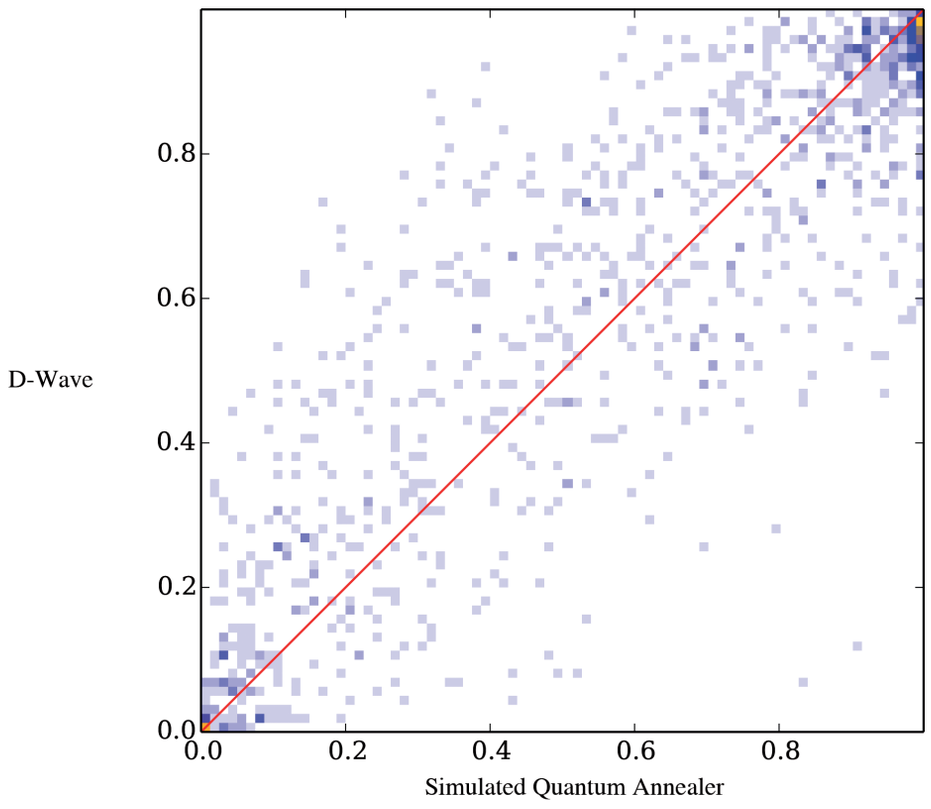
ETH zürich



Computational Science and Engineering (CSE)

Annual Report 2012/2013

CSE

Computational Science and Engineering

Annual Report
2012 / 2013

July 2012 to July 2013

Impressum:

Editors:

Ralf Hiptmair, Kaspar Nipp, Markus Reiher
ETH Zürich

PDF files of this report are available from:

Prof. Dr. Kaspar Nipp
Seminar for Applied Mathematics
Tel.: 41 44 632 3407
E-mail: nipp@math.ethz.ch

or may be downloaded from:

www.rw.ethz.ch/dokumente/cse_annual_report_1213.pdf

CSE curricula at ETH Zürich on the internet:

www.rw.ethz.ch *or* www.cse.ethz.ch

Cover:

Correlations between the success probabilities of finding the solution to a quadratic binary optimization problem in a single iteration on a D-Wave One device and on a simulated quantum annealer. The good correlation is evidence for quantum annealing behavior in the D-Wave device.

Groups having contributed to this report

Research Group	Institute	Projects	Publs.
P. Arbenz	Computer Science	30	204
S. Bonhoeffer	Experimental and Theoretical Biology		206
K. Boulouchos	Engines and Combustion Laboratory	37	208
D. Giardini	Geophysics	41	209
C. Hafner	Electromagnetic Fields	42	210
D. Helbing	Sociology	43	211
H. Herrmann	Building Materials	46	213
R. Hiptmair	Seminar for Applied Mathematics	59	215
P. Hora	Virtual Manufacturing	62	216
P. Hünenberger	Physical Chemistry	68	218
A. Jackson	Geophysics	70	
P. Jenny	Fluid Dynamics	76	220
L. Kleiser	Fluid Dynamics	85	225
M. Kröger	Polymer Physics	89	226
M. Luisier	Integrated Systems Laboratory	90	228
S. Mishra	Seminar for Applied Mathematics	92	229
R. Nesper	Inorganic Chemistry	97	
M. Parrinello	Computational Science & USI	101	231
R. Peikert	Visual Computing	118	
M. Quack	Physical Chemistry	121	233
M. Reiher	Physical Chemistry	133	235
C. Schär	Atmospheric and Climate Science	145	237
C. Schwab	Seminar for Applied Mathematics	146	240
P. Tackley	Geophysics	155	244
M. Troyer	Theoretical Physics		249
W. van Gunsteren	Physical Chemistry	176	252
S. Wiemer	Swiss Seismological Service	195	

Table of Contents

1

Introduction

Interesting people with deep expertise in frontier areas of science and technology and fascinating research agendas abound at ETH Zürich. Not long ago, I was lucky to become acquainted with two of them, Prof. Markus Püschel [1] and Prof. Torsten Höfler [2], who both joined the Computer Science Department rather recently. Even more fortunately, both are engaged in research and teaching that is highly relevant for CSE. M. Püschel describes his research as "program synthesis for performance", which aims at automatic generation of code with best possible performance from a high-level mathematical description of a problem. Inevitably, this involves exploiting the full potential of modern CPUs. M. Püschel regularly teaches the course "How to write fast numerical code" that has drawn ravish comments from participating CSE students. T. Höfler's research interests revolve around the central topic of "Performance-centric Software Development" and include scalable networks, parallel programming techniques, and performance modeling. He is one of the authors of the new MPI-2.2 and MPI-3.0 standards.

Eager to learn more, I arranged to meet both colleagues over lunch and we had a long conversation about computing hardware and its impact on CSE. I would like to give a summary in the form of a (fictitious) interview:

R.H.: **To what extent can compilers relieve the scientific software developer from having to worry about how to tune his code to the underlying hardware?**

T.H.: For particular classes of problems, for instance those based on affine models, compilers can manage to create nearly optimal code by performing optimization. This will probably never be feasible in general.

M.P.: I agree, a compiler will never be able to take care of matching an implementation to the micro-architecture of the hardware completely, for the following reasons; (i) When an idea is turned into code a massive loss of information occurs, information which is vital for optimization. Thus, for want of this knowledge, many problem specific optimizations are beyond the scope of compilers. (ii) It is all but impossible to predict the performance of a complex code, unless it is run with relevant data. Of course, this is usually far too expensive.

R.H.: **What is the point of putting effort into optimizing a code for a particular hardware given the rapid evolution of computer hardware?**

T.H.: The ideal that can never be achieved is "portable performance". The decision about how much effort should be spent on tuning a code for a particular hardware platform, must be guided by "economic" considerations about whether the potential gain in execution speed is worth the investment.

In the future we will see increasing specialization; only small groups of specialists will be able to keep abreast with hardware development. Code developers will increasingly

[1] **Markus Püschel** received his Diploma (M.Sc.) in Mathematics and his Doctorate (Ph.D.) in Computer Science, in 1995 and 1998, respectively, both from the University of Karlsruhe, Germany. From 1998-1999 he was a Postdoctoral Researcher at Mathematics and Computer Science, Drexel University. From 2000-2010 he was with Carnegie Mellon University. In 2010 he accepted the offer of a professorship at D-INFK of ETH Zürich. He is the representative of D-INFK on the steering committee for ETH's RW/CSE BSc and MSc programs. More information can be obtained from M. Püschel's homepage.

[2] **Torsten Höfler** received his Ph.D. in Computer Science from Indiana University in 2008 after he had graduated with a diploma in Computer Science from Chemnitz university in 2004. From 2010 he lead the performance modeling and simulation efforts of parallel petascale applications for the NSF-funded Blue Waters project. Then, in 2011, ETH Zürich hired him as as an Assistant Professor of Computer Science. For more information refer to his homepage.

depend on their advice and support. Computing centers are responding to this trend by creating teams of experts with competence in hardware aware optimization of codes.

M.P.: Any decision about optimizing a code will have to balance two extremes. On the one side, there is hand-tuned code for a specific processor. On the other side, there is fully portable code oblivious of features of the hardware. An important tool in reconciling both extremes are libraries that are incessantly adjusted to the latest hardware by a few experts and used by a large community. Shining examples are provided by BLAS and MPI. Another approach is program synthesis, which generates optimal code from a fully portable problem description. This is the focus of my research, but will probably be limited to special problem domains.

R.H.: **What are your predictions about the future development of computer hardware?**

M.P.: The clock rates having hit a ceiling, the surge in on-chip parallelism will continue, since the number of transistors on a single chip can still be increased. These will also be used for non-programmable special purpose circuits. This development can culminate in the emergence of high performance computers tailored to the efficient execution of one type of algorithm. This is happening: Processors that are particularly suited for graph algorithms are being developed, IBM's Blue Gene L was originally designed as a platform for stencil codes, and the Anton supercomputer has molecular dynamics simulations as its sole purpose.

T.H.: Hardware may become less and less reliable, because of further shrinking of transistor sizes and NTV (near threshold voltage) operation in order to curb power consumption. We will see chips that are lightning fast, energy efficient, but prone to errors. For some applications small errors can be accommodated, for others they are likely to be fatal; thus, reliability will become another resource to be used economically.

In the long run, we may see compilers not only generating code, but also designing hardware well suited for it. Its formal description will be transmitted to a fab, where the circuitry will be produced instantly. This still sounds like science fiction, but the history of 3D printing should teach us not to rule out such developments prematurely. A step in this direction can be hardware that is much more widely configurable than what we know today.

Zürich, November 16, 2013
Ralf Hiptmair, SAM,
Director of Studies CSE, member of the CSE Committee

2

Education

In September 2012, 25 new students started their CSE Bachelor studies, 18 in the first semester and 7 in the third semester. From outside ETH 9 students entered the CSE Master curriculum.

The total number of CSE students enrolled at the end of the academic year 2011/2012 was 92 (64 in the BSc program and 28 in the MSc program).

In the past academic year 27 students have successfully finished a CSE curriculum, 7 Bachelor students and 20 Master students, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/Master thesis and the name and the department of the advisor.

The Willi Studer Preis 2013 for the best CSE Master Diploma in the past academic year was awarded to Adrien Lücker.

Bachelor Theses

Nicolas Andrey:	Overspill avalanching in different networks (Hans Herrmann, D-BAUG)
Martina Beer:	Multiscale edge detection for diffusion tensor MRI (Philipp Grohs, D-MATH)
Raffael Casagrande:	Composite finite element method for cellular solids (Hans Herrmann, D-BAUG)
Dominik Eugster:	High-Speed Motion Tracking for Robot Control (Fumiya Iida, D-MAVT)
Rico Häuselmann:	Lambda-Dynamics in GROMOS11 - Combined with B&S-LEUS for Enhanced Sampling (Philippe Hünenberger, D-CHAB)
Stefan Hegglin:	Networks of space-filling bearings (Hans Herrmann, D-BAUG)
Alan Kaydul:	Solar Flares and Magnetic Self-Reconnection of Flux Loops (Hans Herrmann, D-BAUG)
Jakob Progsch:	A Parallel Hybrid Particle Mesh Framework (Andreas Adelmann, D-INFK, PSI and Ralf Hiptmair, D-MATH)
David Schwarz:	Contour integration techniques for solving large scale eigenvalue problems (Peter Arbenz, D-INFK)
Raphael Stadler:	Jelly blob: a self-propelled deformable solid for 2d computer games (Markus Gross, D-INFK)

Master Theses

Som Datye:	Controlling the Thermal Conductivity of Graphene and Graphene Nanoribbons (Dimos Poulikakos, D-MAVT)
Ruben Dezeure:	P-values for high-dimensional statistics (Peter Bühlmann, D-MATH)
Fabian Kulman:	Wetting Effects for Particle-Based Fluids in Video Games (Markus Gross, D-INFK)
Raoul Bourquin:	Wavepacket propagation in D-dimensional non-adiabatic crossings (Vasile Gradinaru and Ralf Hiptmair, D-MATH)
Gennaro Chirico:	Simulation of shock induced collapse with application to cell membrane poration (Petros Koumoutsakos, D-MAVT)
Andrew Foster:	A Homotopy Method for Multi-Objective Optimization (Peter Arbenz, D-INFK)
Ueli Koch:	Simulation of Plasmonic Particles with Boundary Discretization Methods (Christian Hafner, D-ITET)
Simon Härdi:	Implementierung rheologisch komplexer Materialmodelle in OpenFOAM (Leonhard Kleiser, D-MAVT)
Roman Hellmüller:	Hybrid Adaptive Mesh Partitioning (Andreas Adelmann, D-INFK, PSI and Ralf Hiptmair, D-MATH)
Sandro Mani:	Computational Design of Tensegrity Figures (Markus Gross, D-INFK)
Simon Pintarelli:	Local Multi-trace Boundary Element Formulation for Diffusion Problems (Ralf Hiptmair, D-MATH)
Mischa Obrecht:	Finite Temperature Calculation with Minimally Entangled Typical Thermal States (Matthias Troyer, D-PHYS)
Muhammad Raheem:	Phase change modeling in the presence of non-condensable gas using level-set interface tracking method (Patrik Jenny, D-MAVT)
Tobias Setz:	Bayesian Change Point and Wavelet based Stability Analysis of the Swiss Market (Diethelm Würtz, D-PHYS and Kaspar Nipp, D-MATH)

Alexander Steiner:	Efficient Block Matching on a GPU (Markus Gross, D-INFK)

Listed below are term papers written by the CSE Master students in the past two semesters.

Term Papers

Andrea Arteaga:	Multi-Resolution Simulations of Self-Propelled Swimmers (Petros Koumoutsakos, D-MAVT)
Stefan Bucher:	Simulation Methods to Determine Dynamic Response Functions of Hippocampal Pyramidal Neurons (Boris Gutkin and Sophie Deneve, ENS Paris)
Roman Hellmüller:	Mesh Partitioning with Quadtrees and ParMETIS (Andreas Adelmann, D-INFK, PSI and Ralf Hiptmair, D-MATH)
Dainel Hupp:	Entwicklung eines Black-Scholes Lösers zur Lösung von Finanzderivaten (Ralf Hiptmair, D-MATH)
Stefan Klewenhagen:	A method of Regularized Stokeslets based on the Force Coupling Method (Leonhard Kleiser, D-MAVT)
Karine Osipova:	Amplifier calibration and Geant4 simulation of the read-out for the prototype calorimeter of the PEBS experiment (Günther Dissertori, D-PHYS)

Each semester on Thursdays, 15 - 17 hours, the CSE Case Studies Seminar takes place. Speakers from ETH, from other universities as well as from industry are invited to give a 2x45 minutes talk on an applied topic. The seminar talks of the past academic year are listed in Chapter 3 of the report. Beside the scientific talks the CSE students are asked to give short presentations (10 minutes) on their Bachelor theses or on published papers out of a list. These presentations help the students to practise giving talks. Students are also asked to give talks on their term papers and voluntarily on their Master theses (if there are free time slots).

Zürich, November 6, 2013
Kaspar Nipp,
Advisor of Student Studies CSE and member of the CSE Committee
(Fachberater RW und Mitglied des Ausschusses Rechnergestützte Wissenschaften)

For detailed information on the RW/CSE curricula at ETH Zürich see:
www.rw.ethz.ch *or* www.cse.ethz.ch

3

CSE Case Studies Seminar

The CSE Case Studies Seminar takes place each semester on Thursdays, 15 - 17 hours. Speakers from ETH, from other universities as well as from industry are invited to give a 2x45 minutes talk on an applied topic. The idea is to show the students a case study of an application problem containing the problem setting, the modelling, the mathematical approach and the simulation on a computer. In addition, such a case study should show what is going on in the field of CSE and what are the job perspectives for a CSE engineer. The seminars of the past academic year are given in the two following lists.

Case Studies Seminar HS12

27.09.12	Henning Zimmer, Computergraphics Optical Flow Estimation in a Nutshell
11.10.12	Markus Püschel, Computer Systems The Issue of Performance in Mathematical Computing
25.10.12	Benjamin Stamm, Université de Pierrre et Marie Curie, Paris VI Reduced Order Models for Parametrized Problems
01.11.12	Christoph Kowitz, TU München The Combination Technique for Plasma Turbulence Simulations
15.11.12	Mathieu Luisier, Integrated Systems Laboratory Nano Electronic Device Simulation: from Schrödinger Equation to HPC
06.12.12	Holger Heumann, Université de Nice - Sophia Antipolis PDE-Constrained Optimization for Controlled Thermonuclear Fusion

Case Studies Seminar FS13

28.02.13	Jens Eller, Paul Scherrer Institut (PSI) In-situ X-ray Tomographic Microscopy of Water in Polymer Electrolyte Fuel Cells: From Pore-Scale Imaging Experiments to 3D Computer Modeling for Emission-free Mobility
07.03.13	Evelyne Knapp, ZHAW, Winterthur Simulation of Charge Transport for the Characterization of Organic Light-Emitting Devices
11.04.13	Mustafa Khammash, Control Theory and Systems Biology Pili Expression in Uropathogenic E. Coli: Stochastic Switching and Epigenetic Control
25.04.13	Oliver Fuhrer, MeteoSwiss, Zürich Numerical Weather and Climate Prediction on Emerging High-Performance Computers
02.05.13	Sascha Schnepp, Electromagnetic Fields and Microwave Electronics Adaptive Methods for Simulating Particle Accelerators - A Prototypical Multi-Scale Multi-Physics Problem

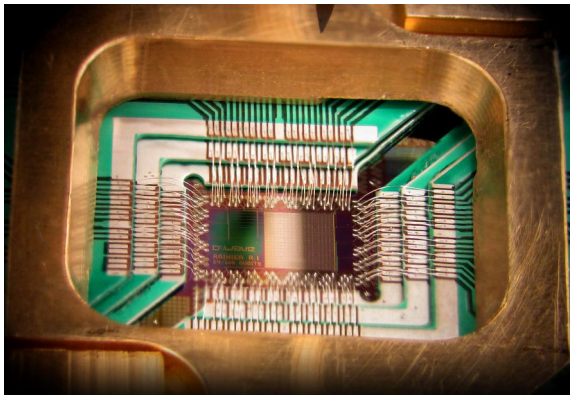
4

Computational Highlight

Quantum Annealing and the D-Wave devices

T.F. Rønnow, S.V. Isakov[1] and M. Troyer, Theoretical Physics, ETH Zürich

Two years ago the Canadian Company D-Wave Systems[2] caused a stir in the media by announcing the sale of the "world's first commercial quantum computing system" to American defense contractor Lockheed Martin. The superconducting chip that is at the core of the machine is shown on the right and contains 128 quantum bits or qubits. This spring there was an even bigger media response when D-Wave announced that second-generation 512-qubit devices had been sold to Lockheed Martin and Google. While scientists were extremely skeptical, if not outright hostile, towards these announcements in light of previous outrageous claims of the company, the media, laypersons and even European and US politicians asked whether the age of quantum computing has finally arrived?



Over the years there have been heated discussions over the company D-Wave and its devices. Experts in quantum computing claimed that these devices cannot be quantum but they are at most classical (if they work at all), while D-Wave just provided further hype and claims that their devices will soon be faster than any classical computer. In this situation we started to plan experimental tests could be run on these devices in order to find out what they are, and to compare their performance capabilities to classical computers. Last summer we visited to the USC-Lockheed Martin Quantum Computing Center[3] at the University of Southern California (USC) in Marina del Rey, a suburb of Los Angeles. There we could take a first look at this mysterious machine and started collaborations, asking them to perform some of the tests that we had devised.

But first let us step back a few decades. The origin of quantum computing is Richard Feynman's proposal in 1982 to use quantum mechanics in a computational device in order to solve the Schrödinger equation, which lies at the heart of quantum mechanics.[4] The Schrödinger equation is a simple linear partial differential equation that describes all of non-relativistic quantum physics, which includes most of physics, chemistry, materials science, and biology. While the equation has been known for almost a century, solving it is hard despite the apparent simplicity of a linear partial differential equation. The problem is the dimensionality of the problem. The so-called "wave function" describing the state of a quantum system with N particles is a complex-valued function in $3N$ dimensions. To solve even a modest problem of a thousand particles, which is trivial nowadays for classical systems, requires the solution of a partial differential equation in three thousand dimensions! Even if we choose only a very small number of d basis functions for each particle the basis

[1] S. Isakov has recently moved to Google to continue research on this topic.
[2] http://www.dwavesys.com
[3] http://www.isi.edu/research_groups/quantum_computing/home
[4] R. Feynman, *Simulating Physics with Computers,* International Journal of Theoretical Physics **21**, 467–488 (1982).

for the $3N$ dimensional space is d^{3N}, and the problem thus exponential in the number of particles. Hence, Feynman proposed to make use of quantum mechanics itself to use these equations.

One way of doing this is to "build" a quantum mechanical model in the laboratory and then perform measurements on the model, just as wind tunnels and scale models are being used for fluid dynamics problems. At ETH Zürich such experiments are done in the group of Tilman Esslinger, who uses laser waves to form a lattice and then loads atomic gases cooled to an amazing temperature of nano-Kelvin (billions of times colder than outer space) to simulate quantum lattice models in the lab.

Such experiments are however, limited to solving restricted classes of models. A general, "universal" quantum computer would be much more powerful. Such a quantum computer would be built based on quantum bits (or *qubits*) for short. Unlike a classical bit, which can take only the values 0 and 1, the quantum bit can be in an arbitrary *superposition* of these two states. Its state is defined not just by a binary variable but by a complex 2-dimensional vector of unit norm. The classical states 0 and 1 are the basis vectors of a 2-dimensional Hilbert space of the quantum system. Similarly the state of N qubits is described by normalized complex vectors in the 2^N-dimensional Hilbert space spanned by the 2^N possible classical states of N bits. Exponentially many classical bits are needed to describe a state of N qubits!

While a quantum computer for solving the Schrödinger equation would be of interest to physicists, its appeal did not extend beyond physics in the first decade. The field of quantum computing really took off in 1994, when Peter Shor, a professor of applied mathematics at the MIT, invented an algorithm[5] by which a quantum computer could factor an N-digit number into its prime factors in a time that only grows polynomially with the number of digits N. While checking whether an N-digit number is prime can be done in polynomial time on a classical computer, no polynomial time classical algorithm is know for finding the prime factors of a number. The hardness of factoring is also the basis of the RSA public key encryption algorithm that is widely used for Internet traffic and e-commerce. In RSA encryption knowing the product of two prime numbers (the "public key") is sufficient to encrypt a message, but the individual prime factors (the "private key") are needed to decrypt the message. Since factoring is hard, knowing the product lets one encrypt but not decrypt a message. A quantum computer, on the other hand, could efficiently factor the public key and thus break the encryption.

While factoring numbers is still one of the main potential uses of a quantum computer, Aram Harrow and collaborators have recently found a quantum algorithm that can solve linear systems of equations in logarithmic time[6] and thus also has an exponential advantage (quantum speedup) over classical algorithms. This algorithm might lead to more interesting applications in the future.

In order for a quantum computer to perform these algorithms the quantum computer has to be "coherent", which means that it has to *perfectly* implement the required operations. The qubits have to be *totally decoupled* from the environment or the quantum computation will be

[5] P.W. Shor, *Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer*, SIAM J. Sci. Statist. Comput. **26,** 1484 (1997).
[6] Aram W. Harrow, Avinatan Hassidim, Seth Lloyd, *Quantum algorithm for solving linear systems of equations,* Phys. Rev. Lett. **15**, 150502 (2009)

destroyed. This is a huge challenge since trillions of operations need to be performed on a quantum computer to solve a problem that cannot be solved on a PC. The current state of the art is far from this requirement. The record at the moment is held by the group of Rainer Blatt in Innsbruck, who used 14 well-isolated ions to realize 14 qubits and perform about one hundred gate operations on them.[7]

D-Wave systems, on the other hand sells 512-qubit quantum computing systems. What is going on here? Has this company achieved a huge breakthrough that has eluded all academic research efforts, similar to Craig Venter sequencing the human genome in his company before any academic effort finished? Or is it a fraud?

The first part of the answer is that the D-Wave devices are *not* universal quantum computers that could, for example, run Shor's algorithm to factor numbers. Instead they are *special purpose analog* devices to solve binary quadratic optimization problems. The problem they are built to solve is a quadratic binary optimization problem (QUBO). This QUBO problem is the minimization of a quadratic cost function

$$C(x_1,...,x_N) = \sum_{i,j=1}^{N} a_{ij} x_i x_j + \sum_{i=1}^{N} b_i x_i$$

where the variables x_i are binary, i.e. they can only take the values 0 and 1. These discrete values make the quadratic problem hard. It is in fact nondeterministic polynomially hard (NP-hard), which means that an efficient way of solving the QUBO problem can be used to solve all problems in the complexity class NP, which includes the traveling salesman problem, graph isomorphisms, factoring, and hundreds of other interesting problems. A quantum device to solve the QUBO problem more efficiently than a classical computer would thus be very interesting.

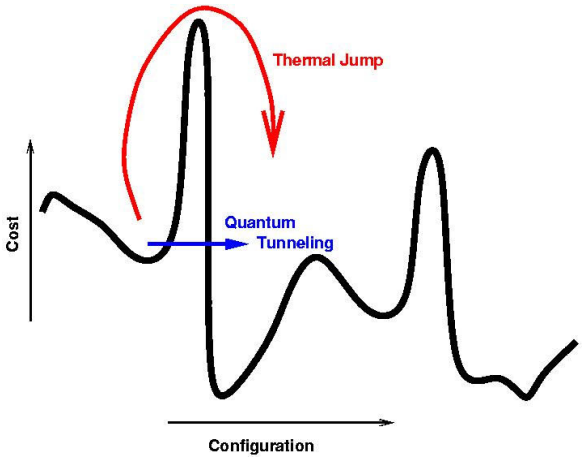
The D-Wave devices are built from superconducting qubits (corresponding to the variables x_i), with programmable couplers between them, realizing the parameters a_{ij} and b_i. They realize a programmable physical system whose energy is given by the cost function of the QUBO. Finding the ground state of this physical system is equivalent to minimizing this cost function. As an analog device there are, of course, limitations. One limitation is that it cannot implement arbitrary couplings a_{ij}, but only between a qubit and six nearby qubits on the chip. Any problem in NP can still be mapped to the device, but one might need N^2 qubits to encode an N-variable problem Another issue is that – as an analog device – there are limitations to the accuracy of the couplers, which currently have a few percent errors.

D-Wave states that their devices find the ground state by a process called "quantum annealing". Annealing is an ancient metallurgical technique that has been used for seven millennia. The properties of a metal or glass can be improved by first heating it, followed by slow cooling. By heating the atoms get more energy and can find a better, lower energy configuration, which is less brittle and stronger. Thirty years ago, Kirkpatrick and coworkers invented *simulated annealing* as an optimization algorithm.[8] This is a simple but powerful and widely used optimization method, mimicking the annealing process. One performs a Monte

[7] T. Monz, *et al. 14-qubit entanglement: creation and coherence*, Phys. Rev. Lett. 106, 130506 (2011).
[8] S. Kirkpatrick, C.D. Gelatt, M.P. Vecchi, *Optimization by Simulated Annealing*, Science **220**, 671–680 (1983).

Carlo simulation on a model that uses the cost function of the optimization problem for the energy. The system explores many configurations, thermally escaping local minima by jumping over energy barriers. By slowly reducing the temperature while performing the Monte Carlo simulation the system finds a local minimum – and with luck in the global minimum after several repetitions.

Quantum annealing is a similar process to annealing, but it works at a very low, almost zero temperature and uses quantum tunneling instead of thermal activation to escape a local minimum. In quantum annealing one starts with a very simple quantum model, which in the device is realized by a strong tunneling term that initializes all qubits to a superposition of 0 and 1. During the quantum annealing process this tunneling term is slowly reduced while the cost function is turned on, and the quantum system slowly adapts to stay close to the ground state of the system, and finally ends up in a local (and hopefully global) minimum of the cost function. The figure on the right, taken from Wikipedia, illustrates the thermal jump over a barrier used in annealing and simulated annealing, and the tunneling through barriers used in quantum annealing.



Quantum annealing can be performed in a material or device, or it can again be employed in a Monte Carlo simulation of a quantum system. The latter has been called *simulated quantum annealing*. There is evidence that simulated quantum annealing is better than simulated classical (thermal) annealing.[9] A physical device implementing quantum annealing might work even better than a simulated classical annealer, since it evolves the state of the quantum system *globally*, while the Monte Carlo simulation only performs local changes. However, not much is known about the powers of a quantum annealer. It is not even known whether a quantum device could, in principle, solve the QUBO problem better than a classical algorithm. While D-Wave's critics point to the missing theoretical foundations, it has been D-Wave's high-risk strategy to simply try it, build a device, sell it, and see what it can do.

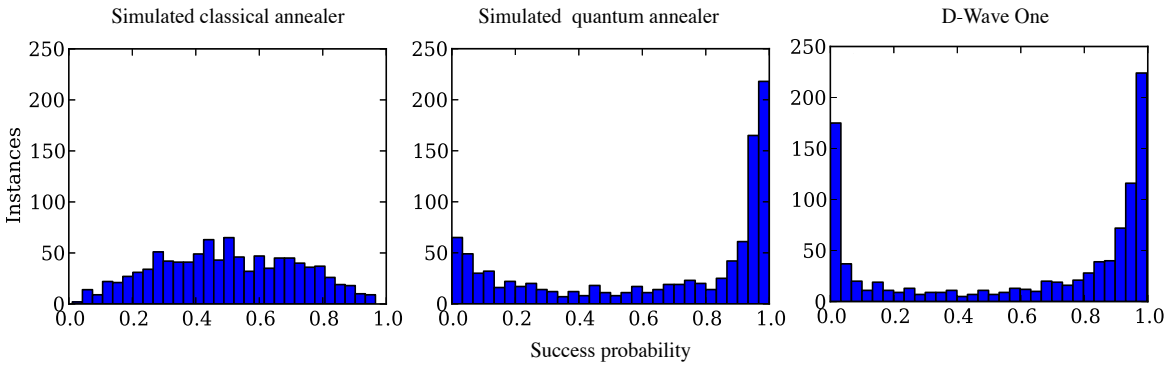
The situation is made even murkier by the fact that D-Wave uses ten year old qubit technology. The reason is that it took a decade to develop the technology to build the device. These qubits, however, couple strongly to the environment and operate at a temperature of about 15 mK. They lose their quantum coherence in a few nanoseconds, a very short time scale compared to the tens of microseconds of the annealing process. Such qubits are clearly unsuitable for a universal quantum computer, which requires perfect coherence, but they might be good enough to implement a quantum annealer. Critics, however, wonder whether the device can actually be called a quantum annealer if the coherence times are so short. They argue that the "qubits" in the device might just be classical bits that flip thermally between 0 and 1 and that the device might actually be doing classical, thermal, annealing instead of quantum annealing.

[9] G. E. Santoro, R. Martoňák, E. Tosatti, R. Car, *Theory of Quantum Annealing of an Ising Spin Glass*, Science **295,** 2427-2430 (2002).

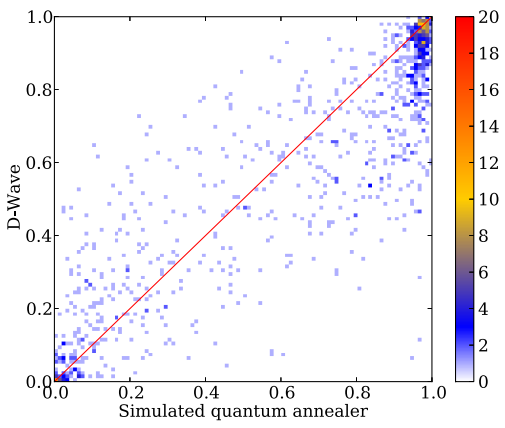
Here our work sets in. Since D-Wave sold a device to Lockheed Martin we could perform the first scientific tests to characterize the performance of the128-qubit and the 512-qubit devices. We set out to check three hypotheses:

1. *It is a classical annealer*, as many scientists believe. If coherence between the qubits is so weak that the device is actually a classical annealer then it should perform similar to a simulated classical annealer.
2. *It is a quantum annealer*, as D-Wave claims. If coherence is strong enough for the device to actually realize a quantum annealer, then it should show similarities to a simulated quantum annealer, that is a quantum Monte Carlo simulation of the annealing process
3. *It shows quantum speedup*. This is the ultimate test. If the time to solution scales better than with the best classical algorithm, then the device is definitely quantum and will be useful.

To test the device we don't try to map real applications to the graph represented by the couplings of the device, since this incurs a large overhead and we can only map pretty simple problems to the current generation D-Wave devices. Instead we look for hard "native" problem instances by picking random couplings of +1 or -1 for any of the couplers on the chip. We first use a slow but exact classical solver to find the global optimum and then run the D-Wave device, a simulated classical annealer and a simulated quantum annealer many times on that problem. For each we count how often a global minimum is found, and from that determine the success probability. Repeating this procedure for many problem instances we finally create histograms of the success probabilities:



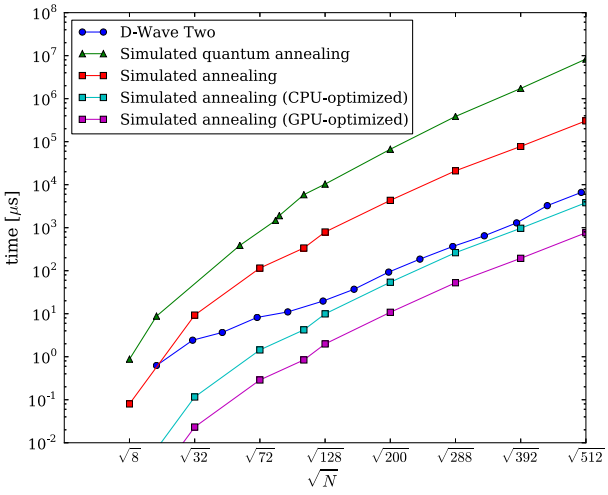
Hard problem instances have low success probabilities, while easy ones have success probabilities close to one. As we can see the distribution for the D-Wave device looks similar to that of the simulated quantum annealer but not the simulated classical annealer. This is a first hint that the device might indeed be quantum, despite the doubts of the community. We next analyze correlations, and find that, as shown in the correlation plot on the right the success probability of finding the global optimum in



one annealing run on the D-Wave device correlates very well with our simulated quantum annealer. Hard problem instances are hard for both the D-Wave device and our simulated quantum annealer, and easy ones are also easy for both. Within calibration errors the D-Wave device is indistinguishable from a simulated quantum annealer. Furthermore we find that hardness depends on a property of the quantum model (the lowest energy gap), and the fact that the D-Wave device is sensitive to that lets us conclude that it is indeed a quantum annealer.[10] But is it useful?

While we have strong experimental evidence that the D-Wave devices are quantum, the 128-qubit D-Wave One Device was also slower than a laptop. Using highly optimized simulated annealers we can solve 128-variable problems in a few microseconds on a classical CPU or GPU, while the D-Wave device needed three seconds just to be programmed. However, this is not the right comparison to make. As Peter Shor pointed out on Scott Aaronson's blog,[11] any journalist who compared the first flight of the Wright brothers with an automobile horse would also have concluded that an automobile is better than an airplane and can go much longer distances.

The really important question to ask is how does the time to solution scale with problem size. If there is quantum speedup, that is, if the scaling is better for a quantum annealer than for any classical algorithm, then ultimately the quantum annealer might win over classical computers. The D-Wave One device was not large enough to explore the asymptotic scaling regime, but the new D-Wave Two devices bought by Lockheed Martin and Google let us run much bigger, 512-variable problems where the classical codes take milliseconds instead of microseconds. While the programming time on the D-Wave device has also been reduced from three seconds to 17 milliseconds, we prefer to focus on the pure annealing time, leaving out constant overheads. This is still work in progress but we have first results. In the figure on the right we show how the median time to solution for benchmark problems with ±1 couplings. For this benchmark we see that at large problem sizes the scaling on the D-Wave device becomes similar to that of as optimized simulated annealer. There is no indication for quantum speedup.



When interpreting this plot one has to keep in mind that our GPU and CPU codes are extremely optimized (as one might expect from a group that teaches high performance computing classes at ETH). The GPU code checks 200 configurations per nanosecond! The fact that an analog device can perform comparably to extremely optimized codes on high-end classical GPUs and CPUs is already quite an achievement. Writing these fast

[10] S. Boixo, T.F. Rønnow, S.V. Isakov, Z. Wang, D. Wecker, D.A. Lidar, J.M. Martinis, M. Troyer, *Quantum annealing with more than one hundred qubits*, arXiv:1304.4595

[11] http://www.scottaaronson.com/blog/?p=1400

codes was also not trivial, and Google and the USC-Lockheed Martin Center were quick to offer jobs to the postdocs working on these codes.

The fact that the scaling is not better is, of course, a disappointment. This may, however, not be the final answer. There are many open questions. The result shown above is just for one class of benchmark problems. Potentially there may be other classes of problems where quantum speedup might show up. Researchers at Google, USC, and D-Wave are working hard to find such problem classes. The observed absence of quantum speedup might also be due to calibration problems. Calibration errors get more severe on larger problem sizes. Maybe there is actually quantum speedup, but it is hidden by problems due to calibration problems?

Another venue to investigate is whether the scaling of the classical optimizers might be misleading? In other related algorithms one has found that they break down beyond a certain size and almost never find the true global minimum anymore. Might this happen also for our codes, but not for a quantum annealer? If we think more optimistically and speculate that quantum speedup might one day be observed, the immediate question to ask will be: can we mimic the features that produce quantum speedup in an efficient classical code and thus beat the machine again? Some students have already successfully started to devise even faster classical optimization codes.

This project has raised many more questions than it has answered and will keep us busy for a long time. Even if it is not clear if the D-Wave machines might ever have an advantage over classical computers, they do lead to exiting scientific questions.

Quantum computing is still in its infancy, and the D-Wave devices should be viewed as being similar to early special-purpose analog classical computers. While analog classical computers were initially much faster than digital classical computers, they suffer from calibration and accuracy problems and are much less flexible than programmable digital computers. That is the reason why ultimately the digital classical computer has won over its analog counterpart. Also for quantum computing we expect that, for the same reason, ultimately digital quantum computers will win. Bit one will still need decades of research to develop good enough qubits that will allow a digital, gate based, quantum computer to be built. In the meantime we can already develop quantum algorithms, implement them on quantum computer emulators, and look for applications that are more exciting than helping the NSA break RSA encryption.

5

CSE Research Projects

Title: Multi-level μ-FE analysis for human bone structures

Researchers: Peter Arbenz[⋆]
Cyril Flaig[⋆]
G. Harry van Lenthe[†]
Ralph Müller[†]
Erhan Turan[⋆]
Andreas Wirth[†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Institute for Biomechanics, ETH Zürich

Description:

Micro-structural finite element (μFE) analysis based on high-resolution computed tomography represents the current gold standard to predict bone stiffness and strength. Recent progress in solver technology makes possible simulations on large supercomputers that involve billions of degrees of freedom.
In order to be effectively solved quickly and reliably on state-of-the-art parallel computers, the resulting μFE models require advanced solution techniques. We developed an improved solver that has a significantly smaller memory footprint compared to the currently used solvers. This new approach fully exploits the information that is contained in the underlying CT image itself. It admits to execute all steps in the underlying multigrid-preconditioned conjugate gradient algorithm in matrix-free form.
The reduced memory footprint allows to solve bigger bone models on a given hardware. It is an important step forward to the clinical usage of μFE simulations.

References:

E. Turan, P. Arbenz: *Preconditioning aspects of large scale micro finite element analysis of 3D bone poroelasticity.* Parallel Computing, 2013, doi:10.1016/j.parco.2013.09.002.

P. Arbenz, E. Turan: *Preconditioning for large scale micro finite element analyses of 3D poroelasticity.* In: Applied Parallel and Scientific Computing (PARA 2012). P. Manninen, P. Öster (eds.). Lecture Notes in Computer Science 7782, pp. 361–374. Springer, Heidelberg, 2013.

C. Flaig, P. Arbenz: *A highly scalable matrix-free multigrid solver for μFE analysis based on a pointer-less octree.* In Large Scale Scientific Computing LSSC'11. I. Lirkov, S. Margenov, J. Waśniewski (eds.). Lecture Notes in Computer Science 7116, pp. 498–506. Springer, Heidelberg, 2012.

C. Bekas, A. Curioni, P. Arbenz, C. Flaig, G.H. van Lenthe, R. Müller, A.J. Wirth: *Massively parallel graph partitioning: A case in human bone simulations.* In Combinato-

rial Scientific Computing. Uwe Naumann, Olaf Schenk (eds.). Chapman and Hall/CRC, 2012. pp. 407–425.

C. Flaig, P. Arbenz: *A scalable memory efficient multigrid solver for micro-finite element analyses based on CT images*. Parallel Computing 37 (12): 846-854 (2011).

Title: **A self-consistent particle-in-cell finite element time domain solver for large accelerator structures**

Researchers: Peter Arbenz[⋆]
Andreas Adelmann[†]
Yves Ineichen[⋆,†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Paul Scherrer Institute, Villigen

Description:

This research project focuses on efficiently solving self-consistent Maxwell's equations in large and complex shaped accelerator structures primarily in the light of the first part of the PSI-FEL/LEG1 project. Our prime goal is a quantitative and self-consistent modeling of the injector in the PSI-FEL/LEG project.
A novel parallel multi-scale modeling code is developed, using knowledge on parallelization, numerical methods and accelerator modeling developed in recent projects. Particle-in-cell (PIC) methods combined with novel finite element discretization techniques and parallel implementation will enable us to build up the unique capabilities with respect to quantitative modeling, needed in order to predict with sufficient accuracy beam and field properties in the detailed design and optimization of the PSI-FEL/LEG project.
Benchmarking and code comparison will be done in collaboration with researchers from Lawrence Berkeley Laboratory (LBL) and CERN.

References:

Y. Ineichen: *Toward massively parallel multi-objective optimization with application to particle accelerators*, PhD thesis, Computer Science Department, ETH Zurich, January 2013. `http://dx.doi.org/10.3929/ethz-a-009792359`

Y. Ineichen, A. Adelmann, A. Kolano, C. Bekas, A. Curioni, P. Arbenz: *A parallel general purpose multi-objective optimization framework, with application to beam dynamics.* Technical report `arXiv:1302.2889v1 [physics.acc-ph]`, February 2013, `http://arxiv.org/abs/1302.2889`.

Y. Ineichen, A. Adelmann, C. Bekas, A. Curioni, P. Arbenz: *A fast and scalable low dimensional solver for charged particle dynamics in large particle accelerators.* Comput. Sci. Res. Dev. 27 (2012), `doi:10.1007/s00450-012-0216-2`.

Y. Ineichen, A. Adelmann, C. Bekas, A. Curioni, P. Arbenz: *A massively parallel general purpose multi-objective optimization framework, applied to beam dynamic studies.* Proceedings of ICAP2012, Rostock-Warnemünde, Germany, 2012, pp. 62–66.

A. Adelmann, P. Arbenz, Y. Ineichen: *Improvements of a fast parallel Poisson solver on irregular domains*. In Applied Parallel and Scientific Computing (PARA 2010). K. Jónasson (ed.). Part I, Lecture Notes in Computer Science 7133, pp. 65–74. Springer, Heidelberg, 2012.

Title: **A self-consistent particle-in-cell time-domain solver incorporating radiative losses and interaction**

Researchers: Peter Arbenz[⋆]
Andreas Adelmann[†]
Christof Kraus[⋆]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Paul Scherrer Institute, Villigen

Description:

The simulation of radiative interactions in a particle accelerator is a challenging problem. Existing codes reduce the dimensionality of the problem, neglect transient effects or limit the number of particles and the complexity of the geometry. Our plan is to compute the electromagnetic field of the particles in time domain on a hierarchy of meshes. To reduce the memory consumption we plan to embed co-moving finer meshes in a coarser mesh. Even with this reduction the computation of the resulting problem will have to be carried out on thousands of compute nodes.
The resulting tool will be seamlessly integrated into the particle tracker Object Oriented Parallel Accelerator Library (OPAL) that has been developed at PSI allowing for simulations of particle accelerators from start to end (S2E) including magnetic chicanes consisting of four deflecting dipoles.

References:

C. Kraus, A. Adelmann, P. Arbenz: *Perfectly matched layers in a divergence preserving ADI scheme for electromagnetics.* J. Comput. Phys. 231 (1): 39-44 (2012).

Title: **Resonant lossy electromagnetic structures**

Researchers: Peter Arbenz[⋆]
Hua Guo[⋆]
Yoichi Matsuo[⋆‡]
Benedikt Oswald[†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Paul Scherrer Institute, Villigen
[‡]Department of Mathematics, Keio University, Japan

Description:
Resonant electromagnetic cavity structures are used in virtually all types of particle accelerators. The X-ray free electron laser currently under study at the Paul Scherrer Institute, is no exception and will consist of a large variety of radio frequency (RF) structures for guiding and accelerating electrons from the photo-cathode through the linear accelerator section.
We introduce a 3-dimensional electromagnetic eigenmodal algorithm for the theoretical analysis of resonating nano-optical structures. The method, a variant of the Jacobi-Davidson algorithm, solves the electric field vector wave, or curl-curl, equation for the electromagnetic eigenmodes of resonant optical structures with a finite element method. In particular, the method includes transparent boundary conditions that enable the analysis of resonating structures in unbounded space.

References:

H. Guo, P. Arbenz, B. Oswald: *A large-scale nonlinear eigensolver for the analysis of dispersive nanostructures.* Computer Phys. Comm. 184 (8): 1898-1906 (2013).

H. Guo, B. Oswald, P. Arbenz: *3-dimensional eigenmodal analysis of plasmonic nanostructures.* Optics Express. 20 (5): 5481-5500 (2012)

H. Guo, B. Oswald, P. Arbenz: *Realistic 3-dimensional eigenmodal analysis of electromagnetic cavities using surface impedance boundary conditions.* Proceedings of ICAP2012, Rostock-Warnemünde, Germany, 2012, pp. 161–163.

H. Guo, A. Adelmann, P. Arbenz, A. Falone, C. Kraus, B. Oswald: *Computation of electromagnetic modes in the transverse deflecting cavity.* Proceedings of the 2010 International Particle Accelerator Conference, Kyoto, Japan, 2010.

Title: **Parallelization of the time integration for time-periodic flow problems**

Researchers: Peter Arbenz[⋆]
Daniel Hupp[⋆]
Dominik Obrist[†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Institute of Fluid Dynamics, ETH Zürich

Description:
We investigate parallel algorithms for the solution of flow problems that are periodic in time. Finite difference approximations on a mesh in space-time are used. For periodic solutions, the discretized problem can be written as a large non-linear system of equations. This system of equations is solved by a Newton-Krylov method, using a GMRES solvers with a block-cyclic preconditioner. The parallel performance of this algorithm is illustrated by a number of numerical experiments in one and two space dimensions.

References:

P. Arbenz, D. Hupp, D. Obrist: *A parallel solver for the time-periodic Navier–Stokes equations.* In Parallel Processing and Applied Mathematics (PPAM 13). R. Wyrzykowski (ed.). Lecture Notes in Computer Science. To appear.

P. Arbenz, A. Hiltebrand, D. Obrist: *A parallel space-time finite difference solver for periodic solutions of the shallow-water equation.* In Parallel Processing and Applied Mathematics (PPAM 11) Part II. R. Wyrzykowski, J. Dongarra, K. Karczewski, J. Waśniewski (eds.). Lecture Notes in Computer Science 7204, pp. 302–312. Springer, Berlin, 2012.

D. Obrist, R. Henniger, P. Arbenz: *Parallelization of the time integration for time-periodic flow problems.* Proc. Appl. Math. Mech. 10 (1): 567–568 (2010).

Title: Flame dynamics in lean premixed CO/H_2/air combustion in a meso-cale channel

A. Brambilla[1,2], C.E. Frouzakis[1], J. Mantzaras[2], R. Bombach[2], K. Boulouchos[1]

Institute/ Group: [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]Combustion Research Laboratory, Paul Scherrer Institute, Villigen

The dynamics and stabilization of fuel lean premixed CO/H_2/air atmospheric pressure flames in meso-scale channels were investigated numerically, using detailed gas phase chemistry and transport. Experiments in a channel flow reactor by means of chemiluminescence detection of the excited OH radical allowed for model validation at steady conditions and identification of the conditions at which unsteady flame dynamics were present. A detailed parametric study of the influence of wall temperature and CO:H_2 ratio on the ensuing flame dynamics was performed. The numerical results revealed different flame modes which included oscillatory ignition, random ignition spots, as well as steady weak and V-shaped flames. The wall temperature stability intervals of these modes changed with the CO:H_2 ratio. The richest variety was found for molar CO:H_2 ratios between 4 and 10, while at lower ratios the random and the weak modes were absent. At higher ratios all the dynamic modes were suppressed. The Computational Singular Perturbation (CSP) method was used to obtain insights into the physicochemical processes responsible for the weak flames, which were found at relatively high inflow velocities compared to previous studies, and V-shaped flames. A kinetic origin of the phenomena was supported by the CSP results.

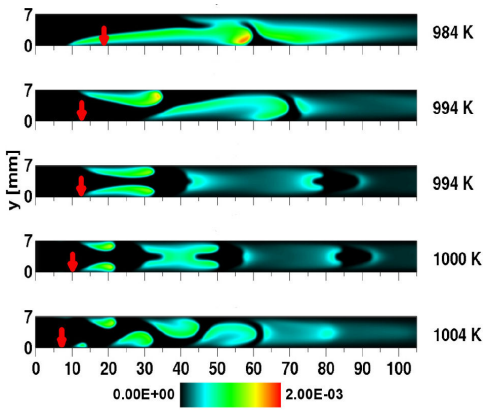


Figure 1: Top to bottom: instantaneous distributions of OH mass fraction of the asymmetric oscillatory flame (wall temperature $T_W = 984$ K), asymmetric oscillatory flame ($T_W = 994$ K), symmetric oscillatory flame ($T_W = 994$ K), symmetric oscillatory flame ($T_W = 1000$ K), asymmetric oscillatory flame ($T_W = 1004$ K), The arrows mark the ignition locations.

References:

• A. Brambilla, C.E. Frouzakis, J. Mantzaras, R. Bombach, K. Boulouchos, Flame dynamics in lean premixed CO/H_2/air combustion in a mesocale channel, *Combust. Flame*, (accepted)

Title: Direct Numerical Simulation of the Autoignition of a Hydrogen Plume in a Turbulent Co-flow of Hot Air

S.G. Kerkemeier[1], C.N. Markides[2], C.E. Frouzakis[1], K. Boulouchos[1]

Institute/ Group: [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]Department of Chemical Engineering, Imperial College, U.K.

The autoignition of an axisymmetric nitrogen-diluted hydrogen plume in a turbulent coflowing stream of high-temperature air was investigated in a laboratory-scale set-up using 3-D numerical simulations with detailed chemistry and transport. The plume was formed by releasing the fuel from an injector with bulk velocity equal to that of the surrounding air coflow. In the 'random spotss regime, autoignition appeared randomly in space and time in the form of scattered localized spots from which post-ignition flamelets propagated outwards in the presence of strong advection. Autoignition spots were found to occur at a favourable mixture fraction close to the most reactive mixture fraction calculated a priori from considerations of homogeneous mixtures based on inert mixing of the fuel and oxidizer streams. The value of the favourable mixture fraction evolved in the domain subject to the effect of the scalar dissipation rate. The hydroperoxyl radical appeared as a precursor to the build-up of the radical pool and the ensuing thermal runaway at the autoignition spots. Subsequently, flamelets propagated in all directions with complex dynamics, without anchoring or forming a continuous flame sheet. These observations, as well as the frequency of and scatter in appearance of the spots, are in good agreement with experiments in a similar set-up. In agreement with experimental observations, an increase in turbulence intensity resulted in a downstream shift of autoignition. The advection of the most reactive mixture through the domain, and hence the history of evolution of the developing radical pools were considered to this effect.

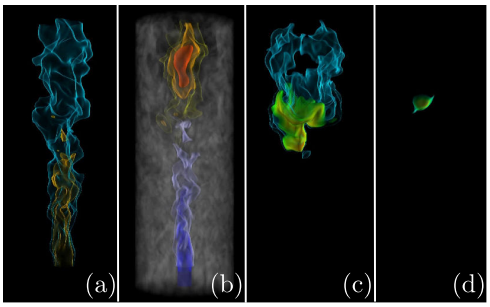


Figure 2: Volume renderings of (a) mixture fraction, (b) temperature, (c) mass fraction of HO_2, (d) reaction rate of OH.

References:

• S. G. Kerkemeier, C. N. Markides, C.E. Frouzakis, K. Boulouchos, Direct Numerical Simulation of the Autoignition of a Hydrogen Plume in a Turbulent Co-flow of Hot Air, *J. Fluid Mech.*, 720, 424-456, 2013

Title: Entropic lattice Boltzmann methods for fluid mechanics

Researchers: I. Karlin[1], S. S. Chikatamarla[1], F. Boesch[1], K. Boulouchos[1]

Institute/ Group: [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ

Lattice Boltzmann methods were introduced in the late 80's - early 90's as a new approach to Computational Fluid Dynamics, and have begun to find wide acceptance during past decade. In LBM, one does not attempt a direct discretization of the Navier?Stokes equations; instead, a kinetic equation of Boltzmann's type for a small number of discrete velocities is solved numerically on a regular grid. Also, the ability of LBM to easily handle complex grid and wall geometries makes them very attractive for novice computational fluid mechanists. However, LBM has inherent instabilities that arise at high Reynolds number and low grid resolutions, thus restricting their applications to highly resolved simulations. Recently, entropic LB models have proven to be a way out of this bottleneck. By deriving a pertinent entropy function and the corresponding equilibria, we had developed a novel version of LBM - the Entropic Lattice Boltzmann method, which enabled stable and thermodynamically consistent LB simulations. Here at LAV, we use ELBM to simulate an array for turbulent flow problems. Some of the current applications are illustrated in Figure 3.

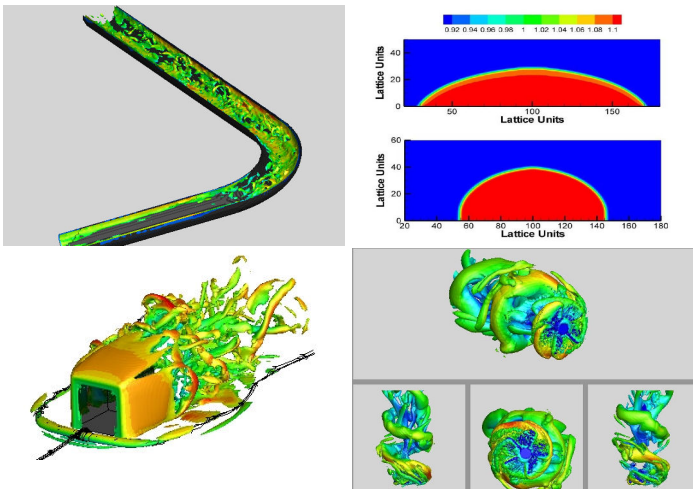


Figure 3: ELBM simulations: (i) Top-Left:Predictive and reliable computation of transition to turbulence in complex geometries. (ii) Bottom-Left: Comparison of ELBM with experimental results obtained from the wind tunnel. (iii) Top-Right: ELBM simulation of liquid droplet on a surface. (iv) Bottom-Right: Simulation of complex moving objects.

References:

• Chikatamarla S. and Karlin I., Entropic lattice Boltzmann method for turbulence: Wall boundary conditions. *Physica A.*, 392,1925-1930 (2013)

• Gu C., Chikatamarla S. and Karlin I., 3D Simulation of turbulent flow past a circular cylinder in resolved and under-resolved regimes using ELBM. *Intl. J. Modern Phys. C*, 25, No. 1, 1340024 (2014).

