ankle joint. Foot drop can be improved by applying functional electrical stimulation (FES) to the common peroneal nerve or to the tibialis anterior muscle during the swing phase of the gait. In this project, instead of using a classical heel switch sensor, which turns ON and OFF the stimulator, a sensor is supposed to communicate with the stimulator network in a preprogrammed stimulation. A wireless inertial sensor with a stimulator network will be closed loop with a feedback coming from the online optimization process. In this regard, the goal of this work is to develop a novel approach for FES using efficient online optimization techniques, i.e. nonlinear model predictive control (NMPC) to modify online the stimulation patterns in order to estimate gait cycle index (GCI), by taking into account different tasks such as turning around, stair climbing, etc. and efficiency of the dorsiflexion. To be usable for the patient's daily life, utilizing the smallest amount of sensors would be desirable. Finally, minimizing the fatigue and metabolic cost in patients would be one of the crucial outcomes of the optimization.

P27 Quantum Chemical Investigation of Charge Transfer States in Donor-Acceptor Copolymers

Mercedes Vanessa Bohnwagner
Theoretical and Computational Chemistry

Optolelectronic devices e.g. photodiodes, photo resistors and solar cells are becoming ever more ubiquitous in our everyday lives. Their special feature is that, when exposed to incident light, they produce electrical energy. The semiconducting material, which is the most important component of such devices, often consist of organic copolymers. Those copolymers contain electron donating and electron withdrawing groups. Absorption of light and simultaneous generation of charge carriers (electrons and holes) is the first step in the power conversion process. Another very important step is the charge transfer (see Figure 1). The energy which is provided by absorption of a photon is used to promote an electron from an energetically low lying state (ground state) located at the donor moiety to an energetically higher lying state (excited state) located at the acceptor moiety (see Figure 1). Simply said, this process can be described as the charge transfer step.
In order to get a better understanding of this fundamental process, quantum chemical methods can be applied. For our quantum chemical investigation of the charge transfer process in donor acceptor (D/A) copolymers, we have chosen small D/A molecules as model compounds.

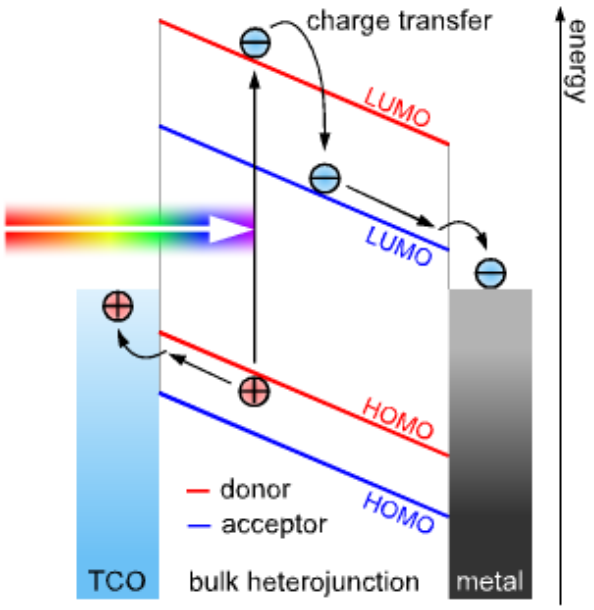

Figure 1: Schematic representation of photoinduced charge transfer in a semiconducting material.

P28 Reduced models for ferromagnetic plates

Florian Nolte
Prof. Knüpfer

In ferromagnetic materials, a huge variety of spatial patterns of the magnetization can be observed. We investigate a transformation between to different magnetization patterns in a ferromagnetic slab, induced by the application of an external field. During the phase transformation, intermediate magnetization patterns occur, that determine the hysteresis and the macroscopic behavior of the material. We study these patterns by investigating a variational model. In particular, the goal is to identify energetically optimal patterns and to derive a reduced model in the framework of Γ-convergence. As a first step, a simplified variational model for a single magnetic domain is investigated. We establish the scaling of the energy in terms of the volume of the domain and show existence, regularity and connectedness of minimizers for the simplified model.

