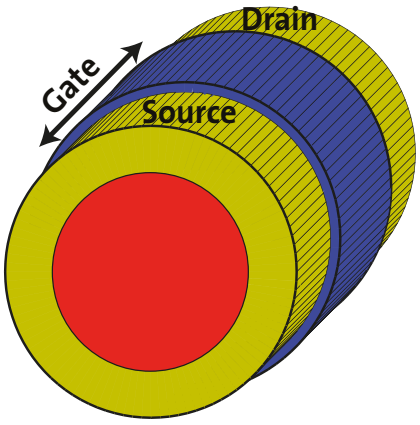
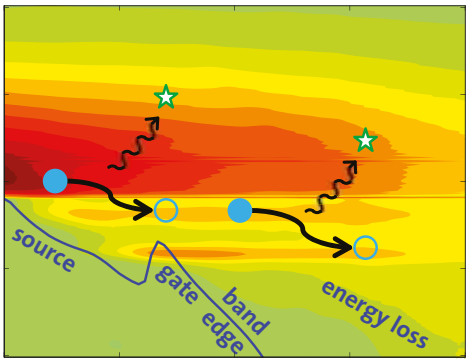
# CSE

Computational Science and Engineering

## Annual Report
## 2011 / 2012




ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

# CSE

Computational Science and Engineering

# Annual Report
# 2011 / 2012

## July 2011 to July 2012

## Impressum:



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*Cover:*

(Left) Schematic view of a gate-all-around nanowire field-effect transistor. The semiconductor channel (red) is surrounded by an oxide layer (yellow/green). The electron flow between source and drain is controlled by a gate-all-around contact (blue). (Right) Spectral current flow through the upper nanowire structure as function of the electron position (horizontal axis) and energy (vertical axis). Red regions indicate high current concentrations, green ones no current. Electrons (blue dots) lose energy when they travel from left (source) to right (drain) by emitting phonon particles (green stars).

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# 1

# Introduction

Last year I elaborated the difficulty of defining the field of "Computational Science and Engineering". This year I make an even bolder bid, attempting to pinpoint what can be regarded as fundamental trends and issues in CSE. An oracle that allowed a glimpse of the future of the field would be invaluable for everybody involved in it, ranging from the graduate student in search for a topic, to the established researcher launching a big project. Since, apparently, modern scientific emphasis on the causality principle has sent oracles into sulking silence, the only available substitutes are experts. So I asked a few of my colleagues to tell me off the top of their heads and in a few catchy words, what they considered major developments and central questions in CSE. Without giving names and, of course, after some editing and rearrangement, I am now going to summarize the responses to the question "What are unfolding key issues in CSE research?"

- *Hardware evolution*: "There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable. There is another theory which states that this has already happened."[1] Well, it seems that this happens all the time concerning the development of high-performance computing hardware, whose complexity is increasing, making it more and more challenging to convert smart algorithms into really fast code. Gradually this emerges as a major research topic. Shifting hardware designs also threaten to render huge implementation efforts obsolete and resources have to be committed to ensure that codes keep up with the development of hardware.

- *Massive parallelism*: Imagine you have more computational cores at your disposal than unknowns in your problem! Of course, this will never come true, but we may be getting closer to this scenario. This may entail a complete reassessment of algorithms and their efficiency.

- *Fault tolerant computing*: If simulations rely on scores of cores some of them will inevitably fail during the execution of the code. It is an exciting research problem to modify existing and design new algorithm so that they can cope with hardware failure efficiently and gracefully.

- *Multi-scale and multi-physics modeling*: There is no bound on the complexity of reality. In particular, physical systems often involve vastly different time- and length-scales, and allow for mathematical modeling on various levels of detail. Brute force resolution of all scales usually proves intractable, which calls for reliable and efficient methods for multi-scale simulation in every respect.

- *Uncertainty quantification*: Under closer scrutiny, inputs (data, parameter, even models) and, therefore, outputs of simulations are random variables; so treat them as such!

[1] D. Adams, The Restaurant at the End of the Universe, 1980

- *Data deluge*: Measurement data, simulation results, ..., in tremendous amounts, useful only after compression, visualization, data mining, statistical post-processing.

Most predictions are either trivial or off the mark, and I leave it to the reader to decide, which applies here.

Zürich, November 16, 2011
Ralf Hiptmair,

Director of Studies CSE, member of the CSE Committee

# 2

# Education

In September 2011, 36 new students started their CSE Bachelor studies, 27 in the first semester and 9 in the third semester. From outside ETH 6 students entered the CSE Master curriculum.

The total number of CSE students enrolled at the end of the academic year 2011/2012 was 109 (64 in the BSc program and 45 in the MSc program).

In the past academic year 33 students have successfully finished a CSE curriculum, 16 Bachelor students and 17 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.