• Karlin I. V, Sichau D, Chikatamarla S. S,Consistent two-population lattice Boltzmann model for thermal flows, *Physical Review E*, (submitted, 2013)
• Chikatamarla S.S, Duenser S, Karlin I.V, ELBM simulation of flow past a surface mounted cube, *Intl. Journal of Modern Physics C*, (in preparation, 2013)
• Boesch, F. and Karlin, I.V., Exact lattice Boltzmann equation, *Phys. Rev. Lett.*, 111, 090601 (2013)
• Mendoza, M., Karlin, I., Succi, S., Herrmann, H.J., Ultrarelativistic transport coefficients in two dimensions, *J. Stat. Mech.* P02036 (2013)
• Mendoza, M., Karlin, I., Succi, S., Herrmann, H.J., Relativistic lattice Boltzmann model with improved dissipation, *Phys. Rev. D.*,87(6), 065027 (2013)
• Singh, S., Krithivasan, S., Karlin, I., Succi, S., Ansumali, S., Energy conserving lattice Boltzmann models for incompressible flow simulations, *Commun. Comput. Phys.* 13(3), 603 (2013)

Title: Whole-mantle radial anisotropy from joint inversion of multi-mode surface wave dispersion and body wave traveltimes

Researchers: L. Auer, L. Boschi, T. Nissen-Meyer

Institute/ Group: Institute of Geophysics
Group for Seismology and Geodynamics

Description:

In the last decades, independently derived seismic tomography models of isotropic Shear wave velocity of the earths mantle have advanced to a state of considerable consistency. It is well known, however, that a simple isotropic description of the elastic properties and their interpretation in terms of fast and slow (cold and hot) velocity anomalies is inadequate and elastic anisotropy is non-negligible at various regions. Global anisotropic tomography is only in its infancy and the few published models of whole-mantle radial anisotropy agree with each other only for low harmonic degrees. In this project, we aim to contribute to the ongoing effort to establish a consensus on a long-spatial-wavelength model of radially anisotropic 3-D whole-mantle structure, by inverting a comprehensive suite of recently published surface and body wave datasets. Additionally, we perform an extensive quantitative comparison of our new results with previously published models. We employ surface wave phase delays from fundamental modes up to the 6th overtone measured in periods between 35 and 300 s, as well as a state of the art cross-correlation datasets of a variety of body wave phases.

Inverting the kernel matrix is computationally intensive and thus we parallelize the involved Cholesky factorization, in a multithreading context, using OpenMP. Our new tomographic solution is based on classical ray-based linearized tomography, a radially anisotropic block parameterization, and non-linear crustal corrections, and shares various features with other independently derived models, such as the intriguing anomaly of faster V_{SH} ($\xi > 1$; horizontal flow) in the Central Pacific and an anomaly of faster V_{SV} ($\xi < 1$; vertical flow) beneath the East Pacific Rise. In the near future we will replace our ray-theoretical sensitivities with numerical finite- frequency kernels, and work is underway to migrate from a uniform inversion grid to a 3-D data-adaptive multi- resolution parameterization, so as to mitigate problems associated with the inhomogeneous distribution of sources and receivers.

References: A manuscript is in preparation for *Geochemistry, Geophysics, Geosystems (G^3)*

Title: Numerical methods for electromagnetics and optimization

Researchers: Christian Hafner
Jürg Fröhlich
Jens Niegemann
Sascha Schnepp
Dimitra Psychogiou
Christian Beyer
Nemat Dolatsha
Mustafa Boyvat
Nikolay Komarvesky
Aytac Alparslan
Mengyu Wang
Christoph Böcklin
Alexander Dorodnyy
Sahar Sargheini
Pegah Souzanghar

Institute Laboratory for Electromagnetic Fields and Microwave Electronics

Description:

We develop various numerical methods and software packages for computational electromagnetics and optimal design with applications ranging from very low up to optical frequencies. These codes, free software (freeFEM++, NGsolve, Concepts) and commercial packages (Comsol, CST, HFSS, etc.) are applied to 1) metamaterials for magnetic field shielding, radar absorption, thermal protection, and efficient solar cells; 2) photonic crystals and dielectric waveguide structures for optical frequencies and for fast interconnects in the mm wave range; 3) design of antenna structures ranging from radio frequencies up to optical frequencies, e.g., plasmonic nano antennas for bio sensing; 4) analysis and design of scanning probe tips for microwaves, optics, and electron emission; 5) devices for biology and medicine; etc.
Currently we develop and combine various field solvers based on boundary discretization methods such as the Multiple Multipole Program (MMP) as well as domain discretization methods in frequency and time domain, namely Finite Elements Methods (FEM), Discontinuous Galerkin (DG), Fourier Modal Method (FMM), etc. The semi-analytic MMP method provides high accuracy, robustness, numerical efficiency for 2D applications, and exhibits no problems with material dispersion and loss. For 3D simulations, TD-FEM and DG-FEM are favorable for the analysis of geometrically complicated structures.
Our MMP and FDTD codes are contained in the OpenMaX platform, which is an OpenSource project (see http://openmax.ethz.ch/).

References:
From fall 2012 till fall 2013, 11 papers on various topics of computational electromagnetics were published in reviewed journals.

Title: QLectives
Researchers: Dirk Helbing et al.
Institute/Group: Chair of Sociology, in particular of Modeling and Simulation

Description:

QLectives is a project bringing together top social modelers, peer-to-peer engineers and physicists to design and deploy next generation self-organising socially intelligent information systems. The project aims to combine three recent trends within information systems:

- Social networks - in which people link to others over the Internet to gain value and facilitate collaboration (think of Facebook)
- Peer production - in which people collectively produce informational products and experiences without traditional hierarchies or market incentives (think of Wikipedia)
- Peer-to-Peer systems - in which software clients running on user machines distribute media and other information without a central server or administrative control (think of BitTorrent)

QLectives aims to bring these together to form Quality Collectives, i.e. functional decentralised communities that self-organise and self-maintain for the benefit of the people who comprise them. We aim to generate theory at the social level, design algorithms and deploy prototypes targeted towards two application domains:

- QMedia - an interactive peer-to-peer media distribution system (including live streaming), providing fully distributed social filtering and recommendation for quality (think of social television 2.0)
- QScience - a distributed platform for scientists allowing them to locate or form new communities and quality reviewing mechanisms, which are transparent and promote quality (think of Slashdot for any particular discipline or sub-discipline)

References:

- Roca, C. P. and Helbing, D. (2011) Emergence of social cohesion in a model society of greedy, mobile individuals. PNAS 108 (28): 11370-11374.
- Wu, J., Lozano, S. and Helbing, D. (2011) Empirical Study of the Growth Dynamics in Real Career H-index Sequences. Journal of Informetrics 5(4), pp. 489-497.
- Helbing, D. and Lozano, S. (2010) Phase transitions to cooperation in the prisoner's dilemma. Physical Review E, 81
- Helbing, D., Szolnoki, A., Perc, M. and Szabó, G. (2010) Evolutionary establishment of moral and double moral standards through spatial interactions. PLoS Computational Biology, 6(4)
- Helbing, D., Szolnoki, A., Perc, M., Szabó, G. (2010) Defector-accelerated cooperativeness and punishment in public goods games with mutations. Physical Review E, 81
- Helbing, D. and Johansson, A. (2010) Evolutionary dynamics of populations with conflicting interactions: Classification and analytical treatment considering asymmetry and power. Physical Review E, 81

Title: Momentum
Researchers: Dirk Helbing et al.
Institute/Group: Chair of Sociology, in particular of Modeling and Simulation

Description:

The Momentum project, funded by an ERC Advanced Investigator Grant with 2.5 million euros, is a five-year project of the SOMS group that has just started. Its central innovation is to explain the emergence of social behavior and institutions from very first principles, making use of large-scale agent-based simulations. These agents will be equipped with artificial brains (neural networks), allowing them to develop and employ new behavioral rules to study under which conditions social institutions can emerge and become globally accepted norms.

Understanding social systems from fundamental principles is one of the most important scientific challenges of the modern area. The main objective of the simulation of sophisticated interacting agents is to show how other-regarding human behavior (characterizing a "homo socialis") can be the result of competition and the co-evolution of social mechanisms. Our models will not assume that actors are equipped with certain social institutions already at the outset of the evolutionary process. We want to demonstrate that, for example, social cooperation and social norms are not static features of societies, but rather emergent outcomes of repeated and multifaceted interactions between many individuals. Rather than *implementing* "homophily", cooperation, norms, inequality, conflict etc. as features of our simulated model societies, we want to understand them as outcomes of a co-evolutionary process in which individual behaviors, social interactions, learning processes and their interplay evolve over time. We seek to develop a model of human societies where each member can invent new behavioral rules, imitate successful behavior of others, and improve existing rules. Thus, besides the complexity that results from the interaction between agents, our model adds a lot of complexity on the level of the individuals, as each individual needs to be equipped with a "brain" that allows her to invent and improve behavioral rules. To simulate these kinds of complex behaviors, our virtual agents will have a small virtual brain in the form of an artificial neural network. We plan to simulate 1,000 agents with 1,000 brains, each running on a separate processor core in a computer cluster.

References:

- Helbing, D., Yu, W., and Rauhut, H. (2011) Self-organization and Emergence in Social Systems: Modeling the Coevolution of Social Environments and Cooperative Behavior. Journal of Mathematical Sociology 35:177-208.
- Helbing, D. and W. Yu (2010) The future of social experimenting. Proceedings of the National Academy of Sciences USA (PNAS) 107(12): 5265-5266.
- Helbing, D. and Yu, W. (2009) The outbreak of cooperation among success-driven individuals under noisy conditions. PNAS 106(10)
- Helbing, D. and A. Johansson (2010) Cooperation, norms, and revolutions: A unified game-theoretical approach. PLoS ONE 5(10): e12530.
- Helbing, D., A. Szolnoki, M. Perc, and G. Szabó (2010) Evolutionary Establishment of Moral and Double Moral Standards through Spatial Interactions. PLoS Computational Biology 6(4): e1000758.

Title: Innovation Accelerator
Researchers: Dirk Helbing et al.
Institute/Group: Chair of Sociology, in particular of Modeling and Simulation

Description:

This project focusses on the long-term vision of creating an "Innovation Accelerator": a general platform to monitor the latest developments in science, detect emerging trends and innovations, find the best experts for projects, and support the distributed generation of new knowledge, thereby promoting innovation.

To that aim, an ecosystem of interconnected, open tools has been developed: Vijo (vijo.inn.ac) is an interface where users can create "virtual journals," consisting of articles published in regular journals but dynamically compiled based on filters defined and shared by individual users or communities. Living Science (livingscience.ethz.ch) is a platform to observe and analyze scientific publications and activities. Living Archive (livingarchive.eu) is an online catalog of open datasets. Nanobrowser (nanobrowser.inn.ac) is an interface for browsing and publishing "nanopublications," i.e. tiny pieces of scientific results represented together with their provenance and metadata in a formal Semantic Web language.

References:

- Helbing, D. and Balietti, S. (2011) How to create an innovation accelerator. EPJ ST 195(1)
- van Harmelen, F., Kampis, G., Börner, K., van den Besselaar, P., Schultes, E. and others. (2012) Theoretical and technological building blocks for an innovation accelerator. EPJ ST 214(1)
- Kuhn, T., Barbano, P.E., Nagy, M.L., and Krauthammer, M. (2013) Broadening the Scope of Nanopublications. Proc. of ESWC 2013
- Kuhn, T. and Krauthammer, M. (2012) Underspecified Scientific Claims in Nanopublications. Proc. of WoLE 2012

Title: From liquid transport in unsaturated granular media to the rheology of dense particle suspensions

Researchers: R. Mani
H.J. Herrmann

Institute/ Institute for Building Materials, ETH Zürich
Group: Computational Physics for Engineering Materials, ETH Zürich

Description:

The addition of small amounts of liquid to granular materials has a great impact on its mechanical and rheological properties. The cohesive forces due to the liquid enable us to build beautiful sandcastles but can also cause severe difficulties when processing wet powders in industries. In a fully saturated granular suspension, the cohesive force is lost. However, suspending fluid may act as a lubricant, which has direct implications on the rheological properties of dense particle suspensions. We model particles and spatial fluid transport as well as the interactions between particles by means of numerical simulations. Spherical hard particles are explicitly modeled using the Contact Dynamics algorithm. The liquid transport is driven by pressure differences between capillary bridges. Numerically calculated Laplace pressures of capillary bridges are used to determine the liquid fluxes between individual capillary bridges. Using this model, we find that liquid is migrating out of shear bands [1] and show how liquid spreading can be optimized in homogenous plane shear [2]. In industries, dense particle suspensions often need to be transported over long distances via pipes. If the particle concentration in the suspension is large enough, the viscosity of the suspension can increase to infinity, which may cause severe damage to industrial facilities. By modeling dense particle suspensions including lubrication between the particle contacts, we were able to propose a novel theory supported by experiments on the shear thickening of dense particle suspension [3]. This theory helps industries to avoid or delay the shear thickening by controlling the friction between particles.

References:

[1] R. Mani, D. Kadau, D. Or, H.J. Herrmann
Fluid depletion in shear bands, Phys. Rev. Lett. **109** (2012) 248001
[2] R. Mani, D. Kadau, H.J. Herrmann
Liquid migration in sheared unsaturated granular media,Granular Matter **15** (2013) 447-454
[3] N. Fernandez, R. Mani, D. Rinaldi, D. Kadau, M. Mosquet, H. Lombois-Burger, J. Cayer-Barrioz, H.J. Herrmann, N. D. Spencer, L.Isa
Microscopic Mechanism for Shear Thickening of Non-Brownian Suspensions
Phys. Rev. Lett. **111** (2013) 108301

Title: Fracturing random media with long range correlations

Researchers: N. Posé
N.A.M. Araújo
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

In statistical physics, percolation has been studied extensively as it exhibits interesting critical properties and have many physical applications. One is especially interested in the geometrical and transport properties of the clusters at criticality [Phys. Rev. E, **86** (2012) 051140]. We want to introduce correlations in the percolation process. To study this problem we consider the general framework of ranked surfaces [Sci. Rep., **2** (2012) 348]. Percolation through invasion clusters can be studied on these surfaces. We study the critical properties of watersheds and other percolation related curves on correlated landscapes. A deeper insight into the critical properties of these curves might be obtained by Stochastic Loewner Evolution (SLE) analysis. This theory has been applied to describe common curves encountered in statistical physics and compute exactly some critical exponents. However, not all the random curves are described by this theory. We study for which curves on correlated landscapes SLE can be established [Phys. Rev. Lett., **109** (2012) 218701]. Generating correlated ranked surfaces and testing the SLE properties of the curves are computationally challenging. The algorithms to obtain the desired curves and to test their properties are complex. Also, as one wants to study carefully the effect of correlations on the obtained curves, one has to generate a large number of curves on large lattice sizes in order to obtain good statistics and reduce the finite size effects. We also need to repeat these measures for several values of the correlation parameter to study the dependency of the properties on the correlation of the surfaces. Therefore one needs to develop efficient algorithms to study these problems.

References:

N. Posé, N.A.M. Araújo, and H.J. Herrmann, *Conductivity of Coniglio-Klein clusters*, Phys. Rev. E, **86** (2012) 051140

K.J. Schrenk, N.A.M. Araújo, J.S. Andrade Jr., and H.J. Herrmann, *Fracturing ranked surfaces*, Sci. Rep., **2** (2012) 348

E. Daryaei, N.A.M. Araújo, K.J. Schrenk, S. Rouhani and H.J. Herrmann, *Watersheds are Schramm-Loewner Evolution curves*, Phys. Rev. Lett., **109** (2012) 218701

Title: Numerical simulation of debris flow and interaction between flow and obstacle via DEM

Researchers: A. Leonardi
M. Mendoza
F.K. Wittel
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Debris flows are dangerous natural hazards that occur in mountainous terrains after heavy rainfall, responsible for casualties and damages reported yearly worldwide. Their heterogeneous composition, with a visco-plastic fluid and the presence of a relevant granular solid phase, determines a non-trivial behavior making them a challenging problem for the physical description of the phenomenon.

A 3D hybrid numerical model is used to simulate them, taking into account the interaction between the two phases [Int. J. for Num. Methods in Eng., **87**, 66–95]. It is developed as a combination of a Discrete Element Method for the description of the solid phase, and a Lattice-Boltzmann Method for the resolution of the fluid phase. For the LBM, the standard BGK collision operator is used, while the fluid-particle interaction is implemented with a modified streaming operator. The non-Newtonian rheology is included with a multiple relaxation time approach. The free surface of the flow is represented with the use of a mass tracking algorithm [J. of Non-Newtonian Fluid Mech., **179-180**, 32–42]. For the DEM, both translational and rotational degrees of freedom are tracked, with the adoption of a standard spring-dashpot-friction contact model to compute collision forces. A realistic particle size distribution is used [Granular Matter, **11**(4), 209–220].

References:

[1] O. Švec, J. Skoček, H. Stang, M.R. Geiker, and N. Roussel (2012). Free surface flow of a suspension of rigid particles in a non-Newtonian fluid: A lattice Boltzmann approach. *Journal of Non-Newtonian Fluid Mechanics*, ***179-180***, 32–42.
[2] D.R.J. Owen, C.R. Leonardi, and Y.T. Feng (2011). An efficient framework for fluid – structure interaction using the lattice Boltzmann method and immersed moving boundaries. *International Journal for Numerical Methods in Engineering*, ***87***, 66–95.
[3] H. Teufelsbauer, Y. Wang, M.C. Chiou, and W. Wu (2009). Flow–obstacle interaction in rapid granular avalanches: DEM simulation and comparison with experiment. *Granular Matter*, **11**(4), 209–220.

Title: Fatigue Particle Fragmentation by Repeated Impact

Researchers: F.K. Wittel
H.J. Herrmann

Institute/ Institute for Building Materials, ETH Zürich
Group: Computational Physics for Engineering Materials, ETH Zürich

Description:

Wanted or unwanted impacts of particles during their comminution or simple transport can cause fragmentation. It is well known that there exists a critical, system dependent energy that separates the damage regime from the fragmentation one by a phase transition [1]. If impact energies are below the fragmentation threshold internal damage and attrition can be caused that lower this threshold. These fatigue effects due to the repeated impact leads to mechanisms for the final breakup that differ from those of single impact fragmentation, usually studied.

We focus on particle agglomerate systems composed of Spherical Discrete Elements (SDE) connected by three-dimensional beam elements, whose fragmentation behavior was well studied for single impact [2-3]. The system is impacted repeatedly at velocities below the bulk fragmentation threshold. After each impact the damaged system is randomly rotated, before it hits the rigid target again. We monitor average particle lifetime as function of velocity as well as the damage accumulation before fragmentation. The occurring fragmentation mechanisms and fragment mass distributions are compared to single impact fragmentations and experiments showing different fragmentation regimes for low and intermediate impact energies. Finally the outcome of alternated impact speeds on the outcome of the fragmentation and powder production is measured that can be used to optimize milling processes with respect to desired fragment mass distributions or reduction of powder production.

References:

[1] F. Kun and H.J. Herrmann, "Transition from damage to fragmentation in collision of solids", *Physical Review E*, **59**, 2623 (1999).
[2] H.A. Carmona, F.K. Wittel, F. Kun, H.J. Herrmann, "Fragmentation processes in impact of spheres", *Physical Review E*, **77**, 051302 (2008).
[3] F.K. Wittel, "Fragmentation of Spheres in Ultrasound Assisted Impact Comminution", *Granular Matter*, **12**, 447-455 (4/2010)

Title: Risk Analysis in Complex Networks

Researchers: V.H.P. Louzada
N.A.M. Araújo
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Natural catastrophes, financial crises, and diseases outbreaks have all been considered as events whose impact could be mitigated through identification of potential threats, as well as fast responses and later effective recovery measures. Usually, all those studies are labeled as 'Risk Analysis', despite the lack of common background, techniques, and vocabulary. Risk is entangled with the concept of complexity. Components forming a system interact in a non-trivial way with emergence of complex behavior, not predicted from the isolated interactions. Hence, the use of Complex Networks or Statistical Physics in general is a powerful way to understand risk [1].

In this project we study the three typical dimensions of Risk Analysis (risk identification [2], mitigation [3], and response [4]) in a complex system. From this, we are developing a theory of Risk Analysis that could be extended for many real applications. As a standard framework to analyze the interplay between topological features and dynamics, we use Kuramoto Oscillators that interact on top of a Complex Network [5].

There is a considerable computational effort when dealing with Kuramoto Oscillators. The dynamics, consisting of non-linear interactions among oscillators (nodes) in a network, has to be followed until a stationary state is achieved. Besides, a number of different realizations of the initial values of the dynamics should be considered in order to avoid finite-size effects and account for statistical fluctuations. As a result, the development of efficient algorithms to tackle this problem is a challenge in itself.

References:

[1] N.A.M. Araújo and H.J. Herrmann, Explosive percolation via control of the largest cluster, Phys. Rev. Lett. 105 (2010) 35701.
[2] V.H.P. Louzada, N.A.M. Araújo, J.S. Andrade, and H.J. Herrmann, Breathing Synchronization in Interconnected Networks, ArXiv: 1304.5177.
[3] V.H.P. Louzada, N.A.M. Araújo, J.S. Andrade, and H.J. Herrmann, How to suppress undesired synchronization, Scientific Reports **2** (2012) 658.
[4] V.H.P. Louzada, F. Daolio, H.J. Herrmann, and M. Tomassini Smart Rewiring for Network Robustness, Journal of Complex Networks, DOI: 10.1093/comnet/cnt010, (to appear).
[5] A. Arenas, A. Diaz-Guilera and C.J. Pérez-Vicente, Synchronization processes in complex networks, Physica D **224** (2006) 27–34.

Title: Extension of the Relativistic Lattice Boltzmann Model for Astrophysical Applications

Researchers: F. Mohseni
M. Mendoza
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

In this project we will extend the range of applications of the current relativistic lattice Boltzmann model [Phys. Rev. Lett. **105** (2010) 14502, Phys. Rev. D **82** (2010) 105008]. To this purpose, we develop a relativistic lattice Boltzmann model capable of describing relativistic fluid dynamics at ultra-high velocities. Hence, we first build a new lattice kinetic scheme by expanding the Maxwell-Jüttner distribution function in an orthogonal basis of polynomials and applying an appropriate quadrature, providing the discrete versions of the relativistic Boltzmann equation and the equilibrium distribution. To achieve ultra-high velocities, we include a flux limiter scheme, and introduce the bulk viscosity by a suitable extension of the discrete relativistic Boltzmann equation. To the best of our knowledge, we, for the first time, simulate viscous shock waves in the highly relativistic regime. Moreover, we show that our model can also be used for near-inviscid flows even at very high velocities. As an astrophysical application, we simulate a relativistic shock wave, generated by, say, a supernova explosion, colliding with a massive interstellar cloud, e.g. molecular gas [Phys. Rev. D **87** (2013) 83003].

Moreover, we extend our model to deal with the ideal gas equation of state by modifying the equilibrium distribution function and collision operator. This helps us to study the relativistic effects on the Richtmyer-Meshkov instability. In addition, in order to investigate more astrophysical applications, we will extend the model to include gravitational fields and we will build a relativistic magnetohydrodynamics lattice Boltzmann model.

References:

[1] M. Mendoza, B.M. Boghasian, H.J. Herrmann, S. Succi, *Fast lattice Boltzmann solver for relativistic hydrodynamic*, Phys. Rev. Lett. **105** (2010) 14502
[2] M. Mendoza, B.M. Boghasian, H.J. Herrmann, S. Succi, *Derivation of the lattice Boltzmann model for relativistic hydrodynamics*, Phys. Rev. D **82** (2010) 105008
[3] F. Mohseni, M. Mendoza, S. Succi, H.J. Herrmann, *Lattice Boltzmann model for ultrarelativistic flows* , Phys. Rev. D **87** (2013) 83003

Title: Neuronal Avalanches: A Statistical Physics Approach to Spontaneous Brain Activity

Researchers: F. Lombardi
H.J. Herrmann
L. de Arcangelis

Institute: Institute for Building Materials, ETH Zürich
Group: Computational Physics for Engineering Materials, ETH Zürich

Description:

In vitro and *in vivo* studies have shown that resting cortical dynamics is characterized by neuronal avalanches, cascades of activity exhibiting a power law in the size and duration distribution, which represents a typical feature of systems acting in a critical state (Eur.Phys.J.Special Topics 205,259-301(2012)). In order to characterize the mechanisms at the origin of neuronal avalanche scaling a detailed analysis of correlations and collective neuronal mechanisms at the basis of the avalanche temporal organization is needed. This implies the analysis of experimental data and simulations of a model inspired by the biology of real neurons (Phys.Rev.Lett.108,228703(2012)).

To obtain numerical results which can be reliably compared with the experimental one, spontaneous brain activity needs to be simulated on large neuronal networks and averages on a large number of samples need to be performed. Given the high non-linearity of the system, consisting of non-linear units interacting in a non-linear way, these simulations require a considerable computational effort. At the same time, in order to detect actual spatio-temporal correlations in experimental data, one has to properly take into account the role of statistical fluctuations, which can be done by means of a recently developed method based on surrogate data techniques (Chaos, Solitons and Fractals 55,102-108(2013)). In the case of fMRI, because of the large dimensionality of the data, this method has a considerable cost in term of computational resources.

References:

[1] D. Plenz, Neuronal avalanches and coherence potentials, Eur. Phys .J. Special Topics 205, 259-301(2012)
[2] F. Lombardi, H.J. Herrmann, C. Perrone-Capano, D. Plenz and L. de Arcangelis, Balance between Excitation and Inhibition Controls the Temporal Organization of Neuronal Avalanches, Phys.Rev.Lett.108, 228703(2012)
[3] F. Lombardi, D.R. Chialvo, H.J. Herrmann and L. de Arcangelis, Strobing brain thunders: functional correlation of extreme activity events, Chaos, Solitons and Fractals, 55(2013), 102-108

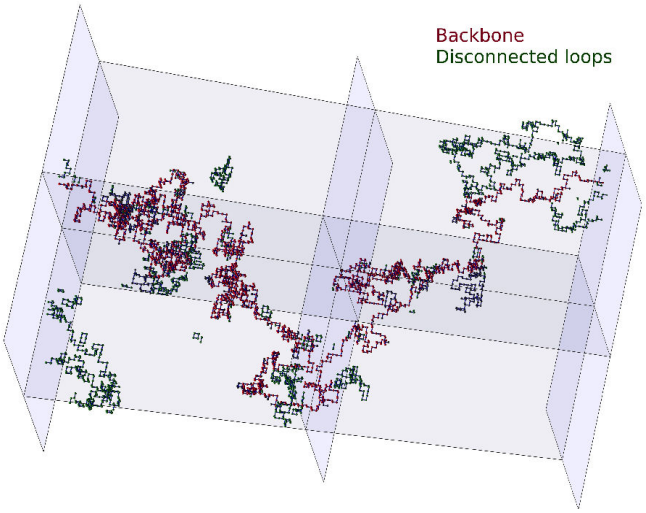
Title: How to Share Underground Reservoirs

Researchers: K.J. Schrenk
N.A.M. Araújo
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Many resources, such as oil, gas, or water, are extracted from porous soils and their exploration is often shared among different companies or nations. We show that the effective shares can be obtained by invading the porous medium simultaneously with various fluids. Partitioning a volume in two parts requires one division surface while the simultaneous boundary between three parts consists of lines. Using Monte Carlo simulations, we identify and characterize these lines, showing that they form a fractal set consisting of a single thread spanning the medium and a surrounding cloud of loops. While the spanning thread has fractal dimension 1.55(3), the set of all lines has dimension 1.69(2). The size distribution of the loops follows a power law and the evolution of the set of lines exhibits a tricritical point described by a crossover with a negative dimension at criticality.



To extract the scale-free properties of the considered fractal sets via finite-size scaling, one has to simulate large lattice sizes, such that this project poses a computational challenge. The figure shows an example of the obtained configurations for a random medium. The spanning backbone is shown in red and the loop cloud in green.

References:

[1] K.J. Schrenk, N.A.M. Araújo, and H.J. Herrmann, *How to share underground reservoirs*, Sci. Rep. **2** (2012) 751
[2] K.J. Schrenk, N.A.M. Araújo, and H.J. Herrmann, *Stacked triangular lattice: Percolation properties*, Phys. Rev. E **87** (2013) 032123

Title: Grain Scale Modelling of Triggering Mechanisms of Rainfall Induced Slope Failures

Researchers: K. Melnikov
F.K. Wittel
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Rainfall induced slope failures are a common phenomenon in mountainous regions after long periods of rains. These failures might lead to creation of landslides which are together with debris flows highly dangerous for both people and infrastructure. The understanding of the slope failures is till now no sufficient to make reliable predictions about the occurrence of these devastating events. Computational facilities of modern computers allow us to improve the understanding by performing large parameter studies that are based on numerical models of underlying processes.

The goal of this research project is to model triggering mechanisms of rainfall induced slope failures at the grain scale level. The triggering mechanisms are investigated in a discrete computational model based on the contact dynamics approach of an initially unsaturated granular material that is infiltrated by water. In order to develop a realistic simulation of this process, capillary forces due to water bridges as well as contact forces between particles are taken into account. It is planned to investigate the influence of the inhomogeneity and structure of granular material on the triggering process. Further important features for the understanding of the triggering mechanisms are the influence of initial void ratio (density) and initial water content. The simulation should help to study effects like the loss of matric suction, crack formation and formation of compaction bands.

Title: Cascading Failures in a Multiplex Network

Researchers: T. Verma
N.A.M. Araújo
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Modern society is established on pillars of infrastructure networks that are robust under ideal conditions. However, these infrastructure networks are extremely vulnerable to malicious attacks, random failure and unpredictable crowd behavior [1]. Examples of such systems are Power Grids, the Internet, Transport Mobility and Waterways among others. Even though transport networks appear to share a similar generic structure [2], they have developed independently of each other. Cities are looked upon as frontiers to accommodate for all the problems of a growing society. Transport systems when coupled together prove to be beneficial for society, simultaneously also are a roadblock towards efficient cooperation. Population density, traffic flows and other operational features play an important role in determining the robustness of these networks. Besides studying the spatial features and design issues, we will focus on an agent-based approach since nodes in a transport network can act independently and give rise to patterns that are both desirable and destructive [3].

We develop a cascading failure model to study the effects of coupling between train and airline networks and analyze the robustness of such couplings. We explore the spatial design, the transportation capacities and the mobility dynamics. We incorporate agent based dynamics and game theoretic models to understand how cooperation can be achieved in a large number of agents that are part of different coupled networks. Through this study we understand better how systems that have formed independently can cooperate and effectively provide for society and quantify the risk involved in doing so.

There is a considerable computational effort when dealing with agents that are capable of forming their own decisions irrespective of the system-wide view. The dynamics of such a system that follows a non-linear transition from the microscopic changes to the macroscopic evolution will require great deliberation and computational capacity.

References:

[1] C.M. Schneider, A Moreira, J.S. Andrade, S. Havlin, and H.J. Herrmann. *Mitigation of malicious attacks on networks*. Proceedings of the National Academy of Sciences, **10** (2011) 3838-3841
[2] C. Roth, S.M. Kang, M. Batty, and M. Barthelemy. *A long-time limit for world subway networks*. Journal of The Royal Society Interface, **9** (2012) 2540-2550
[3] J. Gómez-Gardeñes, I. Reinares, A. Arenas, and L.M. Floría. *Evolution of cooperation in multiplex networks*. Scientific reports, **2** (2012)

Title: Packing of Slender Objects in Deformable Confinements

Researchers: R. Vetter
F.K. Wittel
H.J. Herrmann

Institute/ Group: Institute for Building Materials (IfB), ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

Morphogenesis can be intriguingly complex in nature, and the variety of morphologies emerging from simple geometrical constraints is often compelling in self-organized systems. Elastic wires, for instance, coil and pack in fundamentally different ways depending on their thinness, friction and torsion when pushed into a spherical cavity [1]. However, we have carried out finite element simulations showing that also the shape of such confinement can have dramatic influence on the packing process [2]. Indeed, nature's tight spatial constraints are seldom exactly spherical or rigid. Rather, cell walls, buds and blood vessels are quite soft and may give way when acting as containers for stiffer objects. How do thin bodies crumple, fold and pack in such deformable confinements? How can the non-linear interplay between touching soft thin structures be characterized, and what morphologies emerge from such interactions? We seek to answer these questions using numerical simulations of tightly packed, mutually interacting slender objects, accompanied by experiments conducted on various materials. Soft confinement is modeled using a highly efficient thin shell finite element approach using Loop subdivision surfaces [3].

References:

[1] N. Stoop, J. Najafi, F.K. Wittel, M. Habibi, and H.J. Herrmann, *Packing of Elastic Wires in Spherical Cavities*, Phys. Rev. Lett. **106**, 214102 (2011)
[2] R. Vetter, F.K. Wittel, N. Stoop, and H.J. Herrmann, *Finite element simulation of dense wire packings*, Eur. J. Mech. A **37**, 160-171 (2013)
[3] R. Vetter, N. Stoop, T. Jenni, F.K. Wittel, and H.J. Herrmann, *Subdivision shell elements with anisotropic growth*, Int. J. Numer. Meth. Eng. **95**, 791-810 (2013)

Title: Bursts in intermittent Aeolian saltation

Researchers: M.V. Carneiro
K.R. Rasmussen
H.J. Herrmann

Institute/ Group: Institute for Building Materials, ETH Zürich
Computational Physics for Engineering Materials, ETH Zürich

Description:

We simulate aeolian sand transport using the Discrete Elements Method. Our model simulates the behavior of a disordered particle bed under the influence of a logarithmic wind profile. Close to the onset of Aeolian particle transport through saltation we find in wind tunnel experiments a regime of intermittent flux characterized by bursts of activity.A saltation model including the wind-entrainment from the turbulent fluctuations can reproduce these observations and gives insight about their origin. Bursts occurrance follow an exponential probability distribution. The time intervals between each burst decrease on average as the wind shear velocity increases until the sand flux becomes continuous. Experimentally, we verify in the wind tunnel the fluid and dynamic thresholds at $u_* = 0.17$ m/s and $u_* = 0.145$ m/s, displaying hysteresis for low wind shear velocities.

References:

[1] M.V. Carneiro, T. Pähtz, H. Herrmann, Jump at the onset of saltation, Phys. Rev. Lett. 107, 098001 (2011).

Title: Morphogenesis and fluid-structure interaction of pollen tubes

Researchers: G. Munglani
F.K. Wittel
H.J. Herrmann

Institute/ Group: Computational Physics for Engineering Materials
Institute for Building Materials, ETH Zürich

Description:

A large proportion of our food, fuel and fiber are derived from plants. Greater understanding of the fundamental morphology of plants is therefore essential for their optimal use. One of the major research areas that remains relatively poorly understood is plant growth. This process can be best characterized by studying the morphogenesis of plants at the base cellular level. Experiments have shown that these cells undergo large deformations and growth of ist cell wall, which lead to the formation of long tubular structures called pollen tubes. These highly stable tubes grow in a self-similar manner, and are used for fertilization in seed plants. Understanding the mechanics of these unusually robust structures will lead to greater insight into the morphology of the cell wall. The aim of the project is to create numerical models of this pollen tube morphogenesis. A novel finite element method using subdivision surface thin shell elements has been implemented [Int. J. Numer. Meth. Eng. **95**, 791-810 (2013)] for thin membranes. In order to effectively recreate the cell wall behavior, this implementation needs to be extended to take into account material anisotropies, non-linear material constitutive laws, as well as fluid-structure interaction with the cytoplasm. This project is in conjunction with the Institute of Plant Biology at the University of Zurich and the Institute of Robotics and Intelligent Systems group at ETH. These groups perform the experiments to measure the material parameters that we hope to validate with our computational studies [The Plant Journal, **73(4)**, 617-627 (2013)]. This collaboration will allow us to gain a better understanding of the role of turgor pressure (internal cell pressure), wall material properties, and the dynamic integration of new material into the cell wall, which in turn will give us fundamental answers about plant cell growth.

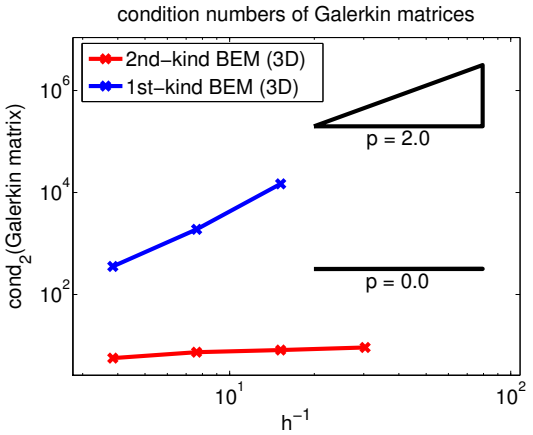
References:

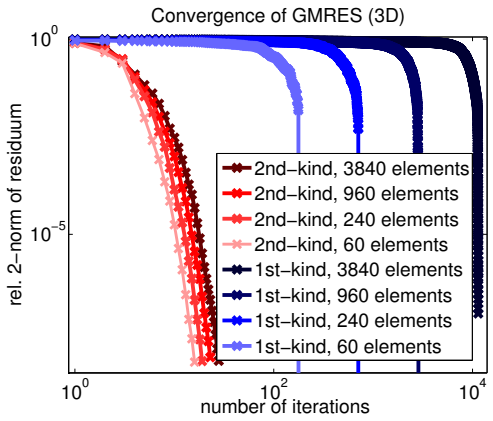
[1] R. Vetter, N. Stoop, T. Jenni, F.K. Wittel, and H.J. Herrmann, *Subdivision shell elements with anisotropic growth*, Int. J. Numer. Meth. Eng. **95**, 791-810 (2013)
[2] H. Vogler, C. Draeger, A. Weber, D. Felekis, C. Eichenberger, A. Routier-Kierzkowska, A. Boisson-Dernier, C. Ringli, B.J. Nelson, R.S. Smith, U. Grossniklaus, *The pollen tube: a soft shell with a hard core*, The Plant Journal, **73(4)**, 617-627 (2013)

Title:	Well-Conditioned Second Kind Single Trace BEM for Acoustic Scattering
Researchers:	Xavier Claeys (Paris UPMC), Prof. Ralf Hiptmair (SAM), Elke Spindler (SAM)
Institute:	Seminar for Applied Mathematics, ETH Zürich
Funding:	SNF Grant 200021_137873

Description:

We consider acoustic scattering at composite objects with Lipschitz boundary. The classical first-kind approach is ill-conditioned and no preconditioner is available. In contrast to this, a new intrinsically well-conditioned second-kind boundary element formulation has been discovered by Xavier Claeys (Paris IV) [1]. We adopt this idea and extend it by lifting the formulation from the trace spaces $H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma)$ into the space $L^2(\Gamma) \times L^2(\Gamma)$. This enables us to solely work with discontinuous ansatz functions in order to approximate the unknown boundary data.
Implementations of this new approach have been done for 2D acoustic scattering in MATLAB. A 3D implementation based on the C++ Boundary Element Template Library (BETL) by Lars Kielhorn (SAM) is ongoing work but will be available soon.
So far we did experiments for 2D and 3D scattering using piecewise constant ansatz functions for the traces. The results show competitive accuracy of the new approach, bounded condition numbers of the Galerkin matrices and superior convergence of GMRES. Several tests also indicate the absence of spurious modes in our new formulation. The below results are based on a model problem of a ball with radius $r = 0.5$ consisting of two half balls with wave numbers $\kappa_1 = 2, \kappa_2 = 3$ and wave number $\kappa_0 = 1$ in the exterior.





Publications:

[1] X. CLAEYS, *A single trace integral formulation of the second-kind for multiple subdomain scattering*, Tech. Rep. 2011-14, Seminar for Applied Mathematics, ETH Zürich, Zürich, Switzerland, 2011.

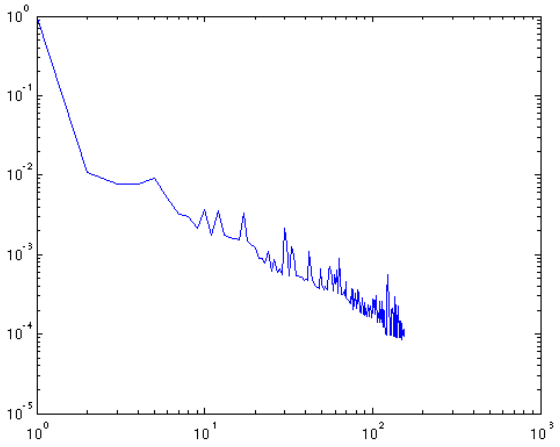
[2] X. CLAEYS, R. HIPTMAIR, AND E. SPINDLER, *A second-kind galerkin boundary element method for scattering at composite objects*, Tech. Rep. 2013-13, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013.

Title: Deterministic uncertainty quantification in Nano-Optics

Researchers: Prof. Ralf Hiptmair
Prof. Christoph Schwab
Dr. Claudia Schillings
Laura Scarabosio

Institute: Seminar for Applied Mathematics, D-MATH, ETH Zürich

Description: The aim of this project is to investigate how the shape uncertainty of nano-devices due to fabrication defects affects their optical response. In this context, a so-called deterministic approach is preferable to Monte-Carlo because of its higher convergence rates. The boundary of the device is parametrized by a Fourier expansion with random variables as coefficients; each coefficient is considered as one entry of a vector-valued random variable, with image space the product of the image spaces of the random coefficients. The shape is thus described by a high-dimensional deterministic parameter, each value corresponding to a realization of this vector-valued random variable. Considering many realizations, one can then compute statistics (mean, variance, ...) of physical quantities which are relevant to describe the response of the system upon excitation, e.g. electric field or linear functionals of it.
To select the realizations, we use an adaptive sparse Smolyak algorithm; this allows to break the so-called curse of dimensionality due to the high dimension of the deterministic parameter, thanks to convergence rates just depending on the sparsity class of the unknown (i.e. speed of decay of the coefficients in the series expansion for the shape).



Convergence of the Smolyak algorithm for the 2D Far Field computation.

References

[1] C. Schwab and C. J. Gittelson, *Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs*, Acta Numerica , 20 (2011), pp. 291–467.

[2] C. Schillings and C. Schwab, *Sparse, Adaptive Smolyak Algorithms for Bayesian Inverse Problems*, Report 2012–37, SAM, ETH Zürich, 2012.

[3] D. Xiu and D.M. Tartakovsky, *Numerical methods for differential equations in random domains*, SIAM J. Sci. Comput. 27 (3) (2005), pp. 1118–1139.

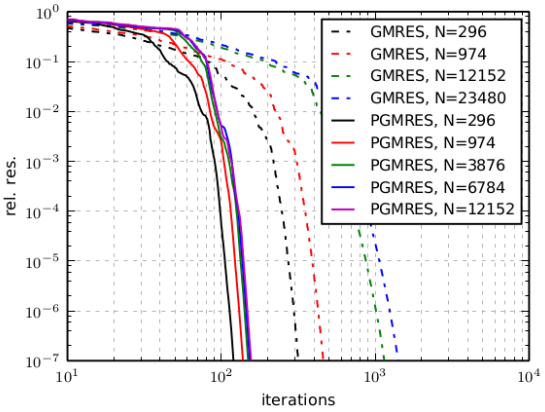
Title: Multi-Trace Boundary Element Methods

Researchers: Ralf Hiptmair (SAM ETH Zürich)
Prof. Xavier Claeys (UPMC, Paris, France),
Prof. Carlos Jerez-Hanckes (PUC, Santiago, Chile)
Simon Pintarelli (SAM, ETH Zürich)

Institute: Seminar for Applied Mathematics (SAM), D-MATH, ETH Zürich

Description: The *multi-trace approach* is a novel way to convert transmission problems for second-order partial differential equations with piecewise constant coefficients into boundary integral equations. They feature two pairs of Cauchy traces on each interface as unknowns and two variants have been devised: (i) Global multi-trace formulations (MTFs) that arise from introducing a virtual gap between sub-domains, and (ii) local MTFs obtained through introducing transmission conditions into weak boundary integral equations arising from Calderón identities.

The big benefit of MTFs is the possibility to apply parallel local Calderón preconditioning in order to obtain well-conditioned linear systems from a boundary element Galerkin discretization. This has been confirmed by numerical experiments based on the C++ boundary element library BETL (http://www.sam.math.ethz.ch/betl/). The extension of MTFs to settings with essential boundary conditions on the surface of some sub-domains has also been accomplished.



The figure shows relative decrease of Euclidean norm of the residual during GMRES iterations for a multi-trace boundary element discretization of a scalar scattering problem. The scatterer was a sphere endowed with different wave numbers ($\kappa_1 = 1$, $\kappa_2 = 2$) in its two halves. In the unbounded exterior region $\kappa_0 = 0$ was used. GMRES stands for the iteration without preconditioner, PGMRES uses local Calderón preconditioning based on dual meshes.

References

[1] X. Claeys and R. Hiptmair, *Multi-trace boundary integral formulation for acoustic scattering by composite structures*, Communications on Pure and Applied Mathematics, 66 (2013), pp. 1163–1201.

[2] X. Claeys, R. Hiptmair, and C. Jerez-Hanckes, *Multi-trace boundary integral equations*, in Direct and Inverse Problems in Wave Propagation and Applications, I. Graham, U. Langer, J. Melenk, and M. Sini, eds., vol. 14 of Radon Series on Computational and Applied Mathematics, De Gruyter, Berlin/Boston, 2013, pp. 51–100.

[3] R. Hiptmair, C. Jerez-Hanckes, J.-F. Lee, and Z. Peng, *Domain decomposition for boundary integral equations via local multi-trace formulations*, Report 2013-08, SAM, ETH Zürich, 2013.

Title Advanced yield locus models taking into account anisotropic hardening effects for the simulation of sheet metal material

Researchers: P.Peters, P. Hora

Institute / Group: Institute of virtual manufacturing

Description:

The requirements for products made from metal sheets are increasingly higher. In particular, the automotive industry is forced to cut weight of the body parts to improve fuel economy. However, this should not happen at the expense of occupant protection, design or comfort.

In order to save weight in car bodies, the usage of advanced materials like aluminum alloys and high strength steels is drastically increasing. Because the production processes for car body parts are nowadays planned virtually by means of finite element computations, constitutive models, which describe the deformation behavior of these materials.

In the framework of this project, anisotropic hardening effects are taken into account. Anisotropic hardening means the change of anisotropy after a foregoing defamation. Three anisotropic hardening effects, namely the nonproportional loading under monotonic strain paths in different directions, the Bauschinger effect as well as cross-hardening/softening effects are focused on. The model used to describe all those effects at once is a combination of an enhanced Yld2000 model [1] and the newly developed HAH model [2]. The model has been implemented and validated by means of the comparison of simulated strain distributions with measurements on a real part. The simulation results were in good agreement

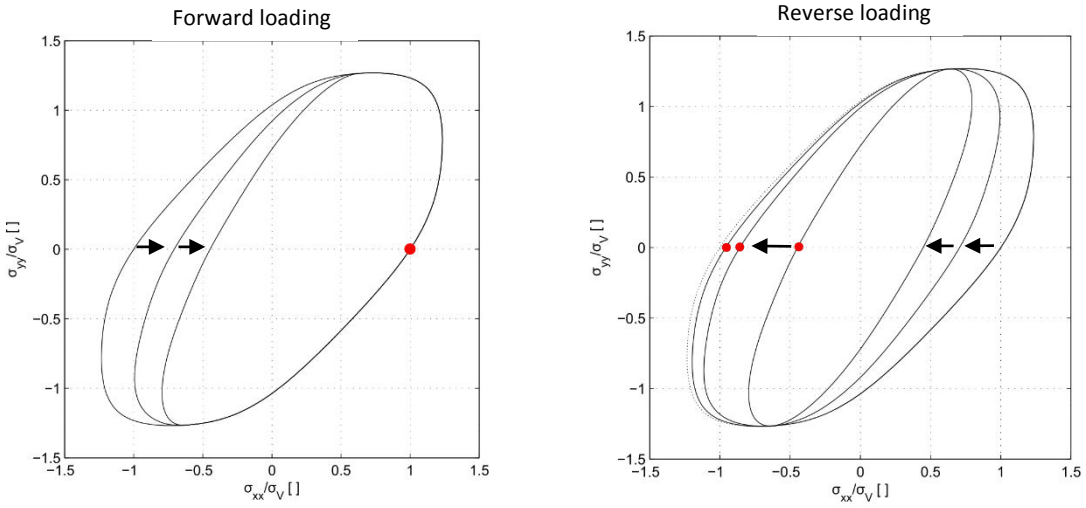


Fig. 1: yield locus distortion after forward and reverse loading using the HAH model

References

[1] Peters, P.; Manopulo, N.; Lange, C.; Hora, P.: *A strain rate dependent anisotropic hardening model and its validation through deep drawing experiments*. Int. J. Mater. Form., 2013

[2] Barlat, F.; Gracio, J.J.; Lee, M.G.; Rauch, E.F.; Vincze, G.: *An alternative to kinematic hardening in classical plasticity.* Intern. J. Plast., Vol. 27, Issue 9, pp. 1309-1327, 2011

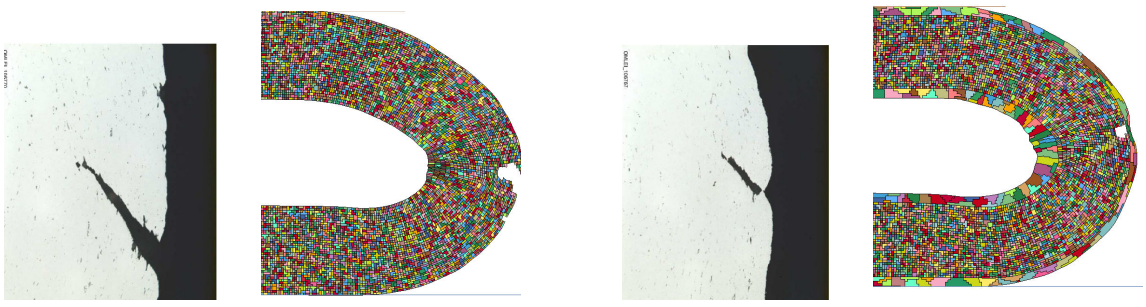
Title	Numerical Models for the Prediction of Failure for Multilayer Fusion Al-Alloy Sheets
Researchers:	M. Gorji, B. Berisha, P. Hora
Institute / Group:	Institute of Virtual Manufacturing

Description:

Demands on structural materials with better performance on strength and formability for manufacturing of lightweight materials, especially in automobile bodies, are increasing. A new technology for improving the formability of aluminum sheet, called “Fusion Technology”, has been presented by the company Novelis [1]. Three layers of aluminum alloys are cast simultaneously into one ingot. This ingot consists of a core and two outer layers. Alloys used for the two outer layers provides the additional very good formability performance, especially for bending processes.

Initiation and propagation of cracks in monolithic and Fusion aluminum alloys are investigated based on bending experiments and 2D-plane strain simulations including grain inhomogeneities. Microstructure of materials is taken into account by introducing a random grain distribution over the sheet thickness as well as a random distribution of the measured yield curve. For this purpose, a Voronoi pattern is mapped to the specimen’s geometry to specify a polycrystalline material microstructure. Afterwards, these patterns are converted into quad elements and, hence made them readable for the FE software [2].

The performed experiments and the introduced FE-Model are appropriate methods to highlight the advantages of the Fusion material, especially for bending processes. This study shows that during hemming process, crack initiates in the surface of monolithic material, whereas in Fusion material crack nucleates and propagates in the core toward the surface and is blunted by the ductile clad material.



[Left] Experiment and simulation of monolithic AA6016 material and [Right] Experiment and simulation of multilayer material Fusion; Experiments are taken from [3].

References

[1] D.J. Lloyd, M. Gallerneault, R.B. Wagstaff, The deformation of clad aluminum sheet produced by direct chill casting, Metallurgical and Materials Transactions A, 41A, 2093-2103, 2010.

[2] M. Gorji, B. Berisha, P. Hora, Numerical models for the prediction of failure for multilayer fusion Al-alloy sheets, In Proceedings of Numisheet 2014, 2014

[3] J. Timm, E. Combaz, W. Hotz, Internal report Sep. 2013: Project meeting (CTI-Project No.: 13082.1 PFIW-IW), 2013.

Title An advanced friction model for aluminium extrusion simulation

Researchers: C. Becker, P. Hora

Institute / Group: Institute of Virtual Manufacturing

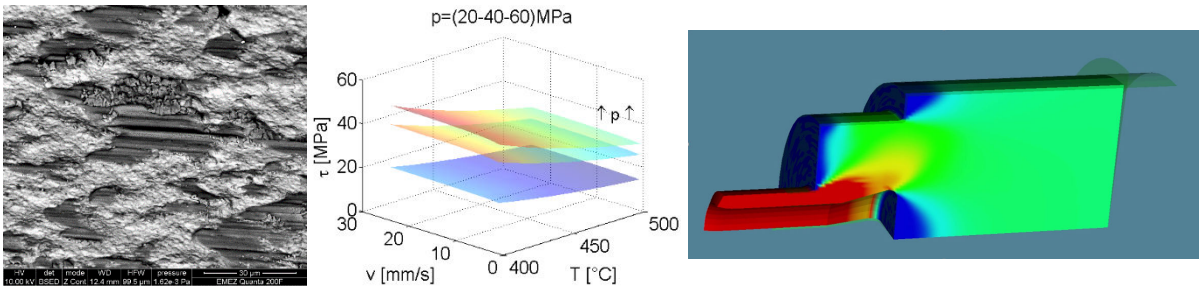
Description:

During extrusion processes complex frictional conditions in the bearing region of the extrusion die occur. Decreasing surfaces pressures in the direction of the profile flow and a non-constant temperature and velocity distribution along the die due to the forming process have an impact on friction. Standard friction models like Coulomb or Shear Friction do not take the process parameters temperature, velocity and surface pressure entirely into account.

To describe the friction conditions in a correct way, the influence of all process parameters has to be considered and an advanced friction model has to be developed and implemented to FEM software. Based on Tribo-Torsion-Test experiments a frictional model, considering the process parameters temperature, velocity and surface pressure has been proposed.

This friction model is based on the Hocket-Sherby approach with physical minimum and maximum boundary values depending on the temperature and strain rate dependent yield stress behavior of the investigated aluminium material.

$$\tau(T,v,p) = \left\{\tau_{max} - (\tau_{max} - \tau_{min}) exp\left[-m\left(\frac{p}{p_0}\right)^n\right]\right\}\left(\frac{v}{v_0}\right)^k \left(\frac{T}{T_0}\right)^l$$



Adhered surface (left), friction model (middle) and subsequent extrusion simulations (right).

A regularization method has been developed to convert the friction behavior from the experiments to a mesh-size independent friction model for simulation purpose. By using the Shear-Friction model the shear stress from above is transferred to the friction parameter $m(T,v,p)$ using experimental yield stress data and the maximum boundary strain rate $\dot{\varepsilon}_{max}$. In FEM software the shear stress is then recalculated using the friction parameter and the yield stress behavior based on the mesh-dependent strain rate. The model has been implemented to the institutes ivpFEM code Pressform3D, but can be implemented to commercial tools (Forge3D, DeForm), too. Finally a friction-sensitive extrusion experiment has been conducted to validate the accuracy of the proposed model.

References

C. Becker, P. Hora, J. Maier, S. Müller, Experimental investigations of friction carried out with the Tribo-Torsion-Test and frictional modelling, Key Engineering Materials, Vol. 585, pp 25-32, 2014.

P. Hora, C. Becker, L. Tong, J. Maier, S. Müller, Advanced frictional models for extrusion application, Key Engineering Materials, Vol. 585, pp 41-48, 2014.

Title: Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: A molecular dynamics study of cellobiose stereoisomers.

Researchers: D. Wang*
M.L. Ámundadótir*
W.F. van Gunsteren*
P.H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

It is often assumed that intramolecular hydrogen-bonding (H-bonding) exerts a significant influence on the conformational properties of aqueous (bio-)polymers. To discuss this statement, one should however distinguish between solvent-exposed and buried H-bonds, and between their respective roles in promoting stability (*i.e.* as driving force) and specificity (for which the term steering force is introduced here). In this study, the role of solvent-exposed H-bonding in carbohydrates as a driving or steering force is probed using explicit-solvent molecular dynamics (MD) simulations with local elevation umbrella sampling (LEUS) in the simple context of cellobiose stereoisomers. More specifically, four $\beta(1\rightarrow4)$-linked D-aldohexopyranose disaccharides are considered, which present a different stereochemisty of the potentially H-bonding groups neighboring the glycosidic linkage. Although the epimerization may largely alter the intramolecular *trans*-glycosidic H-bonding pattern, it is found to have only very limited influence on the Rachamachandran free-energy map of the disaccharide, a loss of intramolecular H-bonding being merely compensated for by an enhancement of the interaction with the solvent molecules. This finding suggests that solvent-exposed *trans*-glycosidic H-bonding (and in particular the $HO'_3\rightarrow O_5$ H-bond) is not the cause of the 2_1-helical secondary structure characteristic of cellooligosaccharides, but rather the opportunistic consequence of a sterically and stereoelectronically dictated conformational preference. In other words, for these compounds, solvent-exposed H-bonding appears to represent a minor (possibly adverse) conformational driving as well as steering force.