P29 The Galerkin-Polynomial Chaos Method for Dynamic Optimization under Uncertainty

Lilli Bergner
JRG Optimization of uncertain systems

Decision making under uncertainty deals with the problem of optimizing some functional while taking incomplete knowledge about the system into account. Such uncertainties in model parameters and initial conditions can be due to limited understanding, measurement and manufacturing inaccuracy or intrinsic variability. It effects the dynamic system in a way that the model variables as well as the objective function and constraints cannot be predicted deterministically. One possibility to quantify the resulting uncertainty of the system output is to probabilistically model the initial uncertainty and propagate it through the model. We demonstrate that the well known Polynomial Chaos expansion is a suitable method for this task and can deal with the specific numerical context of nonlinear, dynamic systems with nonstandard probability distributions and large variations. We further provide an interpretation and implementation of objective and constraint functions under uncertainty.

P30 Modeling and optimal control of compliant robots

Yue Hu
Optimization in Robotics and Biomechanics

Humanoid robots are expected to play a main role in the service robots of the near future, but at the current state there is no humanoid robot yet that walks in a stable and versatile way as humans do. This PhD is part of the EU Project KoroiBot, which objective is to study how humans walk and how to improve humanoid walking by human-inspired mathematical models, optimization and learning.

Most of the existing state of the art humanoid robots employ stiff actuation and have high positioning precision, inspired by industrial robots. The drawbacks of these robots is that they cannot safely interact with the environment and humans and they can hardly reproduce natural looking walking motions. This led to the development of compliant robots, which are demonstrated to be also more energy efficient. In this PhD topic the compliance in human beings will be addressed in walking motions, considering both free walking in even terrain and constrained walking in complex environments. Then the model of the lower limb of the humanoid robot iCub will be developed to carry out experiments. iCub is a robot produced by the Istituto Italiano di Tecnologia (IIT) in Italy and it has four compliant joints with Series Elastic Actuators (SEA). Within this robot the role of compliance in humanoid robots will also be studied.

P31 Tailored Real-Time Mixed-Integer Optimal Control for Exhaust Heat Recovery System in Heavy Duty Trucks

Enrique Guerrero
JRG Kirches

In a renewed effort to apply environmentally friendly technologies and win the market through more efficient products, the heavy duty truck industry is in demand for new control approaches that make a better use of the fuel needed to travel a certain distance. In a conventional approach, fuel is burnt in a Diesel engine. The exhaust gas is released to the environment through the exhaust pipe. A considerable amount of heat can however be captured and used to vaporize a proper working fluid to power up an expander that used as a second way to drive the powertrain. This is similar in spirit to what is done in a conventional Rankine cycle used in fossil fuel or geothermal power plants. To this end, Nonlinear Model Predictive Control (NMPC) is seen as an adequate technique that allows to quickly compute optimal trajectories for controls and states. However, this feature is challenged in this problem by several integer controls that greatly increase the complexity of the problem. Moreover, thermodynamic properties of the different system components have to be interpolated are non-differentiable. In this talk, we present a PhD project with the goal to overcome this difficulties and achieve transient NMPC for an environmentally friendly next-generation heavy duty truck control system. We introduce and analyze fully-implicit DAE truck models of our cooperation partner Daimler AG, considering pertinent additions, parameter estimation, and offline optimal control before proceeding to NMPC.

Abstracts of Invited Talks

I1 Big Data - Little Impact? Raising the bar for "Data Science"

Alexander Lang
IBM

Just because you have a mountain of #bigdata doesn't mean there is gold in these hills (Jeff Jonas, IBM) Size matters - but insights matter even more. To really harness the data around us, be it big or small, in all shapes and sizes, we need to re-think our approach to data analysis: big data will not make a really big impact until it can be put to work by almost everybody. This session will show how IBM technology enables people to have a "conversation with data" around their specific problem, and describe the skills, roles and technologies that we think will help to make a real impact with data.