*Bachelor Theses*

| | |
|---|---|
| Andrea Arteaga | Implementation of a C++ Library for Data Exchange with MATLAB<br>Ralf Hiptmair (D-MATH) |
| Fabian Bösch | Human Computer Interface for Microrobotic Manipulation<br>Brad Nelson (D-MAVT) |
| Raoul Bourquin | Simulation of some non-adiabatic transitions<br>Ralf Hiptmair (D-MATH) |
| Gennaro Chirico | Implementation of the immersed-boundary procedure for infinitely thin membranes<br>Patrick Jenny (D-MAVT) |
| Robert Gantner | Rayleigh Quotient Multigrid<br>Ralf Hiptmair (D-MATH) |
| Roman Hellmüller | Improving robustness of networks with a genetic algorithm approach<br>Prof. Hans Herrmann (D-BAUG) |
| Sandro Mani | A controller for a surfboard on hydrofoils<br>Manfred Morari (D-ITET) |
| Manuel Nescher | Collapse of Snow under Gravity<br>Hans Herrmann (D-BAUG) |
| Mischa Obrecht | Collapse of Snow under Gravity<br>Hans Herrmann (D-BAUG) |
| Sebastian Scherer | Knochensimulationen speichereffizient implementiert mit Hilfe von raumfüllenden Kurven<br>Peter Arbenz (D-INFK) |

| | |
|---|---|
| Tobias Setz | HFN (High Precision Floating Point) port from IBM CELL to Intel SSE<br>Wesley Petersen (D-MATH) |
| Michael Steinlechner | A boundary element method for solving eigenvalue PDEs<br>Daniel Kressner (D-MATH) |
| Severin Thöni | Programming a Humanoid<br>Robert Riener (D-MAVT) |
| Patrick Wyss | Flexibility of Robust Risk Portfolios<br>Hans-Jakob Lüthi (D-MATH) |

*Master Theses*

| | |
|---|---|
| Nadzeya Bedziuk | Correlation skew modelling<br>Cristoph Schwab (D-MATH) |
| Raphael Das Gupta | Sparse Representations for SD objects<br>Markus Gross (D-INFK) |
| Rajdeep Deb | Modelling molecular mixing in spatially inhomogeneous turbulent flow<br>Patrick Jenny (D-MAVT) |
| Roman Fuchs | Sediment-laden freshwater on top of clear sea water: 3D DNS investigation<br>Leonhard Kleiser (D-MAVT) |
| Rafael Hostettler | Agile Brachiation Control<br>Markus Gross (D-INFK) |
| Farhan Imtiaz | Emergence of Reflexive Behavior from Single Muscle Twitches<br>Fumiya Iida (D-MAVT) |
| Joohva Lee | Coarse-scale Moment Closure of Unstable Miscible Flow in Porous media<br>Patrick Jenny (D-MAVT) |
| Pascal Merz | Molecular Dynamics Simulation in Artificial Ensembles<br>Wilfred van Gunsteren (D-CHAB) |
| Gian-Peider Moll | Can measured residual dipolar couplings be sensibly used for structure refinement of proteins<br>Wilfred van Gunsteren (D-CHAB) |

| | |
|---|---|
| Andres Rosero | Numerics of Stochastic Partial Differential Equations and the Heath-Jarrow-Morton Equation with Levy-Noise<br>Josef Teichmann (D-MATH) |
| Yves Didier Salathé | Towards Gigahertz Bandwidth Digital Signal Processing in Circuit Quantum Electrodynamics<br>Andreas Wallraff (D-PHYS) |
| Roman Schärer | Numerical Solutions of Kinetic Equatons for Plasma Applications<br>Patrick Jenny (D-MAVT) |
| Sebastian Scherer | User-Independent 3D Object Recognition and Classification for Cellular Systems<br>Joachim Buhmann (D-INFK) |
| Philipp Simmler | Lighting methods for Over Coat<br>Markus Gross (D-INFK) |
| Michael Steinlechner | Locating Minimum-Energy Crossing Points in Spin-Forbidden Reactions<br>Markus Reiher (D-CHAB) |
| Zack Zhu | Watching YouTube: A Content-Driven Online Social Network<br>Roger Wattenhofer (ITET) |
| Nathaniel Zollinger | Multilevel Monte Carlo for elliptic SPDEs<br>Cristoph Schwab (D-MATH) |

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

*Term Papers*

| | |
|---|---|
| Raoul Bourquin | Spawning of wave-packets in 1d non-adiabatic transitions<br>Ralf Hiptmair (D-MATH) |
| Raffael Casagrande | Implementation of impedance boundary conditions in HADAPT<br>Ralf Hiptmair (D-MATH) |
| Gennaro Chirico | GPU computation of surface tension forces for two-phase compressible flow simulations<br>Petros Koumoutsakos (D-MAVT) |
| Ruben Dezeure | A runtime study: Algorithms for causal inference in R and c + x<br>Peter L. Bühlmann (D-MATH) |