References: D. Wang, M.L. Ámundadótir, W.F. van Gunsteren and P.H. Hünenberger
Eur. Biophys. J. **42** (2013) 521-537.

Title: Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects.

Researchers: G.J. Rocklin[**]
D.L. Mobley[***]
K.A. Dill[****]
P.H. Hünenberger[*]

Institute/ Group:
[*] Laboratory of Physical Chemistry
[**] Departmentof Pharmaceutical Chemistry, University of California San Francisco, San Francisco, USA
[***] Departments of Pharmaceutical Sciences and Chemistry, University of California Irvine, Irvine, USA
[****] Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, USA

Description :

The calculation of a protein-ligand binding free energy based on molecular dynamics (MD) simulations generally relies on a thermodynamic cycle in which the ligand is alchemically inserted into the system, both in the solvated protein and free in solution. The corresponding ligand-insertion free energies are typically calculated in nanoscale computational boxes simulated under periodic boundary conditions and considering electrostatic interactions defined by a periodic lattice-sum. This is distinct from the ideal bulk situation of a system of macroscopic size simulated under non-periodic boundary conditions with Coulombic electrostatic interactions. This discrepancy results in finite-size effects, which affect primarily the charging component of the insertion free energy, are dependent on the box size, and can be large when the ligand bears a net charge, especially if the protein is charged as well. This article investigates finite-size effects on calculated charging free energies using as a test case the binding of the ligand 2-amino-5-methylthiazole (net charge +1 e) to a mutant form of yeast cytochrome c peroxidase in water. Considering different charge isoforms of the protein , either in the absence or the presence of neutralizing counter-ions, and sizes of the cubic computational box , the potentially large magnitude of finite-size effects on the raw charging free energies is demonstrated. Two correction schemes are then proposed to eliminate these effects, a numerical and an analytical one. Both schemes are based on a continuum-electrostatic analysis and require performing Poisson-Boltzmann (PB) calculations on the protein-ligand system. While the numerical scheme requires PB calculations under both non-periodic and periodic boundary conditions, the latter at the box size considered in the MD simulations, the analytical scheme only requires three non-periodic PB calculations for a given system, its dependence on the box size being analytical. The latter scheme also provides insight into the physical origin of the finite-size effects. These two schemes also encompass a correction for discrete solvent effects that persists even in the limit of infinite box sizes. Application of either scheme essentially eliminates the size dependence of the corrected charging free energies.

References: G.J. Rocklin, D.L. Mobley, K.A. Dill and P.H. Hünenberger
J. Chem. Phys. (2013), in press.

Title: Precession driven dynamo in a full sphere

Researchers: Y. Lin
P. Marti
J. Noir
A. Jackson

Institute/ Institute of Geophysics
Group: Earth and Planetary Magnetism Group

Description:

Precession is a change in the orientation of the rotation axis of a rotating body. The earth goes through one full precessional period over a duration of approximately 26000 years due to the luni-solar tidal torque acting on the Earth's equatorial bulge. From an energetic point of view, precession is a possible driving mechanism for the generation of Earth's magnetic field, the so-called geodynamo. Recent numerical simulations have shown that precession driven flows can power dynamos in spherical and spheroidal containers. But it is still an open question whether precession is responsible for the geodynamo because numerical models are far away from the Earth's parameter regime. In this project, we aim at exploring the dynamo action driven by precession in a sphere at lower Ekman numbers (the typical ratio of viscous to Coriolis forces) and lower Magnetic Prandtl numbers (the ratio of viscous and magnetic diffusivities), which is believed to be the case in the Earth's outer core. We will use a very efficient and highly parallelized spectral code developed by Marti (2012). The study will focus on the magnetic field morphology and scaling laws of precession driven dynamos to shed some lights on the role of precession in the magnetic field generation of the Earth.

References:

Marti, P., "Convection and boundary driven flows in a sphere," *PhD thesis, ETH Zurich*, (2012).

Title: Towards more realistic self-consistent dynamo action

Researchers: Andrey Sheyko
Christopher Finlay
Philippe Marti
Andrew Jackson

Institute/ Group: Earth and Planetary magnetism (EPM)
Institute of Geophysics

Description:

Earth's magnetic field is believed to be generated by self-exciting dynamo action in its fluid core. Fluid motions are driven by a heat flux at the inner core boundary and by cooling of the core, equivalent to a distributed source of heat in the entire outer core. Current simulations are limited by the extreme parameter regimes of the core — the body spins extremely rapidly but the liquid iron nevertheless has very low viscosity, equivalent to that of water. We have carried out state of the art simulations using the world-class infrastructure of CSCS that have allowed us to reduce the Ekman number, measuring the ratio of viscous to Coriolis forces, to 10^{-7}. As a result of this we have also been able to reduce the magnetic Prandtl number, measuring the rate of viscous diffusion compared to magnetic diffusion, to 0.05, again lower than ever before. We are currently analysing the results of a suite of six different simulations, analysing dissipation mechanisms, spectra and magnetic field generation physics. Of considerable interest is the agreement of these simulations with suggested scaling laws that govern the rms flow speeds and rms magnetic field strengths as a function of thermal forcing.

Title: Oscillatory and Steady Flows in a Rapidly Rotating, Longitudinally Librating Sphere

Researchers: R. Hollerbach,
Y. Lin,
J. Noir

Institute/ Group: Earth and Planetary magnetism (EPM)
Institute of Geophysics

Description:

We numerically consider the flow in a rapidly rotating sphere that additionally undergoes a slight oscillation in its rotation rate, a so-called longitudinal libration, such that its instantaneous rotation rate is given by $\Omega_0(1 + \epsilon \cos \omega t)$. The problem is defined by three parameters: the Ekman number $E = \nu/\Omega_0 R^2$ measuring the overall rotation Ω_0 (ν is the viscosity and R the sphere's radius), and the nondimensional libration frequency $\hat{\omega} = \omega/\Omega_0$ and amplitude ϵ. We focus attention on the regime $E \ll 1$, $0 < \hat{\omega} \leq 2$, $\epsilon \ll 1$ that is of greatest interest in the interiors of planets or moons. In the weakly nonlinear limit where the dependence on ϵ is treated essentially analytically, we are able to reduce the Ekman number down to 10^{-10}. As $E \to 0$, we show that the linear, oscillatory response exhibits a fractal dependence on $\hat{\omega}$, with increasingly fine peaks and troughs in the kinetic energy. The weakly nonlinear, steady response exhibits a similar structure, although there is not necessarily a 1-to-1 correspondence between peaks and troughs for the two. The full details of these solutions are currently being investigated further, and will be written up for publication in the near future.

Title: Numerical study of planetary core flows using an unstructured finite-volume code

Researchers: S. Vantieghem
A. Jackson

Institute: Institut für Geophysik
Group: Earth and Planetary Magnetism

Description:

The aim of our research is to understand planetary core flows and their ability to generate and sustain magnetic fields. In mathematical terms, this mechanism is described by the incompressible magnetohydrodynamic equations, a set of strongly coupled non-linear partial differential equations. To date, most numerical tools devoted to the solution of these equations are spectral, i.e. they assume that planetary cores are spherically symmetric in shape.
However, due to their rapid rotation, and to gravitational interactions with other celestial bodies, planetary cores are flattened and/or tidally deformed. These phenomena may have two important consequences: 1) Mechanical forces such as precession or libration are transmitted to the fluid in a much more efficient way than in a spherically symmetric core. 2) They promote the occurence of hydrodynamic instabilities and turbulence.
In order to study the effects of this departure from spherical symmetry, one has to recur to so-called local codes that allow investigating the dynamics of flows within enclosures of arbitrary shape, but come at higher computational cost. We have developed an unstructured MPI-parallel finite-volume code for the solution of the MHD equations. The parallelization is based on a domain-decomposition approach. It has been succesfully validated in the context of two different community benchmarks (Jackson et al., Marti et al.). Furthermore, we have used this code to investigate the instability triggered by multipolar deformations of the core in the presence of libration (Cébron et al.). This study addressed both the linear onset of the instability, in excellent agreement with theoretical predictions, and its non-linear saturation.

References:

Jackson, A., Sheyko, A., Marti, P., Tilgner, A., C'ebron D., Vantieghema, S., Simitev, R., Busse, F., Zhan, X., Schubert, G., Takehiro, S., Sasaki, Y., Hayashi, Y.-Y., Ribeiro, A., Nore, C., Guermond, J-L, A spherical shell numerical dynamo benchmark with pseudo vacuum magnetic boundary conditions, *Geophys. J. Int.* Accepted.

P. Marti, N. Schaeffer, R. Hollerbach, D. Cebron, C. Nore, F. Luddens, J-L. Guermond, J. Aubert, S. Takehiro, Y. Sasaki, Y. Hayashi, R. Simitev, F.H. Busse, S. Vantieghem, A. Jackson. Full sphere hydrodynamic and dynamo benchmarks. *Geophys. J. Int.* In Review.

D. Cebron, S. Vantieghem, W. Herreman. Libration driven multipolar instability. *J. Fluid Mech.* In review.

Title: Global 3-D imaging of mantle electrical conductivity from space and ground

Researchers: A. Kuvshinov
S. Koch
C. Puethe

Institute/ Group: Institute of Geophysics
Earth and Planetary Magnetism Group

Description:

We are developing frequency domain inversion schemes that aim to map the three-dimensional (3-D) mantle electrical conductivity distribution on a global scale. As applied to satellite data, two approaches are proposed. One is based on an inversion of time spectra of spherical harmonic (SH) coefficients describing the induced part of the magnetic potential. This approach has been elaborating to interpret the data from forthcoming *Swarm* multi-satellite geomagnetic mission. The second approach deals with an inversion of the responses that connect inducing and induced SH coefficients. As applied to ground (observatory) data, an inversion scheme based on the simultaneous determination of the source structure and the 3-D conductivity distribution is proposed.

References:

Kuvshinov, A, A. Semenov, 2012, Global 3-D imaging of mantle electrical conductivity based on inversion of observatory C-responses - I. An approach and its verification, Geophys. J. Int., 189, 1335–1352, doi:10.1111/j.1365-246X.2011.05349.x .

Koch S. and A. Kuvshinov, 2013. Global 3-D EM inversion of Sq variations based on simultaneous source and conductivity determination. Concept validation and resolution studies. Geophys. J. Int., doi: 10.1093/gji/ggt227

Puethe C. and A. Kuvshinov, 2013. Determination of the 3-D distribution of electrical conductivity in Earth's mantle from Swarm satellite data: Frequency domain approach based on inversion of induced coefficients. Earth, Planets, Space, in press.

Puethe C. and A. Kuvshinov, 2013. Mapping 3-D mantle electrical conductivity from space. A new 3-D inversion scheme based on analysis of matrix Q-responses. Geophys. J. Int., submitted.

Title: Towards magnetic sounding of the Earth's core by an adjoint method

Researchers: K. Li [(1)]
A. Jackson [(1)]
P. W. Livermore [(2)]

Institute/ Group: (1). Institut fur Geophysik, ETH Zurich, Switzerland
(2). School of Earth and Environment, Institute of Geophysics and Tectonics, University of Leeds, UK

Description:

Earth's magnetic field is generated and sustained by the so called geodynamo system in the core. Measurements of the geomagnetic field taken at the surface, downwards continued through the electrically insulating mantle to the core-mantle boundary (CMB), provide important constraints on the time evolution of the velocity, magnetic field and temperature anomaly in the fluid outer core. The aim of any study in data assimilation applied to the Earth's core is to produce a time-dependent model consistent with these observations. This method is broadly used in seismology and meteorology, however, its application to Earth's dynamo system just began recently. In this study, we aim to develop the the variational data assimilation for studying Earth's core fields evolution, which involves the following steps. (1). developing the variational data assimilation framework for the initial value problem of the geodynamo system (finished), (2). designing the numerically stable algorithm for computation and testing on illustrative problems (finished) (3). developing a complete variational data assimilation model of geodynamo for high performance computation, i.e., the numerical models for computing the forward and the adjoint dynamo system in parallel (ongoing) (4). studying the optimal strategy for uniquely determining the true trajectory of the geodynamo (ongoing) and (5). applying the real observed data to the system (in future).

Reference:

Li, K., Livermore, P.W. and Jackson, A. (2011) Variational data assimilation for the initial value dynamo problem, Phys. Rev. E , Vol. 84, 056321.

Title: Turbulence modeling and turbulent reactive flow

Researchers: Heng Xiao (now AP TT at Virginia Tech)
Michael Wild (now at Andritz Hydro AG)
Benjamin Zoller (now at Alstom)
Daniel Meyer
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

General description:
Most flows involving human made devices or flows in the environment are turbulent and involve a large range of length and time scales. Consequently such flows are expensive to solve numerically. To reduce the computational burden, methods are applied that solve only for a fraction of these scales but require turbulence models to incorporate effects that result from neglected scales. Most important are Reynolds-averaged Navier-Stokes (RANS) models, large eddy simulation (LES) and probability density function (PDF) methods.
Worldwide, more than 80% of the consumed energy is converted by burning fossil fuels. Therefore, improving emission rates and efficiency of combustion devices automatically has a significant impact on our environment and is of crucial importance. To achieve such improvements, however, the capability of accurately predicting the governing physical processes (which involve turbulence-reaction interaction) is essential. A modeling approach, which proved to be very general and powerful, is based on solving a joint PDF transport equation. Opposed to other approaches, such PDF methods require no model for turbulent convection and there exist no closure issues with averaging the reaction source terms.

Development of PDF solution algorithms: Compared with RANS models, PDF methods are computationally more expensive and challenging. Due to its high dimensionality, the PDF transport equation is solved by a particle method.
Currently, with the objective to address more realistic reactive flow problems, a new hybrid FV/MC solution algorithm is developed and implemented in OpenFOAM.

Turbulent combustion modeling: In terms of modeling, we focus on five topics: multi-scalar mixing of reactive scalars, non-premixed turbulent combustion with local extinction and re-ignition, premixed turbulent combustion, spray combustion and NO_x formation. In all projects we employ a hybrid particle/finite-volume PDF framework and employ scale separation ideas to describe the statistics at the unresolved fine scales.
Recent developments are a new model, where reaction and mixing are treated simultaneously, a mixing model conditional on velocities, a model for turbulence modulation due to sprays, and a PDF model for premixed combustion based on flame surface density propagation.

Hybrid LES/RANS modeling framework: While LES is a very powerful approach to model turbulent flows, it is not yet widely used in industrial workflows. This is mainly due to the

high computational cost, which is Reynolds number dependent, if wall turbulence is involved. Another difficulty is the choice of an appropriate computational grid. Motivated by these shortcomings, various hybrid LES/RANS methods have been proposed. A major challenge thereby is to determine the RANS and LES regions and to provide valid boundary conditions between them. We follow a new approach which is based on simultaneous LES and RANS simulations, which are coupled via forcing terms to ensure internal consistency. This allows to overcome most of the problems at RANS/LES interfaces, which are intrinsic in other hybrid methods.
Recently it has been demonstrated that robust and consistent coupling of an LES and a RANS simulation, which employ different grids, can be achieved.

References: [1] [7] [14] [15] [20] [21] [30] [31] [32] [33] [34] [36] [40] [44] [45] [48] [D] [F]

Title: Flow and transport in porous and fractured media

Researchers: Florian Müller
Karim Khayrat
Davide Cortinovis
Rajdeep Deb
Manav Tyagi (now at Alstom)
Hadi Hajibeygi (now AP TT at TU Delft)
Dimitrios Karvounis (now at Swiss Seismological Service, ETH)
Daniel Meyer
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

General description:
Flow and transport in porous media has many applications in earth science, energy science, and many other areas. Examples in which we are interested are oil and gas recovery, CO_2 storage in geological sub-surface formations, geothermal power exploration, and uncertainty assessment of flow and transport.

Multi-scale modeling: This is a collaboration with Dr. Seong Lee (Chevron). One of the major challenges in macroscopic simulations is the correct treatment of complex permeability distributions with strong variations and many length scales. To deal with this issue, various upscaling and multi-scale methods have been developed. In collaboration with therapeutic company Chevron we devised and developed a new multi-scale finite-volume (MSFV) algorithm, which has several advantageous properties compared with previous multi-scale methods. The MSFV method allows for very efficient studies of realistic multi-phase flow scenarios in heterogeneous porous media.
Currently it is investigated how the robustness with regard to permeability contrast and variance can be improved by an appropriate enrichment of the coarse space.

Hierarchical model of fractured reservoirs: This is an interdisciplinary collaboration with various earth scientists of ETH Zürich. In the context of geothermal power production, a modeling framework for flow and transport in fractured porous media has been created. It has proper interfaces which allow to interfere with rock mechanics and rock chemistry models. Moreover, everything is coupled with heat conduction in the rock. Due to the very large number of fractures, only the large ones are resolved. The cloud of small fractures is treated by effective permeabilities.
Recent developments include consistent corrections of transmissibility values and a demonstration study showing the benefit of using shallower (cheaper) reservoirs as preheater.

Uncertainty assessment of flow and transport in porous media: This is a collaboration with Prof. Christoph Schwab, Prof. Siddhartha Mishra (both SAM, ETHZ), Prof. Peter Ar-

benz (D-INF, ETHZ), and Prof. Hamdi Tchelepi (Stanford University). The transport of chemical substances in the subsurface is relevant in many different applications. For example, for the assessment of nuclear waste deposition sites or for the coordination of remediation actions after a contamination hazard, predictive simulation tools are required. These tools have to account for the uncertainty in the soil parameters, since measurements of the subsurface structure are typically very scarcely available. The main goal is to develop a simulation framework for tracer flow and transport that provides probabilistic information about local tracer concentration evolutions. A probability density function (PDF) method was developed that is applicable for highly heterogeneous porous media. It accounts for advective transport, pore-scale dispersion, and chemical reactions. Recently, a generalized transport model has been implemented that enables the inclusion of an arbitrary number of permeability measurements. The resulting flow and transport predictions involve less uncertainty and agree well with Monte Carlo reference data.
In addition, a multi-level Monte Carlo method has been developed, which allows to combine expensive high fidelity methods with cheap approximate solvers to achieve output statistics more efficiently.

Prediction of non-equilibrium multi-phase flow: Currently, storing CO_2 in geological subsurface formations seems to be one of the most promising feasible technologies to stabilize the CO_2 concentration in the Earth's atmosphere. The prime objective of our research is to improve our understanding of how the physics and dynamics at the pore scales is linked to the macroscopic equations, which deal with average values. Therefore we devised new model equations for various statistical moments. For closure, however, empirical information regarding Lagrangian fluid particle evolution is required, and to perform corresponding studies a pore network simulator has been developed.
It was demonstrated that in this way it is possible to account for non-equilibrium effects like hysteresis of relative permeabilities. The current effort deals with a quantitative validation of the approach.
In addition to the outlined non-equilibrium effects at the pore scale, non-equilibrium effects also result from density differences between CO_2-saturated brine and pure brine. With the non-wetting CO_2 phase typically sitting on top of the wetting brine phase, so-called gravity fingers form at the phase interface with CO_2 diffusing into the brine and increasing the brine density. The resulting finger-like structures are much smaller than the scale of observation and therefore cannot be resolved numerically. In our recent research, we have developed a scale analysis that implies opportunities for different modeling approaches. These approaches do not require the resolution of the underlying fine-scale structures.

References: [8] [9] [10] [11] [12] [14] [17] [18] [19] [24] [28] [29] [37] [38] [41] [47] [49] [B] [E]

Title: Fluid dynamics in biological systems and biomedical optics

Researchers: Adrien Lücker
Franca Schmid
Milos Sormaz (now at Alstom)
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

General description:
Fluid dynamics in biological systems is a research area, which is mainly driven by questions related to life sciences. In many cases, the background of biologists and medical doctors is not suited to investigate complex transport processes of various fluid compositions, which often are crucial for a deep understanding of the problems at hand. Therefore, bio-fluid dynamics is a very interdisciplinary field, which necessarily involves tight collaborations between life scientists, physicists and engineers.

Modeling the cerebral blood flow: This is a collaboration with Prof. Bruno Weber (University of Zürich) and Prof. Alfred Buck (University Hospital Zürich). Cerebral blood flow (CBF) can be defined as the rate of delivery of arterial (nutritive) blood to the capillary beds of a particular mass of brain tissue. CBF assumes a fundamental role in homeostasis as it ensures that the brain's spatio-temporally changing demands for glucose and oxygen are always met. Synchrotron radiation based X-ray tomographic microscopy (srXTM) is used to acquire 3D data of the cerebral angioarchitecture of macaque and rat animal models. At 700 nm resolution, the vasculature is fully resolved down to capillary level. A Vascular Graph (VG) model for CBF simulation has been developed that can operate on these vessel networks. The model allows for pressure and flow computations, as well as simulations of advective and diffusive transport within the vasculature and surrounding tissue. Moreover, an upscaling scheme has been devised and tested that significantly reduces the computational cost while preserving the accuracy of the simulations to a high degree. The method is based on replacing the discrete topology of the capillary bed by a coarser representative network of similar fluid-dynamical properties. Recently, a stochastic framework for the generation of artificial but realistic vessel networks has been devised and implemented. The large networks that can be produced in this fashion help to reduce the influence of boundary-condition inaccuracies.
Currently a realistic, large network is created with a small domain in the center, where the real sample shall be studied.

Dynamics of flow with particles (erythrocytes) in capillary networks: This is a collaboration with Dr. Dominik Obrist (Institute of Fluid Dynamics, ETH), Prof. Bruno Weber (University of Zürich) and Prof. Alfred Buck (University Hospital Zürich). The rheological influence of red blood cells (RBCs) is an active field of research. While hematocrit dependent viscosity and other phenomena are well described in the literature, the dramatic impact of RBCs on blood flow in capillary networks has not been sufficiently appreciated. A discrete simula-

tion framework was developed in which the erythrocytes are resolved. The number of RBCs in any given capillary relates linearly to the pressure drop along the vessel. At bifurcations, a simple but well confirmed rule is applied to determine the direction of RBC flow, namely that the red cells follow the path of the steepest (local) pressure gradient. The application of the bifurcation rule and RBC-dependent resistance has strong impact on the flow and transport processes within the capillary network. RBC seeded flow differs fundamentally from pure blood-plasma flow (i.e. different flow patterns rather than simple rescaling). A continuum model was devised in which the average number of red cells in a capillary segment is treated as a real number. It has the advantage of being applicable to large capillary networks, where a discrete treatment of RBCs would be computationally too expensive. The continuum model has been extended to work with vascular networks that contain both capillaries and non-capillaries. The goal was to perform blood flow simulations on large, physiological networks that explicitly take the rheological influence of red cells into account. This provides a unique opportunity to study the fascinating self-regulation of blood flow mediated by RBCs and will have enormous impact on our understanding of cerebral blood flow in general, and oxygen supply in particular.
Currently numerical experiments are performed to test a hypothesis regarding micro flow regulation at capillary level.

Biomedical Optics and Salmonella dynamics: We developed an efficient Monte Carlo algorithm and simulator for scattering of polarized light, which we employ to investigate improved methods for biomedical optics; the same simulator is also applied to study Salmonella dynamics in collaboration with Prof. Wolf-Dietrich Hardt's group (Institute of Microbiology, ETH).

References: [3] [22] [27] [42] [43] [C]

Title: Rarefied gas kinetics

Researchers: Hossein Gorji
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

General description:
It is well known that the Navier-Stokes equations become invalid for large Knudsen numbers, i.e. if the mean free path length is significant compared to the scale of observation. Such scenarios can occur e.g. in nano-scale devices, at re-entry of a space vehicle, in plasma flows and in the presence of very strong shocks.

Stochastic particle method based Fokker-Planck model: This project started as a collaboration with Prof. Manuel Torrilhon (ETH Zürich) and Prof. Stefan Heinz (University of Wyoming). A stochastic model and a solution algorithm to simulate the flow of gases, which are not in thermodynamic equilibrium was developed. For the interaction of a particle with others, statistical moments of the local ensemble have to be evaluated, but unlike in molecular dynamics simulations or DSMC, no collisions between computational particles are considered. In addition, a novel integration technique allows for time steps independent of the stochastic time scale. The stochastic model represents a Fokker-Planck equation in the kinetic description, which can be viewed as an approximation to the Boltzmann equation. This allows for a rigorous investigation of the relation between the new model and classical fluid and kinetic equations. The fluid dynamic equations of Navier-Stokes and Fourier are fully recovered for small relaxation times, while for larger values the new model extends into the kinetic regime. It could be demonstrated that the stochastic model is consistent with Navier-Stokes in that limit, but also that the results become significantly different, if the conditions for equilibrium are invalid. It could also be shown that the mass flow rate through a channel is correctly predicted as a function of the Knudsen number. By introducing a cubic non-linear drift term, the model leads to the correct Prandtl number of 2/3 for monatomic gas, which is crucial to study heat transport phenomena. Moreover, a highly accurate scheme to evolve the computational particles in velocity- and physical space is constructed. An important property of this integration scheme is that it ensures energy conservation and honors the tortuosity of particle trajectories. Especially in situations with small to moderate Knudsen numbers this allows to proceed with much larger time steps than with direct simulation Monte Carlo (DSMC), i.e. the mean collision time not necessarily has to be resolved, and thus leads to more efficient simulations.
Recent developments besides algorithmic improvements are a generalization for diatomic gas mixtures and a wall model, which can account for redistribution of internal energy modes.

References: [4] [5] [6] [14] [35]

Title: Morphing wing aerodynamics

Researchers: Vitaly Dmitriev
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

Description:
The technology of morphing wings has a high potential, since many more degrees of freedom can be employed to adapt and control a wing for different purposes in different environments. This project is a collaboration with Profs. Paolo Ermanni, Eduardo Mazza and Manfred Morari (ETH Zürich). Our role is to build predictive virtual models, which allow to design the required structure and control algorithms.
Recently it was demonstrated that it is possible to extract energy from shear flows, but unfortunately the amount is relatively small in realistic turbulent atmospheres. Currently the aerodynamics of oscillating ring wings is investigated.

References: [2] [23]

Title: Numerical schemes and solution algorithms

Researchers: Florian Müller
Halvor Lund
Jinfen Kang
Giuseppe Bonfigli (now at Andritz Hydro AG)
Patrick Jenny

Institute/ Group: Institute of Fluid Dynamics
Prof. Patrick Jenny

General description:
The numerical integration of the Navier-Stokes equations for incompressible flows has always been a central topic of numerical fluid mechanics. One possible approach consists in computing the pressure and the velocity vector at discrete grid points by solving a system of algebraic equations obtained by discretization of the momentum and continuity equations. Easy analytical manipulations provide then an independent Poisson equation for the pressure. In terms of computational efficiency, the solution of the elliptic pressure equation is the bottle neck in most cases and much effort has been made to improve the computational efficiency for this step. In terms of discretization, a Cartesian grid is favored and in order to deal with complex geometries, immersed boundary techniques have been developed. So far, however, it was not possible to preserve high spatial accuracy at immersed boundaries. Moreover, within the context of immersed boundaries, the efficient solution of the pressure Poisson equation becomes more involved, e.g. if a multi-grid technique is applied, an upscaling step is required.

Multi-scale finite-volume method for incompressible flows: The multi-scale finite-volume (MSFV) method, which we originally developed for multi-phase flow in porous media, was improved to become less sensitive to high permeability contrasts.
The ultimate goal is a robust solver with a convergence rate independent of the permeability field.

Rankine Hugoniot solver: In this finite-volume approach, viscous terms, source terms and cross flux variations (in multi-dimensions) are consistently treated as singularities at the cell centers. It has been proven that this solver is second order accurate and studies reveal that the error is approximately one order of magnitude smaller than other established methods of the same spatial order.
It is planned to extend the scheme for general unstructured grids.

Lattice Boltzmann Methods: At PSI, Jinfen Kang under the supervision of Dr. Ioannis Mantzaras, Dr. Nikolaos Prasianakis and myself is developing new Lattice Boltzmann methods for porous media applications (fuel cells).

References: [1] [14] [16] [19] [24] [25] [26] [39] [41] [46] [50]

Title: Fluid Mechanics of the Inner Ear

Researchers: Francesco Boselli, Elisabeth Edom, Bernhard Grieser, Leonhard Kleiser and Dominik Obrist

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

Description:

The inner ear hosts the senses for balance (vestibular system) and hearing (cochlea). We study the (patho-)physiology of the inner ear by numerical simulations.
Inside each semicircular canal (SCC) of the vestibular system an elastic membranous labyrinth holds a lymphatic fluid (endolymph) which develops a quasi-steady Poiseuille flow profile across the SCC lumen during head rotation. This flow leads to the perception of angular motion, and it results in eye motions that stabilize our vision.
It has been observed that, without head motion, the rare presence of a dehiscence in the bony roof of the canals can cause eye movements (nystagmus) when exposed to sound of a certain amplitude ($> 65 - 75$dB) and frequency (ca. $500 - 1000$Hz), resulting in dizziness and vertigo (Tullio phenomenon) which may originate from an induced flow in the SCCs. Sound waves propagate from the stapes not only through the cochlea, but also toward the dehiscence which serves as a third window. In interaction with the flexible membranous labyrinth we expect nonlinear effects that allow an energy transformation of highly oscillating sound into the low-frequency domain of the balance sense, causing a uni-directional second-order flow inside the SCC.
In another project we compute a particle-laden endolymph flow by the Multilayer Method of Fundamental Solutions (MFS) in combination with the Force Coupling Method (FCM) which was applied to a realistic three-dimensional SCC during head rotation. This setup enabled us to study a pathological condition where free-floating particles disturb the endolymph flow. Such a condition can cause benign paroxysmal positional vertigo (BPPV), which is arguably the most common form of vertigo in humans.
The cochlea converts oscillations of the middle ear ossicles into traveling waves of the perilymphatic fluid and of its sensory structures. These movements lead to hearing. We study the cochlear mechanics with the massively-parallel Navier-Stokes solver IMPACT developed in our group. The mechanical structures and their interaction with the fluid flow are integrated with an immersed boundary approach. We investigate a nonlinear effect of the fluid motion which is known as steady streaming. This flow might stimulate the sensory cells in the cochlea and also help to transport ions in the cochlear fluid which are crucial for the hearing. Further, we address the influence of different stimulation modes on the hearing.

References: See separate list.

Title: Prediction of Jet Flows, Aeroacoustic Jet Noise and Stability of Swirling Jets using Large-Eddy Simulation

Researchers: Stefan Bühler, Tobias Luginsland, Michael Gloor, Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

Description:

The reduction of aeroacoustic noise is an important goal in the design process of modern jet engines. To control the noise production in turbulent flow fields it is important to understand the details of the highly unsteady flow that develops in the exhaust of such engines. In order to study jet noise phenomena, high-order numerical schemes for solving the compressible Navier-Stokes equations were developed.

It is well known that the flow conditions at the jet nozzle exit have a significant impact on the radiated noise. However, little physical insight is currently available on how sound generation mechanisms are influenced by the character of the flow disturbances. We therefore study the flow development and sound emission from initially laminar, transitional and turbulent nozzle boundary layers. Sound pressure spectra obtained in the acoustic near-field agree well with experimental data. A spectral analysis of the flow field uncovers the energy transfer from turbulent hydrodynamic perturbations to acoustic waves that radiate to the far-field.

In addition to the research on isothermal single jets, we study coaxial jet flows with a heated core stream to represent realistic flow conditions in the exhaust of modern bypass jet engines. Large-scale simulations are performed to study the complex flow development in which strong velocity and temperature gradients affect the character of the noise sources. Simplified models based on linear stability theory are being developed to study the sound generation by subsonic instability waves which contribute significantly to the downstream sound radiation.

Furthermore, we investigate the stability and transitional behavior of swirling jets at medium to high swirl numbers. At sufficiently high azimuthal velocity the jets break down and a recirculation zone around the centerline develops. This flow state is governed by strong helical modes dominating the conical shear layers. We study the influence of the nozzle on the breakdown behavior of the swirling jet. The nozzle lip has an important impact on the mode selection in the flow region behind the nozzle together with the azimuthal shear layers within and outside the nozzle. The influence of physical parameters (Re, Ma, swirl number S) on the breakdown behavior is additionally investigated.

References: See separate list.

Title: Instability of the swept Hiemenz boundary layer

Researchers: Michael John, Dominik Obrist and Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

Description:

Flow instability, which leads to turbulence, is one of the canonical problems of fluid dynamics. Results for many situations were obtained by means of linear stability analysis of the laminar base flow, but often also non-linear or secondary mechanisms are important. The swept Hiemenz boundary layer (SHBL) is a model for the flow along the leading edge of swept airplane wings and it is inherently three-dimensional. Its instability is of the so-called "subcritical" type, which means that instabilities due to non-linear secondary effects occur before the flow becomes linearly unstable.
This project comprises two major topics. One is the formulation of a novel exact boundary layer formalism, suitable to better describe the laminar flow and its linear instability. This work is carried out analytically and by using stability solvers. The second topic is secondary stability analysis, which is able to explain a transition mechanism that has been observed in experiments and numerical simulations. Our tools of investigation are direct numerical simulations (DNS) with our high-fidelity in-house simulation code IMPACT.
Recently, we presented a compound formalism, which describes homogeneous flat-plate boundary layer flows. This formalism contains both the SHBL as well as the planar asymptotic suction boundary layer. The application of this formalism to the linear stability problem has unveiled the fact that the known most unstable linear modes of the two problems ("Görtler-Hämmerlin" and "Tollmien-Schlichting") are only different in that they are two different parametric realizations of the same instability mode.
Also, DNS carried out by our group have uncovered a non-linear bypass transition mechanism. The mechanism is qualitatively equal to one known from flat plate boundary layers. The effectivity of this formalism in leading to transition has been investigated and suction has been applied at the wall in order to stabilize the flow.
Together, these two observations lead us to the assumption that the instability of this complicated three-dimensional flow configuration is essentially similar to the known mechanisms for two-dimensional boundary layers - both in a linear and in a non-linear context. This work contributes to the fundamental understanding of the instabilities of homogeneous boundary layer flows. Second, the investigation of the subcritical, non-linear instability of differential equations is of high academic value and real test airplanes carry out experiments with devices that try to reduce the secondary instability. Our work might be able to contribute to the theoretical understanding of such devices.

References: None

Title: Simulation of Particle-Laden Flows

Researchers: Yvonne Reinhardt, Tarun Chadha and Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

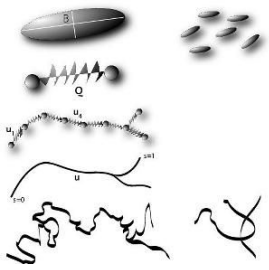
Description:

We study particle-laden flows with direct and large-eddy simulations. The motion of such flows is partially governed by its density differences, which are either due to different densities of the involved fluids or due to suspended particles. For the simulations we use a high order (typically 4^{th} or 6^{th} order) code for incompressible flows which has been developed in-house. It has high scalability with regard to the problem size on massively-parallel computers. It employs compact finite differences on staggered grids in space and a semi-implicit time integration scheme. To further increase the Reynolds number range, we use different sub-grid scale models to perform large-eddy simulations.
To model density differences (e.g. due to salinity or suspended particles), additional transport equations can be solved. In the Eulerian approach the fluid momentum equation has been implemented with an option to be solved with or without the Boussinesq assumption. Further, a Lagrangian particle approach has been implemented where transport equations are solved for each particle. The effect of transported concentrations and particles appears as an additional force term in the Navier-Stokes equations (two-way coupling). Currently, the flow solver is applied to different multiphase flows such as turbidity currents. The effect of various parameters on the front development, energy conversion and the deposit profile is studied. The Lagrangian particle description is used to gather more information on particle-settling mechanisms due to turbulence. Also the results from the Eulerian simulations are compared with those of the more accurate Lagrangian simulations, to determine the range of applicability of the computationally cheaper Eulerian approach.

In a second project we focus on the development and validation of computational methods that can be employed for industrial applications of multiphase flows. Main interest is put on abrasive water jet cutting, which has become increasingly popular for material cutting applications. The aim of this project is to model the mixing process between particles and the jet in the cutting head and the evolution of the flow in the focusing tube.
For the computations, the open-source framework of OpenFOAM is used. High Reynolds numbers and a wide range of particle loadings require the use of Reynolds-averaged Navier–Stokes (RANS) equations and turbulence models for all phases. Wall-bounded single- and two-phase flow simulations were carried out at different Reynolds numbers and particle mass loadings. The influence of mass loading is investigated and various models representing the interactions between the phases were tested to accurately capture the influence of the phases on each other. This includes correct modeling of the momentum exchange and turbulence modulation due to the influence of particles.

References: See separate list.

Title: Nuclear pore complex, actin filaments, multiscale modeling of polymers



Researchers: Prof. Martin Kröger [1]
Prof. Avraham Halperin [2]
Prof. Igal Szleifer & Ying Li [3]
Prof. Andreas Bausch [4]
Prof. Juan J. de Pablo [5]

Institutes: [1] Computational Polymer Physics, D-MATL, ETH Zürich
[2] CEA Grenoble, France
[3] Northwestern University, Chicago, CA, USA
[4] TU Munich, Germany
[5] University of Wisconsin, Madison, WI, USA

Description:

We recently focused our attention on multiscale modeling methods of polymers [1]. We investigated the internal structure of dendronized polymers at the atomistic level [2] and presented computer simulation results of fifth generation dendronized polymers. The data allowed to rate the impact of charge on internal organization [3]. The effect of charge, hydrophobicity and sequence of nucleoporins on the translocation of model particles through the nuclear pore complex was a separate topic [4]. We further addressed the following issues/questions: Application of full flow field reconstruction to a viscoelastic liquid in a 2D cross-slot channel [5]. Direct observation of the dynamics of semiflexible polymers in shear flow [6]. Synthetic regimes due to packing constraints in dendritic molecules confirmed by labelling experiments [7]. Effect of polymer solvent on the mechanical properties of entangled polymer gels: Coarse-grained molecular simulation [8]. Details available at http://www.complexfluids.ethz.ch

[1] Y. Li, B.C. Abberton, M. Kröger, W.K. Liu *Polymers* **5** (2013) 751-832.
[2] O. Bertran, B. Zhang, A.D. Schlüter, A. Halperin, M. Kröger, C. Aleman *RSC Adv.* **3** (2013) 126-140.
[3] O. Bertran, B. Zhang, A. D. Schlüter, M. Kröger, C. Aleman *J. Phys. Chem. B* **117** (2013) 6007-6017.
[4] M. Tagliazucchi, O. Peleg, M. Kröger, Y. Rabin, I. Szleifer *Proc. Natl. Acad. Sci.* **110** (2013) 3363-3368.
[5] M. Sadati, C. Luap, B. Lüthi, M. Kröger, H.C. Öttinger *J. Non-Newtonian Fluid Mech.* **192** (2013) 10-19.
[6] M.B. Harasim, B. Wunderlich, O. Peleg, M. Kröger, A.R. Bausch *Phys. Rev. Lett.* **110** (2013) 108302.
[7] B. Zhang, H. Hu, A.D. Schlüter, A. Halperin, M. Kröger *Nat. Commun.* **4** (2013) 1993.
[8] Y.R. Sliozberg, R.A. Mrozek, J.D. Schieber, M. Kröger, J.L. Lenhart, J.W. Anzelm *Polymer* **54** (2013) 2555-2564.

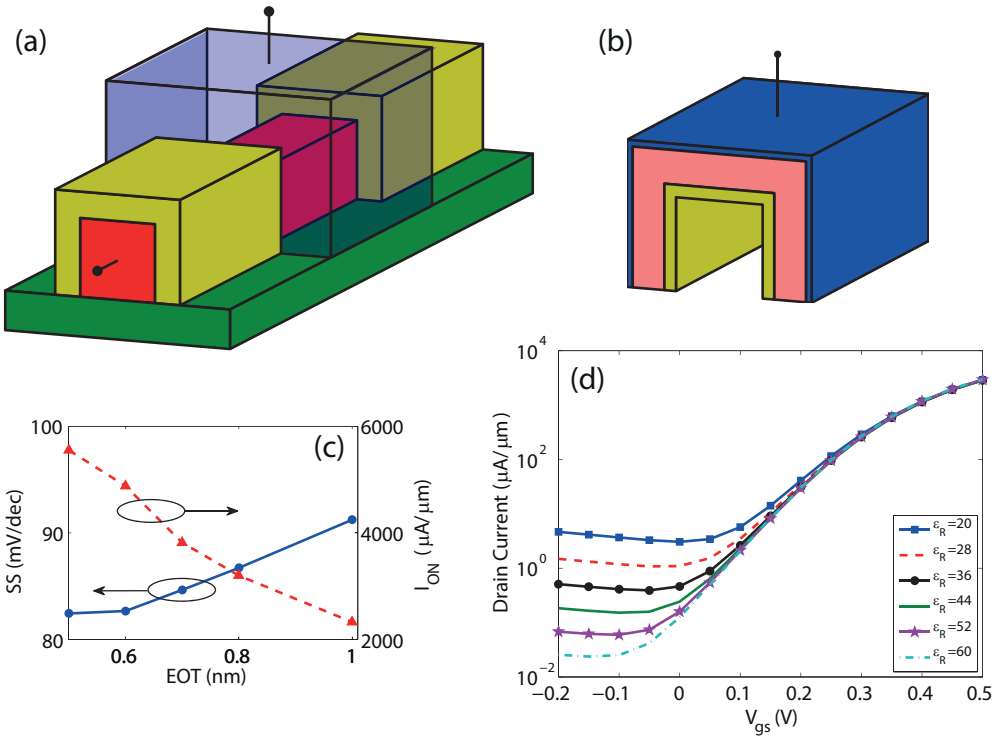
Title: Gate stack engineering in ultra-scaled Si nanowire transistors

Researchers: Mathieu Luisier
Olaf Schenk (USI Lugano)

Institute/ Group: Integrated Systems Laboratory/
Nano-TCAD Group

Description:

In this project the electrical properties of gate stacks composed of an interfacial SiO_x layer and different types of high-κ dielectrics have been theoretically investigated for potential applications as oxide layers in ultra-scaled Si nanowire field-effect transistors (NWFETs) with a gate length of 5 nm. A typical device structure and a schematic of the gate stack are shown in the figure below. As simulation tool, a three-dimensional quantum transport solver based on the effective mass approximation and including gate leakage currents has been employed. Large sparse linear systems of equations must be repeatedly solved to compute the charge and current densities of the considered transistors. First, we have analyzed how the equivalent oxide thickness (EOT) of the gate stack influences the sub-threshold slope and ON-current of the NWFETs: assuming perfectly insulating dielectrics, both quantities improve when the EOT decreases, as illustrated in the subplot (c) below. However, when gate leakage currents are turned-on and the EOT is fixed to 0.5 nm, a dielectric with a large permittivity is needed to maintain the transistor OFF-state current below 0.1 µA/µm, as indicated in subplot (d).



(a) Triple-gate nanowire field-effect transistor with a Si channel (red). (b) Schematic view of the gate stack composed of a SiO_x layer (dark yellow), a high-ϰ layer (light red), and a metallic gate contact (blue). (c) Sub-threshold slope and ON-current of a nanoscale Si transistor as a function of its equivalent oxide thickness (EOT). (d) Transfer characteristic I_d-V_{gs} for six high-ϰ dielectric layers with different permittivity values.

Reference:

M. Luisier and O. Schenk, "Gate-Stack Engineering in *n*-type Ultra-Scaled Si Nanowire Field-Effect Transistors", in press in IEEE Trans. Elec. Dev. (2013).

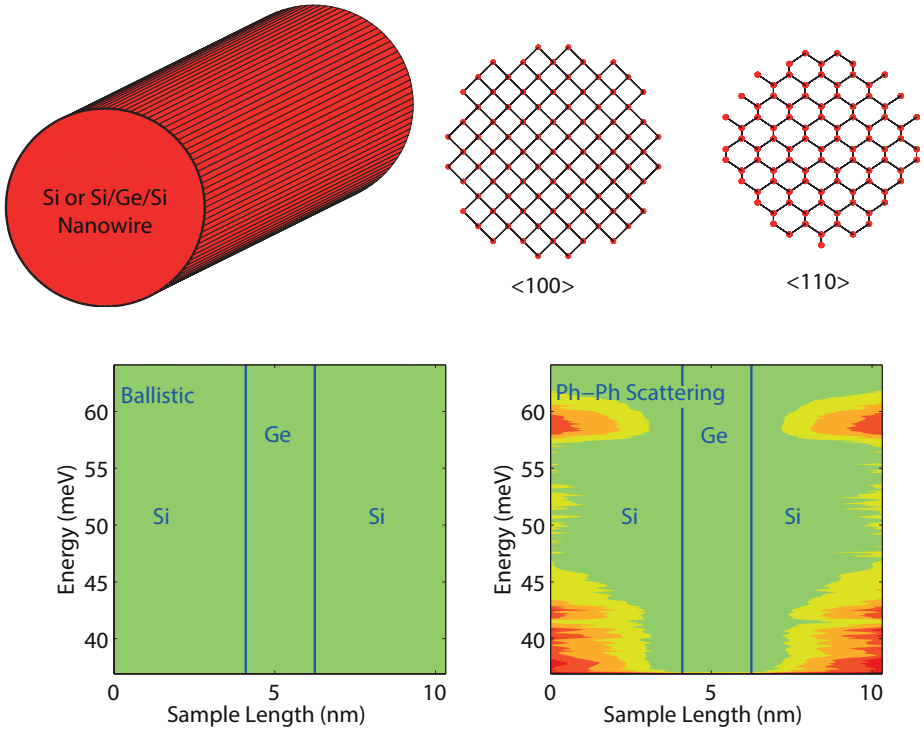
Title: Anharmonic phonon-phonon scattering in Si and Si/Ge/Si nanowires

Researchers: Mathieu Luisier

Institute/ Group: Integrated Systems Laboratory/ Nano-TCAD Group

Description:

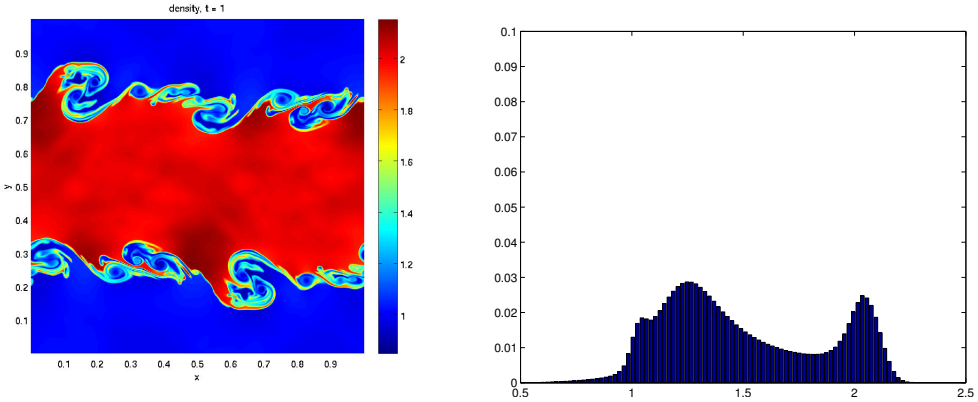
Phonon transport has been simulated in ultra-scaled nanowires in the presence of anharmonic phonon-phonon scattering. A modified valence-force-field model containing four types of bond deformation has been employed to describe the phonon bandstructure. The inclusion of five additional bond deformation potentials has allowed one to account for anharmonic effects. Phonon-phonon interactions have been introduced through inelastic scattering self-energies solved in the self-consistent Born approximation in the Non-equilibrium Green's Function formalism. Such simulations can only be performed on a supercomputer due to the heavy computational burden. After calibrating the model with experimental data, the thermal current, resistance, and conductivity of <100>-, <110>-, and <111>-oriented Si nanowires with different lengths and temperatures have been investigated in the presence of anharmonic phonon-phonon scattering and compared to their ballistic limit. It has been found that all the simulated thermal currents exhibit a peak at temperatures around 200 K if phonon scattering is turned-on while they monotonically increase when this effect is neglected. Finally, phonon transport through Si/Ge/Si nanowires has also been considered, as shown below.



(Top) Schematic view of the circular Si or Si/Ge/Si nanowires considered in this project. The cross sections corresponding to phonon transport along the <100> and <110> crystal axis are also shown. (Bottom) Spectral energy current (energy current as a function of the position along the nanowire and phonon energy) of a Si/Ge/Si nanowire in the ballistic limit of transport (left) and in the presence of anharmonic phonon-phonon scattering (right). Green indicates no current, red high current concentrations.

Reference:

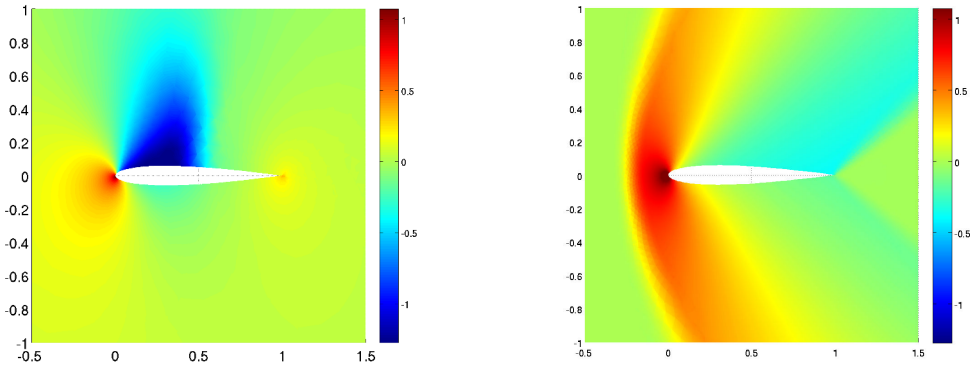
M. Luisier, "Atomistic modeling of anharmonic phonon-phonon scattering in nanowires", Phys. Rev. B 86, 245407 (2012).



Title: Efficient computation of measure valued solutions of hyperbolic conservation laws

Researchers: S. Mishra, R. Käppeli, U.S. Fjordholm (NTNU), E. Tadmor (U. Maryland).
Institute: Seminar for Applied Mathematics (SAM), ETH Zürich.
Description: Entropy solutions of systems of conservation laws may not be well-posed in several space dimensions. We extend and propose a new concept of entropy measure valued solutions and show that these solution exist and can be approximated by a set of numerical methods, satisfying some abstract criteria. Computing the measure valued solutions, amounts to computing one-point statistics in order to characterize the measure. We approximate these statistics efficiently using Monte-Carlo methods.
Publications:

1. U. S. Fjordholm, R. Käppeli, S. Mishra and E. Tadmor, Numerical approximation of entropy measure valued solutions of systems of conservation laws, in preparation, 2013.



Title: Arbitrarily high-order entropy stable space-time discontinuous galerkin (DG) schemes for systems of conservation laws.

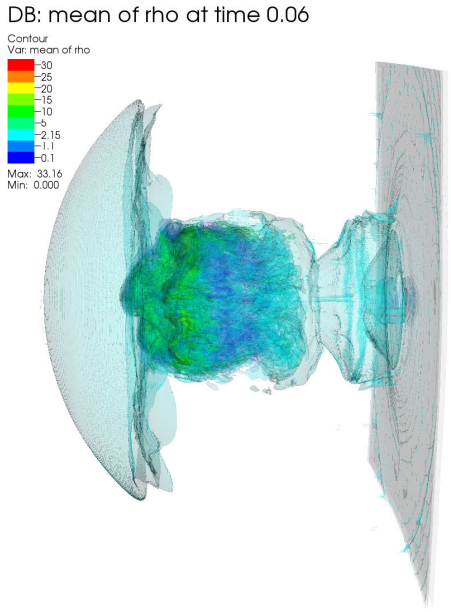
Researchers: S. Mishra, A. Hiltebrand, S. May, U. Koley (U. Wurzburg, Germany)

Institute: Seminar for Applied Mathematics (SAM), ETH Zürich.

Description: Arbitrarily high-order space-time (implicit) DG schemes for systems of conservation laws are designed using the entropy variables as the degrees of freedom. Suitable streamline diffusion and residual based shock capturing operators are need for stability. Various theoretical estimates have been obtained and implementation issues addressed. A proof of convergence to entropy measure valued solutions and the design of efficient preconditioners for improving the efficiency of the solution of resulting nonlinear systems at every time step are highlights. Future work focuses on the extensions of these schemes to the Navier-Stokes equations and goal oriented space-time adaptivity.

Publications:

1. Entropy stable shock capturing streamline diffusion space-time discontinuous Galerkin (DG) methods for systems of conservation laws, A. Hiltebrand and S. Mishra, *Numeriische Mathematik*, to appear, 2013.
2. Efficient pre conditioners for a shock capturing space-time DG method for approximating systems of conservation laws, A. Hiltebrand and S. Mishra, in preparation.

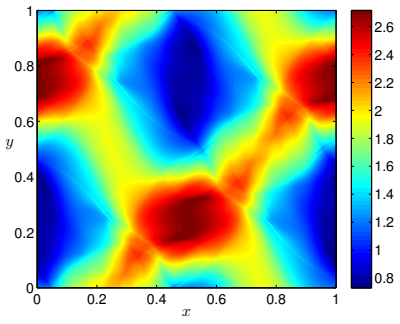


Title: Efficient numerical methods for quantifying uncertainty in hyperbolic PDEs

Researchers: S. Mishra, C. Schwab, J. Sukys, S. Tokareva and N . H. Risebro (U. Oslo)
Institute: Seminar for Applied Mathematics (SAM), ETH Zürich.
Description: Uncertainty quantification (UQ) is a grand challenge in numerical computation of conservation laws. We develop novel MLMC and stochastic collocation finite volume methods to quantify uncertainty efficiently. These methods are far superior to Monte Carlo methods as they have the same (asymptotic) complexity as a single deterministic solve. We have designed a novel load balancing strategy to efficiently parallelize the method such that is scales on massively parallel hardware platforms.
Publications:

1. S. Mishra, N.H. Risebro, Ch. Schwab and S. Tokareva Numerical solution of scalar conservation laws with random flux functions, *Research report 2012-35*, SAM ETH Zürich.

2. J . Sukys, Ch. Schwab and S. Mishra Multi-level Monte Carlo finite difference and finite volume methods for stochastic linear hyperbolic system, to appear in the MCQMC proceedings, Sydney 2012.

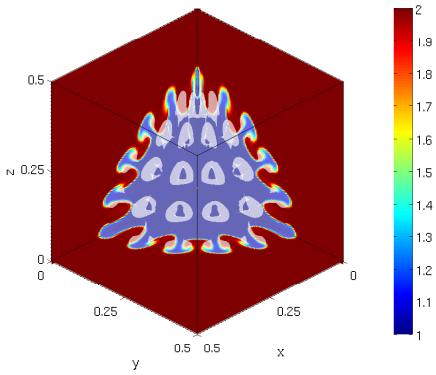


Title: Robust schemes for variational wave equations modeling liquid crystals.

Researchers: S. Mishra,N . H. Risebro F. Weber (U. Oslo), U. Koley (U. Würzburg)
Institute: Seminar for Applied Mathematics (SAM), ETH Zürich.
Description: Robust finite difference and discontinuous Galerkin finite element methods are designed to approximate nonlinear variational wave equations that arise in the modeling of nematic liquid crystals. Energy conservation or dissipation are the main design criteria and the resulting schemes are able to approximate both the conservative as well as dissipative weak solutions efficiently.
Publications:

1. S. Mishra, N. H. Risebro and F. R. Weber, Convergence of finite difference schemes for the wave equation with rough coefficients, Preprint, 2013.

2. U. Koley, S. Mishra, F. R. Weber, Robust finite difference schemes for approximating a nonlinear wave equation modeling liquid crystal, Preprint, 2013.



Title: Structure preserving schemes for systems of conservation laws.

Researchers: S. Mishra, R, Käppeli, E. Tadmor (U. Maryland)
Institute: Seminar for Applied Mathematics (SAM), ETH Zürich.
Description: In addition to the basic properties of conservation and entropy stability, one needs to design schemes for systems of hyperbolic conservation laws that satisfy other criteria, for instance, well-balancing with respect to interesting steady states, the conservation of angular momentum as well as the correct transport of vorticity which is essential for approximating rotation dominated flows.
Publications:

1. R. Käppeli and S. Mishra, Well-balanced schemes for the Euler equations with gravitation, *Research report 2013-05*, SAM ETH Zürich

2. R. Käppeli, S. Mishra and E. Tadmor, Angular momentum preserving schemes for systems of conservation laws, In preparation, 2013.