I2 High-Performance Computing and Uncertainty Quantification

Michael Schick
Heidelberg Institute for Theoretical Studies (HITS)

The increasing demand on the quality and reliability of numerical simulations results in an increased complexity of mathematical models and methods. Especially, the knowledge for the description and definition of model relevant parameters is often subject to uncertainties, such as for example data generated from inexact measurements. Taking such uncertainties into account results in the curse of dimensionality: the number of variables grows exponentially quickly leading to "big data" problems in scientific computing. As a consequence the efficient use of High-Performance Computing becomes are crucial task. One challenge is to combine fast iterative methods with a parallel and scalable memory distributed computation to tackle the memory requirements of large scale computations. In this talk, we provide the basic foundations of Uncertainty Quantification with an emphasis on the stochastic Galerkin projection and demonstrate its use with application in fluid mechanics / meteorology.

I3 Big Data in Scientific Practice

Christopher Jung
KIT Karlsruhe – Steinbuch Center for Computing

Big Data, usually defined by the 5 Vs (volume, variety, velocity, value and veracity), has become very important in many scientific disciplines. Usually, it is driven by rapidly increasing amounts of data from experiments, observations and simulations, but also by policies like Open Access, data privacy and sustainability.

Scientific disciplines differ in their requirements, procedures and cultures. Therefore, generic data management methods need to be complemented by community-specific tools for data management and analysis.

After a review of scientific users' motivation for Data Science, this presentation will focus on data life cycle management in different scientific fields. Also, examples of Big Data facilities will be discussed. The presentation will conclude with experiences and lessons learned.

I4 Big Data in Enterprise Business Processes

Michael Dietz
SAP

Big Data scenarios exist in numerous business processes within enterprises. Europe's largest software company SAP, located in the area of Heidelberg, is the leading supplier of software to support all kinds of business processes in companies. In this context Big Data enables new ways to solve common challenges and offers new opportunities to improve business activities. This presentation gives some insights into the world of business processes and various related Big Data use, which have been realized based with the software and technology provided by SAP.

I5 What a Mathematician can do at Boston Consulting Group

Michael Schmälzle
The Boston Consulting Group

The Boston Consulting Group, as a worldwide leader in strategic consulting, stands for the innovative solutions that we carry out in collaboration with our clients. Founded in the U.S. in 1963, BCG today maintains 81 offices in 45 countries throughout the world. Eight offices and 1500 consultants are based in Germany and Austria. In our presentation, you'll find out what we do, how we work, and why we are the world's leading strategy consultants. We'll show you how we develop strategies for sustainable success together with our clients. You'll also discover how you, as a mathematician, can put your expertise to use at the world's leading strategy consulting firm while advancing your personal and career development. We will use different project examples to demonstrate the diversity of BCG's work and why your academic background is a big plus.

List of Posters

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P9 Antonia Stank
P10 Augusto Sanches
P11 Davide Corradi
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P26 Maedeh Aram
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P29 Lilli Bergner
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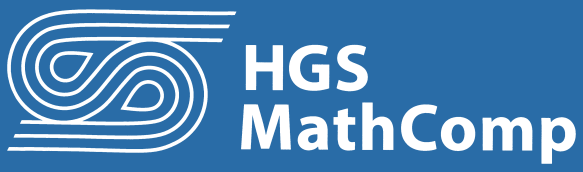
Notes



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Wednesday: 10:00h – 12:00h / 14:00h - 16:00h
Tuesday & Friday: closed

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HEIDELBERG
Zukunft. Seit 1386.

"Mapping the global Twitter heartbeat: The geography of Twitter"
by Kalev H. Leetaru, Shaowen Wang, Guofeng Cao, Anand Padmanabhan, and Eric Shook