| | |
|---|---|
| Robert Gantner | Expnential Integrators<br>Vasile Gradinaru (D-MATH) |
| Simon Härdi | Parallelization of a Radiative Transport Solver<br>Christoph Schwab (D-MATH) |
| Roman Hellmüller | Checkpoint/Restart of massively parallel simulations<br>Ivo Sbalzarini (D-ITET) |
| Rafael Hostettler | Cellar Images from white light through dispersion and binary filters<br>Markus Gross (D-INFK) |
| Ueli Koch | Adoptive Low-Storage Runge-Kutta Methods for Discontinuous Galerkin Time-Domain Simulations<br>Christian Hafner (D-ITET) |
| Nicolò Lardelli | Development of technical Testsuite v2.0 for COSMO atmospheric model<br>Christoph Schär (D-UWIS) |
| Fabian Kulman | Eye tracking using Kinect<br>Markus Gross (D-INFK) |
| Adrien Lücker | Implementing a consistent particle transport scheme for a hybrid TRANS/PDF method<br>Daniel Werner Meyer-Massetti (D-MAVT) |
| Mischa Obrecht | Iterative Methods for Solving High-Dimensional Eigenvalue Problems Using Low-Rank Tensor Approximations<br>Daniel Kressner (D-MATH) |
| Muhammad Raheem | Phase change modeling in the presence of non-condensable gas using level-set interface tracking method<br>Patrick Jenny (D-MAVT) |
| Andres Rosero | Spurious Solutions for transient Maxwell equations in 2D<br>Ralf Hiptmair (D-MATH) |
| Pintarelli Simon | Assessment of extrapolation schemes for the density matrix renormalization group algorithm<br>Markus Reiher (D-CHAB) |

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, October 12, 2012
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 HS11

| | |
|---|---|
| 29.09.11 | Nils Risebro, CMA, Uni Oslo and SAM<br>Flow in porous media and reservoir simulation |
| 13.10.11 | Lars Kielhorn, Applied Mathematics (SAM)<br>Boundary element methods: Fundamentals, implementation and applications |
| 03.11.11 | Xavier Lapillonne, C2SM and MeteoSwiss<br>Adapting numerical weather prediction models to future hardware technologies: Running the COSMO code on Graphical Processor Units (GPUs) |
| 24.11.11 | Eric Sonnendrücker, IRMA, Université de Strasbourg<br>Simulation of charged particles in an accelerator |
| 08.12.11 | Erik Saenger, Geology<br>Digital rock physics |
| 15.12.11 | Peter Bühlmann, Statistics<br>Causal statistical inference for large-scale biological systems |

## Case Studies Seminar FS12

| | |
|---|---|
| 01.03.12 | Jens Niegemann, Electromagnetic Fields and Microwave Electronics (IFH)<br>The Discontinuous Galerkin Time-Domain Method in Nanophotonics |
| 08.03.12 | Olga Sorkine, Visual Computing<br>Modeling and Animation of Shapes for Computer Graphics Using Discrete Differential Geometry Tools |
| 19.04.12 | Frank Vogel, inuTech GmbH, Nürnberg<br>inuTech - Innovative Numerical Technologies |
| 10.05.12 | Philipp Grohs, Seminar for Applied Mathematics (SAM)<br>Mathematica and Computational Methods in Signal Processing |
| 24.05.12 | Wolfgang Langhans, Climate Systems Modeling<br>Numerical Weather Prediction: Factors governing convergence |

# 4

# Computational Highlight

# Quantum Transport Modeling of Next-Generation Nanoelectronic Devices

Mathieu Luisier

Integrated Systems Laboratory

**Abstract**

An advanced, multi-dimensional, and massively parallel simulation approach based on quantum mechanical concepts is introduced and its numerical algorithms briefly summarized. It has been implemented in a computer aided design tool called OMEN, specifically dedicated to next generation nanoelectronic devices. OMEN can treat electron, hole, and phonon (thermal) transport in realistically sized ultra-scaled transistors and thermogenerators with an atomistic resolution of the simulation domain. Its accuracy, usefulness, and parallel performance are demonstrated with the help of four device applications.

## 1 Introduction

During the last four decades the functionality of electronic systems such as audio players, televisions, personal computers, and cellular phones has kept improving due to breakthrough innovations, but also due to a continuous increase of the transistor density per integrated circuit (IC): the number of transistors per IC doubles almost every 2 years according to Moore's scaling law [1]. This exponential increase has been responsible for an aggressive scaling of the transistor dimensions, which nowadays do not exceed a few nanometers so that their active region is composed of a countable number of atoms. Quantum mechanical effects such as energy quantization, confinement, and electron tunneling are already playing a very important role in the currently manufactured transistors. They will completely dominate the behavior of next generation nanoelectronic devices. Hence, the greatest challenges that the semiconductor industry will face in the next couple of years consist in demonstrating and fabricating devices that will (i) work "because" and not "in spite" of quantum mechanical effects, (ii) allow for an extension of Moore's scaling as far as possible, (iii) outperform the currently manufactured silicon metal-oxide-semiconductor field-effect transistors (MOSFETs), and (iv) drastically reduce the IC power consumption and heat dissipation.

Computer aided design (CAD) and experimental efforts can be combined to efficiently address these issues and accelerate the development of new transistor technologies. In effect, physics-based computer simulations represent a powerful methodology to investigate the performance of novel electronic devices prior to their fabrication, reveal internal quantities that cannot be directly measured, identify intrinsic deficiencies early enough to save time and money, or explore new device ideas. Semi-classical approaches like the drift-diffusion model [2, 3, 4] and Monte Carlo simulations [5, 6, 7] have proved their utility in the past. Now that the active region