Title: Unusual bonding in solids. Understanding the chemical bonding, by means of electronic structure calculations, and its representation by the electron localization function (ELF)

Researchers: E. Cuervo-Reyes
A. Slabon
M. Kotyrba
R. Nesper

Institute/ Group: Laboratory of Inorganic Chemistry
Solid State Chemistry

Description:

This project involves a series of studies where we try to understand unusual bonding patterns, observed in recently synthesized materials. First principles calculations of electronic structure are a fundamental tool in this project. We employ the band structure representation of energy levels, and the electron localization function, in order to understand both bonding and physical properties, as well as structure-property relationships. We have found highly charged anions in a lithium rich solid phase. We are also studying novel metal-aluminium carbides (YAlC, Y_3AlC_3, and $Y_5Al_3C_4$) which show interesting electronic interplay between aluminium and carbon, beyond classical bonding patterns. Due to this they may become useful in future carbide applications.
These studies result from a close collaboration with experimentalist in our research group.

References:

[1] A. Slabon, S. Budnyk, E. Cuervo-Reyes, M. Wörle, C. Mensing, and R. Nesper, Angew. Chem. Int. Ed. **51**, 11594 (2012). "Copper silicides with the highest lithium content: Li_7CuSi_2 containing the 16-electron group $[CuSi_2]^{7-}$, and $Li_{7.3}CuSi_3$ with heterographene nets ${}^{2}_{\infty}[CuSi]^{3.3-}$".

Title: Electronic structure, chemical bonding, and magnetic interactions in Zintl phases

Researchers: E. Cuervo Reyes
A. Slabon
R. Nesper

Institute/ Group: Laboratory of Inorganic Chemistry
Solid State Chemistry

Description:

The long known Zintl phases are still a growing family. They are particularly interesting because they commonly contain divalent cations, which can be replaced by chemically equivalent Eu^{2+} magnetic centres. These are linked by bulky and very polarizable Zintl anions. Complex phase systems appear with surprising magnetic and magneto-transport properties. By means of electronic structure calculations we try to model their physical properties, and try to make sense of the experimental observations. We also employ the electron localization function (derived from the electronic wave function) in order to understand the chemical bonding in these solids, and its possible effects on the magnetic behavior.
This projects runs through a strong collaboration with experimentalist of our research group, and with other institutions such as the University of Münster, and the Max Plank Institute for Chemical Physics in Dresden.

References:

[1] A. Slabon, C. Mensing, C. Kubata, E. Cuervo-Reyes, and R. Nesper, Angew. Chem. Int. Ed. **52**, 2122 (2013). "Field-induced inversion of the magnetoresistive effect in the Zintl phase $Eu_{5+x}Mg_{18-x}Si_{13}$ ($x = 2.2$)".
[2] A. Slabon, E. Cuervo-Reyes, C. Kubata, C. Mensing, and R. Nesper, Z. Anorg. Allg. Chem. **638**, 2020 (2012). "Exploring the borders of the Zintl-Klemm concept: on the isopunctual phases $Eu_{5+x}Mg_{18-x}Ge_{13}$ and $Eu_8Mg_{16}Ge_{12}$ ".
[3] A. Slabon, E. Cuervo-Reyes, C. Kubata, M. Wörle, C. Mensing, and R. Nesper, Z. Anorg. Allg. Chem. **638**, 1417 (2012). "Synthesis, crystal, and electronic structure of the new ternary Zintl phase $Eu_{2-x}Mg_{2-y}Ge_3$ ($x = 0.1$, $y = 0.5$)".
[4] I. Schellenberg, M. Eul, C. Schwickert, C. M. Kubata, E. Cuervo-Reyes, R. Nesper, U. Vh. Rodewald, and R. Pöttgen, Z. Anorg. Allg. Chem. **638**, 1976 (2012). "The Zintl phases $Eu_3Mg_5Si_5$ and $Eu_3Mg_5Ge_5$".

Title: Computer-assisted evaluations of crystal structures of novel intermetallic compounds, and modelling of their electronic properties

Researchers: E. Cuervo-Reyes
R. Nesper

Institute/ Group: Laboratory of Inorganic Chemistry
Solid State Chemistry

Description:

A common problem when a new intermetallic compound is obtained, is the identification of atomic positions. In contrast to the random site distribution in alloys, intermetallics show preferred positions for different atomic species. However, it difficult or sometimes even impossible to fully resolve these preferences performing a crystal structure determination by X-ray diffraction. To this end, first-principles total energy calculations are very useful, since we can calculate and compare the total energy of a finite number of most likely atomic distributions. In this project, we apply this idea to recently synthesized ternary intermetallics that have large unit cells with very low symmetry.
We also investigate much more symmetric (tetragonal) ternary intermetallic compounds, and their solid solutions, trying to understand their magnetic phase diagrams.
In the first part of this project we collaborate with researchers from the Technical University of Lund.

References:

Papers in preparation

Title: First-principles materials design of functional inorganic compounds for energy applications

Researcher: Dr Riccarda Caputo

Institute: Laboratory of Inorganic Chemistry, ETH Zürich
Research groups: Prof R. Nesper and Prof M. Kovalenko

Description:

The design of innovative materials with targeted properties for specific applications go hand in hand with the acquisition of a detailed understanding of structure and electronic properties at atomic level. In parallel to experiments, the prediction of unknown or not-yet synthesized compounds, from the sole knowledge of the chemical formula, represents, in fact, one of the most fundamental challenges in materials design. Our approach to the computational design of inorganic compounds is rooted in the crystal structure prediction by using first-principles methodologies. The general issue of crystal structure prediction can be divided in two computational problems: (i) the variable composition problem: $aA^{\alpha} + bB^{\beta} \rightarrow A_aB_b^{\gamma}$; and (ii) the variable structure problem at constant composition: $A_aB_b^{\gamma} \rightarrow A_aB_b^{\delta}$. The first comprises the crystal structure determination of binary phases, solid solutions and the absorption sites in the absorption processes, together with the prediction of the relative thermodynamic (enthalpy of formation, $\Delta_f H(c)$, as a function of composition, c) and lattice (phonon calculations) stability. The second pertains the prediction of possible, in terms of relative total energies, polymorphic structures of a compound with a given stoichiometry. The methodology is based on the cluster modelling via cluster expansion, random searching and simulated annealing algorithms coupled with total energy calculations at the level of Density Functional Theory.

References:

[1] R. Caputo, *Exploring the structure-composition phase space of lithium borocarbide,* Li_xBC *for* $x \leq 1$, RSC Advances, **3**, 10230 (2013)

[2] R. Caputo, A. Kupczak, W. Sikora and A. Tekin, *Ab initio crystal structure prediction by combining symmetry analysis representations and total energy calculations. An insight into the structure of* $Mg(BH_4)_2$, Phys. Chem. Chem. Phys., **15**, 1471 (2013)

[3] M. Yarema, R. Caputo and M.V. Kovalenko, *Precision synthesis of colloidal inorganic nanocrystals using metal and metalloids amides*, Nanoscale **5**, 8398 (2013)

[4] G. Zeng, R. Caputo, D. Carriazo, L. Luo and M. Niederberger, *Tailoring two polymorphs of* $LiFePO_4$ *by efficient microwave-assisted synthesis: A combined experimental and theoretical study*, Chem. Mater. **25**, 3399 (2013)

Title: Density functional simulations of Sb-rich GeSbTe phase change alloys

Researchers: S. Gabardi[1]
S. Caravati[2]
M. Bernasconi[1]
M. Parrinello[2]

Institute/Group: [1]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125, Milano, Italy
[2]Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

We generated models of the amorphous phase of Sb-rich GeSbTe phase change alloys by quenching from the melt within density functional molecular dynamics. We considered the two compositions $Ge_1Sb_1Te_1$ and $Ge_2Sb_4Te_5$. Comparison with previous results on the most studied $Ge_2Sb_2Te_5$ allowed us to draw some conclusions on the dependence of the structural properties of the amorphous phase on the alloy composition. Vibrational and electronic properties were also scrutinized. Phonons at high frequencies above 200 cm^{-1} are localized in tetrahedra around Ge atoms in Sb-rich compounds as well as in $Ge_2Sb_2Te_5$. All compounds are semiconducting in the amorphous phase, with a band gap in the range 0.7–1.0 eV.

References: *J. Phys.: Condens. Matter, 2012,* 24, 385803
DOI:10.1088/0953-8984/24/38/385803

Title: Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives

Researchers: M. Salvalaglio[1,2]
T. Vetter[1]
F. Giberti[2]
M. Mazzotti[1]
M. Parrinello[2]

Institute/Group: [1]Institute of Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland
[2]Department of Chemistry and Applied Biosciences, ETH Zurich, Facolta di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via G. Buffi 13, 6900 Lugano Switzerland

Description:

Controlling the shape of crystals is of great practical relevance in fields like pharmacology and fine chemistry. Here we examine the paradigmatic case of urea which is known to crystallize from water with a needle-like morphology. To prevent this undesired effect, inhibitors that selectively favor or discourage the growth of specific crystal faces can be used. In urea the most relevant faces are the {001} and the {110} which are known to grow fast and slow, respectively. The relevant growth speed difference between these two crystal faces is responsible for the needle-like structure of crystals grown in water solution. To prevent this effect, additives are used to slow down the growth of one face relative to another, thus controlling the shape of the crystal. We study the growth of fast {001} and slow {110} faces in water solution and the effect of shape controlling inhibitors like biuret. Extensive sampling through molecular dynamics simulations provides a microscopic picture of the growth mechanism and of the role of the additives. We find a continuous growth mechanism on the {001} face, while the slow growing {110} face evolves through a birth and spread process, in which the rate-determining step is the formation on the surface of a two-dimensional crystalline nucleus. On the {001} face, growth inhibitors like biuret compete with urea for the adsorption on surface lattice sites; on the {110} face instead additives cannot interact specifically with surface sites and play a marginal sterical hindrance of the crystal growth. The free energies of adsorption of additives and urea are evaluated with advanced simulation methods (well-tempered metadynamics) allowing a microscopic understanding of the selective effect of additives. Based on this case study, general principles for the understanding of the anisotropic growth of molecular crystals from solutions are laid out. Our work is a step toward a rational development of novel shape-affecting additives.

References: *J. Am. Chem. Soc.*, 2012, 134 (41), pp 17221–17233
DOI**:** 10.1021/ja307408x

Title: Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives

Researchers: V. Verdolino[1]
L. Baldini[2]
F. Palazzesi[1]
M. Parrinello[1]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via G. Buffi 13, 6900 Lugano, Switzerland
[2] Dipartimento di Chimica Organica e Industriale, Università di Parma, Parco Area delle Scienze 17/A, I-43124 Parma, Italy

Description:

A combined computational and experimental study of a complex supramolecular system constituted by calix[4]arene derivatives that dimerize upon CO_2 binding is presented. The theoretical investigation includes ab initio density functional theory, molecular dynamics, and metadynamics analysis of both monomers and dimers. The ab initio calculation of the dimerization energy demonstrates the exergonic character of the process, due to the formation of a strong hydrogen bond network between ammonium and carbamate groups. The dimerization is driven by −31.1 kcal/mol in the case of the fully outward orientation of the carbamic hydrogens, while it results in a weaker process when different carbamic orientations are considered. The molecular dynamics simulations show the critical conformational degrees of freedom driving monomers and dimers toward common structures. These conformations show tilted orientations of the carbamic groups highlighting the fundamental role of dynamics in evaluating the most stable configurations. Metadynamics simulations describe, in agreement with the other computational tools, the conformational free energy surface of these calix[4]arenes defining three stable conformational families. ROESY and variable temperature ^{1}H NMR experiments are in agreement with our simulations. The presented approach aims to be the reference for investigating complex supramolecular systems.

References: *J. Phys. Chem. C*, 2012, 116 (44), pp 23441–23452
DOI: 10.1021/jp307895x

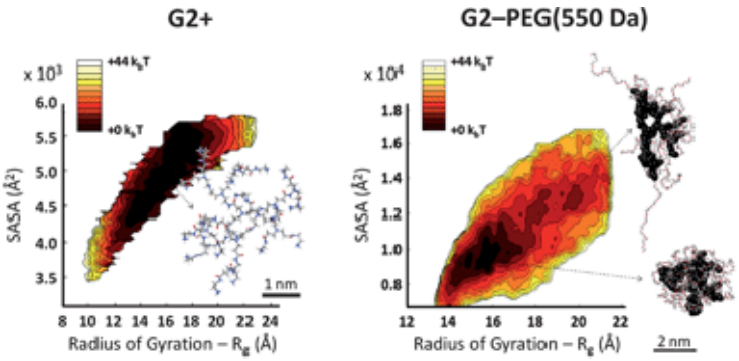
Title: Combining metadynamics simulation and experiments to characterize dendrimers in solution

Researchers: G. Pavan[1]
A. Barducci[2,3]
L. Albertazzi[4]
M. Parrinello[2,3]

Institute/Group: [1]Department of Innovative Technologies, University of Applied Science of Southern Switzerland, Galleria 2, Manno 6928, Switzerland
[2]ETH Zurich, Department of Chemistry and Applied Biosciences, c/o USI Campus, Via Giuseppe Buffi 13, Lugano 6900, Switzerland
[3]Università della Svizzera Italiana, Facoltà di Informatica, Istituto di Scienze Computazionali, Via Giuseppe Buffi 13, Lugano 6900, Switzerland
[4]Institute for Complex Molecular Systems and Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

Description:

We report a combined theoretical–experimental approach to characterize dendrimers and Polyethylene Glycol (PEG)–dendrimer hybrids in solution. Well-tempered metadynamics simulation allows for an exhaustive sampling of the conformational fluctuations in solution. In contrast to classical molecular dynamics, molecular flexibility can also be captured. Simulations are in agreement with our dynamic light scattering experiments providing a complete picture of these semi-flexible molecules in solution.



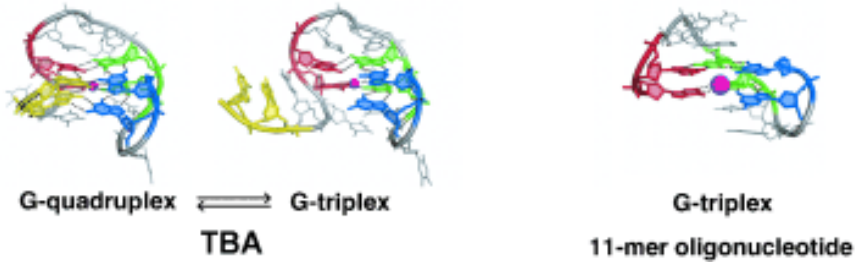
References: *Soft Matter*, 2013, 9, pp 2593-2597,
DOI: 10.1039/C3SM27706B

Title: The G-Triplex DNA

Researchers: Vittorio Limongelli[1,2,3]
Stefano De Tito[1], Linda Cerofolini[4,5]
Marco Fragai[4,5], Bruno Pagano[1]
Roberta Trotta[1,], Sandro Cosconati[1]
Luciana Marinelli[1], Ettore Novellino[1]
Ivano Bertini[4,5], Antonio Randazzo[1]
Claudio Luchinat[4,5], Michele Parrinello[2,3]

Institute/Group: [1]Department of Pharmacy, University of Naples "Federico II", Via D. Montesano, 49, 80131 Naples (Italy)
[2]Department of Chemistry and Applied Biosciences, ETH Zurich
[3]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via Giuseppe Buffi 13, 6900 Lugano (Switzerland)
[4]Magnetic Resonance Center (CERM), University of Florence, 50019 Sesto Fiorentino, Florence (Italy)
[5]Department of Chemistry, University of Florence, 50019 Sesto Fiorentino, Florence (Italy)

Description:



Triplex with a twist: Through metadynamics calculations, the thrombin binding aptamer (TBA) has been shown to adopt a stable G-triplex structural motif, in addition to the usual G-quadruplex (see scheme). An 11-mer oligonucleotide was also shown to form a stable G-triplex, whose structural and thermodynamic properties have been characterized.

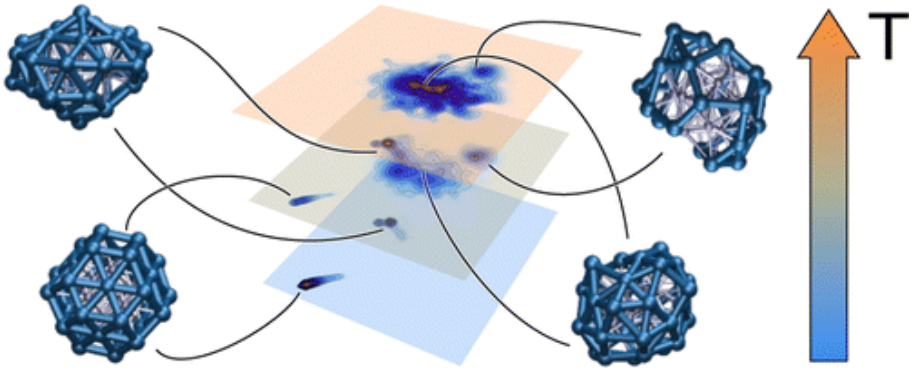
References: *Angewandte Chemie International Edition*, 2013, 52 (8), pp 2269–2273
DOI: 10.1002/anie.201206522

Title: Demonstrating the Transferability and the Descriptive Power of Sketch-Map

Researchers: M. Ceriotti[1]
G. A. Tribello[2]
M. Parrinello[2]

Institute/Group: [1]Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QZ, United Kingdom
[2]Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich and Facoltà di Informatica, Instituto di Scienza Computationali, Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900, Lugano, Switzerland

Description:



Increasingly, it is recognized that new automated forms of analysis are required to understand the high-dimensional output obtained from atomistic simulations. Recently, we introduced a new dimensionality reduction algorithm, sketch-map, that was designed specifically to work with data from molecular dynamics trajectories. In what follows, we provide more details on how this algorithm works and on how to set its parameters. We also test it on two well-studied Lennard-Jones clusters and show that the coordinates we extract using this algorithm are extremely robust. In particular, we demonstrate that the coordinates constructed for one particular Lennard-Jones cluster can be used to describe the configurations adopted by a second, different cluster and even to tell apart different phases of bulk Lennard-Jonesium.

References: *J. Chem. Theory Comput.*, 2013, 9 (3), pp 1521–1532
DOI: 10.1021/ct3010563

Title: Density functional simulations of hexagonal $Ge^2Sb^2Te^5$ at high pressure

Researchers: S. Caravati[1]
G. C. Sosso[2]
M. Bernasconi[2]
M. Parrinello[1]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana Via G. Buffi 13, 6900 Lugano Switzerland
[2]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125 Milano, Italy

Description:

We investigated the structural transformations of the hexagonal phase of $Ge_2Sb_2Te_5$ under pressure by means of *ab initio* molecular dynamics with a variable simulation cell. To overcome the enthalpy barriers between the different phases we used metadynamics techniques. We reproduced the hexagonal-to-bcc transformation under pressure found experimentally. The bcc phase retains a partial chemical order, as opposed to a second bcc phase we generated by pressuring the amorphous phase. This structural difference is suggested to be responsible for the memory effect uncovered experimentally, the bcc phase reverting to the amorphous or to the hexagonal phase upon decompression, depending on the type of precursor phase it originates from.

References: *Phys. Rev. B*, 2013, 87 (9), pp 094117-094128
DOI: 10.1103/PhysRevB.87.094117
Phys. Rev. B, 2013, 88 (1), p 019903
DOI: 10.1103/PhysRevB.88.019903

Title: Funnel metadynamics as accurate binding free-energy method

Researchers: V. Limongelli[1,3,4]
M. Bonomi[2]
M. Parrinello[3,4]

Institute/Group: [1]Department of Pharmacy, University of Naples Federico II, I-80131 Naples, Italy;
[2]Department of Bioengineering and Therapeutic Sciences, and California Institute of Quantitative Biosciences, University of California, San Francisco, CA 94158;
[3]Department of Chemistry and Applied Biosciences, Eidgenössiche Technische Hochschule (ETH), 8006 Zürich, Switzerland; and
[4]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, CH-6900 Lugano, Switzerland

Description:

A detailed description of the events ruling ligand/protein interaction and an accurate estimation of the drug affinity to its target is of great help in speeding drug discovery strategies. We have developed a metadynamics-based approach, named funnel metadynamics, that allows the ligand to enhance the sampling of the target binding sites and its solvated states. This method leads to an efficient characterization of the binding free-energy surface and an accurate calculation of the absolute protein–ligand binding free energy. We illustrate our protocol in two systems, benzamidine/trypsin and SC-558/cyclooxygenase 2. In both cases, the X-ray conformation has been found as the lowest free-energy pose, and the computed protein–ligand binding free energy in good agreement with experiments. Furthermore, funnel metadynamics unveils important information about the binding process, such as the presence of alternative binding modes and the role of waters. The results achieved at an affordable computational cost make funnel metadynamics a valuable method for drug discovery and for dealing with a variety of problems in chemistry, physics, and material science.

References: *PNAS,* 2013*,* 110 (16), pp 6358–6363
DOI: 10.1073/pnas.1303186110

Title: Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations

Researchers: E. Molina-Montes[1]
D. Donadio[2]
A. Hérnandez-Laguna[3]
M. Parrinello[4,5]
C. I. Sainz-Diaz[3]

Institute/Group: [1]Escuela Andaluza de Salud Pública, Cuesta del Observatorio 4, 18080-Granada, Spain, and Ciber Epidemiología y Salud Pública, CIBERESP, Spain
[2]Department of Chemistry, University of California at Davis, One Shields Avenue, Davis, California 95616, United States
[3]Instituto Andaluz de Ciencias de la Tierra, CSIC-Universidad de Granada, Avenida de las Palmeras, 4, 18100-Armilla, Granada, Spain
[4]Department of Chemistry and Applied Biosciences, Eidgenössiche Technische Hochschule (ETH), 8006 Zürich, Switzerland; and
[5]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, CH-6900 Lugano, Switzerland

Description:

We have investigated one of the most controversial aspects of the dehydroxylation–rehydroxylation process of dioctahedral 2:1 phyllosilicates, that is the release of water from the internal structure of the mineral. We simulate the release of water from a periodic crystal model of pyrophyllite by Car–Parrinello molecular dynamics based on Density Functional Theory. The metadynamics algorithm is employed to accelerate activated processes and compute free energy surfaces. We found that, in spite of the strong hydrogen bonds anchoring water molecules in the tetrahedral cavity, the energy barrier for water release is lower than that for the chemical formation of water molecules from the hydroxyl groups. We then conclude that water release is not the rate-limiting step of the dehydration mechanism.

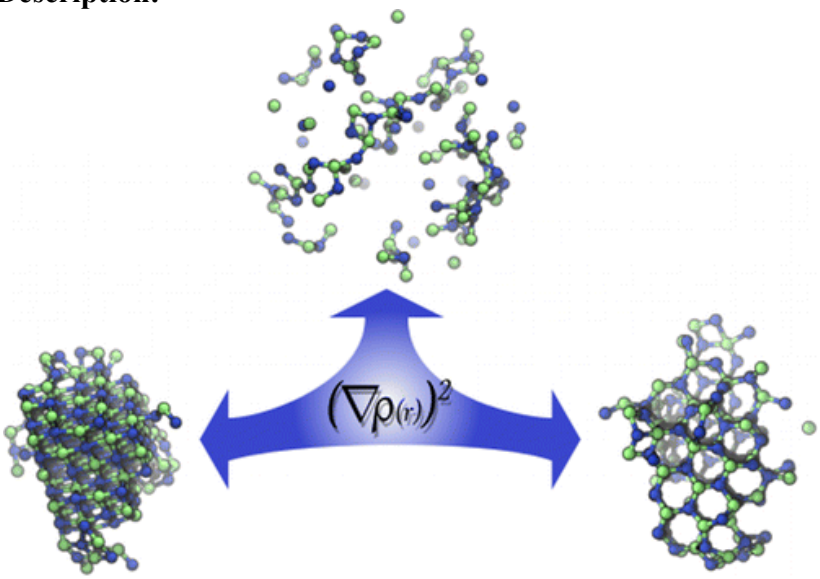
References: *J. Phys. Chem. C*, 2013, 117 (15), pp 7526–7532
DOI: 10.1021/jp310739y

Title: Transient Polymorphism in NaCl

Researchers: F. Giberti[1]
G. A. Tribello[1,2]
M. Parrinello[1]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano Switzerland
[2]Atomistic Simulation Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast, BT7 1NN, Northern Ireland, United Kingdom

Description:



We introduce a new collective variable (CV) that can be used to increase the frequency with which nucleation events are observed in biased atomistic simulations. This CV forces the ions to aggregate into clusters but does not force the ions to order themselves in a particular pattern. We perform metadynamics simulations using this CV in order to examine nucleation in a solution of sodium chloride and find that for small cluster sizes the usual bulk rocksalt structure is less stable than a structure that resembles wurtzite.

References: *J. Chem. Theory Comput.*, 2013, 9 (6), pp 2526–2530
DOI: 10.1021/ct4002027

Title: Proton transfer through the water gossamer

Researchers: A. Hassanali[1]
F. Giberti[1]
J. Cuny[2]
T. D. Kuehne[3,4]
M. Parrinello[1]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, Eidgenössiche Technische Hochschule Zurich and Università della Svizzera Italiana, CH-6900 Lugano, Switzerland;
[2]Laboratoire de Chimie et Physique Quantiques–Unité Mixte de Recherche 5626, F-31062 Toulouse, France;
[3]Institute of Physical Chemistry, University of Mainz, D-55099 Mainz, Germany; and
[4]Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, D-55128 Mainz, Germany

Description:

The diffusion of protons through water is understood within the framework of the Grotthuss mechanism, which requires that they undergo structural diffusion in a stepwise manner throughout the water network. Despite long study, this picture oversimplifies and neglects the complexity of the supramolecular structure of water. We use first-principles simulations and demonstrate that the currently accepted picture of proton diffusion is in need of revision. We show that proton and hydroxide diffusion occurs through periods of intense activity involving concerted proton hopping followed by periods of rest. The picture that emerges is that proton transfer is a multiscale and multidynamical process involving a broader distribution of pathways and timescales than currently assumed. To rationalize these phenomena, we look at the 3D water network as a distribution of closed directed rings, which reveals the presence of medium-range directional correlations in the liquid. One of the natural consequences of this feature is that both the hydronium and hydroxide ion are decorated with proton wires. These wires serve as conduits for long proton jumps over several hydrogen bonds.

References: *PNAS,* 2013, 110 (34), pp 13723-13728
DOI:10.1073/pnas.1312350110

Title: The allosteric communication pathways in KIX domain of CBP

Researchers: F. Palazzesi[1,2]
A. Barducci[3]
M. Tollinger[4]
M. Parrinello[1,2]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland
[2]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[3]Laboratoire de Biophysique Statistique, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
[4]Institute of Organic Chemistry, Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, 6020 Innsbruck, Austria

Description:

Allosteric regulation plays an important role in a myriad of biomacromolecular processes. Specifically, in a protein, the process of allostery refers to the transmission of a local perturbation, such as ligand binding, to a distant site. Decades after the discovery of this phenomenon, models built on static images of proteins are being reconsidered with the knowledge that protein dynamics plays an important role in its function. Molecular dynamics simulations are a valuable tool for studying complex biomolecular systems, providing an atomistic description of their structure and dynamics. Unfortunately, their predictive power has been limited by the complexity of the biomolecule free-energy surface and by the length of the allosteric timescale (in the order of milliseconds). In this work, we are able to probe the origins of the allosteric changes that transcription factor mixed lineage leukemia (MLL) causes to the interactions of KIX domain of CREB-binding protein (CBP) with phosphorylated kinase inducible domain (pKID), by combing all-atom molecular dynamics with enhanced sampling methods recently developed in our group. We discuss our results in relation to previous NMR studies. We also develop a general simulations protocol to study allosteric phenomena and many other biological processes that occur in the micro/milliseconds timescale.

References: *PNAS,* 2013, 110 (35), pp 14237-14242
DOI: 10.1073/pnas.1313548110

Title: Chiral, Racemic, and meso-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis

Researchers: H. H.-M Yeung[1]
M. Kosa[2]
M. Parrinello[3,4]
A. K. Cheetham[1]

Institute/Group: [1]Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge, U.K., CB2 3QZ
[2]Department of Chemistry, Bar Ilan University, Faculty of Exact Sciences, Ramat Gan IL-52900, Israel
[3]Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland
[4]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

Description:

Following our previous report of five anhydrous lithium tartrates **1**–**5** (tart = $C_4H_4O_6^{2-}$), we have synthesized and solved the single crystal structures of four new I^1O^2 inorganic–organic frameworks, all with the same chemical formula, Li_2(tart). Reactions between lithium acetate and the meso, chiral, and racemic isomers of tartaric acid in water:ethanol mixtures have yielded two new polymorphs of Li_2(*meso*-tart) in space groups $P2_1/c$ **6** and Cc **7**, racemic Li_2(d,l-tart) in $P2_1/c$ **8**, and chiral Li_2(l-tart) in $C2$ **9**. Hydrogen bond graph set analysis was adapted for use with framework materials and employed here to examine the motifs displayed by the eight anhydrous dilithium tartrates **2**–**9**. A variety of hydrogen-bonding patterns and dimensionalities are observed in this system, and the relative hydrogen bond strengths are found to correlate well with O–H stretching frequency shifts in the FTIR spectra. The relative formation energies of the framework isomers have been calculated by DFT methods, using schemes that include dispersion correction, zero-point vibrational energy, and thermal vibrations at room temperature. Although the energy ordering depends slightly on the scheme used, it is generally found to relate to the differences in crystallographic density and hydrogen bond strength rather than other structural features.

References: *Cryst. Growth Des.*, 2013, 13 (8), pp 3705–3715
DOI: 10.1021/cg400741b

Title: From Metadynamics to Dynamics

Researchers: P. Tiwary
M. Parrinello

Institute/Group: Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

Description:

Metadynamics is a commonly used and successful enhanced sampling method. By the introduction of a history dependent bias which depends on a restricted number of collective variables(CVs) it can explore complex free energy surfaces characterized by several metastable states separated by large free energy barriers. Here we extend its scope by introducing a simple yet powerful method for calculating the rates of transition between different metastable states. The method does not rely on a previous knowledge of the transition states or reaction co-ordinates, as long as CVs are known that can distinguish between the various stable minima in free energy space. We demonstrate that our method recovers the correct escape rates out of these stable states and also preserves the correct sequence of state-to-state transitions, with minimal extra computational effort needed over ordinary metadynamics. We apply the formalism to three different problems and in each case find excellent agreement with the results of long unbiased molecular dynamics runs.

References: A manuscript has been submitted to *Phys. Rev. Lett*., 2013

Title: Thermodynamical Description of a Quasi First-Order Phase-Transition from the Well-Tempered Ensemble

Researchers: O. Valsson
M. Parrinello

Institute/Group: Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

Description:

We explore the performance of the well-tempered ensemble combined with parallel tempering (PT-WTE) in obtaining a thermodynamical description of a given molecular system. We carefully explain the theoretical procedure employed to extract all the relevant thermodynamical quantities from a PT-WTE simulation. As a specific molecular system, we consider a Lennard-Jones cluster of 147 particles, which is a prototypical case of a finite-size system exhibiting a quasi first-order phase-transition, characterised by a range of temperatures where two distinct phases are thermodynamically stable and coexists. Two separate PT-WTE simulation, which investigate the thermodynamic behaviour on different levels of detail, give equally accurate description of the critical phase-coexistence region, indicating the good quality of PT-WTE results. The positive performance observed here clearly demonstrates that the PT-WTE approach is an effective option when thermodynamical properties are needed.

References: A manuscript has been submitted to *J. Chem. Theory Comput.*, 2013

Title: Controlling and Predicting Crystal Shapes: The Case of Urea

Researchers: M. Salvalaglio[1,3]
T. Vetter[3]
M. Mazzotti[3]
M. Parrinello[1,2]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland and
[2]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[3]Institute of Process Engineering, Eidgenössisch Technische Hochschule Zürich, CH-8093 Zurich, Switzerland

Description:

Understanding crystal growth from solution is crucial to control the evolution of crystal morphologies. Since the interaction of crystals with their environment occurs through their surface, their shape controls a wide variety of properties [1, 2, 3]. This is particularly important not only in nanotechnology, where shape-function relations play a key role, but also in medicine where, i.e., changing the morphology of particles allows for instance for a better targeting of cancer cells [4]. In this work we combine experiments, molecular simulations and theory to examine the morphology of urea crystals grown in di erent solutions. In order to get a rational representation of all the possible habits we introduce a Shape Diagram in which the habit dependence on the relative growth rates is illustrated. A wide portion of the habit space can be experi- mentally explored by varying the composition of the mother solution.
By doing so in the case of urea we obtain morphologies ranging from the paradigmatic needle-like habit in water to regular tetrahedra in ace- tonitrile/biuret mixtures. By combining advanced molecular simulation techniques and theory we can predict urea steady state crystal habits and their dependence on additive concentration and/or supersaturation, thus paving the way towards a rational control of the habit of crystals grown from solution.

References: A manuscript is in press**:** *Angew. Chem. Int. Ed*., 2013,

Title: 1,3,5-tris(4-bromophenyl)benzene prenucleation clusters from metadynamics

Researchers: M. Salvalaglio[1,3]
F. Giberti[1,2]
M. Parrinello[1,2]

Institute/Group: [1]Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland and
[2]Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[3]Department of Process Engineering, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland

Description:

Recent experimental evidence has shown that the nucleation of 1,3,5-tris(4- bromophenyl)benzene (3BrY) follows a two step nucleation mechanism. In this work the formation of clusters of 3BrY from homogeneous water and methanol solution is simulated using metadynamics. The local structure of 3BrY molecules in the clusters is then compared to the low temperature crystal structure of 3BrY, as well as to an alternative 3BrY high pressure crystal packing obtained through Parrinello- Rahaman Molecular Dynamics simulations. We find that the interactions between the aromatic core of 3BrY represent the main supramolecular motif observed in both the local structure of prenucleation clusters as well as in the crystal state. In the clusters these interactions lead to the presence of dimers and trimers locally arranged in crystal-like configurations.

References: A manuscript is in press**:** *Acta Crystallographica Section C*, 2013

Title: Lagrangian Coherent Structures for Design Analysis of Revolving Doors

Researchers: B. Schindler, R. Fuchs, R. Carnecky and R. Peikert

Institute/ Group: Information Technology and Education / Scientific Visualization Group

Description:

Room air flow and air exchange are important aspects for the design of energy-efficient buildings. As a result, simulations are increasingly used prior to construction to achieve an energy-efficient design. We present a visual analysis of air flow generated at building entrances, which uses a combination of revolving doors and air curtains. The resulting flow pattern is challenging because of two interacting flow patterns: On the one hand, the revolving door acts as a pump, on the other hand, the air curtain creates a layer of uniformly moving warm air between the interior of the building and the revolving door. Lagrangian coherent structures (LCS), which by definition are flow barriers, are the method of choice for visualizing the separation and recirculation behavior of warm and cold air flow. The extraction of LCS is based on the finite-time Lyapunov exponent (FTLE) and makes use of a ridge definition which is consistent with the concept of weak LCS. Both FTLE computation and ridge extraction are done in a robust and efficient way by making use of the fast Fourier transform for computing scale-space derivatives.

References: IEEE Transactions on Visualization and Computer Graphics, 18(12), pp. 2159-2168, 2012.

Title: Smart transparency for illustrative visualization of complex flow surfaces

Researchers: R. Carnecky, R. Fuchs, Y. Jang and R. Peikert

Institute/ Group: Information Technology and Education / Scientific Visualization Group

Description:

The perception of transparency and the underlying neural mechanisms have been subject to extensive research in the cognitive sciences. However, we have yet to develop visualization techniques that optimally convey the inner structure of complex transparent shapes. In this paper, we apply the findings of perception research to develop a novel illustrative rendering method that enhances surface transparency non-locally. Rendering of transparent geometry is computationally expensive since many optimizations, such as visibility culling, are not applicable and fragments have to be sorted by depth for correct blending. In order to overcome these difficulties efficiently, we propose the illustration buffer. This novel data structure combines the ideas of the A and G-buffers to store a list of all surface layers for each pixel. A set of local and nonlocal operators is then used to process these depth lists to generate the final image. Our technique is interactive on current graphics hardware and is only limited by the available graphics memory. Based on this framework, we present an efficient algorithm for a nonlocal transparency enhancement that creates expressive renderings of transparent surfaces. A controlled quantitative double blind user study shows that the presented approach improves the understanding of complex transparent surfaces significantly.

References: IEEE Transactions on Visualization and Computer Graphics, 19(5), pp. 838-851, 2013.

Title: Multiverse data-flow control

Researchers: B. Schindler, R. Fuchs, R. Peikert

Institute/ Group: Information Technology and Education / Scientific Visualization Group

Description:

In this paper, we present a data-flow system which supports comparative analysis of time-dependent data and interactive simulation steering. The system creates data on-the-fly to allow for the exploration of different parameters and the investigation of multiple scenarios. Existing data-flow architectures provide no generic approach to handle modules that perform complex temporal processing such as particle tracing or statistical analysis over time. Moreover, there is no solution to create and manage module data, which is associated with alternative scenarios. Our solution is based on generic data-flow algorithms to automate this process, enabling elaborate data-flow procedures, such as simulation, temporal integration or data aggregation over many time steps in many worlds. To hide the complexity from the user, we extend the World Lines interaction techniques to control the novel data-flow architecture. The concept of multiple, special-purpose cursors is introduced to let users intuitively navigate through time and alternative scenarios. Users specify only what they want to see, the decision which data are required is handled automatically. The concepts are explained by taking the example of the simulation and analysis of material transport in levee-breach scenarios. To strengthen the general applicability, we demonstrate the investigation of vortices in an offline-simulated dam-break data set.

References: IEEE Transactions on Visualization and Computer Graphics, 19(6), pp. 1005-1019, 2013.

Title: Tunneling and tunneling switching dynamics in phenol (C_6H_5OH) and its isotopomers from high resolution FTIR spectroscopy with synchrotron radiation in the THz range and theory

Researchers: S. Albert*
R. Prentner*
P. Lerch**
M. Quack

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Swiss Light Source, Paul-Scherrer-Institute, Villigen

Description:
Tunneling and chemical reactions by tunneling switching are reported for phenol and *ortho*-deuterophenol on the basis of high-resolution FTIR spectroscopy. Tunneling splittings are measured for the torsional motion in the ground and several vibrationally excited states of phenol. Tunneling times range from 10 ns to 1 ps, depending on excitation. For more-highly excited torsional levels in *ortho*-deuterophenol, delocalization and chemical reaction by tunneling switching is found by *ab initio* calculations and using the quasiadiabatic channel reaction path hamiltonian.

References:
S. Albert, Ph. Lerch, R. Prentner and M. Quack, Angew. Chem. Intl. Ed. (English) **52**, 346 – 349 (2013), Angew. Chem. 2013, **125**, 364 – 367 (2013)

Title: High resolution spectroscopy and first global analysis of the Tetradecad region of methane $^{12}CH_4$

Researchers: A. Nikitin[a,b]
V. Boudon[c],
C. Wenger[c],
S. Albert[d],
L. Brown[e],
S. Bauerecker[d,f],
M. Quack[d]

Institute/Group:
[a] Laboratory of Theoretical Spectroscopy, Institute of Atmospheric, Optics, Russian Academy of Sciences, 634055 Tomsk, Russia
[b] Laboratoire GSMA, UMR 6089 CNRS-Université de Reims Champagne Ardenne, Moulin de la Housse, BP 1039, Cases 16-17, F-51687 Reims Cedex 2, France
[c] Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, 9 avenue Alain Savary, B.P. 47870, F-21078 Dijon Cedex, France
[d] Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland
[e] Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, USA
[f] Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106, Germany

Description:

We present the first detailed analysis of the infrared spectrum of methane $^{12}CH_4$ in the so-called Tetradecad region from 2.1 to 1.6 μm (4760–6250 cm^{-1}). New experimental high resolution FTIR spectra at 78 K and at room temperature combined with improved theoretical modeling have allowed quantum assignments to be greatly extended in this region. A global fit of all assigned lines of $^{12}CH_4$ in the 0–6200 cm^{-1} region has been performed. In the end, 3012 line positions and 1387 intensities of 45 individual subbands of the Tetradecad were modeled up to $J = 14$. The root mean square deviations were 0.023 cm^{-1} for line positions and 13.86% for line intensities in the Tetradecad region itself. Although this analysis is still preliminary, it is already sufficient to characterize the stronger bands throughout the whole of the Tetradecad. The calculated integrated intensity of the polyad is 1.399×10^{-19} cm^{-1}/(molecule cm^{-2}) at 296 K. A "definitive" theoretical modeling of this spectral region of methane requires further work, but the present success substantially improves our understanding of methane spectroscopy as needed to interpret planetary atmospheres. Lines pertaining to three-fourths of the 60 sub-vibrational bands in this polyad have been assigned.

References:

A. Nikitin, V. Boudon, C. Wenger, S. Albert, L. Brown, S. Bauerecker, M. Quack,
Phys. Chem. Chem. Phys., **15**, 10071 – 10093 (2013)

Title: Nuclear spin symmetry conservation and relaxation in water ($^1H_2{}^{16}O$) studied by Cavity Ring-Down (CRD) spectroscopy of supersonic jets

Researchers: C. Manca Tanner
M. Quack
D. Schmidiger

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:
We report high resolution near-infrared laser spectra of water seeded in a supersonic jet expansion of argon probed by cavity ring-down spectroscopy (CRDS) in the R branch of the $2\nu_3$ band (above 7500 cm^{-1}) at several effective temperatures $T < 30$ K. Our goal is to study nuclear spin symmetry conservation and relaxation. For low mole fractions of water in the gas mixture, we obtained the lowest rotational temperatures and observed nuclear spin symmetry conservation, in agreement with theoretical expectation for inelastic collisions of isolated H_2O molecules with Ar and similar to a previous series of experiments with other small molecules in supersonic jet expansions. However, for the highest mole fractions of water, which we used ($x_{H2O} < 1.6\%$), we obtained slightly higher rotational temperatures and observed nuclear spin symmetry relaxation, which cannot be explained by the intramolecular quantum relaxation mechanism in the monomer H_2O. The nuclear spin symmetry relaxation observed is, indeed, seen to be related to the formation of water clusters at the early stage of the supersonic jet expansion. Under these conditions, two mechanisms can contribute to nuclear spin symmetry relaxation. The results are discussed in relation to claims of the stability of nuclear spin isomers of H_2O in the condensed phase and briefly also to astrophysical spectroscopy. The spectra are modelled numerically.

References:
C. Manca Tanner, M. Quack, D. Schmidiger, J. Phys. Chem. A, **117**, 10105-10118, (2013).

Title: Global Analytical Potential Energy Surface for the Electronic Ground State of NH_3 from High Level ab Initio Calculations

Researchers:
R. Marquardt[a],
K. Sagui[b]
J. Zheng[c]
W. Thiel[c]
D. Luckhaus[d]
S. Yurchenko[e]
F. Mariotti[f]
M. Quack[f]

Institute/Group:
[a] Laboratoire de Chimie Quantique, Institut de Chimie, Université de Strasbourg, France
[b] Laboratoire de Chimie Theorique, Université de Marne-la-Vallée
[c] Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
[d] Chemistry Department, University of British Columbia, Canada
[e] Department of Physics and Astronomy, University College London, UK
[f] Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, Switzerland

Description:
The analytical, full-dimensional, and global representation of the potential energy surface of NH_3 in the lowest adiabatic electronic state developed previously [1] is improved by adjustment of parameters to an enlarged set of electronic energies from ab initio calculations using the coupled cluster method with single and double substitutions and a perturbative treatment of connected triple excitations (CCSD(T)) and the method of multireference configuration interaction (MRCI). CCSD(T) data were obtained from an extrapolation of aug-cc-pVXZ results to the basis set limit (CBS), as described in a previous work [2]; they cover the region around the NH_3 equilibrium structures up to 20 000 hc cm^{-1}. MRCI energies were computed using the aug-cc-pVQZ basis to describe both low lying singlet dissociation channels. Adjustment was performed simultaneously to energies obtained from the different ab initio methods using a merging strategy that includes 10 000 geometries at the CCSD(T) level and 500 geometries at the MRCI level. Characteristic features of this improved representation are NH_3 equilibrium geometry $r^{eq}(NH_3) \approx 101.28$ pm, $\alpha^{eq}(NH_3) \approx 107.03°$, the inversion barrier at $r^{inv}(NH_3) \approx 99.88$ pm and 1774 hc cm^{-1} above the NH_3 minimum, and dissociation channel energies 41 051 hc cm^{-1} (for $NH_3 \rightarrow (^2B_2)NH_2 + (^2S_{1/2})H$) and 38 450 hc cm^{-1} (for $NH_3 \rightarrow (^3\Sigma^-)NH + (^1\Sigma_g^+)H_2$); the average agreement between calculated and experimental vibrational line positions is 11 cm^{-1} for $^{14}N^1H_3$ in the spectral region up to 5000 cm^{-1}. A survey of our current knowledge on the vibrational spectroscopy of ammonia and its isotopomers is also given [3].

References:
[1] R. Marquardt, K. Sagui, W. Klopper and M. Quack, J. Phys. Chem. B **109**, 8439 – 8451 (2005)

[2] S. N. Yurchenko, J. Zheng, H. Lin, P. Jensen, W. Thiel, J. Chem. Phys. **123**, 134308 (2005).
[3] R. Marquardt, K. Sagui, J. Zheng, W. Thiel, D. Luckhaus, S. Yurchenko, F. Mariotti, M. Quack, J. Phys. Chem. A, **117**, 7502-7522 (2013).

Title: Physical Chemistry and Chemical Physics: A Survey

Researchers: R. Marquardt[a]
M. Quack[b]

Institute/Group: [a] Laboratoire de Chimie Quantique, Institut de Chimie, Université de Strasbourg, France
[b] Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:
We provide a survey of physical chemistry as represented in the database, including theoretical and numerical aspects.

References:

R. Marquardt, M. Quack, Physical Chemistry and Chemical Physics: A Survey
in "Chemistry, Molecular Sciences and Chemical Engineering", Online reference Database Elsevier (2013), CMSE:5402, doi: 10.1016/B978-0-12-409547-2.05402-0

Title: Synchrotron based rotationally resolved high resolution FTIR spectroscopy of azulene and the unidentified infrared bands of astronomy

Researchers: S. Albert*
P. Lerch**
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Swiss Light Source, Paul-Scherrer-Institute, Villigen

Description:
We report the first rotationally resolved high resolution infrared spectrum of azulene using synchrotron FTIR spectroscopy including a rovibrational analysis of the out-of-plane fundamental ν_{44}. Comparisons of azulene, naphthalene, indole and biphenyl infrared bands lead to coincidences with UIR bands at 12.8 μm with naphthalene and at 13.55 and 14.6 μm with biphenyl bands, but excluding azulene as a strong absorber. The spectra are simulated numerically.

References:
S. Albert, P. Lerch and M. Quack, ChemPhysChem. **14**, 3204 - 3208 (2013).

Title: Methane line parameters in the HITRAN2012 database,

Researchers: L.R. Brown[a], K. Sung[a], D.C. Benner[b], V.M. Devi[b], V. Boudon[c], T. Gabard[c], C. Wenger[c], A. Campargue[d], O. Leshchishina[d], S. Kassi[d], D. Mondelain[d], L. Wang[d], L. Daumont[e], L. Régalia[e], M. Rey[e], X. Thomas[e], Vl. G. Tyuterev[e], O.M. Lyulin[f], A.V. Nikitin[f], H.M. Niederer[g], S. Albert[g], S. Bauerecker[g], M. Quack[g], J.J. O'Brien[h], I.E. Gordon[i], L.S. Rothman[i], H. Sasada[j], A. Coustenis[k], M.A.H. Smith[l], T. Carrington Jr.[m], X.-G. Wang[m], A.W. Mantz[n], P.T. Spickler[o]

Institute/Group: [a] Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA
[b] Department of Physics, The College of William and Mary, Williamsburg, VA 23187, USA
[c] Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS–Université de Bourgogne, Dijon, France
[d] Université Grenoble 1/CNRS, UMR5588 LIPhy, Grenoble, France
[e] Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 7331, Université de Reims, 4. U.F.R. Sciences, 51687 Reims, France
[f] Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, SB RAS, Tomsk, Russia
[g] Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland
[h] Department of Chemistry and Biochemistry, University of Missouri, St. Louis, MO, USA
[i] Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge, MA, USA
[j] Department of Physics, Faculty of Science and Technology, Keio University, 3-14-1, Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan
[k] Laboratoire d'Etudes Spatiales et d'Instrumentation en Astrophysique (LESIA), Observatoire de Paris, CNRS, UPMC Univ. Paris 06, Univ. Paris-Diderot, 5, 92195 Meudon, France
[l] Science Directorate, NASA Langley Research Center, Hampton, VA 23681, USA
[m] Chemistry Department, Queen's University, Kingston, Ontario, Canada K7L 3N6
[n] Department of Physics, Astronomy and Geophysics, Connecticut College, 270 Mohegan Avenue, New London, CT, USA
[o] Department of Physics, Bridgewater College, Bridgewater, VA, USA

Description:

The compilation of methane molecular line parameters was updated to include new global analyses and measurements for $^{12}CH_4$, $^{13}CH_4$ and $^{12}CH_3D$. Over 70% of the methane parameters in HITRAN2008 were replaced; existing parameters retained were the microwave lines and the Dyad of $^{13}CH_4$ near 7 μm and ν_6 of $^{13}CH_3D$ near 8.7 μm, $^{12}CH_3D$ (7–4076 cm^{-1}), hot bands of $^{12}CH_4$ (1887–3370 cm^{-1}) and normal sample CH_4 (4800–5550 cm^{-1} and 8000–9200 cm^{-1}). With a minimum intensity at 296 K in units of cm^{-1}/(molecule cm^{-2}) set to 10^{-37}

for the far-IR and 10^{-29} for the mid- and near-IR, the methane database increased from 290,091 lines in HITRAN2008 to 468,013 lines, and three-fourths of these involved the main isotopologue. For $^{12}CH_4$ and $^{13}CH_4$, bands from the ground state were revised up to 4800 cm^{-1}. For the first time, $^{13}CH_4$ and $^{12}CH_3D$ line parameters near 2.3 μm were included. Above 5550 cm^{-1}, the new compilation was based on empirical measurements. Prior laboratory results were replaced with extensive new measurements using FTIR (5550–5852 cm^{-1}), differential absorption spectroscopy (DAS) and Cavity Ring Down Spectroscopy (CRDS) (5852–7912 cm^{-1}). Ground state *J* values for nearly half of the measured lines in this range were obtained, either by confirming quantum assignments of analyses or by using spectra at 80 and 296 K. Finally, over 11,000 measured positions, intensities and empirical lower state energies (obtained using cold CH_4) were also added for the first time between 10,923 and 11,502 cm^{-1}. Available pressure broadening measurements from HITRAN2008 were transferred into the new compilation, but 99% of the lines were given crudely-estimated coefficients. New measured intensities and broadening coefficients were included for far-IR transitions, and high accuracy line positions were inserted for the stronger P, Q and R branch transitions of ν_3 at 3.3 μm and $2\nu_3$ at 1.66 μm.

References:

L. R. Brown, K. Sung, D. C. Benner, V. M. Devi, V. Boudon, T. Gabard, C. Wenger, A. Campargue, O. Leshchishina, S. Kassi, D. Mondelain, L. Wang, L. Daumont, L. Régalia, M. Rey, X. Thomas, V. G. Tyuterev, O. M. Lyulin, A. V. Nikitin, H. M. Niederer, S. Albert, S. Bauerecker, M. Quack, J. J. O'Brien, I. E. Gordon, L. S. Rothman, H. Sasada, A. Coustenis, M. A. H. Smith, T. Carrington Jr, X. G. Wang, A. W. Mantz, P. T. Spickler
Methane line parameters in the HITRAN2012 database,
J. Quant. Spectrosc. Radiat. Transfer **130**, 201–219 (2013).

Title: Analysis of the rovibrational spectrum of $^{13}CH_4$ in the Octad range

Researchers: H.-M. Niederer[a]
X.-G. Wang[b]
T. Carrington Jr[b*]
S. Albert[a]
S. Bauerecker[a,c]
V. Boudon[d]
M. Quack[a*]

Institute/Group:
[a] Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland
[b] Chemistry Department, Queen's University, Kingston, Ontario, K7L 3N6, Canada
[c] Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, Germany
[d] Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, Dijon, France
* authors for correspondence

Description:

We have measured the infrared spectrum of methane $^{13}CH_4$ from 1100 cm^{-1} (33 THz), below the fundamental range, to about 12000 cm^{-1} (360 THz) in the high overtone region at temperatures ranging from 80 K to 300 K by high resolution Fourier transform infrared (FTIR) spectroscopy. With instrumental bandwidths between 0.0027 cm^{-1} (80 MHz) and 0.01 cm^{-1} (300 MHz) this provides close to Doppler-limited spectra, using the Zürich prototype spectrometer (ZP2001, Bruker 125HR) combined with a multipath collisional cooling cell. Using perturbation theory and an accurate empirically adjusted potential we have computed ro-vibrational energy levels of $^{13}CH_4$ and $^{12}CH_4$ in the same energy range. Exploiting the synergy between theory and experiment, we analyze here specifically the experimental spectra in the Octad range (~3700–4700 cm^{-1}, or 110 to 140 THz), using the theoretical results to guide the fitting of parameters of a Dijon effective Hamiltonian theory. With the aid of the theoretical results it is possible to analyse the Octad of $^{13}CH_4$ with much less effort than without such information. In the end 1144 purely experimental line positions were fitted with root mean square deviations $d_{rms} \leqslant 2.6 \times 10^{-3}$ cm^{-1} (5548 data including theoretical results, with similar d_{rms}).

References:

1. H.-M. Niederer, X.-G. Wang, T. Carrington Jr, S. Albert, S. Bauerecker, V. Boudon, M. Quack, J. Mol. Spectrosc. **291**, 33-47 (2013).

Title: On Biomolecular Homochirality as a Quasi-Fossil of the Evolution of Life

Researchers: M. Quack

Institute/Group: Physical Chemistry, ETH Zürich

Description:
We provide a review of the title subject including also theoretical and experimental aspects of molecular parity violation.

References:
M. Quack, Adv. Chem. Phys. (2013) in press

Title: On the Emergence of Simple Structures in Complex Phenomena: Concepts and Some Numerical Examples

Researchers: M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:
We provide a conceptual review of the title subject, illustrated with numerical examples.

References:
M. Quack, Adv. Chem. Phys. (2013) in press

Title: Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts

Researchers: Thomas Weymuth
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

Within an inverse design approach applied to a nitrogen-fixation catalyst we discuss options for calculating "jacket" potentials that fulfill a purpose-oriented target requirement. As a target requirement we choose the vanishing geometric gradients on all atoms of a subsystem consisting of a metal center binding the small molecule to be activated — in our case dinitrogen. The additional potential can be represented within a full quantum model or by a sequence of approximations of which a field of electrostatic point charges is the simplest. In order to analyze the feasibility of this approach, we dissect a known dinitrogen-fixating complex and analyze its ligand environment expressed by the "jacket" potential. It is discussed how this ligand-by-potential replacement can be generalized for future applications that eventually allow us to find a competitive synthetic nitrogen-fixation transition metal complex. It can be expected that such a ligand-by-potential replacement approach will be applicable to any type of host-guest chemical process.

References: T. Weymuth, M. Reiher, *MRS Proceedings*, **2013**, *1524*, DOI: 10.1557/opl.2012.1764.

Title: Entanglement Measures for Single- and Multireference Correlation Effects

Researchers: Katharina Boguslawski
Pawel Tecmer
Örs Legeza
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

Electron correlation effects are essential for an accurate ab initio description of molecules. A quantitative a priori knowledge of the single- or multireference nature of electronic structures as well as of the dominant contributions to the correlation energy can facilitate the decision regarding the optimum quantum chemical method of choice. We proposed concepts from quantum information theory as orbital entanglement measures that allowed us to evaluate the single- and multireference character of any molecular structure in a given orbital basis set. By studying these measures, possible artifacts of small active spaces can be detected.

References: K. Boguslawski, P. Tecmer, Ö. Legeza, M. Reiher, *J. Phys. Chem. Lett.*, **2012**, *3*, 3129–3135.