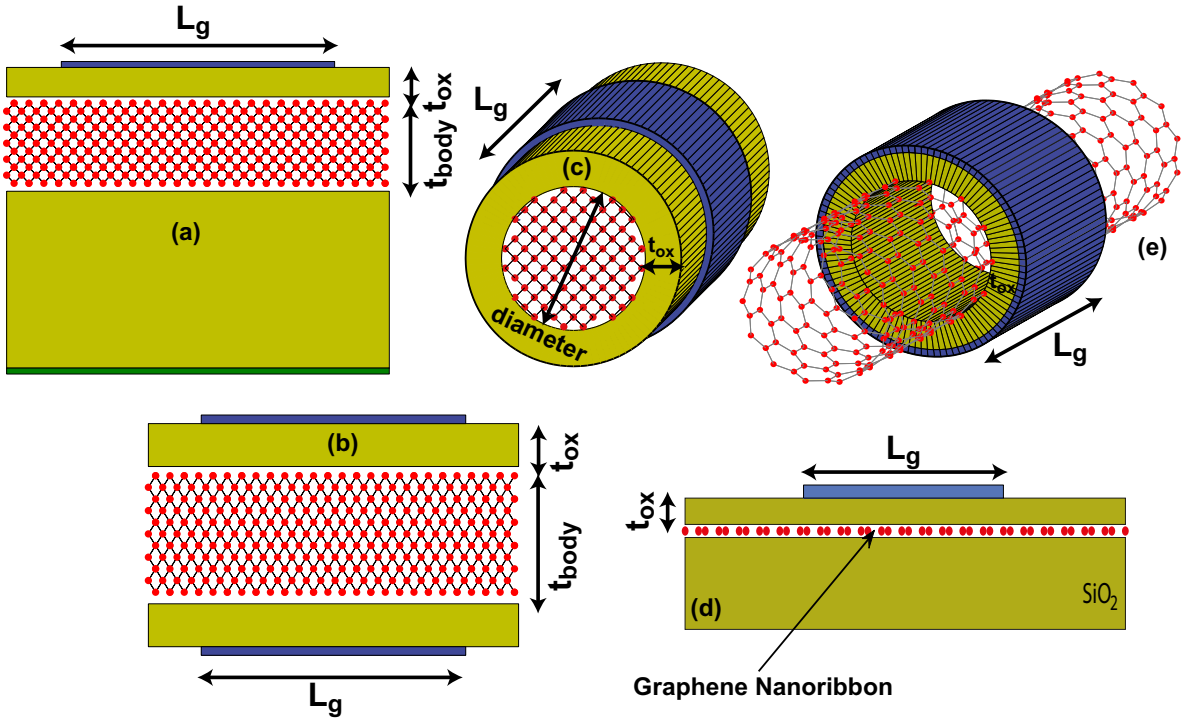


Figure 1: Schematic view of device structures that OMEN can simulate: (a) Single-Gate Ultra-Thin-Body (SG UTB), (b) Double-Gate Ultra-Thin-Body (DG UTB), (c) Gate-All-Around Nanowire (GAA NW), (d) Single-Gate Graphene Nanoribbon (SG GNR), and (e) Coaxially-Gated Carbon Nanotube (CG CNT). The UTB and NW transistors can be made of Si, Ge, or III-V semiconductors. The parameter $L_g$ refers to the gate length, $t_{body}$ to the body thickness, and $t_{ox}$ to the oxide layer thickness.

of transistors is getting closer to the atomic scale and their behavior completely dominated by quantum mechanical effects, the semiconductor industry presses for new modeling concepts to support the development of ultra-scaled devices.

A direct and self-consistent solution of the single-electron Schrödinger equation with open boundary conditions is more accurate than drift-diffusion and Monte Carlo approaches at the nanometer scale. Furthermore, it fulfills the quantum mechanical requirement, but demands more computational power. However, the continuous increase of the CPU performance in recent years offers a fantastic opportunity to re-think nanoelectronic device simulation and go multiple steps beyond standard approaches. In this context, we have developed OMEN, a next generation, multi-dimensional CAD tool based on quantum mechanics and dedicated to the simulation of nanoelectronic devices [8]. Due to multiple parallelization levels, it can benefit from the largest available supercomputers to investigate electrical and thermal transport through nanostructures with an atomistic resolution.

The implementation of OMEN started in 2005 at the ETH Zürich, continued from 2008 to 2011 at Purdue University, and it now again pursued at the ETH Zürich. Since 2005, it has been used to study electron and phonon transport in a broad range of device structures, some of them being shown in Fig. 1. Its usefulness has been demonstrated in various applications such as studying the transport properties and the gate length scaling behavior of ideal and

rough Si triple-gate nanowires with different crystal orientations, comparing the output characteristics of $n$- and $p$-doped Si double-gate ultra-thin-body field-effect transistors (FETs) with different transport and confinement directions, reproducing the experimental data of existing InGaAs high-electron mobility transistors (HEMTs), investigating line-edge roughness in armchair graphene nanoribbons, analyzing and optimizing the performances of different types of band-to-band tunneling transistors (TFETs), understanding the effect of electron-phonon scattering in nanowires and extracting their phonon-limited mobilities, or investigating thermal transport through rough Si nanowires.

In all these applications, the time-to-solution as well as the potential to treat large structures are critical parameters that must be properly handled. The Non-equilibrium Green's Function (NEGF) formalism is very popular among the device modeling community to solve the Schrödinger equation with open boundary conditions [9], but it is computationally intensive, difficult to parallelize, and if not carefully implemented, limited to small device structures. Here, it will be shown how NEGF can be used in OMEN to treat electron-phonon and anharmonic phonon-phonon scattering in realistically large nanostructures and how it can be replaced by a so-called Wave Function approach [8] in coherent transport simulations. As key achievements, very good agreements with experimental data extracted from different device types as well as a sustained performance of 1.44 PFlop/s on 221,400 cores of the former CRAY-XT5 Jaguar at Oak Ridge National Laboratory are reported here.

This research highlight is organized as follows: in Section 2, an overview of the simulation approach is given, followed by its application to four device structures in Section 3. The parallel scheme and performance of OMEN are described and analyzed in Section 4 before the paper is concluded in Section 5.

# 2 Overview of the Simulation Approach

## 2.1 Formulation of the quantum transport problem

OMEN solves multi-dimensional Schrödinger equations with open boundary conditions (OBCs) in the Non-Equilibrium Green's Function (NEGF) or Wave Function (WF) formalism. It is based on different flavors of the nearest-neighbor tight-binding model [10] (single $s$-orbital, $p_z$, $sp^3$, $sp^3s^*$, or $sp^3d^5s^*$, with or without spin-orbit coupling) for electrons and holes and on a modified valence-force-field method for phonons [11]. The carrier and current densities of the simulated nanostructures are obtained by self-consistently coupling the solution of the Schrödinger and Poisson equations till convergence is reached. This must be repeated for multiple bias points in order to obtain *I-V* (current vs. voltage) characteristics.

The core operation in OMEN is to solve the Schrödinger equation for each electron/hole/phonon energy $E$ and momentum $k$. In bulk-like structures (1-D), transport occurs along the $x$ direction (convention) and the $y$ and $z$ axis are assumed periodic so that the momentum vector $k$=$(k_y, k_z)$ is two-dimensional. In quantum wells or ultra-thin-bodies (2-D), $y$ is a direction of confinement along the body or quantum well thickness and $z$ is assumed periodic. In this case, the momentum vector $k$ reduces to a single component $k$=$k_z$. Finally, in nanowires (3-D), $y$ and $z$ are directions of confinement and $k$=0 (no momentum dependence).

Open boundary conditions are introduced to couple the simulation domain to its surrounding environment (semi-infinite contacts or reservoirs) and allow for electrons/holes/phonons to enter and exit a finite domain. One of the most popular ways of treating the Schrödinger equation with

OBCs is the NEGF formalism [9], which consists in solving the following system of equations for electrons or holes

$$\big(\mathbf{E} - \mathbf{H}(k) - \mathbf{V} - \mathbf{\Sigma}^{RB}(E,k) - \mathbf{\Sigma}^{RS}(E,k)\big) \cdot \mathbf{G}^{R}(E,k) \;=\; \mathbf{I} \tag{1}$$

$$\mathbf{G}^{<}(E,k) \;=\; \mathbf{G}^{R}(E,k) \cdot \big(\mathbf{\Sigma}^{<B}(E,k) + \mathbf{\Sigma}^{<S}(E,k)\big) \cdot \mathbf{G}^{A}(E,k). \tag{2}$$

In Eq. (1) and (2), the unknowns are the retarded $\mathbf{G}^{R}(E,k)$ and lesser $\mathbf{G}^{<}(E,k)$ Green's functions at energy $E$ and momentum $k$. They are matrices of size $N_A \times N_{orb}$ where $N_A$ is the number of atoms composing the simulation domain and $N_{orb}$ the number of orbitals describing the properties of each atoms. For example, $N_{orb}$=10 in the $sp^3d^5s*$ tight-binding model without spin orbit coupling, 1 $s$ orbital, 3 $p$ orbitals, 1 excited $s$ orbital called $s*$, and 5 $d$ orbitals. If spin-orbit coupling is included, $N_{orb}$ increases to 20.

The single elements of the retarded $G_{ij}^{R\sigma_1\sigma_2}(E,k)$ and lesser $G_{ij}^{<\sigma_1\sigma_2}(E,k)$ Green's Functions represent the coupling or correlation between two orbitals $\sigma_1$ and $\sigma_2$ situated on two atoms $i$ and $j$. The diagonal matrix $\mathbf{E}$ contains the electron/hole energy $E$, $\mathbf{I}$ is the identity matrix, $\mathbf{H}(k)$ refers to the device Hamiltonian matrix, which includes the orbital on-site energies as well as the coupling elements between different orbitals and atoms ($H_{ij}^{\sigma_1\sigma_2}$). The entries of the diagonal matrix $\mathbf{V}$ are the electrostatic potential at each atomic site. The open boundary conditions are cast into the matrices $\mathbf{\Sigma}^{RB}(E,k)$ and $\mathbf{\Sigma}^{<B}(E,k)$. Finally, the scattering mechanisms such as electron-phonon are described by the scattering self-energies $\mathbf{\Sigma}^{RS}(E,k)$ and $\mathbf{\Sigma}^{<S}(E,k)$. Note that $G_{ij}^{A\sigma_1\sigma_2}(E,k)$=conj($G_{ji}^{R\sigma_2\sigma_1}(E,k)$) and that a greater Green's Function $\mathbf{G}^{>}(E,k)$ exists, defined as in Eq. (2), except that $<$ is replaced by $>$.