Title: Real-time Quantum Chemistry

Researchers: Moritz P. Haag
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

Significant progress in the development of efficient and fast algorithms for quantum chemical calculations has been made in the past two decades. The main focus has always been the desire to be able to treat ever larger molecules or molecular assemblies—especially linear and sublinear scaling techniques are devoted to the accomplishment of this goal. However, as many chemical reactions are rather local, they usually involve only a limited number of atoms so that models of about 200 (or even less) atoms embedded in a suitable environment are sufficient to study their mechanisms. Thus, the system size does not need to be enlarged, but remains constant for reactions of this type that can be described by less than 200 atoms. The question then arises how fast one can obtain the quantum chemical results. This question is not directly answered by linear-scaling techniques. In fact, ideas such as haptic quantum chemistry (HQC) or interactive quantum chemistry require an immediate provision of quantum chemical information which demands the calculation of data in "real time". In this perspective, we aim at a definition of real-time quantum chemistry, explore its realm and eventually discuss applications in the field of HQC. For the latter, we elaborate whether a direct approach is possible by virtue of real-time quantum chemistry.

References: M. P. Haag, M. Reiher, *Int. J. Quantum Chem.*, **2013**, *113*, 8.

Title: Optimized unrestricted Kohn–Sham potentials from ab initio spin densities

Researchers: Katharina Boguslawski
Christoph R. Jacob
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

The reconstruction of the exchange–correlation potential from accurate ab initio electron densities can provide insights into the limitations of the currently available approximate functionals and provide guidance for devising improved approximations for density-functional theory (DFT). For open-shell systems, the spin density is introduced as an additional fundamental variable in spin-DFT. Here, we consider the reconstruction of the corresponding unrestricted Kohn–Sham (KS) potentials from accurate ab initio spin densities. In particular, we investigate whether it is possible to reconstruct the spin exchange–correlation potential, which determines the spin density in unrestricted KS-DFT, despite the numerical difficulties inherent to the optimization of potentials with finite orbital basis sets. We find that the recently developed scheme for unambiguously singling out an optimal optimized potential can provide such spin potentials accurately. This was demonstrated for two test cases, the lithium atom and the dioxygen molecule, and target (spin) densities from full configuration interaction and complete active space self-consistent field calculations, respectively.

References: K. Boguslawski, C. R. Jacob, M. Reiher, *J. Chem. Phys.*, **2013**, *138*, 044111.

Title: Analysis of differences in oxygen sensitivity of Fe-S clusters.

Researchers: Marta K. Bruska
Martin T. Stiebritz
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

Many but not all iron–sulphur clusters in metalloproteins are known to be sensitive to molecular oxygen with dramatic consequences for their biological function. We performed a systematic quantum chemical investigation that sheds light on the differences in oxygen sensitivity depending on charge and spin states of these clusters as well as on their spatial fixation by the enzyme's scaffold. We find that significant structural distortions are required to bind O_2 exothermically to $[Fe_2S_2]$ and $[Fe_3S_4]$ clusters, while only small conformational changes allow for the thermodynamically favorable coordination of molecular oxygen to $[Fe_4S_4]$ cubanes and $[Fe_4S_3]$ clusters.

References: Marta K. Bruska, Martin T. Stiebritz, M. Reiher, *Dalton Trans.*, **2013**, *42*, 8729.

Title: Kinetic Modeling of Hydrogen Conversion at [Fe] Hydrogenase Active-Site Models

Researchers: Arndt R. Finkelmann
Martin T. Stiebritz
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

By means of density functional theory we investigated the catalytic cycle of active-site model complexes of [Fe] hydrogenase and studied how ligand substitutions in the first coordination sphere of the reactive Fe center affect the free-energy surface of the whole reaction pathway. Interestingly, dispersion interactions between the active site and the hydride acceptor MPT^+ render the hydride transfer step less endergonic and lower its barrier. Substitution of CO by CN^-, which resembles [FeFe] hydrogenase-like coordination, inverts the elementary steps H^- transfer and H_2 cleavage. A simplified kinetic model revealed the specifics of the interplay between active-site composition and catalysis. Apparently, the catalytic efficiency of [Fe] hydrogenase can be attributed to a flat energy profile throughout the catalytic cycle. Intermediates that are too stable, as they occur e.g. when one CO ligand is substituted by CN^-, significantly slow down the turnover rate of the enzyme. The catalytic activity of the wild-type form of the active-site model could, however, be enhanced by a PH_3 ligand substitution of the CO ligand.

References: Arndt R. Finkelmann, Martin T. Stiebritz, M. Reiher, *J. Phys. Chem. B*, **2013**, *117*, 4806–4817.

Title: Elimination of the Translational Kinetic Energy Contamination in pre-Born–Oppenheimer Calculations

Researchers: Benjamin Simmen
Edit Mátyus
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

We present a simple strategy for the elimination of the translational kinetic energy contamination of the total energy in pre-Born–Oppenheimer calculations carried out in laboratory-fixed Cartesian coordinates (LFCCs). The simple expressions for the coordinates and the operators are thus preserved throughout the calculations, while the mathematical form and the parametrisation of the basis functions are chosen so that the translational and rotational invariances are respected. The basis functions are constructed using explicitly correlated Gaussian functions (ECGs) and the global vector representation.
First, we observe that it is not possible to parametrise the ECGs so that the system is at rest in LFCCs and at the same time the basis functions are square-integrable with a non-vanishing norm. Then, we work out a practical strategy to circumvent this problem by making use of the properties of the linear transformation between the LFCCs and translationally invariant and center-of-mass Cartesian coordinates as well as the transformation properties of the corresponding basis function parameter matrices.
By exploiting these formal mathematical relationships we can identify and separate the translational contamination terms in the matrix representation of the kinetic energy operator in the LFCC formalism.
We present numerical examples for the translational contamination and its elimination for the two lowest rotational energy levels of the singlet hydrogen molecule, corresponding to para- and ortho-H_2, respectively, treated as four-particle quantum systems.

References: B. Simmen, E. Mátyus, M. Reiher, *Mol. Phys.*, **2013**, *111*, 2086.

Title: An efficient implementation of two-component relativistic exact-decoupling methods for large molecules

Researchers: Daoling Peng
Nils Middendorf
Florian Weigend
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

An efficient algorithm for one- and two-component relativistic exact-decoupling calculations was presented. Spin-orbit coupling was thus taken into account for the evaluation of relativistically transformed (one-electron) Hamiltonian. As the relativistic decoupling transformation has to be evaluated with primitive functions, the construction of the relativistic one-electron Hamiltonian becomes the bottleneck of the whole calculation for large molecules. For the established exact-decoupling protocols, a minimal matrix operation count was established and discussed in detail. Furthermore, a local DLU scheme was applied to accelerate this step. With the new implementation two-component relativistic density functional calculations can be performed invoking the resolution-of-identity density-fitting approximation and (Abelian as well as non-Abelian) point group symmetry to accelerate both the exact-decoupling and the two-electron part. The capability of the implementation was illustrated at the example of silver clusters with up to 309 atoms, for which the cohesive energy is calculated and extrapolated to the bulk.

References: D. Peng, N. Middendorf, F. Weigend, M. Reiher,, *J. Chem. Phys.*, **2013**, *138*, 184105.

Title: Orbital Entanglement in Bond-Formation Processes

Researchers: Katharina Boguslawski
Pawel Tecmer
Gergely Barcza
Örs Legeza
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

The accurate calculation of the (differential) correlation energy is central to the quantum chemical description of bond-formation and bond-dissociation processes. In order to estimate the quality of single- and multireference approaches for this purpose, various diagnostic tools have been developed. One- and two-orbital-based entanglement measures provide quantitative means for the assessment and classification of electron correlation effects among molecular orbitals. The dissociation behavior of some prototypical diatomic molecules features all types of correlation effects relevant for chemical bonding. The entanglement analysis is convenient to dissect these electron correlation effects and to provide a conceptual understanding of bond-forming and bond-breaking processes from the point of view of quantum information theory.

References: K. Boguslawski, P. Tecmer, G. Barcza, Ö. Legeza, M. Reiher, *J. Chem. Theory Comput.*, **2013**, *9*, 2959–2973.

Title: Electric-Field Effects on the [FeFe]-Hydrogenase Active Site

Researchers: Arndt R. Finkelmann
Martin T. Stiebritz
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

The effect of a homogeneous electric field — as exerted by the protein environment and by an electrode potential — on the reactivity of the active site of [FeFe] hydrogenases was unravelled by density functional theory calculations. The electric field of the protein was derived from the electrostatic potential which was obtained by numerical solution of the Poisson-Boltzmann equation for the crystal structure of [FeFe] hydrogenase from *Clostridium pasteurianum*.

References: Arndt R. Finkelmann, Martin T. Stiebritz, M. Reiher, *Chem. Commun.*, **2013**, *49*, 8099-8101.

Title: Structure–Property Relationships of Fe_4S_4 Clusters

Researchers: Maike Bergeler
Martin T. Stiebritz
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

In this theoretical study, the sensitivity of Fe_4S_4 cluster properties, such as potential energy, spin coupling, adiabatic detachment energy, inner-sphere reorganization energy, and reactivity, to structural distortions is investigated. $[Fe_4S_4(SH)_4]^{3-/2-/1-}$ model clusters anchored by fixed hydrogen atoms are compared with Fe_4S_4 clusters coordinated by ethyl thiolates with fixations according to cysteine residues in crystal structures. For the model system, a dependence of the ground-state spin-coupling scheme on the hydrogen–hydrogen distances is observed. The minima of the potential energy surface of $[Fe_4S_4(SH)_4]^{2-/1-}$ clusters are located at slightly smaller hydrogen–hydrogen distances than those of the $[Fe_4S_4(SH)_4]^{3-}$ cluster. For inner-sphere reorganization energies the spin-coupling scheme adopted by the broken-symmetry wave function plays an important role, since it can change the reorganization energies by up to 13 kcal mol^{-1}. For most structures, $[Fe_4S_4(SR)_4]^{2-}$ and $[Fe_4S_4(SR)_4]^{1-}$ (R = H or ethyl, derived from cysteine) favor the same coupling scheme. Therefore, the reorganization energies for this redox couple are relatively low (6–12 kcal mol^{-1}) compared with the 2−/3− redox couple favoring different spin-coupling schemes before and after electron transfer (14–18 kcal mol^{-1}). However, one may argue that more reliable reorganization energies are obtained if always the same spin-coupling pattern is enforced. All theoretical observations and insights are discussed in the light of experimental results distilled from the literature.

References: M. Bergeler, M. T. Stiebritz, M. Reiher, *ChemPlusChem*, **2013**, *78*, 1082-1098.

Title: Characteristic Raman Optical Activity Signatures of Protein β-Sheets

Researchers: Thomas Weymuth
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
Reiher Research Group

Description:

In this study, we compute and analyze theoretical Raman optical activity spectra of large model β-sheets in order to identify reliable signatures for this important secondary structure element. We first review signatures that have already been proposed to be indicative of β-sheets. From these signatures, we find that only the couplet in the amide I region can be regarded as a truly reliable signature. In addition, we propose a strong negative peak at 1350 cm^{-1} to be another good signature for parallel as well as antiparallel β-sheets. We study the robustness of these signatures with respect to perturbations induced by the amino acid side chains, the overall conformation of the sheet structure, and microsolvation. It is found that the latter effects can be very well understood and separated employing the concept of localized modes. Finally, we investigate whether Raman optical activity is capable of discriminating between parallel and antiparallel β-sheets. The amide III region turns out to be most promising for this purpose.

References: T. Weymuth, M. Reiher, *J. Phys. Chem. B*, **2013**,
DOI: 10.1021/jp405981h.

Title: Climate change and the water cycle: processes and scenarios

Researchers: Nikolina Ban, Omar Bellprat, Tanja Dallafior, Erich Fischer, Doris Folini, Maria Hakuba, Hanieh Hassanzadeh, Michael Keller, Sven Kotlarski, Nico Kröner, Wolfgang Langhans, David Leutwyler, Daniel Lüthi, Anna Possner, Jan Rajczak, Christoph Schär, Linda Schlemmer, Jürg Schmidli, Ana Sesartic, Martin Wild.

Institute/Group: Institute for Atmospheric and Climate Science
Group of Christoph Schär

Description:

We are using global and regional atmospheric models on a wide range of temporal and spatial scales. The high-resolution regional modeling uses the COSMO-CLM limited-area atmospheric model. Comprehensive European-scale climate-change scenario simulations were conducted in the framework of the COordinated Regional climate Downscaling Experiment (CORDEX) at horizontal resolutions of 12 and 50 km covering the period 1950-2100. Current work is addressing the calibration of the model, the analysis of changes in heat-wave and heavy precipitation events, snow cover, the height-dependence of the climate change signals, the representation of aerosol effects, and the quantification of different drivers behind the European summer climate. In parallel, we are developing a high-resolution climate simulation capability with a horizontal resolution of 2 km. Both idealized and real-case simulations are conducted. 10 year long simulations for present and future climate conditions for the whole Alpine area are performed at this resolution. The long simulations are complemented by detailed analyses of convective processes over mountainous terrain using a combination of satellite data and idealized large-eddy simulations using the Weather Research and Forecasting (WRF) model. The main motivation behind this work is the desire to explicitly simulate convective clouds (as opposed to using convective cloud parameterization schemes in lower-resolution models). We have also started using a recent GPU version of the COSMO model (jointly developed in HP2C projects by MeteoSwiss, ETH/C2SM and CSCS). The use of the COSMO-CLM is coordinated by Drs. D. Lüthi, J. Schmidli and S. Kotlarski.

The global scale simulations are carried out with the climate model ECHAM6-HAM, developed at the Max Planck Institute in Hamburg, Germany. This work is led by Prof. Martin Wild and Dr. Doris Folini, and it also exploits collaborations with the group of Prof. Ulrike Lohmann. The model contains sophisticated aerosol and cloud microphysics schemes. These are essential for realistic simulations of radiation and precipitation processes in the atmosphere. This model is used to study the link between anthropogenic and natural perturbations of the radiation balance and the intensity of the hydrological cycle. The time period under consideration covers 1870-2100. The global model simulations provide also boundary conditions to drive the regional model. Currently, ECHAM6-HAM is expanded into a coupled atmosphere-ocean climate modeling system, which allows to exploit the full response of the climate system in general and the water cycle in particular to the imposed radiative forcings in transient mode.

References:
A series of papers has been published (see references for further details).

Title: Numerical analysis of martingale driven stochastic evolution equations

Researchers: Andrea Barth, Annika Lang, Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description:

The project deals with the error analysis of approximations of different types of stochastic partial differential equations driven by square integrable martingales. Stochastic partial differential equations are considered in the context of stochastic differential equations taking values in an appropriate Hilbert space. Mean square, L^p, almost sure, and weak errors are considered. The time discretization schemes include Euler–Maruyama and Milstein methods in combination with backward Euler and Crank–Nicolson approaches. Finite dimensional approximations are employed for the space discretization which can for example be realized by Galerkin methods. The noise approximation is attached to the space discretization by an adequate truncation of the corresponding Karhunen–Loève expansion. For weak error approximations, computationally efficient multilevel Monte Carlo methods are introduced. Since stochastic processes with values in Hilbert spaces can be interpreted as random fields, attention to regularity and fast simulation of random fields on domains as well as manifolds is paid. These are important for the simulation and regularity of the driving noise.

[1] R. Andreev and A. Lang, *Kolmogorov–Chentsov theorem and differentiability of random fields on manifolds*. arXiv:1307.4886 [math.PR] SAM-Report 2013-22, July 2013.

[2] A. Barth, *A Finite Element method for martingale-driven stochastic partial differential equations*, Comm. Stoch. Anal., 4 (2010), pp. 355–375.

[3] A. Barth and A. Lang, *Milstein approximation for advection-diffusion equations driven by multiplicative noncontinuous martingale noises*, Appl. Math. Opt., 66 (2012), pp. 387–413.

[4] ——, *Multilevel Monte Carlo method with applications to stochastic partial differential equations*, Int. J. Comp. Math., 89 (2012), pp. 2479–2498.

[5] ——, *Simulation of stochastic partial differential equations using finite element methods*, Stochastics, 84 (2012), pp. 217–231.

[6] ——, *L^p and almost sure convergence of a Milstein scheme for stochastic partial differential equations*, Stoch. Process. Appl., 123 (2013), pp. 1563–1587.

[7] A. Barth, A. Lang, and C. Schwab, *Multilevel Monte Carlo Finite Element method for parabolic stochastic partial differential equations*, BIT Num. Math., 53 (2013), pp. 3–27.

[8] A. Lang, *A Lax equivalence theorem for stochastic differential equations*, J. Comput. Appl. Math., 234 (2010), pp. 3387–3396.

[9] ——, *Mean square convergence of a semidiscrete scheme for SPDEs of Zakai type driven by square integrable martingales*, Procedia Computer Science, 1 (2010), pp. 1609–1617. ICCS 2010.

[10] ——, *Almost sure convergence of a Galerkin approximation for SPDEs of Zakai type driven by square integrable martingales*, J. Comput. Appl. Math., 236 (2012), pp. 1724–1732.

[11] ——, *Isotropic Gaussian random fields on the sphere.* Oberwolfach Report, SAM Report 2013-26, August 2013.

[12] A. Lang, P.-L. Chow, and J. Potthoff, *Almost sure convergence of a semidiscrete Milstein scheme for SPDEs of Zakai type*, Stochastics, 82 (2010), pp. 315–326.

[13] ——, *Erratum: Almost sure convergence of a semi-discrete Milstein scheme for SPDEs of Zakai type*, Stochastics, 84 (2012), p. 561.

[14] A. Lang, S. Larsson, and C. Schwab, *Covariance structure of parabolic stochastic partial differential equations*, Stoch. PDE: Anal. Comp., 1 (2013), pp. 351–364.

[15] A. Lang and J. Potthoff, *Erratum: Fast simulation of Gaussian random fields*, Monte Carlo Methods Appl., 19 (2013), pp. 73–75.

[16] A. Lang and C. Schwab, *Isotropic Gaussian random fields on the sphere: regularity, fast simulation, and stochastic partial differential equations.* arXiv:1305.1170 [math.PR] SAM Report 2013-15, May 2013.

Title: Sparse Tensor Approximation Methods for High-Dimensional Transport Problems

Researchers: Prof. Ralf Hiptmair
Prof. Christoph Schwab
Prof. Philipp Grohs
Eivind Fonn
Konstantin Grella
Axel Obermeier

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

We investigate high dimensional transport problems such as the stationary monochromatic radiative transfer equation or the Boltzmann transport equation. Due to the high dimensionality of the problems, novel methods are required to reduce the workload while maintaining accuracy.

For the solution of the spatially homogeneous Boltzmann equation, we have developed a MATLAB implementation using Fourier spectral discretization, both full and sparse (hyperbolic cross) varieties. A novel polar discretization has also been implemented in parallel C++, which can produce more physically accurate and conservative solutions at the cost of somewhat higher time complexity.

For the radiative transfer problem, we have developed sparse tensor versions of the popular spherical harmonics method and the discrete ordinates method (DOM) as well as a randomized sparse DOM. A parallel C++ implementation enables us to solve large 3+2D radiative transfer problems essentially at the cost of a 3D problem on HPC hardware (e. g. the ETH cluster Brutus).

Finally, we have implemented a new method using a frame that is very well-adapted to linear transport problems ("Ridgelets"). This allows linear-time approximate matrix-vector-multiplication through an adaptive algorithm, which has been implemented in parallel Matlab. The algorithm can be proven to converge with linear complexity. Furthermore, another implementation using ridgelets – the discrete ridgelet transform (realised with `fft`) – has been implemented as well and tested successfully on several model problems in radiative transport.

References:

[1] K. Grella and Ch. Schwab.
Sparse tensor spherical harmonics approximation in radiative transfer.
Journal of Computational Physics (2011), 230(23), 8452–8473.

[2] K. Grella and Ch. Schwab.
Sparse Discrete Ordinates Method in Radiative Transfer.
Computational Methods in Applied Mathematics (2011), 11(3), 305–326.

[3] E. Fonn, P. Grohs and R. Hiptmair.
Hyperbolic cross approximation for the spatially homogeneous Boltzmann equation.
SAM report 2012-28, (2012). Pending review.

Title: Tensor-structured solution of high-dimensional ODEs and PDEs

Researchers: Vladimir Kazeev, Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description:

The project focuses on the numerical solution of high-dimensional ODEs and PDEs in low-parametric representations known as *tensor decompositions*. The key idea is the application of non-linear approximations based on the separation of variables to the representation of the solution, operator and other data involved, discretized by means of the FDM or FEM constructed on extremely fine uniform tensor-product meshes. The full discretizations are not supposed to be dealt with immediately; instead, adaptive algorithms of the low-rank tensor compression, which have to underlie any tensor-structured computation, are exploited as the tool extracting the "effective" degrees of freedom.

The tensor format we employ is the newly introduced *tensor train decomposition*, which generalizes the SVD of matrices differently from the well-known *canonical polyadic* and *Tucker representations*. It enjoys the major advantages of the two, which are, first, linear (with respect to the dimensionality) complexity and, second, the availability of stable algorithms based on standard matrix decompositions (SVD and QR, in particular). Being coupled with *quantization*, which means splitting each "physical" dimension of a vector or matrix into multiple "virtual" dimensions, it gives rise to the *quantized tensor train decomposition*. The latter, in some cases, allows to achieve even logarithmic (with respect to the number of "uncompressed" degrees of freedom) complexity of representing the data and performing the basic operations of linear algebra on it.

The major challenges within the project are: theoretical analysis of the TT and QTT structure of the operators and solutions; investigation of appropriate discretizations in space and time (for evolution problems); solution of linear systems in the TT format; high-performance implementation of the TT arithmetics.

[1] V. Kazeev, M. Khammash, M. Nip, and C. Schwab, *Direct solution of the Chemical Master Equation using Quantized Tensor Trains*, Research Report 4, Seminar for Applied Mathematics, ETH Zürich, 2013.

[2] V. Kazeev and I. Oseledets, *The tensor structure of a class of adaptive algebraic wavelet transforms*, Research Report 28, Seminar for Applied Mathematics, ETH Zürich, 2013.

[3] V. Kazeev, O. Reichmann, and C. Schwab, *hp-DG-QTT solution of high-dimensional degenerate diffusion equations*, Report 11, Seminar for Applied Mathematics, ETH Zürich, 2012.

[4] ——, *Low-rank tensor structure of linear diffusion operators in the TT and QTT formats*, Linear Algebra and its Applications, 438 (2013), pp. 4204–4221.

[5] V. Kazeev and C. Schwab, *Tensor approximation of stationary distributions of chemical reaction networks*, Research Report 18, Seminar for Applied Mathematics, ETH Zürich, 2013.

Title: Finite Elements with mesh refinement for linear, second-order hyperbolic PDEs on polygonal and polyhedral domains.

Researchers: Fabian Müller, Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Linear, second-order hyperbolic PDEs play an important role in modeling various evolution phenomena in applications, such as acoustic, seismic and electromagnetic wave propagation. Simulations are usually performed using a method of lines with semi-discretization in space done by Finite Elements, followed by a time-stepping scheme.

The convergence rates of this discretization strategy depend on the regularity of the exact solution. On polygonal domains, or in the presence of jumps in the material coefficients ("interface problem"), this is an issue yielding severly reduced convergence rates.

In this project, we investigate mesh refinement techniques to recover quasi-optimal convergence rates for the h-version of Finite Elements. For the semi-discretization in space, similar classes of locally refined meshes as known for stationary cases can be applied. Moreover, we study the use of local space-time refinements in order to resolve singularities in the time-variable and investigate the convergence of the resulting fully discretized method for the acoustic and the elastic wave equation with smooth coefficients on polygonal domains and the acoustic interface problem.

[1] F. Müller and C. Schwab, *Finite elements with mesh refinement for wave equations in polygons*, Tech. Rep. 2013-11, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013.

Title: Sparse techniques for parametric differential equations

Researchers: Markus Hansen, Claudia Schillings, Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description:

The focus of the project is on the efficient numerical approximation of parametric differential equations. In particular, we are interested in methods which are dimensionally robust, i.e. whose efficiency (meaning accuracy versus computational cost measured in terms of the total number of floating point operations to achieve this accuracy) is provably robust with respect to the number of parameters.

In order to allow for efficient approximations of the parametric solutions on the entire, possibly infinite dimensional parameter space, some form of sparsity in the parametric dependence of the solution is necessary. Problem classes are identified, so that the solutions of the parametric problems admit sparse expansions in terms of tensorized polynomial systems in the infinite dimensional parameter space, under the provision of sparsity of the random input. We deduce rates of convergence of N-term truncated approximations of expansions of the parametric solutions.

Based on the theoretical results, a major goal of the project is to develop numerical algorithms which allow to exploit computationally the sparse parameter dependence of the solutions and, hence, to achieve the optimal complexity by the sparse approximations. In the references below, we present an adaptive approach for computing sparse, approximate representations of the parametric solutions in large parameter dimensions. The algorithm iteratively localizes a sequence of monotone sets, which, although possibly not optimal in the sense of best N-term approximation, will deliver the optimal rate for given summability of the parametric inputs.

In [5, 6], we propose a novel, deterministic approach to inverse problems for identification of parameters in differential equations from noisy measurements. For forward problems belonging to a certain sparsity class, we quantify analytic regularity of the Bayesian posterior and prove that the parametric, deterministic density of the Bayesian posterior belongs to the same sparsity class. These results suggest in particular dimension-independent convergence rates for data-adaptive Smolyak integration algorithms.

[1] M. Hansen, C. Schillings, and C. Schwab, *Sparse approximation algorithms for high dimensional parametric initial value problems*, in Proceedings 5th Conf. High Performance Computing, Hanoi, Springer LNCSE, 2013.

[2] M. Hansen and C. Schwab, *Analytic regularity and best n-term approximation of high dimensional parametric initial value problems*, Vietnam Journ. Math., 1 (2011), pp. 1–35.

[3] M. Hansen and C. Schwab, *Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic pdes*, Mathematische Nachrichten, 286 (2013), pp. 832–860.

[4] C. Schillings, *A note on sparse, adaptive Smolyak quadratures for Bayesian inverse problems*, Tech. Rep. 2013-06, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013.

[5] C. Schillings and C. Schwab, *Sparse, adaptive Smolyak quadratures for Bayesian inverse problems*, Inverse Problems, 29 (2013), p. 065011.

[6] C. Schillings and C. Schwab, *Sparsity in Bayesian inversion of parametric operator equations*, Tech. Rep. 2013-17, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013.

[7] C. Schwab and C. Schillings, *Sparse quadrature approach to Bayesian inverse problems*, Tech. Rep. 2013-27, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013.

Title: High order numerical methods for stochastic hyperbolic conservation laws

Researchers: Svetlana Tokareva
Siddhartha Mishra, Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description:

The project encompasses the analysis and implementation of algorithms for the numerical solution of hyperbolic conservation laws with stochastic fluxes, initial and boundary data.

We study the conservation laws with Riemann initial data and show that in case of an uncertain initial discontinuity position the statistical mean, variance, spatio-temporal correlation functions as well as the coefficients of the gPC expansions have higher degree of regularity compared to the solution of the deterministic Riemann problem. We study the effects of the extra smoothness of the gPC coefficients on the convergence rates of the Stochastic Galerkin method combined with high order finite volume WENO schemes and demonstrate the high convergence rates in the approximation of gPC expansion terms.

The parametrization of the probability space allows to construct the Stochastic Finite Volume method (SFV) applicable for the uncertainty quantification in stochastic hyperbolic conservation laws. The SFV method is potentially superior to Monte Carlo type methods in terms of error vs work efficiency. We design the algorithm of SFV method based on high order ENO/WENO solvers.

The SFV approach can be generalized for the efficient application of high-order approximation techniques on unstructured grids in physical domains with complicated geometry. To this end, the Discontinuous Galerkin (DG) method can be used to discretize the equations in the physical space, combined with the finite-volume discretization in the stochastic variables.

The algorithm allows efficient parallelization based on the domain decomposition method which is applied in both physical and stochastic space.

[1] S. Mishra, N. H. Risebro, C. Schwab, and S. Tokareva, *Numerical solution of scalar conservation laws with random flux functions*, SAM report 2012-35. `http://www.sam.math.ethz.ch/reports/2012/35`.

[2] C. Schwab and S. Tokareva, *High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data*, ESAIM: M2AN, 47 (2013), pp. 807–835.

[3] S. Tokareva, *Stochastic finite volume methods for computational uncertainty quantification in hyperbolic conservation laws*, PhD thesis, ETH Zürich, 2013.

Title: Free Surface Influence on Plate Tectonics and Mantle Convection

Researchers: F. Crameri
P. J. Tackley
B. Kaus
T. Gerya

Institute/ Group: Institute of Geophysics
Geophysical Fluid Dynamics

Description:

In the mantle of a planet like Earth the viscosity is strongly dependent on temperature, such that the cold upper boundary layer of the convecting system becomes stagnant, if no other complexity is accounted for. On Earth, however, this cold, stiff layer, named the lithosphere, is broken into several plates that move relative to each other. In numerical models of mantle convection, this process can be approximated by introducing plastic yielding, which generates weak plate boundaries in the lithosphere and allows spreading centers and subduction zones to form. However, the simulated subduction zones are typically double-sided (symmetrical) whereas on Earth they are distinctly single sided. In this project we investigate the influence of surface boundary condition on this process, comparing a free-slip surface (i.e., zero vertical velocity and shear stress) with the more realistic free surface (zero stress but finite velocity). We find that this makes a first-order difference to the style of subduction zones, with single-sided subduction arising naturally (see figure). In continuing research, we are also investigating the influence of a layer of hydrated sediments, which forms a weak layer between the subducting and overriding plates, mechanically decoupling them.

Figure. Convection with strongly temperature- and yield stress-dependent viscosity and a free outer surface. Earth-like single-sided subduction is obtained.

References: (i) Crameri F., P. J. Tackley, I. Meilick, T. V. Gerya and B. J. P. Kaus, 2012, A free plate surface and weak oceanic crust produce single-sided subduction on Earth, *Geophys. Res. Lett.* 39, L03306, doi:10.1029/2011GL050046A. (ii) PhD Thesis, Fabio Crameri 2013. (iii) Two manuscripts are in preparation based on Dr. Crameri's PhD thesis results.

Title: Numerical modelling of continental collision zones

Researchers: Taras Gerya, Thibault Duretz, Elena Sizova, Jonas Ruh, Ria Fisher, Chen Lin

Institute: Institute of Geophysics, D-ERDW, ETH-Zurich

Group: Geophysical Fluid Dynamics

Description:
Various aspects of subduction and collision zones dynamics, magmatic activities and fluid regimes are modelled in 2D and 3D with the use of the original codes I2ELVIS and I3ELVIS combining finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations:

- Reviewing models for ultrahigh-pressure terrains (Hacker and Gerya, 2013; Hacker et al., 2013)
- Dynamics of thrust wedges (Ruh et al., 2013)
- Dynamics of slab detachment (Duretz and Gerya, 2013)
- Collision of continental corner (Fig. 2)(Li et al., 2013)
- Steep convergent intracontinental margins (Chen et al., 2013a,b)
- Styles of Precambrian collision (Sizova et al., 2013)

Fig. 2. Collision of continental corner (Li et al., 2013).

References:

Chen, L., Gerya, T., Zhang, Z., Aitken, A., Li, Z., Liang, X. (2013b) Formation mechanism of steep convergent intracontinental margins: Insights from numerical modeling. Geophysical Research Letters, DOI: DOI: 10.1002/grl.50446

Chen, L., Gerya, T., Zhang, Z., Zhu, G., Duretz, T., Jacoby, W.R. (2013a) Numerical modeling of eastern Tibetan-type margin: Influences of surface processes, lithospheric structure and crustal rheology. Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2013.01.003

Duretz, T., Gerya, T.V. (2013) Slab detachment during continental collision: Influence of crustal rheology and interaction with lithospheric delamination. Tectonophysics, DOI: http://dx.doi.org/10.1016/j.tecto.2012.12.024.

Hacker, B.R., Gerya, T.V. (2013) Paradigms, new and old, for ultrahigh-pressure tectonism. Tectonophysics, 603, 79-88.

Hacker, B.R., Gerya, T.V., Gilotti, J.A. (2013) Formation and exhumation of ultrahigh-pressure terranes. Elements, 9, 289-293

Li, Z., Xu, Z., Gerya, T., Burg, J.-P. (2013) Collision of continental corner from 3-D numerical modeling. Earth and Planetary Science Letters, 380, 98–111. 2013_EPSL_Zhonghai.pdf

Ruh, J.B., Gerya, T., Burg, J.-P. (2013) High-resolution 3D numerical modeling of thrust wedges: Influence of decollement strength on transfer zones. Geochem. Geophys. Geosys., doi:10.1002/ggge.20085

Sizova, E.V., Gerya, T.V., Brown, M. (2013) Contrasting styles of Phanerozoic and Precambrian continental collision, Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.12.011

Title: Development of new numerical geodynamic modeling techniques

Researchers: Taras Gerya, Dave May, Ria Fisher, Christoph Püthe

Institute: Institute of Geophysics, D-ERDW, ETH-Zurich

Group: Geophysical Fluid Dynamics

Description:
Further development of numerical modeling approaches for variable viscosity problems based on staggered finite differences and marker in cell technique:

- An adaptive staggered grid finite difference method (Geryat et al., 2013)
- A multigrid staggered grid solver on a GPU for Stokes equations (Zheng et al., 2013)

Fig. 3. An adaptive staggered grid finite difference model (Gerya et al., 2013)

References:

Gerya, T.V., May, D.A., Duretz, T. (2013) An adaptive staggered grid finite difference method for modeling geodynamic Stokes flows with strongly variable viscosity, Geochemistry, Geophysics, Geosystems, DOI: 10.1002/ggge.20078

Zheng, L., Zhang, H., Gerya, T., Knepley, M., Yuen, D.A., Shi, Y. (2013) Implementation of a multigrid solver on a GPU for Stokes equations with strongly variable viscosity based on Matlab and CUDA. The International Journal of High Performance Computing Applications, DOI: 10.1177/1094342013478640

Title: Numerical modelling of lithospheric extension and faulting processes
Researchers: Taras Gerya, Filippo Schenker, Jie Liao, Christoph Puthe

Institute: Institute of Geophysics, D-ERDW, ETH-Zurich

Group: Geophysical Fluid Dynamics

Description:
Various aspects of lithospheric extension processes are modelled in 2D and 3D with the use of the original codes I2ELVIS and I3ELVIS combining finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations:

- Intrusion of felsic magma in the crust (Schubert et al., 2013)
- Continental breakup and transition to oceanic spreading (Fig.3) (Gerya, 2013a,b)
- Development of spreading patterns at mid-ocean ridges (Püthe and Gerya, 2013)

Fig. 3. Types of mid-ocean spreading patterns (Püthe and Gerya, 2013)

References:

Gerya, T.V. (2013a) Initiation of transform faults at rifted continental margins: 3D petrological–thermomechanical modeling and comparison to the Woodlark Basin. Petrology, 21, 550–560.

Gerya, T.V. (2013b) Three-dimensional thermomechanical modeling of oceanic spreading initiation and evolution.Phys. Earth Planet. Interiors, DOI: http://dx.doi.org/10.1016/j.pepi.2012.10.007

Püthe, C., Gerya, T.V. (2013) Dependence of mid-ocean ridge morphology on spreading rate in numerical 3-D models. Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2013.04.005

Schubert, M., Driesner, T., Gerya, T.V., Ulmer, P. (2013) Mafic injection as a trigger for felsic magmatism: A numerical study. Geochemistry, Geophysics, Geosystems, 14, doi:10.1002/ggge.20124.

Title: Coupled modelling of atmosphere and mantle evolution

Researchers: C. Gillmann, P. J. Tackley, G. J. Golabek

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

We use Venus as test bed for our numerical model of the evolution of the atmosphere of terrestrial planets, as an intermediary between life-sustaining Earth and yet to be discovered exoplanets. Here, we focus on mechanisms that deplete or replenish the atmosphere: volcanic degassing and atmospheric escape. These processes are linked together to obtain a coupled model, using retroaction of the atmosphere on the mantle. We study potential divergent evolutions this could cause. Two aspects of the atmospheric escape are taken into account. During early evolution, hydrodynamic escape is dominant. We use a model developed to take into account the linked escape of Hydrogen and Oxygen. A significant portion of the early atmosphere can be removed this way. For later evolution, we focus on non-thermal escape. Post 4 Ga escape is low. Water escapes moderately, while we are not able to detect the present-day escape of CO_2. The atmosphere is replenished by volcanic degassing, bringing volatiles from the mantle to the surface. Volcanic activity is obtained by adapting the finite difference/finite volume code StagYY for Venus. Volatile fluxes are estimated for different mantle compositions and partitioning ratios.Surface conditions are estimated by tracking the amount of CO_2 and water in the atmosphere and computing the surface temperature with a gray radiative-convective atmosphere model. These surface conditions in turn act as a boundary condition for the mantle dynamic model and have an influence on convection, volcanism and subsequent degassing. Our results show that we are able to obtain a Venus-like behavior for the solid planet, with resurfacing events which constitute an efficient way of losing Venus' internal heat. We are able to create evolution leading to present conditions. CO2 pressure seems unlikely to vary much over the history of the planet, only slightly increasing due to degassing. A late build-up of the atmosphere with several resurfacing events seems unlikely. On the other hand, water pressure is strongly sensitive to volcanic activity and varies rapidly. This leads to variations in surface temperatures of up to 200K, which have been identified to have an effect on volcanic activity. While a positive feedback (increasing atmosphere temperature leading to increasing mantle temperatures and melting) is not immediately apparent, we observe a clear link between temperature changes and volcanic spikes, in particular a strong correlation between large temperature drops and increased volcanism. Mobilization of the upper layers occurs, which imply that our coupling is not complete without taking into account rehydratation of the mantle. This depends on the surface alteration processes and could have important effects.

Title: Numerical models of the thermomechanical evolution of planetesimals: Application to the acapulcoite-lodranite parent body

Researchers: G. J. Golabek, B. Bourdon, T. V. Gerya

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

The acapulcoite-lodranite meteorites are members of the primitive achondrite class. The observation of partial melting and resulting partial removal of Fe-FeS indicates that this meteorite group could be an important link between achondrite and iron meteorites on the one hand and chondrite meteorites on the other. Thus a better understanding of the thermomechanical evolution of the parent body of this meteorite group can help to improve our understanding of the evolution of early planetesimals. Here we use 2D and 3D finite-difference numerical models to determine the formation time, initial radius of the parent body of the acapulcoite-lodranite meteorites and their formation depth inside the body by applying available geochronological, thermal and textural constraints to our numerical data. Our results indicate that the best fit to the data can be obtained for a parent body with 35-65 km radius, which formed around 1.3 Ma after CAI. The 3D results indicate possible formation depths of the acapulcoite-lodranite meteorites of 19 and 22-23 km, respectively. Our data also suggest that other meteorite classes could form at different depths inside the same parent body, supporting recently proposed models.

Figure: 3D model of early thermomechanical evolution of an early-formed planetesimal.

References:

Manuscript submitted to *Meteoritics and Planetary Science*.

Title: Towards coupled giant impact and long term interior evolution models

Researchers: G. J. Golabek, M. Jutzi, T. V. Gerya, E. I. Asphaug

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

The crustal dichotomy is the dominant geological feature on planet Mars. The exogenic approach to the origin of the crustal dichotomy (Wilhelms and Squyres, 1984; Frey and Schultz, 1988; Andrews-Hanna et al., 2008; Marinova et al., 2008; Nimmo et al., 2008) assumes that the northern lowlands correspond to a giant impact basin formed after primordial crust formation. However these simulations only consider the impact phase without studying the long-term repercussions of such a collision. The endogenic approach, suggesting a degree-1 mantle upwelling underneath the southern highlands, relies on a high Rayleigh number and a particular viscosity profile to form a low degree convective pattern within the geological constraints for the dichotomy formation. Such vigorous convection, however, results in continuous magmatic resurfacing, destroying the initially dichotomous crustal structure in the long-term. A further option is a hybrid exogenic–endogenic approach, which proposes an impact-induced magma ocean and subsequent superplume in the southern hemisphere. However these models rely on simple scaling laws to impose the thermal effects of the collision. Here we performed impact simulations with a SPH code and coupled it serially with geodynamical computations performed using the code I3VIS to improve the latter approach and test it against observations. We are exploring collisions varying the impactor velocities, impact angles and target body properties, and are gauging the sensitivity to the handoff from SPH to I3VIS. As expected, our first results indicate the formation of a transient hemispherical magma ocean in the impacted hemisphere, and the merging of the cores. We also find that impact angle and velocity have a strong effect on the post-impact temperature field and on the timescale and nature of core merger.

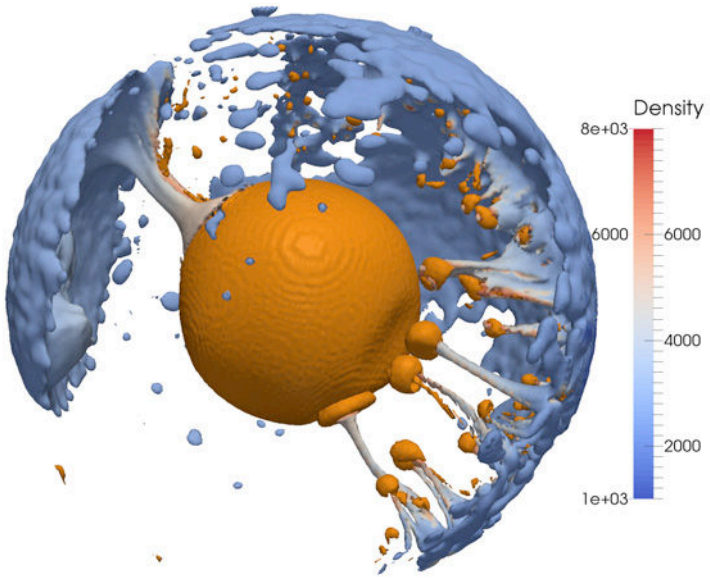


Figure: Long-term evolution of magma ocean and impactor core after giant impact.

Title: Combined modelling of planetary accretion and differentiation

Researchers: G. J. Golabek, R. Morishima, T. V. Gerya, P. J. Tackley, S. Labrosse

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Results of current 1D models on planetesimal accretion yield an onion-like thermal structure with very high internal temperatures due to powerful short-lived radiogenic heating in the planetesimals. These lead to extensive silicate melting in the parent bodies. Yet, magma ocean and impact processes are not considered in these models and core formation is, if taken into account, assumed to be instantaneous with no feedback on the mantle evolution. It was pointed out that impacts can not only deposit heat deep into the target body, which is later buried by ejecta of further impacts, but also that impacts expose in the crater region originally deep-seated layers, thus cooling the interior. This combination of impact effects becomes even more important when we consider that planetesimals of all masses contribute to planetary accretion. This leads occasionally to collisions between bodies with large ratios between impactor and target mass. Thus, all these processes can be expected to have a profound effect on the thermal evolution during the epoch of planetary accretion and may have implications for the onset of mantle convection and cannot be described properly in 1D geometry. Here we present a new methodology, which can be used to simulate the internal evolution of a planetary body during accretion and differentiation: Using the N-body code PKDGRAV we simulate the accretion of planetary embryos from an initial annulus of several thousand planetesimals. The growth history of the largest resulting planetary embryo is used as an input for the thermomechanical 2D code I2ELVIS. The thermomechanical model takes recent parametrizations of impact processes like impact heating and crater excavation into account. Results show that late-formed planetesimals do not experience silicate melting and avoid thermal alteration, whereas in early-formed bodies accretion and iron core growth occur almost simultaneously and magma oceans develop in the interior of these bodies. These tend to form first close to the core-mantle boundary and migrate upwards with growing internal pressure.

Figure: 2D model of thermochemical evolution of an accreting protoplanet.

Title: 3D Modelling of Continental Break-Up at Oblique Margins

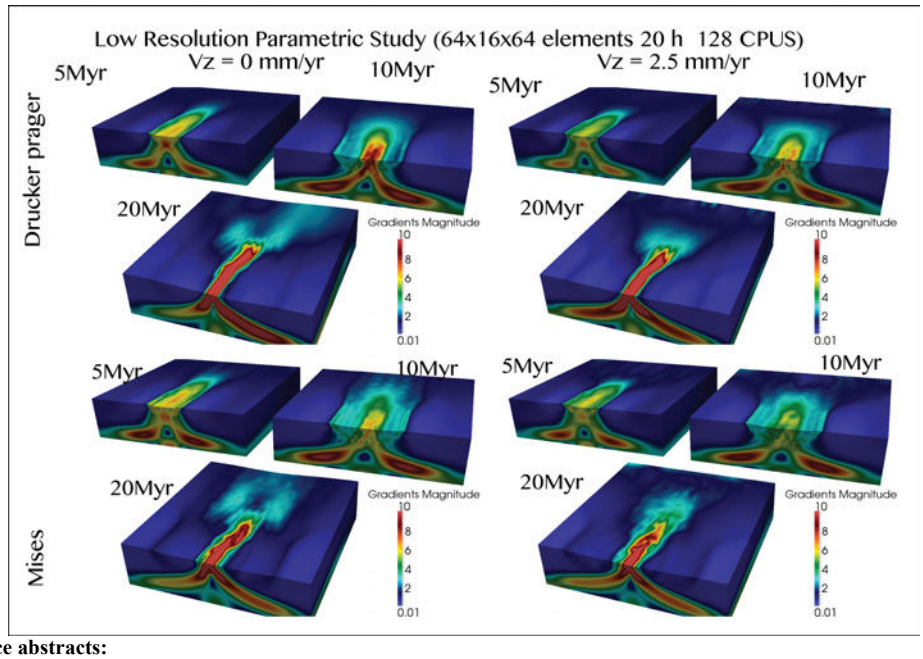
Researchers: Laetitia Le Pourhiet (1), Dave A. May(2)

Institute/ (1) UPMC/ISTEP
Group: (2) Department of Earth Sciences/Geophysical Fluid Dynamics

Description: When the rupture of the continental crust propagates, it does not propagate straight like an elastic crack but rather by step over which might be very large (100-1000 km), giving rise to either transform margins or more subtle (10-100 km) oblique margins. In order to better understand how continental break-up and boundary conditions influence the state of stress and the direction of propagation of continental rifting, it is very important to account for non linear rheologies such as pressure dependant yield stress (Drucker-Prager), a free surface and temperature dependant viscosity. The last point is crucial to the understanding of continental rifting and this aspect cannot be investigated via analogue modelling.

In this project, we make use of newly developed finite-element / particle-in-cell code *pTatin3d* to investigate the formation of transforms and oblique boundary with a special target of explaining the opening of the Equatorial Atlantic Ocean.

Preliminary results show that obliquity might develop self-consistently at the tip of the propagating break-up with out forcing from boundary conditions (left on figure). We also find that pressure dependant mantle favours the asymmetry of the propagation (top left). Forcing the obliquity from boundary conditions leads to oblique continental margin but break up tends to propagate in a straighter manner (right panel on figure).



Conference abstracts:

Le Pourhiet L. and **May D.**, 3D thermo-mechanical models of continental break up, Geophysical Research Abstracts, Vol. 15, EGU2013-8434-1, EGU General Assembly 2013
Le Pourhiet L. and **May D.,** sollicited, From 2D to 3D modelling in long term tectonics: Modelling challenges and HPC solutions, AGU Fall Meeting 2013
Mercier de Lépinay M. , **L. Le Pourhiet**, L. Loncke, B. Vendeville, C. Basile, A. Maillard, W. R. Roest, V. Gaullier, P. de Clarens, **May D.**; 3D Thermo-mechanical models of Equatorial Atlantic rifting and opening and the oblique/transform continental margins formation and evolution – Preliminary results; AGU Fall Meeting 2013

Title: Robust non-linear methods to study shear band structures in 3D

Researchers: Dave A. May

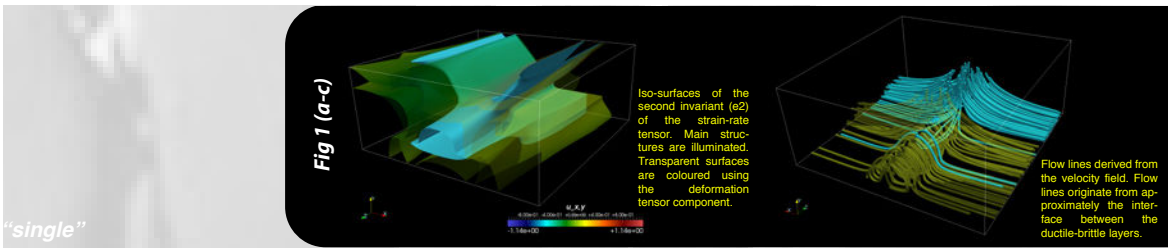
Institute/ Group: Geophysical Fluid Dynamics
Department of Earth Sciences

Description:

Understanding the development and evolution of individual faults, and fault systems is a fundamental aspect of lithospheric deformation. Many studies treating the lithosphere as a visco-plastic (Mises or Drucker Prager) material have been conducted in 2D. However, natural systems are inherently three-dimensional, thus to study non-cylindrical structures requires 3D numerical simulations. The additional spatial dimension permits a much wider choice of boundary conditions and allows for the possibility to have 6 modes of deformation, thereby leading to more complex fault systems compared to 2D models.

To date, little research has been conducted using numerical models which examine the behaviour of visco-plastic fault systems in 3D. This is primarily due to the complexity associated with solving the discrete non-linear Stokes flow problem at sufficiently high resolution. A new parallel finite element code pTatin3d, has been developed to address this limitation.

To develop our understanding of the behaviour of visco-plastic shear band formation, in this work we consider a simple model of the lower and upper crust. The model consists of a two layer ductile-brittle system subject to extensional boundary conditions. Here I explore how the geometry of the heterogeneity used to initiate localisation influences the topology of the resulting fault system.



References:

D. A. May, J. Brown & L. Le Pourhiet, A scalable, matrix-free Stokes discretisation for geodynamic applications, Computer Methods in Applied Mechanics and Engineering (2013) [in preparation]

Title: N-body simulations of oligarchic growth of Mars: Implications for Hf-W chronology.

Researchers: R. Morishima, G. J. Golabek, H. Samuel

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Dauphas and Pourmand (2011) estimated the accretion timescale of Mars to be 0.8 - 2.7 Ma from the W isotopes of martian meteorites. This timescale was derived assuming perfect metal-silicate equilibration between the impactor and the target's mantle. However, in case of a small impactor most likely only a fraction of the target's mantle is involved in the equilibration, while only a small part of the impactor's core equilibrates in the case of a giant impact. We examined the effects of imperfect equilibration using results of high-resolution N-body simulations for the oligarchic growth stage. It was found that with plausible assumptions these effects are small. The former effect is small due to the low Hf/W ratio of the martian mantle. The latter effect is small because a large fraction of the embryo mass is delivered from small planetesimals, which are likely to fully equilibrate with the embryo mantle. The accretion timescale of Mars indicated by the Hf-W chronology is shorter than that expected for the minimum mass solar nebula model. This probably indicates that the local surface densities of solid and gas in the protosolar nebula were higher than those for the minimum mass model.

Figure: N-body results on the growth of planetary embryos from an annulus of planetesimals.

References:

Morishima, R., G. J. Golabek and H. Samuel, N-body simulations of oligarchic growth of Mars: Implications for Hf-W chronology, *Earth Planet. Sci. Lett.*, 366, 6-16, http://dx.doi.org/10.1016/j.epsl.2013.01.036, 2013.

Title: Implications of High Core Thermal Conductivity on Earth's Coupled Mantle and Core Evolution

Researchers: T. Nakagawa, P. J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Description:

Mineral physicists recently determined that the thermal conductivity of Earth's metallic core (which generates the magnetic field through dynamo action) is 2-3 times higher than previously thought. We investigate the influence of this on the evolution of Earth's core and mantle over billions of years using numerical simulations of two-dimensional thermo-chemical mantle convection coupled to a parameterised core heat balance model. The value of core thermal conductivity has no effect on mantle evolution but a significant effect on core evolution. The core-mantle boundary heat flow starts high and decreases with time to ~13 TW, which is below the core adiabatic heat flux for the largest thermal conductivity tested (200 W/m/K), meaning that a purely thermal dynamo is not viable. However, gravitational energy release and latent heat associated with inner core growth become important in the last ~0.9 Gyr and allow continuous geodynamo generation despite high core thermal conductivity, although we estimate a subadiabatic region at the top of the core of the order of hundreds of kilometers.

Figure. Time evolution of (a) core-mantle boundary temperature, (b) core-mantle boundary heat flow, (c) size of solid inner core, (d) magnetic dissipation.

References: Nakagawa, T. and P. J. Tackley (2013) Implications of high core thermal conductivity on Earth's coupled mantle and core evolution, Geophys. Res. Lett. 40, doi:10.1002/grl.50574..

Title: Single viscous layer folding interplay and linkage. A 3D-FEM modelling approach

Researchers: Thomas A. Philippe , Dave A. May, Marcel Frehner

Institute/ Group: Institute of Geophysics / Geophysical Fluid Dynamics

Description:

Recent fieldwork observations and numerical experiments have demonstrated that large fold-belt systems do not necessarily grow uniformly in a cylindrical manner but arise from the lateral connection (parallel to the fold axis) of smaller embryonic folds. From these observations, the cylindrical assumption often assumed in folding experiments has to be relaxed and a fully 3D numerical model has to be used in order to understand the fold linkage process.

We solved the problem using a finite element method employing a high-resolution mesh which required massive parallel computing resources.

We tested first the ability of the marker-and-cell (MAC) method, coupled with the finite element method (FEM) to accurately model folding process for large strain. The advantage of the MAC-FEM is that a regular mesh can be used independently on how strongly folded the domain is because the properties are carried by the markers and not by the elements anymore. It avoids developing a lithology dependent remeshing algorithm which is difficult to make robust for large deformation experiments.

The mechanical feasibility of the fork-linkage or more generally the triple-linkage (three isolated embryonic folds linking laterally together) has been then studied. To address this issue, a template for modelling the triple-linkage was introduced, which consists of a solitary embryonic fold opposite to a binary perturbation. The folding and linkage process were then tackled considering the vorticity field and it turned out to be a very interesting and fruitful framework that makes the linkage patterns and embryonic fold interplays simple to understand. Based on the 3D analytical solution for the finite amplitude folding of a single viscous layer embedded in a matrix, the planar-vorticity dominant wavelength (in the viscous layer plane) was computed numerically. This planar-vorticity dominant wavelength came out to be distinct from the dominant amplification wavelength and it appeared to be the characteristic length controlling the linkage process. In light of these observations, a new interpretation and explanation has been given for the simple-linkage previously studied and the perspective for the general case has been finally discussed.

References:

T. A. Philippe, Single viscous layer folding interplay and linkage. A 3D-FEM modelling approach. (2013) [master thesis]

Title: Modelling the Influence of Continents on Plate Tectonics

Researchers: T. Rolf
P. J. Tackley
N. Coltice

Institute/ Group: Institute of Geophysics
Geophysical Fluid Dynamics, D-ERDW

Description:

Earth's tectonic plates have two components: oceanic and continental. Previous mantle convection simulations with continents have revealed that they have a first-order influence on mantle convection, affecting convective wavelength and surface heat loss. In this study we model 3D spherical mantle convection with self-consistent plate tectonics and a mobile, strong continent to gain insight into the effect of continents on plate tectonics. Stable continents affect the convective regime by thermal blanketing and stress focussing at the continental margins, which facilitates the formation of subduction zones by increasing convective stresses at the margins, which allows for plate tectonics at higher yield strength. Combining continents with ocean plates leads to an Earth-like area-age distribution of oceanic floor, with time-dependence also similar to that of Earths. Supercontinent cycles are observed under some conditions but not all.