For phonons, Eq. (1) and (2) are slightly modified and take the following form

$$\big(\omega^2 - \mathbf{\Phi}(q) - \mathbf{\Pi}^{RB}(\omega,q) - \mathbf{\Pi}^{RS}(\omega,q)\big) \cdot \mathbf{D}^{R}(\omega,q) \;=\; \mathbf{I} \tag{3}$$

$$\mathbf{D}^{<}(\omega,q) \;=\; \mathbf{D}^{R}(\omega,q) \cdot \big(\mathbf{\Pi}^{<B}(\omega,q) + \mathbf{\Pi}^{<S}(\omega,q)\big) \cdot \mathbf{D}^{A}(\omega,q). \tag{4}$$

The main differences with Eq. (1) and (2) comes from the notation of the phonon Green's Functions, $\mathbf{D}^{<,>,R,A}(\omega,q)$ instead of $\mathbf{G}^{<,>,R,A}(\omega,k)$ and of the self-energies $\mathbf{\Pi}^{<,>,R,A}(\omega,q)$. The electron/hole energy $E$ is replaced by $\omega^2$, the square of the phonon frequency, the phonon momentum is denoted by $q$ instead of $k$, and the Hamiltonian matrix $\mathbf{H}(k)$ becomes a dynamical matrix $\mathbf{\Phi}(q)$ of size $3\times N_A$. The valence-force-field method is employed to construct $\mathbf{\Phi}(q)$.

Equations (1)-(4), which have the form "A·B=C", must be solved for each possible energy $E$ or frequency $\omega$ and momentum $k$ ($q$). This can be done with a recursive Green's Function (RGF) algorithm instead of directly inverting or multiplying large matrices [12]. Although much more efficient than brute-force solutions, the RGF algorithm still induces high computational costs and limits the size of the device structure that can be treated. Furthermore, the presence of dissipative scattering mechanisms, cast into the self-energies $\mathbf{\Sigma}^{R,>,<,S}(E,k)$ and $\mathbf{\Pi}^{R,>,<,S}(\omega,q)$, couple different energies or frequencies and momentum altogether, adding another level of complexity to the problem.

Ballistic simulations represent a special case of Eq. (1)-(4) since all the scattering self-energies disappear and the equation for each energy and momentum can be treated independently from the others. Beside that simplification, the NEGF formalism can be replaced by a Wave Function approach where a single system of equations must be solved

$$\big(\mathbf{E} - \mathbf{H}(k) - \mathbf{\Sigma}^{RB}(k,E)\big) \cdot \mathbf{C}(k,E) \;=\; \mathbf{Inj}(k,E) \tag{5}$$

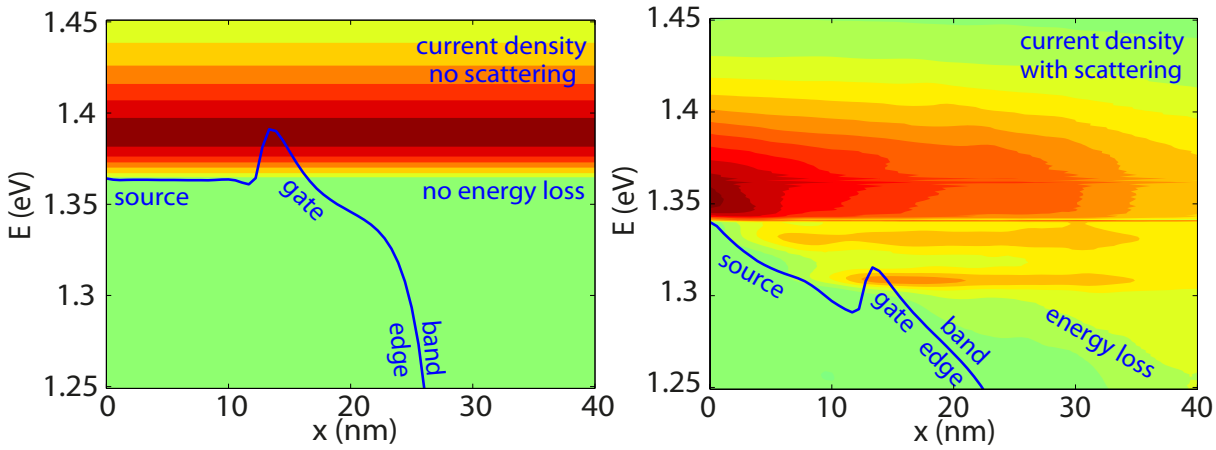


Figure 2: Spectral distribution of the electron current flowing through a nanowire transistor. (left) Ballistic limit of transport. (right) With electron-phonon scattering. Red indicates a high current concentration, green no current. The blue lines refer to the conduction band edge of these transistors.

for electrons and holes. A similar equation can be derived for phonons. The multiple right-hand-side vector $\mathbf{Inj}(k, E)$ contains all the electronic states that are injected into the device structure from the contact regions. The advantage of Eq. (5) over Eq. (1) to (4) resides its form, a sparse linear system of equations "Ax=b", where the unknown is the coefficient vector $\mathbf{C}(k, E)$. Equation (5) can therefore be solved more efficiently using direct sparse linear solvers such as Umfpack [13], Pardiso [14], SuperLU$_{dist}$ [15], MUMPS [16], or a home-made block cyclic reduction (BCR) of the matrix "A" [17]. The Wave Function formalism thus allows for rapid simulations of large nanostructures, but only works in ballistic cases.

## 2.2 Electron-phonon and phonon-phonon scattering

Very short devices do not necessarily operate close to their ballistic limit of transport (no interaction with their environment). Historically, it has been observed that Si transistors, irrespective of their gate length, operate at about 50% or less of their theoretical limit. Other semiconductor materials such as InGaAs can reach higher values (80-90%), but never 100%. It is therefore mandatory to include the interactions of electrons, holes, and phonons with each other and with their environment into the modeling effort in order to produce a tool capable of predicting the performance of nanoelectronic devices. Especially, the dissipative electron/hole-phonon and anharmonic phonon-phonon scattering mechanisms play an essential role at the nanoscale and should not be neglected. They have been therefore implemented in OMEN.

Electron-phonon scattering is expected to drastically reduce the ON-current of ultra-scaled transistors due to an effect known as backscattering [18]. By absorbing or emitting phonons, electrons are reflected back to their origin instead of propagating along one single direction. Electron-phonon scattering also modifies the spectral distribution of the current within a device structure and affects the electrostatic potential, as indicated in Fig. 2: while moving from the source to the drain contact of a transistor, electrons may loose energy by emitting phonons. Hence, in the presence of dissipative scattering, they enter and leave the device structure at a different energy. In the ballistic limit, each electron keeps the same energy and momentum from the beginning till the end of its trajectory.

In the NEGF formalism the scattering self-energies $\mathbf{\Sigma}^{\gtrless S}(E,k)$ and $\mathbf{\Sigma}^{RS}(E,k)$ have the following form to account for electron-phonon scattering [19]

$$\begin{aligned}\mathbf{\Sigma}^{\gtrless S}_{nn}(E,k) &= \sum_{l,i,j}\sum_{q}\sum_{\omega_{ph}} \mathcal{V}^{ij}_{nlln}(\omega_{ph},q)\cdot\nabla_i\mathbf{H}_{nl}\cdot\Big(n^{ph}(\omega_{ph})\cdot\mathbf{G}^{\gtrless}_{ll}(E\pm\hbar\omega_{ph},k-q)+ \\ &\qquad (n^{ph}(\omega_{ph})+1)\cdot\mathbf{G}^{\gtrless}_{ll}(E\mp\hbar\omega_{ph},k-q)\Big)\cdot\nabla_j\mathbf{H}_{ln}, \\ \mathbf{\Sigma}^{RS}_{nn}(E,k) &\approx \frac{1}{2}(\mathbf{\Sigma}^{>S}_{nn}(E,k)-\mathbf{\Sigma}^{<S}_{nn}(E,k)). \end{aligned} \tag{6}$$

All $\mathbf{\Sigma}$'s are block diagonal matrices, where each block $\mathbf{\Sigma}^{S}_{nn}(E,k)$ is of size $N_{orb}\times N_{orb}$. In Eq. (6), $\omega_{ph}$ is the confined phonon frequency, $n^{ph}(\omega_{ph})$ the Bose distribution of equilibrium phonons with frequency $\omega_{ph}$ and momentum $q$. The quantity $\nabla_i\mathbf{H}_{nm}$ represents the derivative of the nearest-neighbor coupling matrix $\mathbf{H}_{nm}$ with respect to the coordinate $i$=$x$, $y$, or $z$ along the bond $\mathbf{R}_m-\mathbf{R}_n$ connecting the atoms $n$ and $m$. To simplify the calculation, all the self-energies are assumed local in position, i. e. only the diagonal $\mathbf{\Sigma}^{S}_{nn}(E,k)$ elements are considered [19]. The form factor $\mathcal{V}^{ij}_{nmmn}(\omega_{ph},q)$ contains information about the phonon modes.

It becomes clear from Eq. (6) that one energy-momentum $(E,k)$ pair is connected to many other $(E-E',k-q)$. If the computation of the energy and momentum points is parallelized, as shown later, the required exchange of information between CPUs storing different $(E',k')$ configurations makes the solution of Eq. (6) more tedious from a numerical point of view. Since also the expression for the scattering self-energy $\mathbf{\Sigma}^{\gtrless S}(E,k)$ in Eq. (6) depends on the Green's Function $\mathbf{G}^{\gtrless}(E-E',k-q)$ in Eq. (2), these two equations must be iteratively solved till convergence is achieved. This procedure is known as self-consistent Born approximation. It requires $N_{SC,iter}$ iterations to convergence, where $N_{SC,iter}$ might vary from 5 to 50 and is not known at the beginning of a simulation.