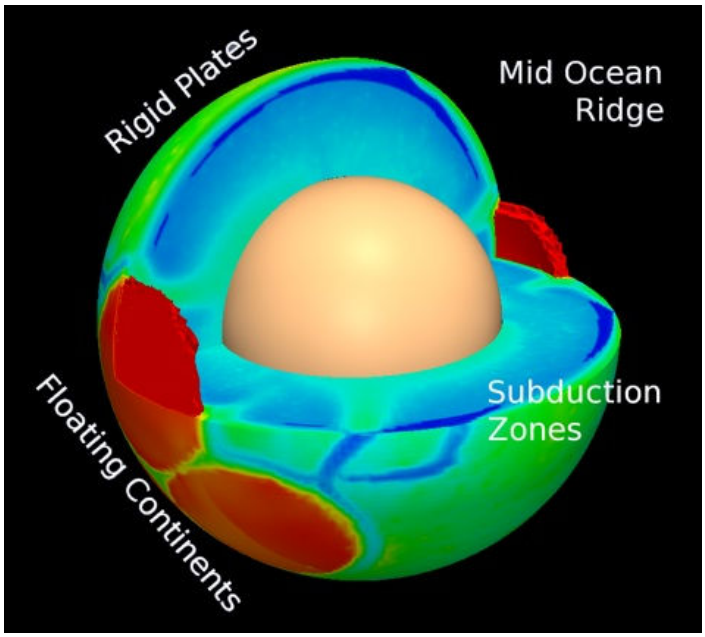


Figure. Numerical simulation of plate tectonics with buoyant continents in 3-D spherical geometry. Plotted is effective viscosity (red=high to blue=low).

References: Rolf, T., N. Coltice and P. J. Tackley (2012) EPSL. 351-352. 134-146.; (ii) Coltice, N., T. Rolf, P. J. Tackley and S. Labrosse (2012) Science 336, 6079, 335-338, (iii) Coltice, N., M. Seton, T. Rolf, R.D. Müller and P.J. Tackley, in press, EPSL, (iv) Coltice, N., T. Rolf and P. J. Tackley, submitted to Geology, (v) Rolf, T., N. Coltice and P. J. Tackley, submitted to Geology.

Title: Self-consistent generation of single-plume state for Enceladus using non-Newtonian rheology

Researchers: A. Rozel, J. Besserer, G.J. Golabek, M. Kaplan, T.W. Becker and P.J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

The thermal dichotomy of Enceladus suggests an asymmetrical structure in its global heat transfer. So far, most of the models proposed that obtained such a distribution have prescribed an a priori asymmetry, i.e. a mechanical anomaly in the south polar ice shell. We present here the first set of numerical simulations of convection that yield a stable single-plume state for Enceladus without prescribed mechanical asymmetry.

Using the convection code StagYY in a 2D-spherical annulus geometry, we show that a non-Newtonian rheology is sufficient to create a localized, single hot plume surrounded by a conductive ice mantle. We obtain a self-sustained state in which a region of small angular extent has a sufficiently low viscosity to allow convection to occur due to the stress-dependent part of the rheological law. We find that the single-plume state is very unlikely to remain stable if the rheology is Newtonian, confirming what has been found by previous studies. Additional simulations with tidal heating (see figure) show that the gravitational influence of Saturn increase the stability field of the single-plume state.

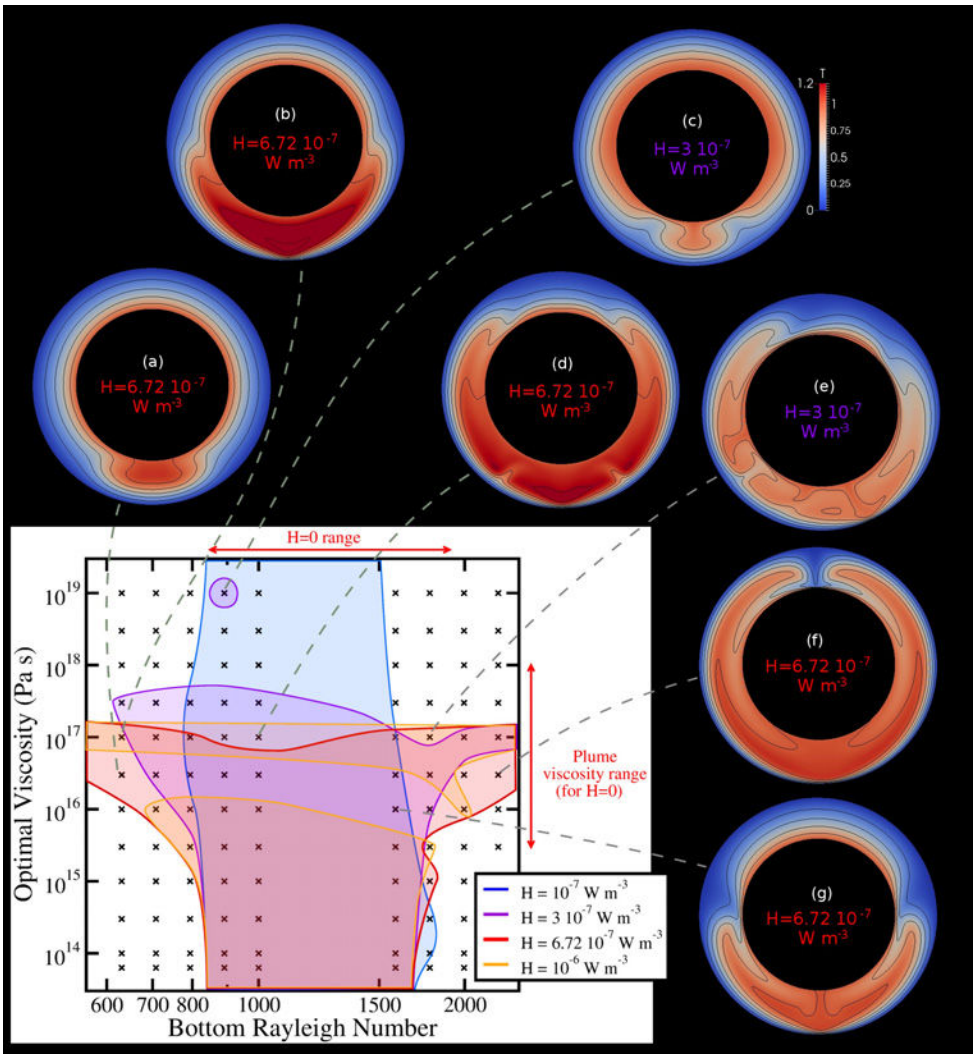


Figure: Stability fields of the single-plume state for different heating rates.

Title: Grain size evolution and convection regimes of the terrestrial planets

Researchers: A. Rozel, G. J. Golabek, E. Boutonnet

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

A new model of grain size evolution has recently been proposed. This new approach stipulates that the grain size dynamics is governed by two additive and simultaneous processes: grain growth and dynamic recrystallization. We use the usual normal grain growth laws for the growth part. For dynamic recrystallization, reducing the mean grain size increases the total area of grain boundaries. Grain boundaries carry some surface tension, so some energy is required to decrease the mean grain size. We consider that this energy is available during mechanical work. It is usually considered to produce some heat via viscous dissipation. A partitioning parameter f is then required to know what amount of energy is dissipated and what part is converted in surface tension.
This study gives a new calibration of the partitioning parameter on major Earth materials involved in the dynamic of the terrestrial planets. Our calibration is in adequation with the published piezometric relations available in the literature (equilibrium grain size versus shear stress). We test this new model of grain size evolution in a set of numerical computations of the dynamics of the Earth using StagYY. We show that the grain size evolution has a major effect on the convection regimes of terrestrial planets.

Figure: Long-term evolution of mantle convection considering the influence of grain size evolution.

Title: Mantle Dynamics on Super-Earths

Researchers: P. J. Tackley
+ external collaborators

Institute/ Group: Institute of Geophysics
Geophysical Fluid Dynamics, D-ERDW

Description:

The discovery of extra-solar ‘‘super-Earth’’ planets with sizes up to twice that of Earth has prompted interest in their possible plate tectonics, mantle dynamics and evolution. The pressures inside these planets are very large, which has a strong influence on the physical properties, particularly viscosity. Here we perform density functional theory (DFT) calculations of the diffusion-creep rheology of the most important rock phase up to a pressure of 1 Tpa, then use this in numerical simulations of super-Earth dynamics for planets with up to 10 Earth masses. Along an adiabat our calculated viscosity would increase by at least 7 order of magnitude. Results confirm the likelihood of plate tectonics for planets with Earth-like surface conditions (temperature and water) and show a self-regulation of deep mantle temperature. The deep mantle is not adiabatic; instead feedback between internal heating, temperature and viscosity regulates the temperature such that the viscosity has the value needed to facilitate convective loss of the radiogenic heat. Convection in large super-Earths is characterised by large upwellings (even with zero basal heating) and small, time-dependent downwellings, which for large super-Earths merge into broad downwellings.

Figure. Temperature (top) and viscosity (bottom) for numerical simulations of super-Earths with from 1 to 10 Earth masses.

References: Tackley, P. J., M. Ammann, J. P. Brodholt, D. P. Dobson and D. Valencia (2013) Mantle dynamics in super-Earths: Post-perovskite rheology and self-regulation of viscosity, Icarus 225(1), 50-61, doi:10.1016/j.icarus.2013.03.013..

Title: Solid-state deformation by large-scale mantle downwellings in asteroid 4 Vesta

Researchers: B.J. Tkalcec, G. J. Golabek, F. E. Brenker

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Diogenites are thought to represent mantle rocks formed as cumulates in magma chambers on 4 Vesta or a very similar differentiated asteroid. Northwest Africa (NWA) 5480 is a rare harzburgitic diogenite meteorite. In contrast to expectations, the results from the olivine-dominated zones can be explained neither by cumulate formation, nor by impact reprocessing near the asteroid's surface. Rather they represent high-temperature solid-state plastic deformation by pencil-glide. This type of lattice-preferred orientation is well known from dry ultramafic rocks on Earth typically formed by mantle convection at temperatures between 1273 and 1523 K. Corresponding 2D finite-difference models indicate that these observations may be explained by large-scale downwellings occurring in the Vestan mantle within the first 50 Ma after formation of Ca–Al-rich inclusions. The discovery of solid-state plastic deformation in an asteroidal ultramafic rock represents the first evidence of dynamic planet-like processes in asteroids. Implications include long-lasting effective mass exchange occurring in the dynamic interiors of differentiated asteroids, such as Vesta, enabling accelerated chemical, structural and thermal equilibration.

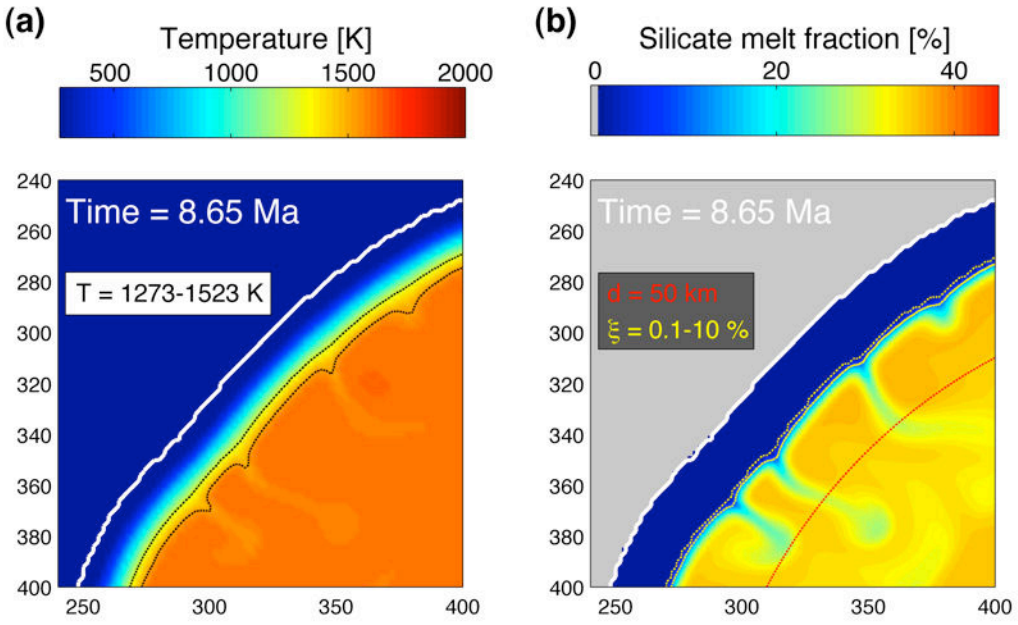


Figure: Early thermochemical evolution of a Vesta-like body displaying regions from which meteorite NWA 5480 could be derived from.

References:

Tkalcec, B. J., G. J. Golabek and F. E. Brenker, Solid-state plastic deformation in the dynamic interior of a differentiated asteroid, *Nature Geosci.*, 6, 93-97, doi:10.1038/ngeo1710, 2013.

Title: Numerical modelling of subduction zones

Researchers: Guizhi Zhu, Katharina Vogt, Taras Gerya, Diana Dymkova, Thibault Duretz, Bettina Baitsch-Ghirardello, Ria Fisher, Sam Chapman, Dave May

Institute: Institute of Geophysics, D-ERDW, ETH-Zurich

Group: Geophysical Fluid Dynamics

Description:
Various aspects of subduction zones dynamics, magmatic activities and fluid regimes are modelled in 2D and 3D with the use of the original codes I2ELVIS and I3ELVIS combining finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations:

- Crustal growth in magmatic arcs (Fig.1) (Zhu et al., 2013; Castro et al., 2013)
- Tectonic transport of sediments by oblique subduction (Malatesta et al., 2012)
- Seismicity of subduction zones (van Dinther et al., 2013; Mikhailov et al., 2013)
- Normal faulting in bending slabs (Naliboff et al., 2013)
- Subduction initiation at passive margins (Marques et al., 2013)
- Subduction of oceanic plateaus (Vogt and Gerya, 2013)
- Reviewing models of Precambrian geodynamics (Gerya, 2013)
- Intra-oceanic subduction styles (Baitsch-Ghirardello et al., 2013)

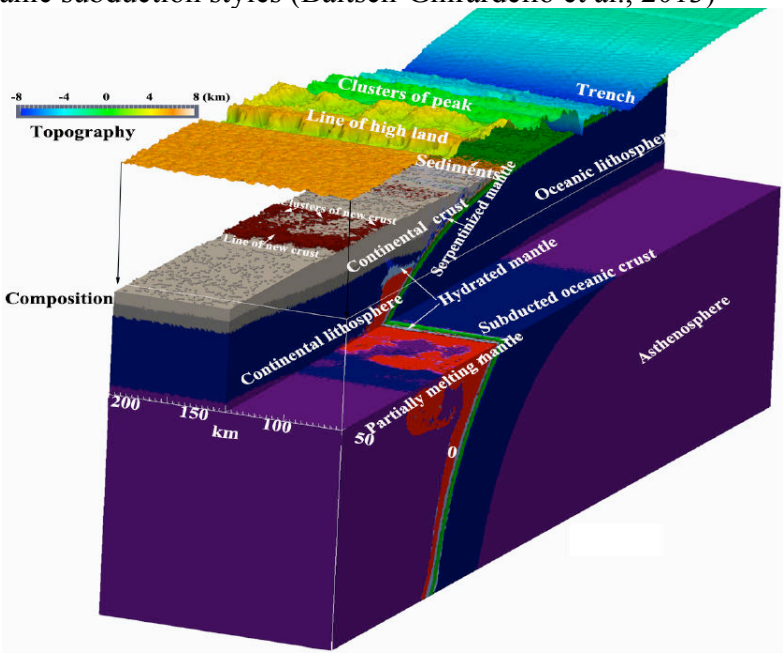


Fig. 1. Crustal growth in subduction zone (Zhu et al., 2013).

References:

Baitsch-Ghirardello, B., Gerya, T.V., Burg, J.-P. (2013) Geodynamic regimes of intra-oceanic subduction: Implications forearc extension vs. shortening processes. Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.11.003

Castro, A., Vogt, K., Gerya, T. (2013) Generation of new continental crust by sublithospheric silicic-magma relamination in arcs: A test of Taylor's andesite model. Gondwana Research, http://dx.doi.org/10.1016/j.gr.2012.07.004. 2012_GR_Antonio.pdf

Gerya, T.V. (2013) Precambrian geodynamics: Concepts and models. Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.11.008

Malatesta, C., Gerya, T., Crispini, L., Federico, L., Capponi, G. (2013) Oblique subduction modelling indicates along-trench tectonic transport of sediments. Nature Communications, 4, Article number: 2456.

Marques, F.O., Nikolaeva, K., Assumpcao, M., Gerya, T.V, Bezerra, F.H.R., do Nascimento, A.F., Ferreira, J.M. (2013) Testing the influence of far-field topographic forcing on subduction initiation at a passive margin. Tectonophysics, DOI: doi:10.1016/j.tecto.2013.08.035a.

Mikhailov, V., Lyakhovsky, V., Panet, I., van Dinther, Y., Diament, M., Gerya, T.V., deViron, O., and Timoshkina, E. (2013). Numerical modelling of post-seismic rupture propagation after the Sumatra 26.12.2004 earthquake constrained by GRACE gravity data, Geophysical Journal International, 194 (2): 640-650, doi:10.1093/gji/ggt145. 2013_GJI_Sumatra.pdf

Naliboff, J.B., Billen, M.I., Gerya, T., Saunders, J. (2013) Dynamics of outer rise faulting in oceanic-continental subduction systems. Geochemistry, Geophysics, Geosystems, DOI: 10.1002/ggge.20155. 2013_G3_John.pdf

van Dinther, Y., Gerya, T.V., Dalguer, L.A., Corbi, F., Funiciello, F., Mai, P.M. (2013) The seismic cycle at subduction thrusts: 2. Dynamic implications of geodynamic simulations validated with laboratory models. J. Geophys. Res., DOI: 10.1029/2012JB009479.

Vogt, K., Gerya, T.V. (2013) From oceanic plateaus to allochthonous terranes: Numerical modelling, Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.11.002 2012_GR_Katharina.pdf

Zhu, G., Gerya, T.V., Tackley, P.J., Kissling, E. (2013) 4-D Numerical modeling of crustal growth at active continental margins. Journal of Geophysical Research, DOI: 10.1002/jgrb.50357.

Title: Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12

Researchers: L.J. Smith
W.F. van Gunsteren*
J.R. Allison*

Institute/ Group: Inorganic Chemistry Laboratory, University of Oxford, United Kingdom
Laboratory of Physical Chemistry, ETH Zürich, Switzerland*

Description:

Molecular dynamics simulations have been used to characterise the binding of the fatty acid ligand palmitate in the barley lipid transfer protein 1 (LTP) internal cavity. Two different palmitate binding modes (1 and 2), with similar protein-ligand interaction energies, have been identified using a variety of simulation strategies. These strategies include applying experimental protein-ligand atom-atom distance restraints during the simulation, or protonating the palmitate ligand, or using the vacuum GROMOS 54B7 force-field parameter set for the ligand during the initial stages of the simulations. In both the binding modes identified the palmitate carboxylate head group hydrogen bonds with main chain amide groups in helix A, residues 4 to 19, of the protein. In binding mode 1 the hydrogen bonds are to Lys 11, Cys 13, and Leu 14 and in binding mode 2 to Thr 15, Tyr 16, Val 17, Ser 24 and also to the OH of Thr 15. In both cases palmitate binding exploits irregularity of the intrahelical hydrogen-bonding pattern in helix A of barley LTP due to the presence of Pro 12. Simulations of two variants of barley LTP, namely the single mutant Pro12Val and the double mutant Pro12Val Pro70Val, show that Pro12 is required for persistent palmitate binding in the LTP cavity. Overall, the work identifies key MD simulation approaches for characterizing the details of protein-ligand interactions in complexes where NMR data provide insufficient restraints.

References: *Prot. Sci.* **22** (2013) 56-64, incl. supp. mat.
DOI: 10.1002/pro.2184

Title: Free enthalpy differences between α-, π-, and 3_{10}-helices of an atomic level fine-grained alanine deca-peptide solvated in supra-molecular coarse-grained water

Researchers: Z. Lin
S. Riniker
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

Atomistic molecular dynamics simulations of peptides or proteins in aqueous solution are still limited to the multi-nanosecond time scale and multi-nanometer range by computational cost. Combining atomic solutes with a supramolecular solvent model in hybrid fine-grained/coarse-grained (FG/CG) simulations allows atomic detail in the region of interest while being computationally more efficient. We used enveloping distribution sampling (EDS) to calculate the free enthalpy differences between different helical conformations, i.e., α-, π-, and 310-helices, of an atomic level FG alanine decapeptide solvated in a supramolecular CG water solvent. The free enthalpy differences obtained show that by replacing the FG solvent by the CG solvent, the π-helix is destabilized with respect to the α-helix by about 2.5 kJ mol−1, and the 310-helix is stabilized with respect to the α-helix by about 9 kJ mol−1. In addition, the dynamics of the peptide becomes faster. By introducing a FG water layer of 0.8 nm around the peptide, both thermodynamic and dynamic properties are recovered, while the hybrid FG/CG simulations are still four times more efficient than the atomistic simulations, even when the cutoff radius for the nonbonded interactions is increased from 1.4 to 2.0 nm. Hence, the hybrid FG/CG model, which yields an appropriate balance between reduced accuracy and enhanced computational speed, is very suitable for molecular dynamics simulation investigations of biomolecules.

References: *J. Chem. Theory Comput.* **9** (2013) 1328-1333
DOI: 10.1021/ct3010497

Title: Efficient combination of environment change and alchemical perturbation within the enveloping distribution sampling (EDS) scheme: twin system EDS and application to the determination of octanol-water partition coefficients

Researchers: N. Hansen
P.H. Hünenberger
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

The methodology of Enveloping Distribution Sampling (EDS) is extended to probe a single-simulation alternative to the thermodynamic cycle that is standardly used for measuring the effect of a modification of a chemical compound, e.g. from a given species to a chemical derivative for a ligand or solute molecule, on the free-enthalpy change associated with a change in environment, e.g. from the unbound state to the bound state for a protein-ligand system or from one solvent to another one for a solute molecule. This alternative approach relies on the coupled simulation of two systems (computational boxes) 1 and 2, and the method is therefore referred to as twin-system EDS. Systems 1 and 2 account for the two choices of environment. The end states of the alchemical perturbation for the twin-system associate the two alternative forms X and Y of the molecule to systems 1 and 2 or 2 and 1, respectively. In this way, the processes of transforming one molecule into the other are carried out simultaneously in opposite directions in the two environments, leading to a change in free enthalpy that is smaller than for the two individual processes and to an energy-difference distribution that is more symmetric. As an illustration, the method is applied to the calculation of octanol-water partition coefficients for C_4 to C_8 alkanes, 1-hexanol and 1,2-dimethoxyethane. It is shown in particular that the consideration of the residual hydration of octanol leads to calculated partition coefficients that are in better agreement with reported experimental numbers.

References: *J. Chem. Theory Comput.* **9** (2013) 1334-1346, incl. supp. mat.
DOI: 10.1021/ct300933y,

Title: Combination of enveloping distribution sampling (EDS) of a soft-core reference-state Hamiltonian with one-step perturbation to predict the effect of side chain substitution on the relative stability of right- and left-helical folds of β-peptides

Researchers: Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

Folding free enthalpies of many not too different polypeptides can be efficiently and accurately predicted with the one-step perturbation (OSP) method using only one or a few molecular dynamics (MD) simulations. In this article, we introduce a combination of enveloping distribution sampling (EDS) and the OSP method (EDSOSP) and apply it to predict the free enthalpy differences between a right-handed 2.7 $_{10/12}$-helix and a left-handed 3_{14}-helix for 16 β-peptides with slightly different side-chain substitution patterns. An EDS simulation of a designed softcore reference-state peptide was carried out in which both helices were sampled. Then, the soft-core atoms were perturbed into physical atoms. Thus, free enthalpy differences between the two helices for the 16 β-peptides can be predicted from only one simulation. The results predicted by EDS-OSP and a previous OSP study are very similar, i.e., the deviations between the results of the 16 peptides are mostly within the order of k_BT, and the average absolute deviation is 1.2 kJ mol^{-1}. Together with the EDS parameter update simulation, about 128ns of MD simulations needed to be carried out using the EDS-OSP method, while 700ns of MD simulations were required in the previous OSP study where two separate reference-state simulations and an additional long time MD simulation of one of the 16 β-peptides were carried out. Thus, the computational effort was significantly reduced, i.e., by more than a factor of 5, using the EDS-OSP method. Hence, we consider this method an efficient tool to predict conformational free enthalpy differences from MD simulations

References: *J. Chem. Theory Comput*. **9** (2013) 126-134
DOI: 10.1021/ct300929q

Title: Structure of hen egg-white lysozyme solvated in TFE/water: a molecular dynamics simulation study based on NMR data

Researchers: A.P. Eichenberger
W.F. van Gunsteren
L.J. Smith*

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland
Inorganic Chemistry Laboratory, University of Oxford, United Kingdom*

Description:

Various experimental studies of hen egg white lysozyme (HEWL) in water and TFE/water clearly indicate structural differences between the native state and TFE state of HEWL, e.g. the helical content of the protein in the TFE state is much higher than in the native state. However, the available detailed NMR studies were not sufficient to determine fully a structure of HEWL in the TFE state. Different molecular dynamics (MD) simulations, i.e. at room temperature, at increased temperature and using proton–proton distance restraints derived from NMR NOE data, have been used to generate configurational ensembles corresponding to the TFE state of HEWL. The configurational ensemble obtained at room temperature using atomatom distance restraints measured for HEWL in TFE/water solution satisfies the experimental data and has the lowest protein energy. In this ensemble residues 50–58, which are part of the β-sheet in native HEWL, adopt fluctuating α-helical secondary structure.

References: *J. Biomol. NMR* **55** (2013) 339-353, incl. supp. mat.
DOI: 10.1007/s10858-013-9717-y

Title: Influence of variation of a side chain on the folding equilibrium of a β-peptide: limitations of one-step perturbation

Researchers: Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

In a recent study (Lin et al., Helv. Chim. Acta 2011, 94, 597), the one-step perturbation method was applied to tackle a challenging computational problem, that is, the calculation of the folding free enthalpies $\Delta G_{F,U}$ of six hepta-β-peptides with different, Ala, Val, Leu, Ile, Ser, or Thr, side chains in the fifth residue. The $\Delta G_{F,U}$ values obtained using one-step perturbation based on a single molecular dynamics simulation of a judiciously chosen reference state with soft-core atoms in the side chain of the fifth residue showed an overall accuracy of about k_BT for the four peptides with nonpolar side chains, but twice as large deviations were observed for the peptides with polar side chains. Here, alternative reference-state Hamiltonians that better cover the conformational space relevant to these peptides are investigated, and post simulation rotational sampling of the χ_1 and χ_2 torsional angles of the fifth residue is carried out to sample different orientations of the side chain. A reference state with rather soft atoms yields accurate $\Delta G_{F,U}$ values for the peptides with the Ser and Thr side chains, but it failed to correctly predict the folding free enthalpy for one peptide with a nonpolar side chain, that is, Leu. Based on the results and those of earlier studies, possible ways to improve the accuracy of the efficient one-step perturbation technique to compute free enthalpies of folding are discussed.

References: *J. Comput. Chem.* **34** (2013) 1899-1906
DOI: 10.1002/jcc.23331

Title: Relative free enthalpies for point mutations in two proteins with highly similar sequence but different folds

Researchers: N. Hansen
J.R. Allison*
F. Hodel
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland
Centre for Theoretical Chemistry and Physics, Massey University Albany, Auckland, New Zealand*

Description:

Enveloping distribution sampling was used to calculate freeenthalpy changes associated with single amino acid mutations for a pair of proteins, G_A95 and G_B95, that show 95% sequence identity yet fold into topologically different structures. Of the L → A, I → F, and L → Y mutations at positions 20, 30, and 45, respectively, of the 56-residue sequence, the first and the last contribute the most to the free-enthalpy difference between the native and non-native sequence-structure combinations, in agreement with the experimental findings for this protein pair. The individual free-enthalpy changes are almost sequence-independent in the fourstrand/one-helix structure, the stable form of G_B95, while in the three-helix bundle structure, the stable form of G_A95, an interplay between residues 20 and 45 is observed.

References: *Biochemistry* **52** (2013) 4962–4970, DOI: 10.1021/bi400272q

Title: The effect of branched side chains on the relative stability of α- and π-helices: a combination of the enveloping distribution sampling and one-step perturbation methods

Researchers: Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

The method of enveloping distribution sampling (EDS) to efficiently obtain free enthalpy differences between different molecular systems from a single simulation can also be used to compute free enthalpy differences between two different conformations of a system. A combination (EDS–OSP) of EDS and the one-step perturbation (OSP) method that yields many free enthalpy differences from a single simulation allows for rapid prediction of conformational free enthalpy differences for many not too different molecular systems from a single simulation. Here, we applied EDS–OSP to predict the free enthalpy differences between a π-helix and an α-helix for a set of four deca-peptides with as fifth residue Ala, Val, Leu, or Ile in aqueous solution. First, an EDS simulation of a designed soft-core reference-state Hamiltonian was carried out to sample both helices in a single simulation. Then the soft-core atoms are perturbed into real atoms of each of the four peptides. Thus, the free enthalpy differences between the π-helix and the α-helix for all four perturbed-state, real peptides can be predicted with only one simulation using EDS–OSP. EDS–OSP and the original EDS method gave very similar free enthalpy values, i.e., the average absolute deviation between the two methods for the four peptides is 0.8 kJ mol^{-1}, while EDS–OSP required almost four times less computational effort. Side chains branched at the C β-position were found to slightly decrease the stability of the α-helical conformation with respect to the π-helical one.

References: *Mol. Phys.* **111** (2013) 2126-2130, incl. supp. Mat.
DOI: 10.1080/00268976.2013.793828

Title: On the use of one-step perturbation to investigate the dependence of different properties of liquid water upon a variation of model parameters from a single simulation

Researchers: S.J. Bachmann
J. Dolenc
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

One-step perturbation is an efficient technique to explore the relation between force-field or model parameters and properties of a molecular system in the condensed phase from a single simulation of the latter using a particular set of model parameters. The accuracy of the prediction of different properties as a function of the extent of perturbation of different model parameters is evaluated using liquid water at ambient temperature and pressure as the test system. The accuracy of predicted changes in free enthalpy, energy, radial distribution functions and dielectric permittivity due to variations in geometric, van der Waals or electrostatic interaction parameters is strongly dependent on the type of property analysed and the type of parameter varied. This is illustrated by the application of one-step perturbation to predict the properties of four models of liquid water from the four ensembles generated for these models.

References: *Mol. Phys.* **111** (2013) 2334-2344,
DOI: 10.1080/00268976.2013.815374

Title: MD simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data

Researchers: L.J. Smith
Y. Roby
J.R. Allison*
W.F. van Gunsteren*

Institute/ Group: Inorganic Chemistry Laboratory, University of Oxford, United Kingdom
Laboratory of Physical Chemistry, ETH Zürich, Switzerland*

Description:

Experimental studies of barley and maize lipid transfer proteins (LTPs) show that the two proteins bind the ligand palmitate in opposite orientations in their internal cavities. Moreover, maize LTP is reported to bind the ligand caprate in the internal cavity in a mixture of two orientations with approximately equal occupancy. Six 30 ns molecular dynamics (MD) simulations of maize and barley LTP with ligands bound in two orientations (modes M and B) have been used to understand the different ligand binding preferences. The simulations show that both maize and barley LTP could bind palmitate in the orientation observed experimentally for maize LTP (mode M), with the predominant interaction being a salt bridge between the ligand carboxylate headgroup and a conserved arginine side chain. However, the simulation of barley LTP with palmitate in the mode B orientation shows the most favorable protein−ligand interaction energy. In contrast, the simulations of maize LTP with palmitate and with caprate in the mode B orientation show no persistent ligand binding, the ligands leaving the cavity during the simulations. Sequence differences between maize and barley LTP in the AB loop region, in residues at the base of the hydrophobic cavity, and in the helix A region are identified as contributing to the different behavior. The simulations reproduce well the experimentally observed binding preferences for palmitate and suggest that the experimental data for maize LTP with caprate reflect ligand mobility in binding mode M rather than the population of binding modes M and B.

References: *Biochemistry* **52** (2013) 5029-5038
DOI: 10.1021/bi4006573

Title: A comparison of calculated and measured relative free enthalpies of folding of twenty amide-to-ester mutants of a small protein

Researchers: A.P. Eichenberger
N. Hansen
S. Riniker
L. von Ziegler
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

The effect of removing a hydrogen-bond donor from the backbone of the 34-residue WW domain of the protein Pin1 is investigated for 20 residues that are part of the three-stranded β-sheet fold of this protein in aqueous solution. Forty-eight molecular dynamics (MD) simulations of the wild-type protein and 20 amide-to-ester mutants started from the X-ray crystal structure and the NMR solution structure are analysed in terms of backbone-backbone hydrogen bonding and differences in free enthalpies of folding in order to provide a structural interpretation of the experimental chaotrope and thermal denaturation data available for this protein and the 20 mutants. The forty enveloping distribution sampling (EDS) simulations of the 20 mutants link the structural Boltzmann ensembles to relative free enthalpies of folding, $\Delta\Delta G_{mw}^{f,u}$, between mutants and wild-type protein. The contribution of the different β -sheet hydrogen bonds to the relative stability of the mutants with respect to wild type cannot be directly inferred from thermal denaturation temperatures or free enthalpies of chaotrope denaturation for the different mutants, because some β-sheet hydrogen bonds show sizeable variation in occurrence between the different mutants.

References: *J. Am. Chem. Soc. (2013) submitted*

Title: A method to apply bond-angle and dihedral-angle constraints in molecular dynamics simulation

Researchers: A.P. Eichenberger
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

A method to apply bond-angle or dihedral-angle constraints in molecular dynamics simulations of macromolecules is presented. It uses Cartesian coordinates and determines the Lagrangian multipliers necessary for maintaining the constraints iteratively. It constitutes an alternative to the use of only distance constraints between particles to maintain a particular geometry. Since the latter are not suitable to maintain particular, e.g. linear or at, geometries of molecules, the presented method offers an alternative to the methods standardly used in such cases. It can easily handle bond-length, bond-angle and dihedral-angle constraints simultaneously, as when calculating a potential of mean force along a dihedral-angle coordinate while applying bond-length constraints throughout the macromolecule.

References: *J. Comput. Chem. (2013) submitted*

Title: Free enthalpy differences between 3_{10}-, α-, and π-helical conformations of deca-alanine in aqueous solution calculated for different force fields using enveloping distribution sampling (EDS)

Researchers: W. Huang
Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

Different helical conformations such as 3_{10}-, α-, and π-helices show different stability in molecular dynamic (MD) simulations using different biomolecular force fields. The method of enveloping distribution sampling (EDS) can be used to efficiently obtain precise values for the free enthalpy differences $\Delta G_{\beta\alpha}$ between 3_{10}-, α-, and π-helical conformations α and β using an alanine deca-peptide solvated in explicit water as illustration. The mentioned free enthalpy differences are computed for three different force fields, *i.e.* the GROMOS force fields 45A3, $53A6_{OXY+N}$ and 54A7, and the results are compared with those calculated earlier for the GROMOS 53A6 force field and for other force fields as reported in the literature. The $\Delta G_{\beta\alpha}$ values appear to be sensitive to changes of partial charges and van der Waals parameters of the backbone atoms of the Ala-deca-peptide. The parameter set $53A6_{OXY+N}$ of the GROMOS force field does not reproduce the experimentally observed trend in helical propensity between α-helical and other helical structures, as was earlier observed for the CHARMM22 parameter set. The other GROMOS parameter sets do pass this biomolecular force field test. The EDS method thus provides an efficient way to test free enthalpy properties of particular biomolecular conformations.

References: *Prot. Sci. (2013) submitted, incl. supp. mat.*

Title: On the behavior of water at subfreezing temperatures in a protein crystal: evidence of higher mobility than in bulk water

Researchers: D. Wang*
A. Böckmann**
J. Dolenc
B. Meier
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland
Inst. High Energy Physics, Chinese Academy of Sciences, Beijing, China*
Inst. de Biologie et Chimie des Proteines, Universite de Lyon, France**

Description:

NMR experiments have shown that water molecules in the crystal of the protein Crh are still mobile at temperatures well below 273K. In order to investigate this water anomaly, a molecular dynamics simulation study of crystalline Crh was carried through to determine the mobility of water in this crystal. The simulations were carried out at three temperatures, 150, 200 and 291K. Simulations of bulk water at these temperatures were also done in order to obtain the properties of the SPC water model used at these temperatures and to allow a comparison of the properties of water in the Crh crystal with those of bulk water at the same temperatures. According to the simulations, water is immobilised at 150K both in crystal and in bulk water. As expected, at 291K it diffuses and rotates slower in the protein crystal than in bulk water. However, at 200K, the translational and rotational mobility of the water molecules is larger in the crystal than in bulk water. The enhancement of water mobility in the crystal at 200K was further investigated by MD simulations in which the backbone or all protein atoms were positionally restrained, and in which additionally the electrostatic proteinwater interactions were removed. Of these changes in the environment of the water molecules, rigidifying the protein backbones slightly enhanced water diffusion, while it slowed down rotation. In contrast, removal of electrostatic protein-water interactions did not change water diffusion, but enhanced rotational motion significantly. Further investigations are required to delineate particular features of the protein crystal that induce the anomalous behaviour of water at 200K.

References: *J. Phys. Chem. (2013) in press, incl. supp. mat.*

Title: Using enveloping distribution sampling (EDS) to compute the folding free enthalpy of a β-peptide with a very unstable folded conformation in solution: the advantage of focused sampling using EDS

Researchers: Z. Lin
C. Necula
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

Peptides and proteins adopt a dynamic ensemble of conformations rather than a single structure in solution, although this ensemble may be dominated by one or a few particular folds. Computer simulation can be used to simulate the folding equilibria of peptides from which free energy differences between different conformations can be calculated. However, standard molecular dynamics (MD) simulation is rather inefficient when the relative free energy of a rather unstable fold is to be calculated. Here, we show, using a hepta-β-peptide with a very unstable 3_{14}-helical conformation as an example, that the method of enveloping distribution sampling (EDS) offers a much more efficient alternative to compute the relative free energy of different folds. The folding free energies obtained using the EDS method are compared to those obtained from a standard MD simulation, from reweighting trajectories generated using hydrogen-bond restraints to enhance the sampling of a particular fold, and from one-step perturbation. The EDS method yields the widest sampling of relevant conformations and shows the fastest convergence.

References: *Chem. Phys. (2013) submitted*

Title: Refinement of the application of the GROMOS 54A7 force field to β-peptides

Researchers: Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

In this study, a hexa-β-peptide whose conformational equilibrium encompasses two different helical folds, a right-handed $2.7_{10/12}$-helix and a left-handed 3_{14}-helix, is simulated using different GROMOS force-field parameter sets. When applying the recently developed GROMOS 54A7 force field, a significant destabilization effect on the $2.7_{10/12}$-helix of the peptide is observed, and the agreement with the experimental NOE distance bounds is much worse compared with the ones using previous versions of the GROMOS force field. This led us to investigate the free enthalpy difference between the two helices as a function of a variation of different subsets of force-field parameters. Both long time molecular dynamics (MD) simulations and one-step perturbation predictions suggest that the disagreement with the experimental NMR data when using the 54A7 force field is caused by the use for β-peptides of the new backbone φ-/ψ- torsional-angle energy terms introduced in this force field which were based on conformational fitting of backbone φ/ψ angles for a large set of proteins. his means that these parameters of backbone φ- and ψ- torsional-angle terms should not be applied to non-α-peptides such as β-peptides. This modified assignment of torsional-angle energy terms and parameters is denoted as 54A7_β. It corrects the wrong description of the conformational ensemble of the hexa-β-peptide obtained using the previous assignment and yields as good agreement with NMR data for other β-peptides that adopt a single helical or a hairpin fold.

References: *J. Comput. Chem. (2013) in press*

Title: Structure and conformational dynamics of the domain 5 RNA hairpin of a bacterial group II intron revealed by solution NMR and molecular dynamics simulations

Researchers: M. Pechlaner
R.K.O. Sigel
W.F. van Gunsteren*
J. Dolenc*

Institute/ Group: Institute of Inorganic Chemistry, University of Zürich, Switzerland
Laboratory of Physical Chemistry, ETH Zürich, Switzerland*

Description:

NMR NOE data obtained for a 35-nucleotide RNA segment of a bacterial group II intron indicate a helical hairpin structure in which three parts, a terminal pentaloop, a bulge, and a G-A mismatch display no Watson-Crick base pairing. The 668 NOE upper-distance bounds for atom pairs are insufficient to uniquely determine the conformation of these segments. Therefore, molecular dynamics simulations including time-averaged distance restraints have been used to obtain a conformational ensemble compatible with the observed NMR data. The ensemble shows alternating hydrogen-bonding patterns for the mentioned segments. In particular in the pentaloop and in the bulge the hydrogen-bonding networks correspond to distinct conformational clusters which could not be captured by using conventional single-structure refinement techniques. This implies that in order to obtain a realistic picture of the conformational ensemble of such flexible biomolecules it is necessary to properly account for the conformational variability in structure refinement of RNA fragments.

References: *Biochemistry (2013) in press, incl. supp. mat.*

Title: On the sensitivity of peptide nucleic acid duplex formation and crystal dissolution to a variation of force-field parameters

Researchers: S.J. Bachmann*
Z. Lin*
T. Stafforst
W.F. van Gunsteren*
J. Dolenc*/**

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland*
Organic Chemistry, ETH Zürich, Switzerland
Faculty of Chemistry Chemical Techn., Uni. of Ljubljana, Slovenia**

Description:

The technique of one-step perturbation to explore the relation between particular force-field parameters on the one hand and particular properties of a biomolecular system on the other hand from one or a few molecular dynamics simulations is applied to investigate the dependence of the free enthalpy of dimer formation and of crystal dissolution of a self-complementary fragment (*H-CGTACG-NH$_2$*) of peptide nucleic acid, PNA, a mimic of DNA. The simulations result that PNA dimer formation in aqueous solution is favoured by a decrease of the base charges with respect to values of the GROMOS 45A4 force-field, while it is disfavoured by a decrease of the backbone charges. In contrast crystal dissolution of the PNA dimer is favoured by a decrease in base charges, while a variation of backbone charges has a minor effect on this free enthalpy change. These opposite effects in crystalline versus aqueous solution environment can be understood from the different water contents for these systems and have consequences for biomolecular force-field development.

References: *J. Chem. Theory Comput. (2013) submitted*

Title: Enhanced conformational sampling using enveloping distribution sampling

Researchers: Z. Lin
W.F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland

Description:

To lessen the problem of insufficient conformational sampling in biomolecular simulations is still a major challenge in computational biochemistry. In this article, an application of the method of enveloping distribution sampling (EDS) is proposed that addresses this challenge and its sampling efficiency is demonstrated in simulations of a hexa-β-peptide whose conformational equilibrium encompasses two different helical folds, *i.e.* a right-handed $2.7_{10/12}$-helix and a left-handed 3_{14}-helix, separated by a high energy barrier. Standard MD simulations of this peptide using the GROMOS 53A6 force field did not reach convergence of the free enthalpy difference between the two helices even after 500ns of simulation time. The use of soft-core non-bonded interactions in the centre of the peptide did enhance the number of transitions between the helices, but at the same time led to neglect of relevant helical configurations. In the simulations of a two-state EDS reference Hamiltonian that envelops both the physical peptide and the soft-core peptide, sampling of the conformational space of the physical peptide ensures that relevant conformations can be visited, and sampling of the conformational space of the soft-core peptide helps to enhance the transitions between the two helices. The EDS simulations sampled many more transitions between the two helices and showed much faster convergence of the relative free enthalpy of the two helices compared with the standard MD simulations with only a slightly larger computational effort to determine optimal EDS parameters. Combined with various methods to smoothen the potential energy surface, the proposed EDS application will be a powerful technique to enhance the sampling efficiency in biomolecular simulations.

References: *J. Chem. Phys. (2013) in press*

Title: Whole-mantle radial anisotropy from joint inversion of multi-mode surface wave dispersion and body wave traveltimes

Researchers: L. Auer, L. Boschi, T. Nissen-Meyer

Institute/ Group: Institute of Geophysics
Group for Seismology and Geodynamics

Description:

In the last decades, independently derived seismic tomography models of isotropic Shear wave velocity of the earths mantle have advanced to a state of considerable consistency. It is well known, however, that a simple isotropic description of the elastic properties and their interpretation in terms of fast and slow (cold and hot) velocity anomalies is inadequate and elastic anisotropy is non-negligible at various regions. Global anisotropic tomography is only in its infancy and the few published models of whole-mantle radial anisotropy agree with each other only for low harmonic degrees. In this project, we aim to contribute to the ongoing effort to establish a consensus on a long-spatial-wavelength model of radially anisotropic 3-D whole-mantle structure, by inverting a comprehensive suite of recently published surface and body wave datasets. Additionally, we perform an extensive quantitative comparison of our new results with previously published models. We employ surface wave phase delays from fundamental modes up to the 6th overtone measured in periods between 35 and 300 s, as well as a state of the art cross-correlation datasets of a variety of body wave phases.

Inverting the kernel matrix is computationally intensive and thus we parallelize the involved Cholesky factorization, in a multithreading context, using OpenMP. Our new tomographic solution is based on classical ray-based linearized tomography, a radially anisotropic block parameterization, and non-linear crustal corrections, and shares various features with other independently derived models, such as the intriguing anomaly of faster V_{SH} ($\xi > 1$; horizontal flow) in the Central Pacific and an anomaly of faster V_{SV} ($\xi < 1$; vertical flow) beneath the East Pacific Rise. In the near future we will replace our ray-theoretical sensitivities with numerical finite- frequency kernels, and work is underway to migrate from a uniform inversion grid to a 3-D data-adaptive multi- resolution parameterization, so as to mitigate problems associated with the inhomogeneous distribution of sources and receivers.

References: A manuscript is in preparation for *Geochemistry, Geophysics, Geosystems (G^3)*

6

High-performance Hardware

6.1 C4: The Year in Review

The Competence Center for Computational Chemistry (C4) is a network of researchers of the IBM Zürich Research Laboratory, the University of Zürich, and the ETH Zürich. The goal of C4 is to assist the search for new frontiers and opportunities in molecular modeling and simulation, to cater to the flow of know-how within this growing community, and to serve as a platform for the interaction with partners from other areas of science or from outside academia. Today, the C4 network covers a broad spectrum of research activities involving about fifteen research groups from ten different institutes (see also www.c4.ethz.ch).

The C4 Steering Committee
The Steering Committee consists of Prof. Alessandro Curioni, head of computational sciences at IBM Zürich Research, Profs. Jürg Hutter (University of Zürich), and PD Dr. Hans P. Lüthi (ETH Zürich).

C4 Seminar
The actual "backbone" of C4 is its Seminar Program. During the 2012 Fall- and 2013 Spring-Term the C4 Seminar Program covered 11 lectures, again some of them presented by leaders in the field of computational chemistry. The seminar enjoys a remarkable popularity bringing together between forty and sixty students and researchers each time. One C4 seminar was hosted by the IBM Research Lab, another three seminars were hosted by the University of Zürich.

Compute Resource
Since many of the members of the computational chemistry community have their own computing facilities, or were granted compute time by the Centro Svizzero die Calcolo Scientifico (CSCS), the compute resource offered by C4 in recent years became less and less "mission critical". C4 holds a number of nodes on the ETH Brutus cluster that are open to all ETH computational chemists.

C4 Tutorials
With CECAM being established in Switzerland, the offering for tutorials and workshops has increased considerably, both, in number and in the spectrum of topics covered. The CECAM Zurich node is lead by our colleague Prof. Matthias Troyer of the Institute of Theoretical Physics. C4 did not offer its own tutorials.

The IBM Research Award
In 2007, the ETH Schulleitung approved the "IBM Research Forschungspreis", an award for outstanding MSc and PhD theses sponsored by the IBM Zürich Research Laboratory. This year, the prize was awarded to Konrad Marti of the group of Prof. Markus reiher for his PhD thesis entitled "New Electron Correlation Theories and Haptic Exploration of Molecular Systems".

The 2012 Award Ceremony took place at the ETH Tag with the Rector, Prof. Lino Guzzella, handing out the award to the winner. The laureate also presented his research at the occasion of a special C4 Seminar held at the IBM Research Lab in Rüschlikon.

The 7th Molecular Quantum Mechanics Congress, held in Lugano in June of 2013, was the second big global computational chemistry event held in Switzerland after the WATOC 2002. The event, organized by Hans P. Lüthi, traditionally has a strong focus on method

development in electronic structure theory, and brought more than 320 scientists to Switzerland. See also www.mqm2013.ethz.ch.

Outlook
A network such as C4 plays an important role when it comes to the exchange of information within a relatively large and distributed community. Modeling and Simulation have become established tools also for researchers with an experimental background, and the C4 network gives them access to the state-of-the-art methodologies and computational know-how. Also in the next year we will make sure that C4 is a valuable platform for its stakeholders.

Hans P. Lüthi, Leiter C4
November 5, 2013

6.2 Information Technology Services

The following resource is available:

The IT Services operate BRUTUS, a Linux cluster co-financed by over 60 professors in the departments of Chemistry (D-CHAB); Biology (D-BIOL); Physics (D-PHYS); Environmental Sciences (D-USYS); Earth Sciences (D-ERDW); Mathematics (D-MATH); Material Sciences (D-MATL); Mechanical and Process Engineering (D-MAVT); Civil, Environmental and Geomatic Engineering (D-BAUG); Management, Technology and Economics (D-MTEC); Health Sciences and Technology (D-HEST); Computer Science (D-INFK); and Humanities, Social and Political Sciences (D-GESS).

The share of the cluster financed by IT Services is made available to the whole scientific community of ETH at no cost. Other "shareholders" are guaranteed a share of CPU time proportional to their investment.

The BRUTUS cluster consists of the following node types:

Standard nodes
120 nodes with four 12-core AMD Opteron 6174 CPUs and 64 GB of RAM (5'760 cores)
24 nodes with two 12-core AMD Opteron 6174 CPUs and 32 GB of RAM (576 cores)
410 nodes with four quad-core AMD Opteron 8380 CPUs and 32 GB of RAM (6'560 cores)
80 nodes with four quad-core AMD Opteron 8384 CPUs and 32 GB of RAM (1'280 cores)

Large-memory (fat) nodes
6 nodes with four 8-core Intel Xeon E7-8837 CPUs and 1024 GB of RAM (192 cores)
80 nodes with four 12-core AMD Opteron 6174 CPUs and 256 GB of RAM (3'840 cores)
10 nodes with four quad-core AMD Opteron 8380 CPUs and 128 GB of RAM (160 cores)

GPU nodes
18 nodes with two 12-core AMD Opteron 6174 CPUs, 32 GB of RAM and 2 Nvidia Fermi C2050 CPUs (432 cores + 36 GPUs)
2 nodes with two 6-core AMD Opteron 2435 CPUs, 32 GB of RAM and various Nvidia and AMD GPUs (24 cores + 2 GPUs)

Legacy nodes
256 nodes with two dual-core AMD Opteron 2220 CPUs and 16 GB of RAM (1'024 cores)

This is a total of 19'848 cores. The peak performance of the cluster is over 200 teraflops.

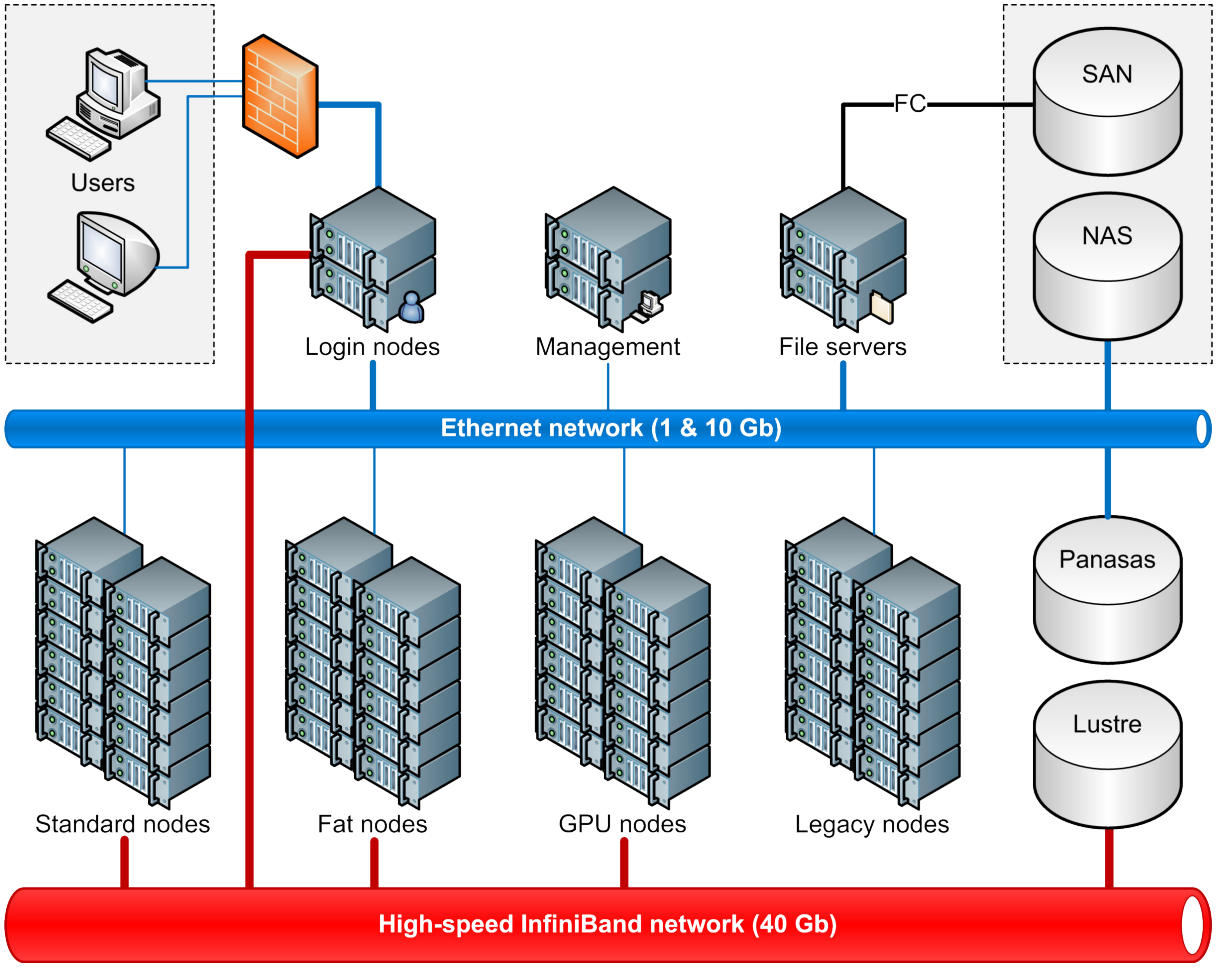
A high performance Lustre parallel file system with a capacity of over 400 TB is available for I/O-intensive computations with large files. A Panasas parallel file system with more than 70 TB of capacity is available for medium and large files.

All compute nodes are connected to the cluster's Ethernet backbone via 1Gb links.
The login nodes are connected to this backbone and to the ETH network via 10Gb links.
All nodes except legacy nodes are connected to a high-speed/low-latency InfiniBand QDR network.

The NFS file servers, the Panasas file system and the ETH's NAS are connected to the cluster's Ethernet backbone via 10Gb links.
The Lustre file system is connected directly to the cluster's InfiniBand QDR network.

Compute nodes connected to the InfiniBand network are intended for parallel computations (typically MPI based) requiring high bandwidth and/or low latency communication. These nodes can also be used for shared-memory applications requiring up to 48 cores and/or 64, 256 or 1024 GB of memory.
Legacy nodes connected via Ethernet only are used for single-processor computations.

Schematic view of the BRUTUS cluster:



7

Publications* in 2012/2013

*only CSE-related articles
in refereed journals

Group of P. Arbenz

H. Guo, P. Arbenz, B. Oswald: *A large-scale nonlinear eigensolver for the analysis of dispersive nanostructures*. Computer Phys. Comm. 184 (8): 1898-1906 (2013).

E. Turan, P. Arbenz: *Preconditioning aspects of large scale micro finite element analysis of 3D bone poroelasticity*. Parallel Computing, 2013, doi:10.1016/j.parco.2013.09.002.

P. Arbenz, E. Turan: *Preconditioning for large scale micro finite element analyses of 3D poroelasticity*. In: Applied Parallel and Scientific Computing (PARA 2012). P. Manninen, P. Öster (eds.). Lecture Notes in Computer Science 7782, pp. 361–374. Springer, Heidelberg, 2013.

P. Arbenz, D. Hupp, D. Obrist: *A parallel solver for the time-periodic Navier–Stokes equations*. In Parallel Processing and Applied Mathematics (PPAM 13). R. Wyrzykowski (ed.). Lecture Notes in Computer Science. To appear.

C. Flaig, P. Arbenz: *A highly scalable matrix-free multigrid solver for μFE analysis based on a pointer-less octree*. In Large Scale Scientific Computing LSSC'11. I. Lirkov, S. Margenov, J. Waśniewski (eds.). Lecture Notes in Computer Science 7116, pp. 498–506. Springer, Heidelberg, 2012.

C. Bekas, A. Curioni, P. Arbenz, C. Flaig, G.H. van Lenthe, R. Müller, A.J. Wirth: *Massively parallel graph partitioning: A case in human bone simulations*. In Combinatorial Scientific Computing. Uwe Naumann, Olaf Schenk (eds.). Chapman and Hall/CRC, 2012. pp. 407–425.

Y. Ineichen, A. Adelmann, C. Bekas, A. Curioni, P. Arbenz: *A fast and scalable low dimensional solver for charged particle dynamics in large particle accelerators*. Comput. Sci. Res. Dev. 27 (2012), doi:10.1007/s00450-012-0216-2.

A. Adelmann, P. Arbenz, Y. Ineichen: *Improvements of a fast parallel Poisson solver on irregular domains*. In Applied Parallel and Scientific Computing (PARA 2010). K. Jónasson (ed.). Part I, Lecture Notes in Computer Science 7133, pp. 65–74. Springer, Heidelberg, 2012.

P. Arbenz, A. Hiltebrand, D. Obrist: *A parallel space-time finite difference solver for periodic solutions of the shallow-water equation*. In Parallel Processing and Applied Mathematics (PPAM 11) Part II. R. Wyrzykowski, J. Dongarra, K. Karczewski, J. Waśniewski (eds.). Lecture Notes in Computer Science 7204, pp. 302–312. Springer, Berlin, 2012.

C. Kraus, A. Adelmann, P. Arbenz: *Perfectly matched layers in a divergence preserving ADI scheme for electromagnetics*. J. Comput. Phys. 231 (1): 39–44 (2012).

H. Guo, B. Oswald, P. Arbenz: *3-dimensional eigenmodal analysis of plasmonic nanostructures*. Optics Express. 20 (5): 5481-5500 (2012)

H. Guo, P. Arbenz, B. Oswald: *Realistic 3-dimensional eigenmodal analysis of electromagnetic cavities using surface impedance boundary conditions.* Proceedings of ICAP2012, Rostock-Warnemünde, Germany, 2012.

A.J. Wirth, J. Goldhahn, C. Flaig, P. Arbenz, R. Müller, G.H. van Lenthe: *Implant stability is affected by local bone microstructural quality.* Bone 49 (3): 473–478 (2011).

C. Flaig, P. Arbenz: *A scalable memory efficient multigrid solver for micro-finite element analyses based on CT images.* Parallel Computing 37 (12): 846-854 (2011).

C. Bekas, A. Curioni, P. Arbenz, C. Flaig, G.H. van Lenthe, R. Müller, A.J. Wirth: *Extreme scalability challenges in micro-finite element simulations of human bone.* Concurrency and Computation: Practice and Experience 22 (16): 2282–2296 (2010).

A.J. Wirth, Th.L. Mueller, W. Vereecken, C. Flaig, P. Arbenz, R. Müller, G.H. van Lenthe: *Mechanical competence of bone-implant systems can accurately be determined by image-based micro-finite element analyses.* Arch. Appl. Mech. 80 (5): 513–525, 2010.

A. Adelmann, P. Arbenz, Y. Ineichen: *A Fast Parallel Poisson Solver on Irregular Domains Applied to Beam Dynamic Simulations*, J. Comp. Phys. 229 (12): 4554–4566 (2010)

H. Guo, A. Adelmann, P. Arbenz, A. Falone, C. Kraus, B. Oswald: *Computation of Electromagnetic Modes in the Transverse Deflecting Cavity.* Proceedings of the 2010 International Particle Accelerator Conference (IPAC), Kyoto, Japan, May 23-28, 2010.

D. Obrist, R. Henniger, P. Arbenz: *Parallelization of the time integration for time-periodic flow problems.* Proc. Appl. Math. Mech. 10 (1): 567–568 (2010).

Group of S. Bonhoeffer

Publication list Group Bonhoeffer

1. Ona, L, Kouyos, RD, Lachmann, M, **Bonhoeffer, S** (2013)
On the role of resonance in drug failure under HIV treatment interruption
THEORETICAL BIOLOGY AND MEDICAL MODELLING 10:-

2. Stadler, T, **Bonhoeffer, S** (2013)
Uncovering epidemiological dynamics in heterogeneous host populations using phylogenetic methods
PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B-BIOLOGICAL SCIENCES 368:-

3. Saenz, RA, **Bonhoeffer, S** (2013)
Nested model reveals potential amplification of an HIV epidemic due to drug resistance
EPIDEMICS 5:34-43

4. Moslonka-Lefebvre, M, **Bonhoeffer, S**, Alizon, S (2013)
Weighting for sex acts to understand the spread of STI on networks (vol 311, pg 46, 2012)
JOURNAL OF THEORETICAL BIOLOGY 317:429-429

5. Stadler, T, Kuhnert, D, **Bonhoeffer, S**, Drummond, AJ (2013)
Birth-death skyline plot reveals temporal changes of epidemic spread in HIV and hepatitis C virus (HCV)
PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA 110:228-233

6. Alexander, HK, **Bonhoeffer, S** (2012)
Pre-existence and emergence of drug resistance in a generalized model of intra-host viral dynamics
EPIDEMICS 4:187-202

7. Moslonka-Lefebvre, M, **Bonhoeffer, S**, Alizon, S (2012)
Weighting for sex acts to understand the spread of STI on networks
JOURNAL OF THEORETICAL BIOLOGY 311:46-53

8. Cadosch, D, **Bonhoeffer, S**, Kouyos, R (2012)
Assessing the impact of adherence to anti-retroviral therapy on treatment failure and resistance evolution in HIV
JOURNAL OF THE ROYAL SOCIETY INTERFACE 9:2309-2320

9. Arnoldini, M, Mostowy, R, **Bonhoeffer, S**, Ackermann, M (2012)
Evolution of Stress Response in the Face of Unreliable Environmental Signals
PLOS COMPUTATIONAL BIOLOGY 8:-

10. Mostowy, R, Kouyos, RD, Hoof, I, Hinkley, T, Haddad, M, Whitcomb, JM, Petropoulos, CJ, Kesmir, C, **Bonhoeffer, S** (2012)
Estimating the Fitness Cost of Escape from HLA Presentation in HIV-1 Protease and Reverse Transcriptase
PLOS COMPUTATIONAL BIOLOGY 8:-

11. Kouyos, RD, Leventhal, GE, Hinkley, T, Haddad, M, Whitcomb, JM, Petropoulos, CJ, **Bonhoeffer, S** (2012)
Exploring the Complexity of the HIV-1 Fitness Landscape
PLOS GENETICS 8:-

12. Leventhal, GE, Kouyos, R, Stadler, T, von Wyl, V, Yerly, S, Boni, J, Cellerai, C, Klimkait, T, Günthard, HF, **Bonhoeffer, S** (2012)
Inferring Epidemic Contact Structure from Phylogenetic Trees
PLOS COMPUTATIONAL BIOLOGY 8:-

13. Stadler, T, Kouyos, R, von Wyl, V, Yerly, S, Boni, J, Burgisser, P, Klimkait, T, Joos, B, Rieder, P, Xie, D, Günthard, HF, Drummond, AJ, **Bonhoeffer, S** (2012)
Estimating the Basic Reproductive Number from Viral Sequence Data
MOLECULAR BIOLOGY AND EVOLUTION 29:347-357

Group of K. Boulouchos publications

1. A. Brambilla, C.E. Frouzakis, J. Mantzaras, R. Bombach, K. Boulouchos, Flame dynamics in lean premixed CO/H_2/air combustion in a mesocale channel, *Combust. Flame*, (accepted)

2. F. Lucci, C.E. Frouzakis, J. Mantzaras, Three-dimensional direct numerical simulation of turbulent channel flow catalytic combustion of hydrogen over platinum, *Proc. Combust. Inst.* 34, 2295-2302, 2013

3. S. G. Kerkemeier, C. N. Markides, C.E. Frouzakis, K. Boulouchos, Direct Numerical Simulation of the Autoignition of a Hydrogen Plume in a Turbulent Co-flow of Hot Air, *J. Fluid Mech.*, 720, 424-456, 2013

4. Chikatamarla S. and Karlin I., Entropic lattice Boltzmann method for turbulence: Wall boundary conditions. *Physica A.*, 392,1925-1930 (2013)

5. Gu C., Chikatamarla S. and Karlin I., 3D Simulation of turbulent flow past a circular cylinder in resolved and under-resolved regimes using ELBM. *Intl. J. Modern Phys. C*, 25, No. 1, 1340024 (2014).

6. Karlin I. V, Sichau D, Chikatamarla S. S,Consistent two-population lattice Boltzmann model for thermal flows, *Physical Review E*, (submitted, 2013)

7. Chikatamarla S.S, Duenser S, Karlin I.V, ELBM simulation of flow past a surface mounted cube, *Intl. Journal of Modern Physics C*, (in preparation, 2013)

8. Boesch, F. and Karlin, I.V., Exact lattice Boltzmann equation, *Phys. Rev. Lett.*, 111, 090601 (2013)

9. Mendoza, M., Karlin, I., Succi, S., Herrmann, H.J., Ultrarelativistic transport coefficients in two dimensions, *J. Stat. Mech.* P02036 (2013)

10. Mendoza, M., Karlin, I., Succi, S., Herrmann, H.J., Relativistic lattice Boltzmann model with improved dissipation, *Phys. Rev. D.*, 87(6), 065027 (2013) (2013)

11. Singh, S., Krithivasan, S., Karlin, I., Succi, S., Ansumali, S., Energy conserving lattice Boltzmann models for incompressible flow simulations, *Commun. Comput. Phys.* 13(3), 603 (2013)

Swiss Seismological Service / Group of S. Wiemer / Group of D. Giardini

P. Galvez, J-P Ampuero, L.A. Dalguer, S. Somala and T. Nissen-Meyer. Dynamic earthquake rupture modeled with an unstructured 3D spectral element method applied to the 2011 Mw9 Tohoku earthquake, to be submitted in Geophysical Journal International (2013).

van Dinther, Y., Gerya, T., Dalguer, L., Corbi, F., Funiciello, F., and Mai, P. (2013). The seismic cycle at subduction thrusts: 2. Dynamic implications of geodynamic simulations validated with laboratory models, JGR, 118(4), 1502–1525, doi:10.1029/2012JB009479.

van Dinther, Y., Gerya, T., Dalguer, L., Mai, P.M., Morra, G., Giardini, D. (in press). The seismic cycle at subduction thrusts: insights from seismo-thermo-mechanical models, JGR.

van Dinther, Y., Gerya, T., Dalguer, L., Mai, P.M., Morra, G., Giardini, D. (submitted). Modeling the seismic cycle in subduction zones: the role of off-megathrust events, GRL.

S. Song, and L.A. Dalguer (2013). Importance of 1-point statistics in earthquake source modeling for ground motion simulation, *Geophys. J. Int.*, 192, 1,255-1,270.

S. Song, L.A. Dalguer, and P.M. Mai (2013). Pseudo-dynamic source modeling with 1-point and 2-point statistics of earthquake source parameters, *Geophys. J. Int.*, in revision.

Group of Ch. Hafner

Reviewed Journals

1. ***D. Psychogiou, Y. Li, J. Hesselbarth, D. Peroulis, C. Hierold, Ch. Hafner****, Continuously variable W-band phase shifters based on MEMS-actuated conductive fingers, International Journal of Microwave and Wireless Technologies, Vol. 5, Issue 04, pp.477-489, August 2013.*
2. ***Y. Li, D. Psychogiou, S. Kuhne, J. Hesselbarth, Ch. Hafner, C. Hierold****, Large Stroke Staggered Vertical Comb-Drive Actuator for the Application of a Millimeter-Wave Tunable Phase Shifter, IEEE Journal of Microelectromechanical Systems, Vol. 22, Issue 4, pp.962-975, August 2013.*
3. ***D. Psychogiou, D. Peroulis****, Reconfigurable bandpass filter with center frequency and bandwidth control, Microwave and Optical Technology Letters, Vol. 55, Issue 11, pp.2745-2750, August 2013.*
4. ***N. Dolatsha, J. Hesselbarth****, Millimeter-wave Antenna Array fed by an Insulated Image Guide Operating in Higher-Order Ex11 Mode, IEEE Trans. Antenna Propagation, Vol. 61, Issue 6, pp.1-5, June 2013.*
5. ***D. Psychogiou, D. Peroulis, Y. Li, Ch. Hafner****, V-band bandpass filter with continuously variable centre frequency, IET Microwaves, Antennas & Propagation, Vol. 7, Issue 8, pp.701 - 707, June 2013.*
6. ***D. Psychogiou, Y. Li, J. Hesselbarth, S. Kühne, D. Peroulis, C. Hierold, Ch. Hafner****, Millimeter-wave phase shifter based on waveguide-mounted RF-MEMS, Microwave and Optical Technology Letters, Vol. 55, Issue 3, pp.465-468, March 2013.*
7. ***C. Beyer, P. Christen, I. Jelesarov, J. Fröhlich****, Experimental System for Real-Time Assessment of Potential Changes in Protein Conformation Induced by Electromagnetic Fields, Bioelectromagnetics, pp.DOI: 10.1002/bem.21795, 2013.*
8. ***Mengyu Wang, Kersten Schmidt, Aytac Alparslan, Christian Hafner****, hp-FEM and PML analysis of plasmonic particles in layered media, PIER (Progress In Electromagnetics Research), Vol. 142, pp.523-544, 2013.*
9. ***M. Boyvat, Ch. Hafner****, Magnetic Field Shielding by Metamaterials, PIER (Progress In Electromagnetics Research), Vol. 136, pp.647-664, 2013.*
10. ***M. Husnik, S. Linden, R. Diehl, J. Niegemann, K. Busch, M. Wegener****, Quantitative experimental determination of scattering and absorption cross-section spectra of individual optical metallic nanoantennas, Phys. Rev. Lett., Vol. 109, Issue 23, pp.233902, December 2012.*
11. ***S. G. Huwiler, C. Beyer, J. Fröhlich, Hauke Hennecke, T. Egli, D. Schürmann, H. Rehrauer, H.-M. Fischer****, Genome-wide transcription analysis of Escherichia coli in response to extremely low-frequency magnetic fields, Bioelectromagnetics, Vol. 33, Issue 6, pp.488-496, September 2012.*

Group of D. Helbing

List of publications in 2012 and 2013:

- D. Brockmann and D. Helbing (2013) “The hidden geometry of complex, network-driven contagion phenomena.” Science, in print.
- D. Helbing (2013). “Globally networked risks and how to respond.” Nature, 497, 51–59.
- Leduc, C., K. Padberg-Gehle, V. Varga, D.Helbing, S. Diez, and J. Howard (2012) “Molecular crowding creates traffic jams of kinesin motors on microtubules.” PNAS 16: 6100-6105.
- R. Bhavnani, K. Donnay, D. Miodownik, M. Mor, and D. Helbing (2013) Group segregation and urban violence. American Journal of Political Science, in print (DOI: 10.1111/ajps.12045).
- F. Winter, H. Rauhut and D. Helbing (2012) “How norms can generate confict: an experiment on the failure of cooperative micro-motives on the macro-level.” Social Forces 90(3): 919-946.
- T. Chadefaux, D. Helbing (2012) “The rationality of prejudices.” PLoS ONE 7(2): e30902.
- R. Berger, H. Rauhut, S. Prade, and D. Helbing (2012) “Bargaining over waiting time in ultimatum game experiments.” Social Science Research 41: 372-379.
- Heliövaara, S., H. Ehtamo, D. Helbing, T. Korhonen (2013) “Patient and impatient pedestrians in a spatial game for egress congestion.” Physical Review E 87: 012802.
- Helbing, D. and P. Mukerji (2012) “Crowd disasters as systemic failures: Analysis of the Love Parade disaster.” EPJ Data Science 1:7.
- Helbing, D. (2013) "Economics 2.0: The natural step towards a self-regulating, participatory market society", Evolutionary and Institutional Economics Review, in print.
- Helbing, D. and A. Kirman (2013) "Rethinking economics using complexity theory", Real-World Economics Review, in print.
- Parisi, D.R., D. Sornette, and D. Helbing (2013) "Financial price dynamics and pedestrian counterflows: A comparison of statistical stylized facts." Physical Review E 87: 012804.
- Preis, T., D. Y. Kenett, H. E. Stanley, D. Helbing, and E. Ben-Jacob (2012)
- “Quantifying the behavior of stock correlations under market stress.” Scientific Reports 2: 752.
- Helbing, D., and A. Carbone, eds. (2012) "Participatory Science and Computing for our Complex World". EPJ Special Topics 214: 1-666.
- Helbing, D. (2012) "The FuturICT knowledge accelerator: Towards a more resilient and sustainable future." EPJ Special Topics 214: 5–9.
- Helbing, D., S. Bishop, R. Conte, P. Lukowicz and J.B. McCarthy (2012) "FuturICT: Participatory computing to understand and manage our complex world in a more sustainable and resilient way." EPJ Special Topics 214: 11–39.
- Helbing, D. (2012) "Accelerating scientific discovery by formulating grand scientific challenges." EPJ Special Topics 214: 41–48.
- Giannotti, F., D. Pedreschi, A. Pentland, P. Lukowicz, D. Kossmann, J. Crowley and D. Helbing (2012) "A planetary nervous system for social mining and collective

awareness." EPJ Special Topics 214: 49–75.

- Buckingham Shum, S., K. Aberer, A. Schmidt, S. Bishop, P. Lukowicz, S. Anderson, Y. Charalabidis, J. Domingue, S. de Freitas, I. Dunwell, B. Edmonds, F. Grey, M. Haklay, M. Jelasity, A. Karpištšenko, J. Kohlhammer, J. Lewis, J. Pitt, R. Sumner and D. Helbing (2012) "Towards a global participatory platform: Democratising open data, complexity science and collective intelligence." EPJ Special Topics 214: 109–152.
- van den Hoven, J., D. Helbing, D. Pedreschi, J. Domingo-Ferrer, F. Gianotti and M. Christen (2012) "FuturICT - The road towards ethical ICT." EPJ Special Topics 214: 153–181.
- van Harmelen, F., G. Kampis, K. Börner, P. van den Besselaar, E. Schultes, C. Goble, P. Groth, B. Mons, S. Anderson, S. Decker, C. Hayes, T. Buecheler and D. Helbing (2012) "Theoretical and technological building blocks for an innovation accelerator." EPJ Special Topics 214: 183–214.
- Johnson, J., S. Buckingham Shum, A. Willis, S. Bishop, T. Zamenopoulos, S. Swithenby, R. MacKay, Y. Merali, A. Lorincz, C. Costea, P. Bourgine, J. Louçã, A. Kapenieks, P. Kelley, S. Caird, J. Bromley, R. Deakin Crick, C. Goldspink, P. Collet, A. Carbone and D. Helbing (2012) "The FuturICT education accelerator." EPJ Special Topics 214: 215–243.
- San Miguel, M., J.H. Johnson, J. Kertesz, K. Kaski, A. Díaz-Guilera, R.S. MacKay, V. Loreto, P. Érdi and D. Helbing (2012) "Challenges in complex systems science." EPJ Special Topics 214: 245–271.
- Doyne Farmer, J., M. Gallegati, C. Hommes, A. Kirman, P. Ormerod, S. Cincotti, A. Sanchez and D. Helbing (2012) "A complex systems approach to constructing better models for managing financial markets and the economy." EPJ Special Topics 214: 295–324.
- Conte, R., N. Gilbert, G. Bonelli, C. Cioffi-Revilla, G. Deffuant, J. Kertesz, V. Loreto, S. Moat, J.-P. Nadal, A. Sanchez, A. Nowak, A. Flache, M. San Miguel and D. Helbing (2012) "Manifesto of computational social science." EPJ Special Topics 214: 325–346.
- Cederman, L.-E., R. Conte, D. Helbing, A. Nowak, F. Schweitzer and A. Vespignani (2012) "Exploratory of society." EPJ Special Topics 214: 347–360.
- Ferscha, A., K. Farrahi, J. van den Hoven, D. Hales, A. Nowak, P. Lukowicz and D. Helbing (2012) "Socio-inspired ICT: Towards a socially grounded society-ICT symbiosis." EPJ Special Topics 214: 401–434.
- Mazloumian, A., D. Helbing, S. Lozano, R. P. Light and K. Börner (2013) “Global multi-level analysis of the ‘Scientific Food Web’.” Scientific Reports 3: 1167.
- Helbing, D. (2013) “Globally Networked Risks and How to Respond.” Nature, 497(7447), 51–59.
- D. Helbing, ed. (2012) Social Self-Organization. Agent-based Simulations and Experiments to Study Emergent Social Behavior (Springer, Berlin).
- Ormerod, P. and D. Helbing (2012) "Back to the Drawing Board for Macroeconomics." In: D. Coyle (ed.) What's the Use of Economics? Teaching the Dismal Science After the Crisis (London Publishing Partnership).
- D. Helbing (2012) "New ways to promote sustainability and social well-being in a complex, strongly interdependent world: The FuturICT approach." Pages 55–60 in: P. Ball, Why Society is a Complex Matter (Springer, Berlin).

Group of H.J. Herrmann

R. Vetter, F.K. Wittel, N. Stoop and H.J. Herrmann
Finite element simulation of dense wire packings
European Journal of Mechanics A/Solids **37** (2013) 160171

R. Vetter, N. Stoop, F.K. Wittel, T. Jenni and H.J. Herrmann
Subdivision Shell Elements with Anisotropic Growth
International Journal for Numerical Methods in Engineering **95** (2013) 791-810

V.H.P. Louzada, F. Daolio, H.J. Herrmann, and M. Tomassini
Smart Rewiring for Network Robustness, Journal of Complex Networks,
doi:10.1093/comnet/cnt010, (to appear).

F. Mohseni, M. Mendoza, S. Succi, H.J. Herrmann
Lattice Boltzmann model for ultrarelativistic flows
Phys. Rev. D **87** (2013) 83003

R. Mani, D. Kadau, D. Or, H.J. Herrmann
Fluid depletion in shear bands
Phys. Rev. Lett. **109** (2012) 248001

R. Mani, D. Kadau, H.J. Herrmann
Liquid migration in sheared unsaturated granular media
Granular Matter **15** (2013) 447-454

N. Fernandez, R. Mani, D. Rinaldi, D. Kadau, M. Mosquet, H. Lombois-Burger,
J. Cayer-Barrioz, H.J. Herrmann, N.D. Spencer, L. Isa
Microscopic Mechanism for Shear Thickening of Non-Brownian Suspensions
Phys. Rev. Lett. **111** (2013) 108301

K.J. Schrenk, N.A.M. Araújo, H.J. Herrmann
How to share underground reservoirs
Sci. Rep. **2** (2012) 751

E. Daryaei, N.A.M. Araújo, K.J. Schrenk, S. Rouhani, H.J. Herrmann
Watersheds are Schramm-Loewner Evolution curves
Phys. Rev. Lett. **109** (2012) 218701

K.J. Schrenk, N.A.M. Araújo, H.J. Herrmann
Stacked triangular lattice: Percolation properties
Phys. Rev. E **87** (2013) 032123

F. Lombardi, D.R. Chialvo, H.J. Herrmann and L. de Arcangelis,
Strobing brain thunders: functional correlation of extreme activity events,
Chaos, Solitons and Fractals 55(2013),102-108

N. Posé, N.A.M. Araújo, and H.J. Herrmann,
Conductivity of Coniglio-Klein clusters, Phys. Rev. E, **86** (2012) 051140

M.V. Carneiro and H.J. Herrmann,
Simulation of aeolian saltation AIP Conf. Proc. 1542, pp. 1051-1054;
doi: http://dx.doi.org/10.1063/1.4812115 (4 pages) POWDERS AND GRAINS 2013: Proceedings of the 7th International Conference on Micromechanics of Granular Media

M.V. Carneiro, N.A.M. Araújo, T.Pähtz, H.J. Herrmann,
Midair Collisions Enhance Saltation
Phys. Rev. Lett. 111, 058001 (2013).

Publications: Group of Prof. Ralf Hiptmair

[1] X. Claeys and R. Hiptmair, *Integral equations on multi-screens*, Integral Equations and Operator Theory, (2013), pp. 1–31.

[2] X. Claeys, R. Hiptmair, and E. Spindler, *A second-kind galerkin boundary element method for scattering at composite objects*, Tech. Rep. 2013-13, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013. Submitted to BIT.

[3] R. Hiptmair, C. Jerez-Hanckes, J.-F. Lee, and Z. Peng, *Domain decomposition for boundary integral equations via local multi-trace formulations*, Report 2013-08, SAM, ETH Zürich, 2013. To appear in Proceedings of XXI International Conference on Domain Decomposition Methods, Rennes, France, June 25-29, 2012.

[4] R. Hiptmair, C. Jerez-Hanckes, and C. Schwab, *Sparse tensor edge elements*, BIT Numerical Mathematics, (2013), pp. 1–15.

[5] R. Hiptmair, A. Moiola, and I. Perugia, *Plane wave discontinuous galerkin methods: Exponential convergence of the hp-version*, Report 2013-31, SAM, ETH Zürich, Switzerland, 2013. Submitted to Found. Comput. Math.

[6] R. Hiptmair, A. Paganini, and S. Sargheini, *Comparison of approximate shape gradients*, Tech. Rep. 2013-30, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2013. Submitted to BIT.

[7] K. Schmidt and R. Hiptmair, *Asymptotic boundary element methods for thin conducting sheets*, Report 2013-19, SAM. ETH Zurich, Switzerland, July 2013. Submitted to Disc. Cont. Dyn. Sys. A.

[8] ——, *Asymptotic boundary element methods for thin conducting sheets in two dimensions*, IEEE Trans. Magnetics, (2013). Matheon report, http://nbn-resolving.de/urn:nbn:de:0296-matheon-12464.

Group of P. Hora

2012

P. Hora, N. Manopulo, L. Tong, Numerical and experimental methods for the prediction of failure in sheet metal forming, 1-10, FTF 2012 Zurich

L. Tong, P. Hora, B. Berisha, Numerical prediction of forming limit curves with consideration of anisotropy and anisotropic hardening effects, 145-149, FTF 2012 Zurich

P. Hora, M. Gorji, J. Maier, Analyzing the Tribological Phenomena in Hot Extrusion Processes by using New Torsion-Tribo Test, Tenth International Aluminum Extrusion Technology Seminar & Exposition (ET '12), 2012

P. Hora, M. Gorji, B. Berisha, Modeling of friction phenomena in extrusion processes by using a new torsion-friction test, Key engineering materials, 129-135, 2012

P. Hora, B. Berisha, M. Gorji, N. Manopulo, A generalized approach for the prediction of necking and rupture phenomena in the sheet metal forming, Proceedings of the IDDRG conference 2012

P. Peters, P. Hora, Effect of anisotropic hardening on deep drawing processes, Proceedings of the IDDRG conference 2012

J. Heingärtner, A. Neumann, P. Hora, D. Hortig, In-line acquisition of material properties of aluminium to increase process robustness, Proceedings of the IDDRG conference 2012

R. Hitz, Diss. 20160 ETH Zürich, 2012, Metamodellbasierte Methodenplanung von Umform- und Feinschneideprozessen

S. Wagner, Verfahren zur schnellen Erstellung und Bewertung von Konzeptmethoden für Blechbauteile, Diss. 20679 ETH Zürich, 2012

J. Krauer, P. Hora, Enhanced material models for the process design of the temperature dependent forming behavior of metastable steels, International Journal of Metal Forming, 361-379, 2012

2013

Th. Wesner, N. Manopulo, P. Hora, Failure prediction methods in 3D ale fine blanking simulations, IDDRG 2013 Conference Proceedings

Ph. Peters, N. Manopulo, Ch. Lange, P. Hora, A strain rate dependent anisotropic hardening model and its validation through deep drawing, International Journal of Material Forming, 2013

Ph. Peters, N. Manopulo, P. Hora, Application of HAH model with extension to cross hardening effects to DC05 deep drawing steel, IDDRG 2013 Conference Proceedings

N. Manopulo, Ph. Peters, P. Hora, Prediction of localized necking for nonlinear strain paths using the modified maximum force criterion (MMFC) and the homogeneous anisotropic hardening model (HAH), IDDRG 2013 Conference Proceedings

P. Hora, Ch. Becker, L. Tong, J. Maier, S. Müller, Advanced frictional models for extrusion application, Key Engineering materials Vol. 585, 41-48, 2013

Ch. Becker, P. Hora, J. Maier, S. Müller, Experimental investigations of friction carried out with the Tribo-Torsion-Test and frictional modelling, Key Engineering materials Vol. 585, 25-31, 2013

Ch. Becker, P. Hora, J. Maier, An optimized tribo-testing method for coating investigations for aluminum extrusion dies, Proceedings Aluminium 2000 Conference, 2013

P. Hora, New software concept for an integral in-line quality control in sheet metal forming, Proceedings 6th FTF 2013

J. Heingärtner, Y. Renkci, P. Hora, Application of non-destructive testing to control material properties of stainless steel in kitchen sink production, IDDRG 2013 Conference Proceedings

J. Heingärtner, Y. Renkci, P. Hora, Non-destructive testing of material properties, Proceedings 6th FTF 2013

J. Heingärtner, Zerstörungsfreie Kontrolle von schwankenden Werkstoffeigenschaften in der Produktion, IWF Kolloquium

P. Hora, Planung, Umsetzung und Betrieb von selbstkorrigierenden Fertigungssystemen in der Umformtechnik, IWF Kolloquium

P. Hora, B. Berisha, M. Gorji, A generalized approach for the prediction of necking and rupture phenomena in the sheet metal forming, Plasticity Symposium 2013

F. Quetting, P. Hora, K. Roll, Increasing the robustness of sheet metal forming processes using an intelligent planning and control system, IDDRG 2013 Conference Proceedings

R. van Ravenswaaij, R. van Tijum, P. Hora, T. van den Boogaard, U. Engel, Towards zero-defect manufacturing of small metal parts, IDDRG 2013 Conference Proceedings

M. Gorji, B. Berisha, P. Hora, Prediction of rupture phenomena in sheet metal forming, IDDRG 2013 Conference Proceedings

Group of P.H. Hünenberger

M.M. Reif, P.H. Hünenberger and C. Oostenbrink
New interaction parameters for charged amino acid side chains in the GROMOS force field.
J. Chem. Theory Comput. **8** (2012) 3705-3723.

B. Dahlgren, M.M. Reif, P.H. Hünenberger and N. Hansen
Calculation of derivative thermodynamic hydration and aqueous partial molar properties of ions based on atomistic simulations.
J. Chem. Theory Comput. **8** (2012) 3542-3564.

P.F.J. Fuchs, H.S. Hansen, P.H. Hünenberger and B.A.C. Horta
A GROMOS parameter set for vicinal diether functions: properties of polyethyleneoxide and polyethyleneglycol.
J. Chem. Theory Comput. **8** (2012) 3943-3963.

P.H. Hünenberger, A.E. Mark and H.J.C. Berendsen
Wilfred van Gunsteren: 35 years of biomolecular simulation.
J. Chem. Theory Comput. **8** (2012) 3425-3429.

M. Laner, B.A.C. Horta and P.H. Hünenberger
Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: Influence of the system size and force-field parameters.
Mol. Simul. **39** (2013) 563-583.

N. Hansen, P.H. Hünenberger and W.F. van Gunsteren.
Efficient combination of environment change and alchemical perturbation within the enveloping distribution sampling (EDS) scheme: Twin-system EDS and application to the determination of octanol-water partition coefficients.
J. Chem. Theory Comput. **9** (2012) 1334-1346.

D. Wang, M.L. Ámundadótir, W.F. van Gunsteren and P.H. Hünenberger.
Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: A molecular dynamics study of cellobiose stereoisomers.
Eur. Biophys. J. **42** (2013) 521-537.

G.J. Rocklin, D.L. Mobley, K.A. Dill and P.H. Hünenberger.
Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects.
J. Chem. Phys. (2013), in press.

Group of P. Jenny

[1] G. Bonfigli. High-order finite-difference implementation of the immersed-boundary technique for incompressible flows. Computers and Fluids, 46, 2011.

[2] V. Dmitriev and P. Jenny. Energy extraction from onflow inhomogeneity in the spanwise direction. a theoretical study. Journal of Intelligent Robotic Systems, 69(1-4):83-89, 2013.

[3] K. M. Erbertseder, J. Reichold, R. Helmig, P. Jenny, and B. Flemisch. A coupled discrete / continuum model for describing cancer therapeutic transport in the lung. PLoS ONE, 7(3), 2012.

[4] H. Gorji and P. Jenny. Continuous stochastic equations for diatomic rarefied gas flows. In Proceedings of the 3rd GASMEMS Workshop - Bertinoro, June 9-11, 2011.

[5] H. Gorji and P. Jenny. A kinetic model for gas mixtures based on Fokker–Planck equation. Journal of Physics: Conference Series, 362, 2012.

[6] H. Gorji, M. Torrilhon, and P. Jenny. Fokker–Planck model for computational studies of monatomic rarefied gas flows. J. Fluid Mech., 680:574–601, 2011.

[7] M. L. Hack and P. Jenny. Joint PDF closure of turbulent premixed flames. In Proceedings of Mediterranean Combustion Symposium, 2011.

[8] H. Hajibeygi, R. Deb, and P. Jenny. Multiscale finite volume method for non-conformal coarse grids arising from faulted porous media. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 142205-PP), 2011.

[9] H. Hajibeygi and P. Jenny. Adaptive iterative multiscale finite volume method. Journal of Computational Physics, 230(3), 2011.

[10] H. Hajibeygi, D. Karvounis, and P. Jenny. A hierarchical fracture model for the iterative multiscale finite volume method. Journal of Computational Physics, 230(24), 2011.

[11] H. Hajibeygi, D. Karvounis, and P. Jenny. A loosely coupled hierarchical fracture model for the iterative multiscale finite volume method. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141991-PP), 2011.

[12] H. Hajibeygi, I. Lunati, and S. H. Lee. Accurate and efficient simulation of multiphase flow in a heterogeneous reservoir by using error estimate and control in the multiscale finite-volume framework. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141954-PP), 2011.

[13] M. Hegetschweiler, B. Zoller, and P. Jenny. Reactive parametrized scalar profile (R-PSP) mixing model for partially premixed combustion. Combustion and Flame, 2011.

[14] P. Jenny and D. W. Meyer. Transported Probability and Mass Density Function (PDF/MDF) Methods for Uncertainty Assessment and Multi-Scale Problems, volume 83 of Lecture Notes in Computational Science and Engineering - Numerical Analysis of Multiscale Problems. Springer, 2011.

[15] P. Jenny, D. Roekaerts, and N. Beishuizen. Modeling of turbulent dilute spray combustion. Progress in Energy and Combustion Science, 38:846–887, 2012.

[16] J. Kang, N. Prasianakis, and J. Mantzaras. Development of an LB model for non-isothermal mixture flows. In Proceedings of 21st Conference on Discrete Simulation of Fluid Dynamics, 2012.

[17] D. Karvounis and P. Jenny. Modeling of flow and transport in enhanced geothermal systems. In Proceedings of Thirty-Sixth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, 2011.

[18] D. Karvounis and P. Jenny. Modeling of flow and transport for EGS cost optimization problems. In Proceedings of Thirty-Seventh Workshop on Geothermal Reservoir Engineering, 2012.

[19] I. Lunati, M. Tyagi, and S. H. Lee. An iterative multiscale finite volume algorithm converging to the exact solution. Journal of Computational Physics, 2011.

[20] D. W. Meyer. Modelling of turbulence modulation in particle- or droplet-laden flows. Journal of Fluid Mechanics, 706, 2012.

[21] D. W. Meyer and R. Deb. Modeling molecular mixing in a spatially inhomogeneous turbulent flow. Physics of Fluids, 24(2), 2012.

[22] B. Misselwitz, N. Barrett, S. Kreibich, P. Vonasch, D. Andritschke, S. Rout, K. Weidner, M. Sormaz, P. Songhet, P. Horvath, M. Chabria, V. Vogel, D. Spori, P. Jenny, and W.-D. Hardt. Near surface swimming of salmonella Typhimurium explains target-site selection and cooperative invasion. PLoS Pathogens, 8(7), 2012.

[23] G. Molinari, M. Quack, V. Dmitriev, M. Morari, P. Jenny, and P. Ermanni. Aero-structural optimisation of morphing aerofoils for adaptive wings. Journal of Intelligent Material Systems and Structures, 22, 2011.

[24] F. Müller, D. W. Meyer, and P. Jenny. Probabilistic collocation and Lagrangian sampling for tracer transport in randomly heterogeneous porous media. Advances in Water Resources, 34(12), 2011.

[25] N. Prasianakis, T. Rosen, J. Kang, J. Eller, J. Mantzaras, and F. N. Büchi. Simulation of 3D porous media flows with application to polymer electrolyte fuel cells. Communications in Computational Physics, 13(3), 2012.

[26] T. Rosen, J. Eller, J. Kang, N. I. Prasianakis, J. Mantzaras, and F. N. Büchi. Saturation dependent effective transport properties of PEFC gas diffusion layers. Journal of The Electrochemical Society, 159(9), 2012.

[27] M. Sormaz and P. Jenny. Empirical model for target depth estimation used in the time-domain subsurface imaging. Journal of Optical Society of America, 29(10), 2012.

[28] M. Tyagi and P. Jenny. Probability density function framework for modeling multi-phase ganglia flow in porous media. Journal of Fluid Mechanics, 688:219-257, 2011.

[29] M. Tyagi and P. Jenny. Probability density function modeling of multi-phase flow in porous media with density-driven gravity currents. Transp. Porous Media, 87(2), 2011.

[30] H. Xiao and P. Jenny. A consistent dual-mesh framework for hybrid LES/RANS modeling. Journal of Computational Physics, 231(4), 2012.

[31] H. Xiao, M. Wild, and P. Jenny. Preliminary evaluation and applications of a consistent hybrid LES/RANS method. In Proceedings of HRLM-4, 2011.

[32] B. T. Zoller, J. Allegrini, U. Maas, and P. Jenny. PDF model for NO calculations with radiation and consistent NO-NO2 chemistry in non-premixed turbulent flames. Combustion and Flame, 158, 2011.

[33] B. T. Zoller, M. L. Hack, and P. Jenny. A PDF combustion model for turbulent premixed flames. In Proceedings of the Combustion Institute, 34(1):15-28, 2013.

[34] B. T. Zoller and P. Jenny. Combustion model to predict local and global extinction of partially premixed flames. In Proceedings of Mediterranean Combustion Symposium, 2011.

[35] H. Gorji and P. Jenny. A Fokker-Planck based model for diatomic rarefied gas flows. Physics of Fluids, 25, 2013.

[36] M. L. Hack and P. Jenny. Joint PDF closure of turbulent premixed flames. Flow, turbulence and combustion, 90(2), 2013.

[37] P. Jenny, J. S. Lee, D. W. Meyer, and H. A. Tchelepi, Scale analysis of miscible density-driven convection in porous media. Journal of Fluid Mechanics, 2013 (submitted).

[38] D. Karvounis and P. Jenny. Adaptive hierarchical fracture model for enhanced geothermal systems. Water Resources Research, 2013 (submitted).

[39] H. Lund, F. Müller, B. Müller, and P. Jenny. Rankine-Hugoniot-Riemann solver for multidimensional conservation laws with source terms. Journal of Computational Physics, 2012 (submitted).

[40] D. W. Meyer and P. Jenny. Accurate and computationally efficient mixing models for the simulation of turbulent mixing with PDF methods. Journal of Computational Physics, 247, 2013.

[41] F. Müller, P. Jenny, and D. W. Meyer. Multilevel Monte Carlo for two phase flow and transport in random heterogeneous porous media. Journal of Computational Physics, 250, 2013.

[42] J. Reichold, D. Obrist, A. Buck, B. Weber, and P. Jenny. Computational modeling of cerebral blood flow including red cell influence and physiological boundary conditions. Journal of Cerebral Blood Flow & Metabolism, 2012 (submitted).

[43] M. Sormaz and P. Jenny. Monte Carlo study of subsurface imaging in the time-domain with co-axial laser-detector setup and a novel scheme for the target reconstruction. Journal of Optical Society of America, 2011 (submitted).

[44] H. Xiao and P. Jenny. Implicitly consistent formulation of a dual-mesh hybrid LES/RANS framework. Journal of Computational Physics, 2012 (submitted).

[45] H. Xiao, Y. Sakai, R. Henniger, M. Wild, and P. Jenny. A consistent hybrid LES/RANS framework with high-order LES solver on Cartesian mesh. Physics of Fluids, 2013 (accepted).

[46] N. I. Prasianakis, T. Rosen, J. Kang, J. Eller, I. Mantzaras, F. N. Büchi. Simulation of 3D porous media flows with application to polymer electrolyte fuel cells. Communications in Computational Physics, 13(3), 2013.

[47] D. W. Meyer, H. A. Tchelepi, and P. Jenny. A fast simulation method for uncertainty quantification of subsurface flow and transport. Water Resources Research, 49(5), 2013.

[48] Y. Reinhardt, N. Meinen, and D. W. Meyer. Modeling anisotropic Reynolds-stress dissipation in particle- or droplet-laden flows. International Journal of Multiphase Flow, 56, 2013.

[49] D. Cortinovis and P. Jenny. Iterative Galerkin-enriched multiscale finite-volume method. Journal of Computational Physics, 2013 (submitted).

[50] J. Kang, N. I. Prasianakis, I. Mantzaras. Lattice Boltzmann model for thermal binary mixture gas flows. Physical Review E, 87, 2013.

Dissertations since 2011:

[A] M. L. Hack. Joint PDF closure for turbulent premixed flames. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

[B] H. Hajibeygi. Iterative multiscale finite volume method for multiphase flow in porous media with complex physics. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

[C] J. Reichold. Cerebral blood flow modeling. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

[D] M. A. Wild. General purpose PDF solution algorithm for reactive flow simulations in OpenFOAM. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2013.

[E] D. C. Karvounis. Simulations of enhanced geothermal systems with an adaptive hierarchical fracture representation. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2013.

[F] B. T. Zoller. Scale separation modeling of turbulent gas-phase combustion using PDF methods. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2013.

Group of L. Kleiser

References

F. Boselli, D. Obrist, and L. Kleiser. A meshless boundary method for Stokes flows with particles. *Int. J. Num. Meth. Biomed. Eng.*, 2013. doi: 10.1002/cnm.2564.

S. Bühler and L. Kleiser. Simulation of a nozzle-jet configuration including the acoustic near-field. *Proc. Appl. Math. Mech.*, 12(1):541–542, 2012.

M. Gloor, D. Obrist, and L. Kleiser. Linear stability and acoustic characteristics of compressible, viscous, subsonic coaxial jet flow. *Phys. Fluids*, 25(8):84102, 2013.

M. O. John, D. Obrist, and L. Kleiser. An exact Navier-Stokes solution for three-dimensional, spanwise-homogeneous boundary layers. *Proc. Appl. Math. Mech.*, 12 (1):477–478, 2012.

T. Luginsland and L. Kleiser. Dynamic mode decomposition for swirling jet flow undergoing vortex breakdown. *Proc. Appl. Math. Mech.*, 12(1):495–496, 2012.

Y. Reinhardt, N. Meinen, and D. W. Meyer. Modeling anisotropic Reynolds-stress dissipation in particle- or droplet-laden flows. *Int. J. Multiphase Flow*, 56:1–3, 2013.

J. Ziefle and L. Kleiser. Numerical investigation of a film-cooling flow structure. *J. Turbomach.*, 135:41001, 2013.

S. Bühler, L. Kleiser, and C. Bogey. Simulation of subsonic turbulent nozzle-jet flow and its near-field sound. *AIAA J.*, 2013. accepted.

E. Edom, D. Obrist, R. Henniger, L. Kleiser, J. H. Sim, and A. Huber. The effect of rocking stapes motions on the fluid flow in the cochlea and on the basilar membrane motion. *J. Acoust. Soc. Am.*, 2013. in press.

Y. Reinhardt and L. Kleiser. Influence of mass loading on particle-laden turbulent pipe flow. *Proc. Appl. Math. Mech.*, 2013. in press.

Martin Kröger

www.complexfluids.ethz.ch

Y. Li, B.C. Abberton, M. Kröger, W.K. Liu, Challenges in multiscale modeling of polymers, *Polymers* **5** (2013) 751-832.

O. Bertran, B. Zhang, A.D. Schlüter, A. Halperin, M. Kröger, C. Aleman, Computer simulations of dendronized polymers: Organization and characterization at the atomistic level, *RSC Adv.* **3** (2013) 126-140.

O. Bertran, B. Zhang, A. D. Schlüter, M. Kröger, C. Aleman, Computer simulation of fifth generation dendronized polymers: Impact of charge on internal organization, *J. Phys. Chem. B* **117** (2013) 6007-6017.

M. Tagliazucchi, O. Peleg, M. Kröger, Y. Rabin, I. Szleifer, Effect of charge, hydrophobicity and sequence of nucleoporins on the translocation of model particles through the nuclear pore complex, *Proc. Natl. Acad. Sci.* **110** (2013) 3363-3368.

M. Sadati, C. Luap, B. Lüthi, M. Kröger, H.C. Öttinger, Application of full flow field reconstruction to a viscoelastic liquid in a 2D cross-slot channel, *J. Non-Newtonian Fluid Mech.* **192** (2013) 10-19.

M.B. Harasim, B. Wunderlich, O. Peleg, M. Kröger, A.R. Bausch, Direct observation of the dynamics of semiflexible polymers in shear flow, *Phys. Rev. Lett.* **110** (2013) 108302.

B. Zhang, H. Hu, A.D. Schlüter, A. Halperin, M. Kröger, Synthetic regimes due to packing constraints in dendritic molecules confirmed by labelling experiments, *Nat. Commun.* **4** (2013) 1993.

Y.R. Sliozberg, R.A. Mrozek, J.D. Schieber, M. Kröger, J.L. Lenhart, J.W. Anzelm, Effect of polymer solvent on the mechanical properties of entangled polymer gels: Coarse-grained molecular simulation, *Polymer* **54** (2013) 2555-2564.

Y. Li, M. Kröger, Viscoelasticity of carbon nanotube buckypaper: Zipping-unzipping mechanism and entanglement effects, *Soft Matter* **8** (2012) 7822-7830.

Y. Li, S. Tang, B.C. Abberton, M. Kröger, C. Burkhart, B. Jiang, G.J. Papakonstantopoulos, M. Poldneff, W.K. Liu, A predictive multiscale computational framework on viscoelastic properties of linear polymers, *Polymer* **53** (2012) 5935-5952.

Y. Li, M. Kröger, A theoretical evaluation of the effects of carbon nanotube entanglement and bundling on structural and mechanical properties of buckypaper,

Carbon **50** (2012) 1793-1806.

Y. Li, M. Kröger, W.K. Liu, Nanoparticle geometrical effect on structure, dynamics and anisotropic viscosities of polyethylene nanocomposites,
Macromolecules **45** (2012) 2099-2112.

Y. Li, M. Kröger, W.K. Liu, Nanoparticle effect on the dynamics of polymer chains and their entanglement network,
Phys. Rev. Lett. **109** (2012) 118001.

Y. Li, M. Kröger, Computational study on the entanglement length and pore size of carbon nanotube buckypaper,
Appl. Phys. Lett. **100** (2012) 021907.

O. Peleg, T. Savin, G.V. Kolmakov, I.G. Salib, A.C. Balazs, M. Kröger, V. Vogel, Fibers with integrated mechano-chemical switches: Minimalistic design principles derived from fibronectin,
Biophys. J. **103** (2012) 1909-1918.

N.C. Karayiannis, R. Malshe, M. Kröger, J.J. de Pablo, M. Laso, Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings,
Soft Matter **8** (2012) 844-858.

A. Karantrantos, R.J. Composto, K.I. Winey, M. Kröger, N. Clarke, Entanglements and dynamics of polymer melts near a SWCNT,
Macromolecules **45** (2012) 7274-7281.

A. Halperin, M. Kröger, Theoretical considerations on mechanisms of harvesting cells cultured on thermoresponsive polymer brushes,
Biomaterials **33** (2012) 4975-4987.

A. Halperin, M. Kröger, Thermoresponsive cell culture substrates based on PNIPAM brushes functionalized with adhesion peptides: Theoretical considerations of mechanism and design,
Langmuir **28** (2012) 16623-16637.

Group of M. Luisier

1. M. Luisier, “Thermal transport and Matthiessen’s rule in ultra-scaled Si nanowires”, App. Phys. Lett. 103, 113103 (2013).

2. Kuzmin, M. Luisier, and O. Schenk, “Fast Methods for Computing Selected Elements of the Green's Function in Massively Parallel Nanoelectronic Device Simulations”, Euro-Par 2013, LNCS 8097, F. Wolf, B. Mohr, and D. an Ney (Eds.), Springer-Verlag Berlin Heidelberg, p. 533-544, 2013.

3. M. Luisier, T. B. Boykin, Z. Ye, A. Martini, G. Klimeck, N. Kharche, X. Jiang, and S. Nayak, “Investigation of ripple-limited low-field mobility in large-scale graphene nanoribbons”, App. Phys. Lett. 102, 253506 (2013).

4. Szabo and M. Luisier, “Under-the-Barrier Model: An Extension of the Top-of-the-Barrier Model to Efficiently and Accurately Simulate Ultrascaled Nanowire Transistors”, IEEE Trans. Elec. Dev. 60, 2353 (2013).

5. M. Luisier, “Atomistic modeling of anharmonic phonon-phonon scattering in nanowires”, Phys. Rev. B 86, 245407 (2012).

6. M. Luisier and O. Schenk, “Gate-Stack Engineering in *n*-type Ultra-Scaled Si Nanowire Field-Effect Transistors”, in press in IEEE Trans. Elec. Dev. (2013).

7. L. De Michielis, N. Dagtekin, A. Biswas, L. Lattanzio, L. Selmi, M. Luisier, H. Riel, and A. M. Ionescu, “An Innovative Band-to-Band Tunneling Analytical Model and Implications in Compact Modeling of Tunneling-Based Devices”, in press in App. Phys. Lett. (2013).

Group of S. Mishra

Published papers

1. U.S. Fjordholm, S. Mishra and E. Tadmor, ENO reconstruction and ENO interpolation are stable, Jl. Found. Comp. Math, 13(2), 2013, 139-159.

2. P. Corti and S. Mishra, Stable finite difference schemes for the magnetic induction equation with Hall effect, BIT Numerical Mathematics, 52 (4), 2012, 905-932.

3. M. Svärd and S. Mishra, Entropy stable scheme for initial-boundary-value-problems for conservation laws, ZAMP, 63 (6), 2012, 985-1003 .

4. M.J. Castro, U.S. Fjordholm, S. Mishra and C. Pares Entropy conservative and entropy stable schemes for non-conservative hyperbolic systems, SIAM Jl. Num. Anal, 51 (3), 1371-1391.

5. S. Mishra, Ch. Schwab and J. Sukys Multi-level Monte Carlo finite volume methods for shallow water equations with uncertain topography in multi-dimensions, SIAM JL. Sci. Comput, 34 (6), 2012, 761-784.

6. U.Koley, S. Mishra, N.H.Risebro and M. Svärd, Higher order SBP-SAT schemes for magnetic induction equations with resistivity, *IMA Jl. Num. Anal.,* 32(3), 2012, 1173-1193.

In Press

7. J. Sukys, Ch. Schwab and S. Mishra Multi-level Monte Carlo finite difference and finite volume methods for stochastic linear hyperbolic systems, *Research report 2012-19*, SAM ETH Zürich, to appear in the MCQMC proceedings, Sydney 2012.

8. F. Fuchs, A. D. McMurry, S. Mishra and N. H. Risebro, Explicit and Implicit finite volume schemes for radiation MHD and the effects of radiation on wave propagation in stratified atmospheres, *Proc. of Hyperbolic conference 2012*, to appear.

9. A. Hiltebrand and S. Mishra, Entropy stable shock capturing streamline diffusion space-time discontinuous Galerkin (DG) methods for systems of conservation laws, *Num. Math.,* to appear, 2013

10. G.M. Coclite, L. Di Ruvo, J. Ernest and S. Mishra, Convergence of vanishing capillarity approximations for scalar conservation laws with discontinuous fluxes, *Netw. Heterog. Media.,* to appear, 2013

Preprints

11. S. Mishra, Ch. Schwab and J. Sukys Monte Carlo and multi-level Monte Carlo finite volume methods for uncertainty quantification in nonlinear systems of balance laws, *Research report 2012-08*, SAM ETH Zürich

12. S. Mishra, N.H. Risebro, Ch. Schwab and S. Tokareva Numerical solution of scalar conservation laws with random flux functions, *Research report 2012-35*, SAM ETH Zürich.

13. I. Averbukh, D. Ben-Zvi, S. Mishra and N. Barkai, Scaling morphogen gradients during tissue growth by a cell division rule.

14. G. M. Coclite, S. Mishra, N. H. Risebro and F. R. Weber, Analysis and numerical approximation of Brinkmann regularization of two phase flows in porous media.

15. R. Käppeli and S. Mishra, Well-balanced schemes for the Euler equations with gravitation, *Research report 2013-05*, SAM ETH Zürich.

16. S. Mishra, N. H. Risebro and F. R. Weber, Convergence of finite difference schemes for the wave equation with rough coefficients.

17. J. Ernest, P. G. LeFloch and S. Mishra, Schemes with well controlled dissipation (WCD)- nonclassical shock waves.

18. U. Koley, S. Mishra, F. R. Weber, Robust finite difference schemes for approximating a nonlinear wave equation modeling liquid crystals.

Group of M. Parrinello

S. Gabardi, S. Caravati, M. Bernasconi and M. Parrinello
Density functional simulations of Sb-rich GeSbTe phase change alloys
J. Physics-Cond. Matter, **24** (38), 385803 (2012), DOI:10.1088/0953-8984/24/38/385803

M. Salvalaglio, T. Vetter, F. Giberti, M. Mazzotti and M. Parrinello
Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives
J. Am. Chem. Soc., **134**, 17221-17233 (2012), DOI: 10.1021/ja307408x

V. Verdolino, L. Baldini, F. Palazzesi, F. Giberti and M. Parrinello
Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives
J. Phys. Chem. C, **116**, 23441-23452 (2012), DOI: 10.1021/jp307895x

G. M. Pavan, A. Barducci, L. Albertazzi and M. Parrinello
Combined metadynamics simulation and experiments to characterize dendrimers in solution
Soft Matter, **9**, 2593-2597(2013), DOI: 10.1039/C3SM27706B

V. Limongelli, S. De Tito, L. Cerofolini, M. Fragai, B. Pagano, R. Trotta, S. Cosconati, L. Marinelli, E. Novellino, I. Bertini, A. Randazzo, C. Luchinat and M. Parrinello
The G-Triplex DNA
Angew. Chem. Int. Ed., **52**, 2269-2273 (2013), DOI: 10.1002/anie.201206522

M. Ceriotti, G. A. Tribello and M. Parrinello
Demonstrating the Transferability and the Descriptive Power of Sketch-Map
J. Chem. Theory Comput., **9**, 1521-1532 (2013), DOI: 10.1021/ct3010563

S. Caravati, G. C. Sosso, M. Bernasconi and M. Parrinello
Density functional simulations of hexagonal $Ge_2Sb_2Te_5$ at high pressure
Physical Rev. B, **87**, 094117 (2013), DOI: 10.1103/PhysRevB.87.094117
Phys. Rev. B, 2013, **88** (1), 019903 (2013), DOI: 10.1103/PhysRevB.88.019903

V. Limongelli, M. Bonomi and M. Parrinello
Funnel metadynamics as accurate binding free-energy method
PNAS, **110** (16), 6358-6363 (2013), DOI: 10.1073/pnas.1303186110

E. Molina-Montes, D. Donadio, A. Hernàndez-Laguna, M. Parrinello and C. I. Sainz-Díaz
Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum mechanical Simulations
J. Phys. Chem., **117**, 7526-7532 (2013), DOI: 10.1021/jp310739y

F. Giberti, G. A. Tribello and M. Parrinello
Transient Polymorphism in NaCl
J. Chem. Theory Comp., **9** (6), 2526-2530 (2013), DOI: 10.1021/ct4002027

A. Hassanali, F. Giberti, J. Cuny, T. D. Kuehne and M. Parrinello
Proton transfer through the water gossamer
PNAS, **110** (34), 13723-13728 (2013), DOI:10.1073/pnas.1312350110

F. Palazzesi, A. Barducci, M. Tollinger and M. Parrinello
The allosteric communication pathways in KIX domain of CBP
PNAS, 110 (35), 14237-14242 (2013), DOI: 10.1073/pnas.1313548110

H. H.-M Yeung, M. Kosa, M. Parrinello, A. K. Cheetham
Chiral, Racemic, and meso-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis
Cryst. Growth Des., 13 (8), 3705–3715 (2013), DOI: 10.1021/cg400741b

Group of M. Quack

S. Albert, Ph. Lerch, R. Prentner and M. Quack
Tunneling and tunneling switching dynamics in phenol (C_6H_5OH) and its isotopomers from high resolution FTIR spectroscopy with synchrotron radiation in the THz range and theory
Angew. Chem. Intl. Ed. (English) **52**, 346 – 349 (2013),
Angew. Chem. 2013, **125**, 364 – 367 (2013)
DOI: 10.1002/anie.201205990, published online 6 December 2012

A. Nikitin, V. Boudon, C. Wenger, S. Albert, L. Brown, S. Bauerecker, M. Quack,
High resolution spectroscopy and first global analysis of the Tetradecad region of methane $^{12}CH_4$,
Phys. Chem. Chem. Phys., **15**, 10071 – 10093 (2013)

C. Manca Tanner, M. Quack, D. Schmidiger,
Nuclear spin symmetry conservation and relaxation in water ($^1H_2{}^{16}O$) studied by Cavity Ring-Down (CRD) spectroscopy of supersonic jets
J. Phys. Chem. A, **117**, 10105-10118 (2013).

R. Marquardt, K. Sagui, J. Zheng, W. Thiel, D. Luckhaus, S. Yurchenko, F. Mariotti, M. Quack
Global Analytical Potential Energy Surface for the Electronic Ground State of NH_3 from High Level ab Initio Calculations
J. Phys. Chem. A, **117**, 7502-7522 (2013).

R. Marquardt, M. Quack
Physical Chemistry and Chemical Physics: A Survey
in "Chemistry, Molecular Sciences and Chemical Engineering", Online reference Database Elsevier (2013), CMSE:5402, doi: 10.1016/B978-0-12-409547-2.05402-0

S. Albert, P. Lerch and M. Quack
Synchrotron based rotationally resolved high resolution FTIR spectroscopy of azulene and the unidentified infrared bands of astronomy
ChemPhysChem. **14**, 3204 - 3208 (2013).

L. R. Brown, K. Sung, D. C. Benner, V. M. Devi, V. Boudon, T. Gabard, C. Wenger, A. Campargue, O. Leshchishina, S. Kassi, D. Mondelain, L. Wang, L. Daumont, L. Régalia, M. Rey, X. Thomas, V. G. Tyuterev, O. M. Lyulin, A. V. Nikitin, H. M. Niederer, S. Albert, S. Bauerecker, M. Quack, J. J. O'Brien, I. E. Gordon, L. S. Rothman, H. Sasada, A. Coustenis, M. A. H. Smith, T. Carrington Jr, X. G. Wang, A. W. Mantz, P. T. Spickler
Methane line parameters in the HITRAN2012 database,
J. Quant. Spectrosc. Radiat. Transfer **130**, 201–219 (2013).

H.-M. Niederer, X.-G. Wang, T. Carrington Jr, S. Albert, S. Bauerecker, V. Boudon, M. Quack
Analysis of the rovibrational spectrum of $^{13}CH_4$ in the Octad range
J. Mol. Spectrosc. **291**, 33-47 (2013).

M. Quack
On Biomolecular Homochirality as a Quasi-Fossil of the Evolution of Life
Adv. Chem. Phys. (2013) in press

M. Quack
On the Emergence of Simple Structures in Complex Phenomena: Concepts and Some Numerical Examples
Adv. Chem. Phys. (2013) in press

Group of M. Reiher

T. Weymuth, M. Reiher,
Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts,
MRS Proceedings, 1524, DOI: 10.1557/opl.2012.1764 (**2013**)

K. Boguslawski, P. Tecmer, Ö. Legeza, M. Reiher,
Entanglement Measures for Single- and Multi-Reference Correlation Effects,
J. Phys. Chem. Lett., 3,3129–3135,(**2012**)

M.P. Haag, M. Reiher,
Real-time Quantum Chemistry,
Int. J. Quantum Chem., 113, 8–20 (**2013**)

K. Boguslawski, C. R. Jacob, M. Reiher,
Optimized unrestricted Kohn–Sham potentials from ab Initio spin densities,
J. Chem. Phys., 138, 044111 (**2013**)

M. K. Bruska, M. T. Stiebritz, M. Reiher,
Analysis of differences in oxygen sensitivity of Fe-S clusters,
Dalton Trans., 42, 8729 (**2013**).

A. R. Finkelmann, M. T. Stiebritz, M. Reiher,
Kinetic Modeling of Hydrogen Conversion at [Fe] Hydrogenase Active-Site Models
J. Phys. Chem. B, 117, 4806–4817 (**2013**)

B. Simmen, E. Mátyus, M. Reiher,
Elimination of the Translational Kinetic Energy Contamination in pre-Born–Oppenheimer Calculations,
Mol. Phys., 111, 2086 (**2013**)

D. Peng, N. Middendorf, F. Weigend, M. Reiher,
An efficient implementation of two-component relativistic exact-decoupling methods for large molecules,
J.Chem. Phys., 138, 184105, (**2013**)

K. Boguslawski, P. Tecmer, G. Barcza, Ö. Legeza, M. Reiher,
Orbital entanglement in bond-formation processes,
J. Chem. Theory Comput., 9, 2959–2973, (**2013**)

A. R. Finkelmann, M. T. Stiebritz, M. Reiher,
Electric-field effects on the [FeFe]-hydrogenase active site
Chem. Commun., 49, 8099–8101 (**2013**)

M. Bergeler, M. T. Stiebritz, M. Reiher,
Structure-Property Relationships of Fe_4S_4 Clusters,
ChemPlusChem, 78, 1082–1098 (**2013**)

T. Weymuth, M. Reiher,
Characteristic Raman Optical Activity Signatures of Protein β-Sheets,
J. Phys. Chem. B, DOI: 10.1021/jp405981h (**2013**)

Group of Christoph Schär

Allen, R.J., Norris, J.R., and Wild, M. 2013: Evaluation of multidecadal variability in CMIP5 surface solar radiation and inferred underestimation of aerosol direct effects over Europe, China, Japan, and India, *J. Geophys. Res. Atmos.*, **118**, 6311–6336, doi:10.1002/jgrd.50426.

Auchmann, R., Arfeuille, F., Wegmann, J., Franke, J., Barriendos, M., Prohom, M., Sanchez-Lorenzo, A., Bhend, J., Wild, M., Folini, D., Stepanek, P., and Brönnimann, S. 2013: Impact of volcanic stratospheric aerosols on diurnal temperature range (DTR) in Europeover the past 200 years:Observations versusmodel simulations, *J. Geophys. Res. Atmos.,* **118**, 9064–9077, doi:10.1002/jgrd.50759.

Bellprat O., D. Lüthi, S. Kotlarski and C. Schär, 2012: Exploring perturbed physics ensembles of a regional climate model. *J. Climate*, **25** (13), 4582-4599. DOI: 10.1175/JCLI-D-11-00275.1

Bellprat O., S. Kotlarski, D. Lüthi, C. Schär, 2012: Objective calibration of regional climate models. *J. Geophys. Res.*, **117**, Art. No . D23115, DOI: 10.1029/2012JD018262

Bellprat O., Kotlarski S., Lüthi D. and Schär C., 2013: Physical constraints for temperature biases in climate models. *Geophys. Res. Letters*, **40** (15), 4042-4047, doi: 10.1002/grl.50737

Bichet, A., Wild, M., Folini, D., and Schär, C., 2012: Causes for decadal variations of wind speed over land: Sensitivity studies with a global climate model, Geophys. Res. Lett. 39, Art. No. L11701, DOI: 10.1029/2012GL051685

Bhend, J., Franke, J., Folini, D., Wild, M., and Brönnimann, S., 2012: An ensemble-based approach to climate reconstructions, Clim. Past, 8, 963-976, DOI: 10.5194/cp-8-963-2012.

Bosshard, T., Carambia, M., Görgen, K., Kotlarski, S., Krahe, P., Zappa, M., Schär, C., 2013: Quantifying uncertainty sources in an ensemble of hydrological climate-impact projections. *Water Resource Research*, **49**, 1–14, doi: 10.1029/2011WR011533

Dutra E., C. Schär, P. Viterbo, and P.M.A. Miranda, 2012: Land-atmosphere coupling associated with snow cover. *Geophys. Res. Letters*, **38**, Art. No. L15707

Fischer, A.M., A.P. Weigel, C.M. Buser, R. Knutti, H.R. Künsch, M.A Liniger, C. Schär, C., Appenzeller, 2012: Climate Change Projections for Switzerland based on a Bayesian Climate Change Projections for Switzerland based on a Bayesian multi-model approach. *Int. J. Climatol.*, 32 (15), 2348-2371 DOI: 10.1002/joc.3396

Fischer, E. M., J. Rajczak, and C. Schär, 2012: Changes in European summer temperature variability revisited. *Geophys. Res. Letters*, 6, Art. No. L19702, doi:10.1029/2012GL052730

Glur L., S.B. Wirth, U. Büntgen, A. Gilli, G.H. Haug, C. Schär, J. Beer and F.S. Anselmetti, 2013: Frequent floods in the European Alps coincide with cooler periods of the past 2500 years. *Sci. Rep.,* **3**, 2770; DOI:10.1038/srep02770

Hakuba, M.Z., D. Folini, M. Wild and C. Schär, 2012: Impact of Greenland's topographic height on precipitation and snow accumulation in idealized simulations. *J. Geophys. Res.*, **117**, Art. No. D09107, doi: 10.1029/2011JD017052

Kothe, S., D. Lüthi, B. Ahrens, 2013: Analysis of the West African Monsoon system in the regional climate model COSMO-CLM. *Int. J. of Climatology*. DOI: 10.1002/joc.3702.

Kotlarski S., T. Bosshard, D. Lüthi, P. Pall, C. Schär, 2012: Elevation Gradients of European Climate Change in the Regional Climate Model COSMO-CLM. Climatic Change, **112**, 189–215, DOI: 10.1007/s10584-011-0195-5

Langhans, W., J. Schmidli and C. Schär, 2012a: Mesoscale impacts of explicit numerical diffusion in a convection-permitting model. *Mon. Wea. Rev.*, **140** (1), 226-244

Langhans, W., J. Schmidli and C. Schär, 2012b: Bulk convergence of kilometer-scale simulations of moist convection over complex terrain, *J. Atmos. Sci.*, **69** (7), 2207-2228

Langhans, E., J. Schmidli, S. Bieri, O. Fuhrer, and C. Schär, 2013: Long-term simulations of thermally driven flows and orographic convection at convection-parameterizing and cloud-resolving resolutions. *J. Appl. Meteor. Clim.*, **52**, 1490-1510, DOI: 10.1175/JAMC-D-12-0167.1

Panitz, H.-J., A. Dosio, M. Büchner, D. Lüthi, K. Keuler, 2013: COSMO-CLM (CCLM) climate simulations over CORDEX Africa domain: analysis of the ERA-Interim driven simulations at 0.44° and 0.22° resolution, *Clim. Dyn.*, DOI 10.1007/s00382-013-1834-5.

Rajczak, J., P. Pall, C. Schär, 2013: Projections of extreme precipitation events in regional climate simulations for Europe and the Alpine region. *J. Geophys. Res. Atmos.,* **118**, 3610–3626, doi:10.1002/jgrd.50297

Schaller, N., Cermak, J., Wild, M., and Knutti, R. 2013: The sensitivity of the modeled energy budget and hydrological cycle to CO2 and solar forcing, *Earth Syst. Dynam.*, **4**, 253-266, doi:10.5194/esd-4-253-2013.

Schlemmer, L., C. Hohenegger, J. Schmidli, C. Schär, 2012: Diurnal equilibrium convection and land surface-atmosphere interactions in an idealized cloud-resolving model. *Quart. J. Roy. Meteorol. Soc.*, **138** (667), 1526-1539 DOI: 10.1002/qj.1892

Steger, C., S. Kotlarski, T. Jonas and C. Schär, 2013: Alpine snow cover in a changing climate: a regional climate model perspective. *Clim. Dyn.*, **41**, 735–754, DOI 10.1007/s00382-012-1545-3

Stephens, G.L., Wild, M., Stackhouse, P., L'Ecuyer, T., Kato, S., 2012: The global character of the flux of downward longwave radiation. Journal of Climate, 25, 2329-2340 DOI: 10.1175/JCLI-D-11-00262.1.

Stephens, G.L., Li, J.-L., Wild, M., Clayson, C.A., Loeb, N., Kato, S., L'Ecuyer, T., Stackhouse, P.W., Andrews, T., 2012b: The energy balance of the Earth's climate system, *Nature Geoscience*, **5**, 691-696.

Wild, M. 2012: Enlightening Global Dimming and Brightening. *Bull. Amer. Meteor. Soc.*, **93**, 27–37, doi:10.1175/BAMS-D-11-00074.1

Wild M., Folini D., Schär C., Loeb N., Dutton E.G., and König-Langlo G., 2013: The global energy balance from a surface perspective. *Clim. Dyn.*, **40**, 3107–3134, DOI 10.1007/s00382-012-1569-8

You, Q., Sanchez-Lorenzo, A., Wild, M., Folini, D., Fraedrich, K., Ren, G., and Kang, S., 2013: Decadal variation of surface solar radiation in the Tibetan Plateau from observations, reanalysis and model simulations, *Clim. Dyn.*, **40**, 2073-2086, DOI: 10.1007/s00382-012-1383-3.

Zwiers F.W., L.V. Alexander, G.C. Hegerl, T.R. Knutson, J.P. Kossin, P. Naveau, N. Nicholls, C. Schär, S.I. Seneviratne, and X. Zhang, 2013: Climate Extremes: Challenges in Estimating and Understanding Recent Changes in the Frequency and Intensity of Extreme Climate and Weather Events. In: *Climate Science for Serving Society.* G.R. Asrar abd J.W. Hurrell (Eds.), Springer Netherlands, DOI 10.1007/978-94-007-6692-1, ISBN 978-94-007-6691-4 and 978-94-007-6692-1, 339-390

In press, accepted, submitted:

Bichet, A., D. Folini, M. Wild, and C. Schär, 2013: Enhanced Central European summer precipitation in the late 19th century: A link to the tropics. *Quart. J. Roy. Meteorol. Soc.*, in press

Bosshard, T., Kotlarksi, S., Zappa, M., Schär, S., 2012: Hydrological climate-impact projections for the Rhine river: GCM-RCM uncertainty and separate temperature and precipitation effects, Journal of Hydrometeorology, submitted

Broennimann S., C. Appenzeller, M. Croci-Maspoli, J. Fuhrer, M. Grosjean, R. Hohmann, K. Ingold, R. Knutti, M. Liniger, C. Raible, R. Röthlisberger, C. Schär, S. Scherrer, K. Strassmann, P. Thalmann, 2013: Climate change in Switzerland: A review of physical, institutional and political aspects. *Wiley Interdisciplinary Reviews: Climate Change*, submitted

Froidevaux, P., L. Schlemmer, J. Schmidli, W. Langhans, and C. Schär, 2013: Influence of background wind on the local spatial soil moisture-precipitation feedback. *J. Atmos. Sci.*, in press.

Kirtman B., S. Power, J.A. Adedoyin, G. Boer, R. Bojariu, I. Camilloni, F.J. Doblas-Reyes, A.M. Fiore, M. Kimoto, G.A. Meehl, M. Prather, A. Sarr, C. Schär, R. Sutton, G.J. van Oldenborgh, G. Vecchi, H.-J. Wang (and contributing authors), 2013: *Near-term Climate Change: Projections and Predictability*. Chapter 11 in: *Climate Change 2013. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change* [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, in press [available from www.climatechange2013.org]

Nabat, P., Somot, S., Mallet, M., Sevault, F., Chiacchio, M., and Wild, M., 2013: Direct and semi-direct aerosol radiative effect on the Mediterranean climate variability using a coupled Regional Climate System Model, *Clim. Dyn.,* submitted

Schmidli, J., 2013: Daytime heat transfer processes over mountainous terrain. *J. Atmos. Sci*., in press.

Group of Christoph Schwab

R. Andreev and A. Lang
Kolmogorov–Chentsov theorem and differentiability of random fields on manifolds
arXiv:1307.4886 [math.PR] SAM-Report 2013-22 (2013)

A. Barth
A Finite Element method for martingale-driven stochastic partial differential equations
Comm. Stoch. Anal., 4(3):355–375 (2010)

A. Barth and A. Lang
Milstein approximation for advection-diffusion equations driven by multiplicative non-continuous martingale noises
Appl. Math. Opt., 66(3):387–413 (2012)

A. Barth and A. Lang
Multilevel Monte Carlo method with applications to stochastic partial differential equations
Int. J. Comp. Math., 89(18):2479–2498 (2012)

A. Barth and A. Lang
Simulation of stochastic partial differential equations using finite element methods
Stochastics, 84(2-3):217–231 (2012)

A. Barth and A. Lang
L^p and almost sure convergence of a Milstein scheme for stochastic partial differential equations
Stoch. Process. Appl., 123(May):1563–1587 (2013)

A. Barth, A. Lang, and C. Schwab
Multilevel Monte Carlo Finite Element method for parabolic stochastic partial differential equations
BIT Num. Math., 53(1):3–27 (2013)

K. Grella and C. Schwab
Sparse discrete ordinates method in radiative transfer
Comp. Meth. in Applied Math., 11(3):305–326 (2011)

K. Grella and C. Schwab
Sparse tensor spherical harmonics approximation in radiative transfer
J. Comput. Phys., 230(23):8452–8473 (2011)

M. Hansen, C. Schillings, and C. Schwab
Sparse approximation algorithms for high dimensional parametric initial value problems
In *Proceedings 5th Conf. High Performance Computing, Hanoi*. Springer LNCSE (2013)

M. Hansen and C. Schwab
Analytic regularity and best n-term approximation of high dimensional parametric initial value problems
Vietnam Journ. Math., 1:1–35 (2011)

M. Hansen and C. Schwab
Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic pdes
Mathematische Nachrichten, 286(8-9):832–860 (2013)

V. Kazeev, M. Khammash, M. Nip, and C. Schwab
Direct solution of the Chemical Master Equation using Quantized Tensor Trains
Technical Report 2013-4, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

V. Kazeev and I. Oseledets
The tensor structure of a class of adaptive algebraic wavelet transforms
Technical Report 2013-28, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

V. Kazeev, O. Reichmann, and C. Schwab
hp-DG-QTT solution of high-dimensional degenerate diffusion equations
Technical Report 2012-11, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2012)

V. Kazeev, O. Reichmann, and C. Schwab
Low-rank tensor structure of linear diffusion operators in the TT and QTT formats
Linear Algebra and its Applications, 438(11):4204–4221 (2013)

V. Kazeev and C. Schwab
Tensor approximation of stationary distributions of chemical reaction networks
Technical Report 2013-18, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

A. Lang
A Lax equivalence theorem for stochastic differential equations
J. Comput. Appl. Math., 234(12):3387–3396 (2010)

A. Lang
Mean square convergence of a semidiscrete scheme for SPDEs of Zakai type driven by square integrable martingales
Procedia Computer Science, 1(1):1609–1617 (2010)

A. Lang
Almost sure convergence of a Galerkin approximation for SPDEs of Zakai type driven by square integrable martingales
J. Comput. Appl. Math., 236(7):1724–1732 (2012)

A. Lang
Isotropic Gaussian random fields on the sphere
Oberwolfach Report, SAM Report 2013-26 (2013)

A. Lang, P.-L. Chow, and J. Potthoff
Almost sure convergence of a semidiscrete Milstein scheme for SPDEs of Zakai type
Stochastics, 82(3):315–326 (2010)

A. Lang, P.-L. Chow, and J. Potthoff
Erratum: Almost sure convergence of a semi-discrete Milstein scheme for SPDEs of Zakai type
Stochastics, 84(4):561 (2012)

A. Lang, S. Larsson, and C. Schwab
Covariance structure of parabolic stochastic partial differential equations
Stoch. PDE: Anal. Comp., 1(2):351–364 (2013)

A. Lang and J. Potthoff
Erratum: Fast simulation of Gaussian random fields
Monte Carlo Methods Appl., 19(1):73–75 (2013)

A. Lang and C. Schwab
Isotropic Gaussian random fields on the sphere: regularity, fast simulation, and stochastic partial differential equations
arXiv:1305.1170 [math.PR] SAM Report 2013-15 (2013)

S. Mishra, N. H. Risebro, C. Schwab, and S. Tokareva
Numerical solution of scalar conservation laws with random flux functions
Technical Report 2012-35, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2012)

F. Müller and C. Schwab
Finite elements with mesh refinement for wave equations in polygons
Technical Report 2013-11, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

C. Schillings
A note on sparse, adaptive Smolyak quadratures for Bayesian inverse problems
Technical Report 2013-06, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

C. Schillings and C. Schwab
Sparse, adaptive Smolyak quadratures for Bayesian inverse problems
Inverse Problems, 29(6):065011 (2013)

C. Schillings and C. Schwab
Sparsity in Bayesian inversion of parametric operator equations
Technical Report 2013-17, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

C. Schwab and C. Schillings
Sparse quadrature approach to Bayesian inverse problems
Technical Report 2013-27, Seminar for Applied Mathematics, ETH Zürich, Switzerland (2013)

C. Schwab and S. Tokareva
High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data
ESAIM: M2AN, 47:807–835 (2013)

S. Tokareva
Stochastic finite volume methods for computational uncertainty quantification in hyperbolic conservation laws
PhD thesis, ETH Zürich (2013)

Group of P. J. Tackley

Armann, M. and P. J. Tackley (2012) Simulating the thermo-chemical magmatic and tectonic evolution of Venus' mantle and lithosphere 1. two-dimensional models, J. Geophys. Res. 117, E12003, doi:10.1029/2012JE004231.

Baitsch-Ghirardello, B., Gerya, T.V., Burg, J.-P. (2013) Geodynamic regimes of intra-oceanic subduction: Implications forearc extension vs. shortening processes. Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.11.003

Brown, J, M.G. Knepley, D.A. May, L.C. McInnes, B. Smith (2012) Composable linear solvers for multi-physics, 11th International Symposium on Parallel and Distributed Computing (ISPDC), IEEE (2012) 55-62

Castro, A., Vogt, K., Gerya, T. (2013) Generation of new continental crust by sublithospheric silicic-magma relamination in arcs: A test of Taylor's andesite model. Gondwana Research, DOI:10.1016/j.gr.2012.07.004.

Chen, L., Gerya, T., Zhang, Z., Aitken, A., Li, Z., Liang, X. (2013) Formation mechanism of steep convergent intracontinental margins: Insights from numerical modeling. Geophysical Research Letters, DOI: 10.1002/grl.50446

Chen, L., Gerya, T., Zhang, Z., Zhu, G., Duretz, T., Jacoby, W.R. (2013) Numerical modeling of eastern Tibetan-type margin: Influences of surface processes, lithospheric structure and crustal rheology. Gondwana Research, DOI:10.1016/j.gr.2013.01.003

Coltice, N., T. Rolf, P. J. Tackley and S. Labrosse (2012) Dynamic causes of the relation between area and age of the ocean floor, Science 336, 6079, 335-338, DOI:10.1126/science.1219120.

Crameri, F., H. Schmeling, G. J. Golabek, T. Duretz, R. Orendt, S. Buiter, D. A. May, B. J. P. Kaus, T. V. Gerya and P. J. Tackley (2012) A benchmark comparison of numerical surface topography calculations in geodynamic modelling, Geophys. J. Int. 189, 1, 38-54, doi:10.1111/j.1365-246X.2012.05388.x.

Crameri F., P. J. Tackley, I. Meilick, T. V. Gerya and B. J. P. Kaus (2012) A free plate surface and weak oceanic crust produce single-sided subduction on Earth, Geophys. Res. Lett. 39, L03306, doi:10.1029/2011GL050046.

Deschamps, F., L. Cobden and P. J. Tackle (2012) The primitive nature of large low shear-wave velocity provinces, Earth Planet. Sci. Lett. 349-350, 198-208.

Deschamps, F., C. Yao, P. J. Tackley and C. Sanchez-Valle (2012) High Rayleigh number thermal convection in volumetrically heated spherical shells, J. Geophys. Res. 117, E09006, doi:10.1029/2012JE004090.

Duretz, T., Gerya, T.V. (2013) Slab detachment during continental collision: Influence of crustal rheology and interaction with lithospheric delamination. Tectonophysics, DOI: 10.1016/j.tecto.2012.12.024.

M. Fox, F. Herman, S.D. Willet, D.A. May (2013) A linear inversion method to infer exhumation rates in space and time from thermochronometric data, Earth Surface Dynamics 1(1) 207-259

Gerya, T.V. (2013) Precambrian geodynamics: Concepts and models. Gondwana Research, DOI:10.1016/j.gr.2012.11.008

Gerya, T.V. (2013a) Initiation of transform faults at rifted continental margins: 3D petrological–thermomechanical modeling and comparison to the Woodlark Basin. Petrology, 21, 550–560.

Gerya, T.V. (2013b) Three-dimensional thermomechanical modeling of oceanic spreading initiation and evolution.Phys. Earth Planet. Interiors, DOI:10.1016/j.pepi.2012.10.007

Gerya, T.V., D.A. May, T. Duretz (2013) An Adaptive Staggered Grid, Finite Difference Method for Modeling Geodynamic Stokes Flows with Strongly Variable Viscosity Geochemistry, Geophysics, Geosystems 14, 1200-1225

Hacker, B.R., Gerya, T.V. (2013) Paradigms, new and old, for ultrahigh-pressure tectonism. Tectonophysics, 603, 79-88.

Hacker, B.R., Gerya, T.V., Gilotti, J.A. (2013) Formation and exhumation of ultrahigh-pressure terranes. Elements, 9, 289-293

Keller, T., D.A. May, B.J.P. Kaus, Numerical modelling of magma dynamics coupled to tectonic deformation of lithosphere and crust, Geophysical Journal International DOI: 10.1093/gji/ggt306 (2013)

Le Pourhiet, L., B. Huet, D.A May, L. Labrousse, L. Jolivet (2012) Kinematic interpretation of the 3D shapes of metamorphic core complexes, Geochemistry, Geophysics, Geosystems 13 Q09002

Li, Z., Xu, Z., Gerya, T., Burg, J.-P. (2013) Collision of continental corner from 3-D numerical modeling. Earth and Planetary Science Letters, 380, 98–111.

Massmeyer, A., A. Davaille, T. Rolf, P. Tackley and E. Di Giuseppe (2013) Numerical simulation of thermal plumes in a Herschel-Bulkley fluid, J. Non-Newtonian Fluid Mechanics 195, 32-45, doi:10.1016/j.jnnfm.2012.12.004

May, D. A., Volume reconstruction of point cloud data sets derived from computational geodynamic simulations, Geochemistry, Geophysics, Geosystems 13 (2012) Q05019

May, D.A., W.P. Schellart, L. Moresi, Overview of adaptive finite element analysis in computational geodynamics, Journal of Geodynamics 70 (2013) 1-20

Malatesta, C., Gerya, T., Crispini, L., Federico, L., Capponi, G. (2013) Oblique subduction modelling indicates along-trench tectonic transport of sediments. Nature Communications, 4, Article number: 2456.

Marques, F.O., Nikolaeva, K., Assumpcao, M., Gerya, T.V, Bezerra, F.H.R., do Nascimento, A.F., Ferreira, J.M. (2013) Testing the influence of far-field topographic forcing on subduction initiation at a passive margin. Tectonophysics, doi:10.1016/j.tecto.2013.08.035a.

Mikhailov, V., Lyakhovsky, V., Panet, I., van Dinther, Y., Diament, M., Gerya, T.V., deViron, O., and Timoshkina, E. (2013). Numerical modelling of post-seismic rupture propagation after the Sumatra 26.12.2004 earthquake constrained by GRACE gravity data, Geophysical Journal International, 194 (2): 640-650, doi:10.1093/gji/ggt145.

Morishima, R., G. J. Golabek and H. Samuel, N-body simulations of oligarchic growth of Mars: Implications for Hf-W chronology, Earth Planet. Sci. Lett., 366, 6-16, 2013.

Morra, G., R. Geller, S. T. Grilli, S. Karato, S. King, S.-M. Lee, P. J. Tackley, and D. Yuen (2013) Subduction Dynamics and Seismic Hazards, EOS, Trans. AGU, 94(13), 121-130.

Nakagawa, T. and P. J. Tackley (2013) Implications of high core thermal conductivity on Earth's coupled mantle and core evolution, Geophys. Res. Lett. 40, doi:10.1002/grl.50574.

Nakagawa, T. and P. J. Tackley, Influence of magmatism on mantle cooling surface heat flow and Urey ratio (2012) Earth Planet. Sci. Lett. 329-330, 1-10, doi:10.1016/j.epsl.2012.02.011.

Nakagawa, T., P. J. Tackley, F. Deschamps and J. A. D. Connolly (2012) Radial 1-D seismic structures in the deep mantle in mantle convection simulations with self-consistently calculated mineralogy, Geochem. Geophys. Geosyst.13, Q11002, doi:10.1029/2012GC004325

Naliboff, J.B., Billen, M.I., Gerya, T., Saunders, J. (2013) Dynamics of outer rise faulting in oceanic-continental subduction systems. Geochemistry, Geophysics, Geosystems, DOI: 10.1002/ggge.20155.

Püthe, C., Gerya, T.V. (2013) Dependence of mid-ocean ridge morphology on spreading rate in numerical 3-D models. Gondwana Research, DOI:1016/j.gr.2013.04.005.

Rolf, T., N. Coltice and P. J. Tackley (2012) Linking continental drift, plate tectonics and the thermal state of the Earth's mantle, Earth Planet. Sci. Lett. 351-352. 134-146.

Ruedas, T., P. J. Tackley and S. C. Solomon (2013) Thermal and compositional evolution of the martian mantle: Effects of water, Phys. Earth Planet. Inter. 220, 50-72, doi:10.1016/j.pepi.2013.04.006.

Ruedas, T., P. J. Tackley and S. C. Solomon (2013) Thermal and compositional evolution of the martian mantle: Effects of phase transitions and melting, Phys. Earth Planet. Inter. 216, 32-58, doi:10.1016/j.pepi.2012.12.002

Ruh, J.B., Gerya, T., Burg, J.-P. (2013) High-resolution 3D numerical modeling of thrust wedges: Influence of decollement strength on transfer zones. Geochem. Geophys. Geosys., doi:10.1002/ggge.20085

Schubert, M., Driesner, T., Gerya, T.V., Ulmer, P. (2013) Mafic injection as a trigger for felsic magmatism: A numerical study. Geochemistry, Geophysics, Geosystems, 14, doi:10.1002/ggge.20124.

Sizova, E.V., Gerya, T.V., Brown, M. (2013) Contrasting styles of Phanerozoic and Precambrian continental collision, Gondwana Research, DOI:10.1016/j.gr.2012.12.011

Tackley, P. J. (2012) Dynamics and evolution of the deep mantle resulting from thermal, chemical, phase and melting effects, Earth Science Reviews 110, 1-25, doi:10.1016/j.earscirev.2011.10.001.

Tackley, P. J., M. Ammann, J. P. Brodholt, D. P. Dobson and D. Valencia (2013) Mantle dynamics in super-Earths: Post-perovskite rheology and self-regulation of viscosity, Icarus 225(1), 50-61, doi:10.1016/j.icarus.2013.03.013.

Tkalcec, B. J., G. J. Golabek and F. E. Brenker, Solid-state plastic deformation in the dynamic interior of a differentiated asteroid, Nature Geosci., 6, 93-97, doi:10.1038/ngeo1710, 2013.

Ulvrova, M., S. Labrosse, N. Coltice, P. Raback and P. J. Tackley (2012) Numerical modeling of convection interacting with a melting and solidification front in geodynamics, Phys. Earth Planet. Inter. 206-207, 51-66.

van Dinther, Y., Gerya, T.V., Dalguer, L.A., Corbi, F., Funiciello, F., Mai, P.M. (2013) The seismic cycle at subduction thrusts: 2. Dynamic implications of geodynamic simulations validated with laboratory models. J. Geophys. Res., DOI: 10.1029/2012JB009479.

Vogt, K., Gerya, T.V. (2013) From oceanic plateaus to allochthonous terranes: Numerical modelling, Gondwana Research, DOI: http://dx.doi.org/10.1016/j.gr.2012.11.002

P. Yamato, R. Tartèse, T. Duretz, D.A. May (2012) Numerical modelling of magma transport in dykes, Tectonophysics 526, 97-109

Zheng, L., Zhang, H., Gerya, T., Knepley, M., Yuen, D.A., Shi, Y. (2013) Implementation of a multigrid solver on a GPU for Stokes equations with strongly variable viscosity based on Matlab and CUDA. The International Journal of High Performance Computing Applications, DOI: 10.1177/1094342013478640

Zhu, G., Gerya, T.V., Tackley, P.J., Kissling, E. (2013) 4-D Numerical modeling of crustal growth at active continental margins. Journal of Geophysical Research, DOI: 10.1002/jgrb.50357

Submitted or in press

Coltice, N., M. Seton, T. Rolf, R.D. Müller and P.J. Tackley, Convergence of tectonic reconstructions and mantle convection models for significant fluctuations in seafloor spreading, Earth Planet. Sci. Lett.

Coltice, N., T. Rolf and P. J. Tackley, Seafloor spreading evolution in response to continental growth, Geology.

Lechmann, S.M., S.M. Schmalholz, G. Hetenyi, D.A. May, B.J.P. Kaus, Towards constraining the dynamics of the India-Asia collision with 3D numerical models Journal of Geophysical Research

Nakagawa, T. and P. J. Tackley, On the origin of long-wavelength structure in compressible mantle convection simulations with plate-like behavior in a 3-D spherical shell, Phys. Earth Planet. Inter.

Rolf, T., N. Coltice and P. J. Tackley, Statistical cyclicity of the supercontinent cycle, Geology.

Rozel, A., Equilibrium internal temperature and heat flux in a super-Earth, J. Geophys. Res.

Rozel, A., J. Besserer, G. J. Golabek, M. Kaplan, T. W. Becker and P. J. Tackley, Self-consistent generation of single plume state for Enceladus using non-Newtonian rheology, J. Geophys. Res.

Zhu, G., T. Gerya, P. J. Tackley and E. Kissling, 4-D numerical modeling of crustal growth at active margins, J. Geophys. Res.

Group of M. Troyer

M.H. Freedman, J. Gukelberger, M.B. Hastings, S. Trebst, M. Troyer, Zhenghan Wang
Galois Conjugates of Topological Phases
Phys. Rev. B **85**, 045414 (2012)

B. Surer, M. Troyer, P. Werner, A.M. Läuchli, TO. Wehling, A. Wilhelm, A. I. Lichtenstein
Multi-orbital Kondo physics of Co in Cu hosts
Phys. Rev. B **85**, 085114 (2012)

B. Bauer, P. Corboz, A. M. Läuchli, L. Messio, K. Penc, M. Troyer, F. Mila
Three-sublattice order in the SU(3) Heisenberg model on the square and triangular lattice
Phys. Rev. B **85** 125116 (2012)

S. Pilati and M. Troyer
The bosonic superfluid-insulator transition in continuous space
Phys. Rev. Lett. **108**, 155301 (2012)

Didier Poilblanc, Matthias Troyer, Eddy Ardonne, Parsa Bonderson
Fractionalization of itinerant anyons in one dimensional chains
Phys. Rev. Lett. **108**, 207201 (2012)

S.V. Streltsov, E. Gull, A.O. Shorikov, M. Troyer, V.I. Anisimov, P. Werner
Magnetic susceptibility of Ce: an LDA+DMFT study
Phys. Rev. B **85**, 195109 (2012)

C. R. Laumann, D. A. Huse, A. W. W. Ludwig, G. Refael, S. Trebst, and M. Troyer
Strong-disorder renormalization for interacting non-Abelian anyon systems in two dimensions
Phys. Rev. B **85**, 224201 (2012)

P.N. Ma, S. Pilati, X. Dai and M. Troyer
Density functional theory for atomic Fermi gases
Nature Physics **8**, 601 (2012).

M. Dolfi, B. Bauer, M. Troyer, Z. Ristivojevic
Multigrid Algorithms for Tensor Network States
Phys. Rev. Lett., **109**, 020604 (2012)

Jia-Wei Huo, Weiqiang Chen, U. Schollwöck, M. Troyer, Fu-Chun Zhang
Dipolar Dynamics for Interacting Ultracold Fermions in a Trapped Optical Lattice
Phys. Rev. A **86**, 033611 (2012)

R.N.C. Pfeifer, O. Buerschaper, S. Trebst, A.W.W. Ludwig, M. Troyer, and G. Vidal
Translation invariance, topology, and protection of criticality in chains of interacting anyons
Phys. Rev. B **86**, 155111 (2012)

Arash Bellafard, Helmut G. Katzgraber, Matthias Troyer, Sudip Chakravarty
Bond disorder induced criticality of the three-color Ashkin-Teller model
Phys. Rev. Lett. **109**, 155701 (2012)

Peter Anders, Philipp Werner, Matthias Troyer, Manfred Sigrist, Lode Pollet
From the Cooper problem to canted super solids in Bose-Fermi mixtures
Phys. Rev. Lett. **109**, 206401 (2012)

Bela Bauer, Roman M. Lutchyn, Matthew B. Hastings, Matthias Troyer
Effect of thermal fluctuations in topological p-wave superconductors
Phys. Rev. B **87**, 014503 (2013)

Didier Poilblanc, Adrian Feiguin, Matthias Troyer, Eddy Ardonne, Parsa Bonderson
One-dimensional itinerant interacting non-Abelian anyons
Phys. Rev. B **87**, 085106 (2013)

T. Uehlinger, D. Greif, G. Jotzu, L. Tarruell, T. Esslinger, Lei Wang, M. Troyer
Double transfer through Dirac points in a tunable honeycomb optical lattice
Eur. Phys. J. Special Topics **217**, 12 (2013)

Lei Wang, Alexey A. Soluyanov, Matthias Troyer
Direct measurement of topological invariants in optical lattices
Phys. Rev. Lett. **110**, 166802 (2013)

Bela Bauer and Liza Huijse and Erez Berg and Matthias Troyer and Kareljan Schoutens
Strong finite-size corrections for lattice fermions at a supersymmetric multicritical point
Preprint, Phys. Rev. B **87**, 165145 (2013)

E. Kozik, E. Burovski, V.W. Scarola, M. Troyer
Néel temperature and thermodynamics of the half-filled 3D Hubbard model by Diagrammatic Determinant Monte Carlo
Phys. Rev. B **87**, 205102 (2013)

C. Gils, E. Ardonne, S. Trebst, D.A. Huse, A.W.W. Ludwig, Matthias Troyer, Z. Wang
Anyonic quantum spin chains: Spin-1 generalizations and topological stability
Phys. Rev. B. **87**, 235120 (2013)

Paul Fendley, Sergei V. Isakov, Matthias Troyer
Fibonacci topological order from quantum nets
Phys. Rev. Lett. **110**, 260408 (2013)

Lei Wang, Matthias Troyer, Xi Dai
Topological charge pumping in a one-dimensional optical lattice
Phys. Rev. Lett. **111**, 026802 (2013)

Hsiang-Hsuan Hung, Lei Wang, Zheng-Cheng Gu, Gregory A. Fiete
Topological phase transition in a generalized Kane-Mele-Hubbard model: A combined Quantum Monte Carlo and Green's function study.
Phys. Rev. B, **87**, 121113, (2013).

Lei Wang, Alexey A. Soluyanov and Matthias Troyer,
Proposal for direct measurement of topological invariants in optical lattices.
Phys. Rev. Lett., **110**, 166802, (2013).

S. Boixo, T. Ronnow, S. Isakov, Z.H. Wang, D. Wecker, D. Lidar, J. Martinis, M. Troyer
Quantum annealing on more than a hundred qubits
Preprint, submitted to Nature Physics

Iztok Pizorn, Viktor Eisler, Sabine Andergassen, Matthias Troyer
Real time evolution at finite temperatures with operator space matrix product states
Preprint, submitted to Phys. Rev. Lett.

Johannes Schachenmayer, Lode Pollet, Matthias Troyer, Andrew John Daley
Spontaneous emissions and thermalization of cold bosons in optical lattices
Preprint, submitted to Phys. Rev. Lett.

Lei Wang, T.F. Rønnow, S. Boixo, S.V. Isakov, Zhihui Wang, D. Wecker, D.A. Lidar, J.M. Martinis, Matthias Troyer
Comment on: "Classical signature of quantum annealing"
arXiv:1305.5837

S. Pilati, I. Zintchenko, M. Troyer
Ferromagnetism of a Repulsive Atomic Fermi gas in an Optical Lattice: a Quantum Monte Carlo study
Preprint, submitted to Phys. Rev. Lett.

Ilia Zintchenko, Lei Wang, Matthias Troyer
Ferromagnetism of the Repulsive Atomic Fermi Gas: three-body recombination and domain formation
Preprint, submitted to Phys. Rev. Lett.

Lei Wang, Matthias Troyer
Seeing Hofstadter's Butterfly in Atomic Fermi Gases
Preprint, submitted to Phys. Rev. Lett.

J. Imriška, M. Iazzi, Lei Wang, E. Gull, D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, M. Troyer
Thermodynamics and magnetic properties of the anisotropic 3D Hubbard model
Preprint, submitted to Phys. Rev. Lett.

Group of W.F. van Gunsteren

D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
Helical content of a β^3-octapeptide in methanol:
Molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data
Chem. Eur. J. 18 (2012), 586-593, DOI: 10.1002/chem.201102667, incl. supp. mat.

A.P. Eichenberger, L.J. Smith, W.F. van Gunsteren
Ester-linked hen egg white lysozyme shows a compact fold in a molecular dynamics simulation -possible causes and sensitivity of experimentally observable quantities to structural changes maintaining this compact fold
FEBS Journal 279 (2012), 299-315, DOI: 10.1111/j.1742-4658.2011.08424.x, incl. supp. mat.

K. Meier, W. Thiel, W.F. van Gunsteren
On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations
J. Comput. Chem. 33 (2012), 363-378, DOI: 10.1002/jcc.21962

A.P.E. Kunz, J.R. Allison, D.P. Geerke, B.A.C. Horta, P.H. Hünenberger, S. Riniker, N. Schmid, W.F. van Gunsteren
New functionalities in the GROMOS biomolecular simulation software
J. Comput. Chem. 33 (2012), 340-353, DOI: 10.1002/jcc.21954

N. Schmid, C.D. Christ, M.Christen, A.P. Eichenberger, W.F. van Gunsteren
Architecture, implementation and parallelization of the GROMOS software for biomolecular simulation
Comp. Phys. Comm. 183 (2012), 890-903, DOI: 10.1016/j.cpc.2011.12.014

N. Hansen, J. Dolenc, M. Knecht, S. Riniker, W.F. van Gunsteren
Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution
J. Comput. Chem. 33 (2012) 640-651, DOI: 10.1002/jcc.22879, incl. supp. mat

J.R. Allison, S. Riniker, W.F. van Gunsteren
Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
J. Chem. Phys. 136 (2012) 054505, DOI: 10.1063/1.3681140, incl. supp. mat.

S. Riniker, B.A.C. Horta, B. Thijssen, S. Gupta, W.F. van Gunsteren, P.H. Hünenberger
Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: A molecular dynamics simulation study
ChemPhysChem 13 (2012) 1182-1190, DOI:10.1002/cphc.201100949

A.P.E. Kunz, Z. Lin, W.F. van Gunsteren
Test of a method for sampling the internal degrees of freedom of a flexible solute molecule based on adiabatic decoupling and temperature or force scaling
Mol. Phys. 110 (2012) 407-417, DOI:10.1080/00268976.2011.650716

D. Steiner, C. Oostenbrink, W.F. van Gunsteren
Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9
J. Comput. Chem. 33 (2012) 1467-1477, DOI: 10.1002/jcc.22972, incl. supp. mat.

D. Steiner, W.F. van Gunsteren
An improved structural characterisation of reduced french bean plastocyanin based on NMR data and local-elevation molecular dynamics simulation
Eur. Biophys. J. 41 (2012) 579-595, DOI: 10.1007/s00249-012-0824-6, incl. supp. mat.

D. Steiner, J.R. Allison, W.F. van Gunsteren
On the calculation of $^{3}J_{\alpha\beta}$-coupling constants for side chains in proteins
J. Biomol. NMR 53 (2012) 223-246, DOI: 10.1007/s10858-012-9634-5, incl. supp. mat.

S. Riniker, W.F. van Gunsteren
Mixing coarse-grained and fine-grained water in molecular dynamics simulations of a single system
J. Chem. Phys. 137 (2012) 044120, DOI: 10.1063/1.4739068

S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Structural effects of an atomic-level layer of water molecules around proteins solvated in supra-molecular coarse-grained water
J. Phys. Chem. B 116 (2012) 8873-8879, DOI: 10.1021/jp304188z, incl. supp. mat.

Z. Lin, T.A. Timmerscheidt, W.F. van Gunsteren
Using enveloping distribution sampling (EDS) to compute the free enthalpy difference between right-and left-handed helices of a β-peptide in solution
J. Chem. Phys.137 (2012) 064108, DOI: 10.1063/1.4742751, incl. supp. mat.

S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations
Eur. Biophys. J. 41 (2012) 647-661, DOI: 10.1007/s00249-012-0837-1

B.A.C. Horta, Z. Lin, W. Huang, S. Riniker, W.F. van Gunsteren, P.H. Hünenberger
Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: influence on the folding properties of two β-peptides in methanol
J. Comput. Chem. 33 (2011) 1907-1917, DOI: 10.1002/jcc.23021

S. Riniker, J.R. Allison, W.F. van Gunsteren
On developing coarse-grained models for biomolecular simulation: a review:
Phys. Chem. Chem. Phys. 14 (2012) 12423-12430, DOI:10.1039/C2CP40934H

W. Huang, A.P. Eichenberger, W.F. van Gunsteren
Molecular dynamics simulation of thionated hen egg white lysozyme
Prot. Sci. 21 (2012) 1153-1161, DOI:10.1002/pro.2102, incl. supp. mat.

K. Meier, N. Schmid, W.F. van Gunsteren
Interfacing the GROMOS (bio) molecular simulation software to quantum-chemical program packages
J. Comput. Chem. 33 (2012) 2108-2117, DOI: 10.1002/jcc.23047

T.S. Hofer, W.F. van Gunsteren
Exploring the properties of small molecule protein binding via molecular simulation: the TRSH – p53 core domain complex
Mol. BioSyst. **8** (2012) 2891-2900, DOI: 10.1039/c2mb25166c, incl. supp. mat.

A. Choutko, W.F. van Gunsteren
Molecular dynamics simulation of the last step of a catalytic cycle: product release from the active site of the enzyme chorismate mutase of mycobacterium tuberculosis
Prot. Sci. **21** (2012) 1672-1681, DOI:10.1002/pro.2143, incl. supp. mat.

J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren, J. Dolenc
Influence of 63Ser phosphorylation and dephosphorylation on the structure of the stathmin helical nucleation sequence: A molecular dynamics study
Biochemistry **51** (2012) 8455-8463, DOI: 10.1021/bi300885y, incl. supp. mat.

W.F. van Gunsteren, J. Dolenc
Thirty-five years of biomolecular simulation: development of methodology, force fields, and software
Mol. Sim. **38** (2012) 1271-1281, DOI: 10.1080/08927022.2012.701744

J. Kleinjung, W.R.P. Scott, J.R. Allison, W.F. van Gunsteren, F. Fraternali
Implicit solvation parameters derived from explicit water forces in large-scale molecular dynamics simulations
J. Chem. Theory Comput. **8** (2012) 2391-2403, DOI: 10.1021/ct200390j, incl. supp. mat.

S. Riniker, L.J. Barandun, F. Diederich, O. Krämer, A. Steffen, W.F. van Gunsteren
Free enthalpies of replacing water molecules in protein binding pockets
J. Computer-Aided Mol. Des. **26** (2012) 1293-1309, incl. supp. mat.

D. Wang, F. Freitag, Z. Gattin, H. Haberkern, B. Jaun, M. Siwko, R. Vyas,
W.F. van Gunsteren, J. Dolenc
Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules
Helv. Chim. Acta **95** (2012) 2562-2577, DOI: 10.1002/hlca.201200534, incl. supp. mat.

D. Wang, W.F. van Gunsteren, Z. Chai
Recent advances in computational actinide chemistry
Chem. Soc. Rev. **41** (2012) 5836–5865, DOI: 10.1039/c2cs15354h
Progress in Chemistry **7** (2011) 1566-1581 (Chinese version)

W.F. van Gunsteren
The seven sins in academic behavior in the natural sciences
Angew. Chem. Int. Ed. **52** (2013) 118-122, DOI: 10.1002/anie.201204076
Angew. Chem. **125** (2013) 128-132, DOI: 10.1002/ange.201204076

L.J. Smith, W.F. van Gunsteren, J.R. Allison
Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12
Prot. Sci. **22** (2013) 56-64, DOI: 10.1002/pro.2184, incl. supp. mat.

M.M. Müller, J.R. Allison, N. Hongdilokkul, L. Gaillon, P. Kast, W.F. van Gunsteren, P. Marliére, D. Hilvert
Directed evolution of a model primordial enzyme provides insights into the development of the genetic code
PLoS Genet **9** (2013) e1003187, DOI:10.1371/journal.pgen.1003187, incl. supp. mat.

A. Choutko, W.F. van Gunsteren
Conformational preferences of a β-octapeptide as function of solvent and force-field parameters
Helv. Chim. Acta **96** (2013) 189-200, DOI: 10.1002/hlca.201200173, incl. supp. mat.

Z. Lin, W.F. van Gunsteren
On the choice of a reference state for one-step perturbation calculations between polar and non-polar molecules in a polar environment
J. Comput. Chem. **34** (2013) 387-393, DOI: 10.1002/jcc.23146, incl. supp. mat.

K. Meier, A. Choutko, J. Dolenc, A.P. Eichenberger, S. Riniker, W.F. van Gunsteren
Multi-resolution simulation of biomolecular systems: a review of methodological issues
Angew. Chem. Int. Ed. **52** (2013) 2820-2834, DOI: 10.1002/anie.201205408
Angew. Chem. **125** (2013) 2-19, DOI: 10.1002/ange.201205408

Z. Lin, S. Riniker, W.F. van Gunsteren
Free enthalpy differences between α-, π-, and 3_{10}-helices of an atomic level fine-grained alanine deca-peptide solvated in supra-molecular coarse-grained water
J. Chem. Theory Comput. **9** (2013) 1328-1333, DOI: 10.1021/ct3010497

N. Hansen, P.H. Hünenberger, W.F. van Gunsteren
Efficient combination of environment change and alchemical perturbation within the enveloping distribution sampling (EDS) scheme: twin system EDS and application to the determination of octanol-water partition coefficients
J. Chem. Theory Comput. **9** (2013) 1334-1346, DOI: 10.1021/ct300933y, incl. supp. mat.

Z. Lin, W.F. van Gunsteren
Combination of enveloping distribution sampling (EDS) of a soft-core reference-state Hamiltonian with one-step perturbation to predict the effect of side chain substitution on the relative stability of right- and left-helical folds of β-peptides
J. Chem. Theory Comput. **9** (2013) 126-134, DOI: 10.1021/ct300929q

K. Meier, W.F. van Gunsteren
On the use of advanced modelling techniques to investigate the conformational discrepancy between two X-ray structures of the AppA BLUF domain
Mol. Sim. **39** (2013) 472-486, DOI: 10.1080/08927022.2012.743659

A.P. Eichenberger, W.F. van Gunsteren, L.J. Smith
Structure of hen egg-white lysozyme solvated in TFE/water: a molecular dynamics simulation study based on NMR data
J. Biomol. NMR **55** (2013) 339-353, DOI: 10.1007/s10858-013-9717-y, incl. supp. mat.

A. Choutko, A.P. Eichenberger, W.F. van Gunsteren, J. Dolenc
Exploration of swapping enzymatic function between two proteins: a simulation study of chorismate mutase and isochorismate pyruvate lyase
Prot. Sci. **22** (2013) 809-822, DOI: 10.1002/pro.2264, incl. supp. mat.

D. Wang, M.L. Amundadottir, W.F. van Gunsteren, P.H. Hünenberger
Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: a molecular dynamics study of cellobiose stereoisomers
Eur. Biophys. J. **42** (2013) 521-537, DOI: 10.1007/s00249-013-0901-5

Z. Lin, W.F. van Gunsteren
Influence of variation of a side chain on the folding equilibrium of a β-peptide: limitations of one-step perturbation
J. Comput. Chem. **34** (2013) 1899-1906, DOI: 10.1002/jcc.23331

N. Hansen, J.R. Allison, F. Hodel, W.F. van Gunsteren
Relative free enthalpies for point mutations in two proteins with highly similar sequence but different folds
Biochemistry **52** (2013) 4962–4970, DOI: 10.1021/bi400272q

Z. Lin, W.F. van Gunsteren
The effect of branched side chains on the relative stability of α- and π- helices: a combination of the enveloping distribution sampling and one-step perturbation methods
Mol. Phys. **111** (2013) 2126-2130, DOI: 10.1080/00268976.2013.793828, incl. supp. mat.

S.J. Bachmann, J. Dolenc, W.F. van Gunsteren
On the use of one-step perturbation to investigate the dependence of different properties of liquid water upon a variation of model parameters from a single simulation
Mol. Phys. 111 (2013) 2334-2344, DOI: 10.1080/00268976.2013.815374

L.J. Smith, Y. Roby, J.R. Allison, W.F. van Gunsteren
MD simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data
Biochemistry **52** (2013) 5029-5038, DOI: 10.1021/bi4006573

In press or submitted

A.P. Eichenberger, N. Hansen, S. Riniker, L. von Ziegler, W.F. van Gunsteren,
A comparison of calculated and measured relative free enthalpies of folding of twenty amide-to-ester mutants of a small protein
J. Am. Chem. Soc. (2013) submitted

A.P. Eichenberger, W.F. van Gunsteren
A method to apply bond-angle and dihedral-angle constraints in molecular dynamics simulation
J. Comput. Chem. (2013) submitted

W. Huang, Z. Lin, W.F. van Gunsteren
Free enthalpy differences between 3_{10}-, α-, and π-helical conformations of deca-alanine in aqueous solution calculated for different force fields using enveloping distribution sampling (EDS)
Prot. Sci. (2013) submitted, incl. supp. mat.

D. Wang, A. Böckmann, B. Meier, W.F. van Gunsteren
On the behavior of water at subfreezing temperatures in a protein crystal: evidence of higher mobility than in neat water
J. Phys. Chem. (2013) in press, incl. supp. mat.

Z. Lin, C. Necula, W.F. van Gunsteren
Using enveloping distribution sampling (EDS) to compute the folding free enthalpy of a β-peptide with a very unstable folded conformation in solution: the advantage of focused sampling using EDS
Chem. Phys. (2013) submitted

Z. Lin, W.F. van Gunsteren
Refinement of the application of the GROMOS 54A7 force field to β-peptides
J. Comput. Chem. (2013) in press

M. Pechlaner, R.K.O. Sigel, W.F. van Gunsteren, J. Dolenc
Structure and conformational dynamics of the domain 5 RNA hairpin of a bacterial group II intron revealed by solution NMR and molecular dynamics simulations
Biochemistry (2013) in press, incl. supp. mat.

S.J. Bachmann, Z. Lin, T. Stafforst, W.F. van Gunsteren, J. Dolenc
On the sensitivity of peptide nucleic acid duplex formation and crystal dissolution to a variation of force-field parameters
J. Chem. Theory Comput. (2013) submitted

Z. Lin, W.F. van Gunsteren
Enhanced conformational sampling using enveloping distribution sampling
J. Chem. Phys. (2013) in press

Computational Science and Engineering (CSE)
Annual Report
2012/2013

ETH Zürich
Rämistrasse 101
8092 Zurich

www.rw.ethz.ch