As electron-phonon scattering affects electronic transport, anharmonic phonon-phonon scattering has a huge influence on thermal transport processes: it strongly reduces the thermal conductivity of materials for temperatures about 100 K. In the framework of NEGF, anharmonic phonon-phonon scattering can be formulated with the help of scattering self-energies $\mathbf{\Pi}^{\gtrless S}(\omega,q)$ and $\mathbf{\Pi}^{RS}(\omega,q)$ defined as [20]

$$\begin{aligned}\mathbf{\Pi}^{\gtrless S}_{nn}(\omega,q) &= 2i\hbar\sum_{lm}\sum_{q'}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}dV^{(3)}_{nlm}(q')dV^{(3)}_{lmn}(q')\mathbf{D}^{\gtrless}_{ll}(\omega+\omega',q+q')\mathbf{D}^{\lessgtr}_{mm}(\omega',q'), \\ \mathbf{\Pi}^{RS}_{nn}(\omega,q) &\approx \frac{1}{2}(\mathbf{\Pi}^{>S}_{nn}(\omega,q)-\mathbf{\Pi}^{<S}_{nn}(\omega,q)). \end{aligned} \tag{7}$$

As for electron-phonon scattering, all the $\mathbf{\Pi}$ are block diagonal matrices. Each block $\mathbf{\Pi}^{S}_{nn}(\omega,q)$ is of size 3×3. In Eq. (7), the term $dV^{(3)}_{lmn}$ refers to the third derivative of the anharmonic potential energy $V^{anh}$ as function of the atom positions $\mathbf{R}_l$, $\mathbf{R}_m$, and $\mathbf{R}_n$ [11]. For phonons too, one frequency-momentum pair ($\omega$,$q$) is connected to many other ($\omega+\omega'$,$q+q'$), making the parallelization of these quantities much more complicated than in ballistic simulations. Also, Eq. (7) depends on Eq. (3) and (4) so that both systems of equations must be solved self-consistently. This iterative process usually converges for $10\leq N_{SC,iter}\leq 100$.

## 2.3 Carrier and current densities

Once that Eq. (1) and (2) have been solved for each electron/hole energy $E$ and momentum $k$, the charge and current densities of the considered systems can be calculated in the NEGF formalism according to the following equations

$$n(\mathbf{r}) \;=\; -i \sum_j \sum_k \int \frac{\mathrm{d}E}{2\pi} \mathrm{tr}\left(\mathbf{G}^<_{jj}(E,k)\right) \delta(\mathbf{r}-\mathbf{R_j}) \tag{8}$$

and

$$J_{i\rightarrow i+1} \;=\; \frac{e}{2\hbar} \sum_{i_1\in i} \sum_{i_2\in i+1} \sum_k \int \frac{\mathrm{d}E}{2\pi} \mathrm{tr}\left(\mathbf{H}_{i_1 i_2}\cdot\mathbf{G}^<_{i_2 i_1}(E,k) - \mathbf{G}^<_{i_1 i_2}(E,k)\cdot\mathbf{H}_{i_2 i_1}\right). \tag{9}$$

The trace operator $\mathrm{tr}$ runs over all the orbitals of an atom situated at $\mathbf{r}=\mathbf{R}_j$ in Eq. (8) and over the orbitals of all the atoms situated in the plane $x$=$x_i$ in Eq. (9). Hence, $J_{i\rightarrow i+1}$ depicts the electron current flowing between the atomic plane $x$=$x_i$ and $x_{i+1}$.

The charge density $n(\mathbf{r})$ in Eq. (8) is then used to compute the electrostatic potential $V(\mathbf{r})$ that forms the diagonal entries of the matrix $\mathbf{V}$ in Eq. (1). This is achieved through Poisson equation that is self-consistently solved with Eq. (1), (2) and (8). This additional loop between $n(\mathbf{r})$ and $V(\mathbf{r})$ typically converges after $N_{Poiss,iter}$=3 to 10 iterations.

For phonons, the quantity of interest is the thermal current that flows through nanostructures whose contacts exhibit different temperatures. It is defined as

$$J_{ph,i->i+1} \;=\; \sum_{i_1\in i} \sum_{i_2\in i+1} \sum_q \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega \;\mathrm{tr}\left(\mathbf{\Phi}_{i_1 i_2}\cdot\mathbf{D}^<_{i_2 i_1}(\omega,q) - \mathbf{D}^<_{i_1 i_2}(\omega,q)\cdot\mathbf{\Phi}_{i_2 i_1}\right). \tag{10}$$

In Eq. (10), the trace operator runs over the 3 degrees of freedom along which atoms can oscillate, $x$, $y$, and $z$. The phonon density, contrary to the electron density, does not play an important role since there is no Poisson equation to solve here. Hence, it is not calculated.

# 3 Application to Nanoelectronic Devices

The models that have been implemented in OMEN and described in Section 2 serve as the basis to simulate next generation nanoelectronic devices and predict their performance before they are even fabricated. To achieve this ambitious goal, it should first be demonstrated than OMEN can reproduce available experimental data. This will be done by comparing simulation results and experimental measurement for four different types of nanoscale applications.

## 3.1 III-V high electron mobility transistor

The first application deals with a multi-quantum well InAs high electron mobility transistor (HEMT) as schematized in Fig. 3. Due to their excellent transport properties, 10 to 15 times better than Si, III-V semiconductors are attracting a lot of attention as potential replacement for Si in 5 to 10 years from now. However, currently, the III-V technology is not mature enough to build the core of metal-oxide-semiconductor field-effect transistors (MOSFETs) with equivalent or better characteristics than Si, but progresses are regularly made. The major difficulties to

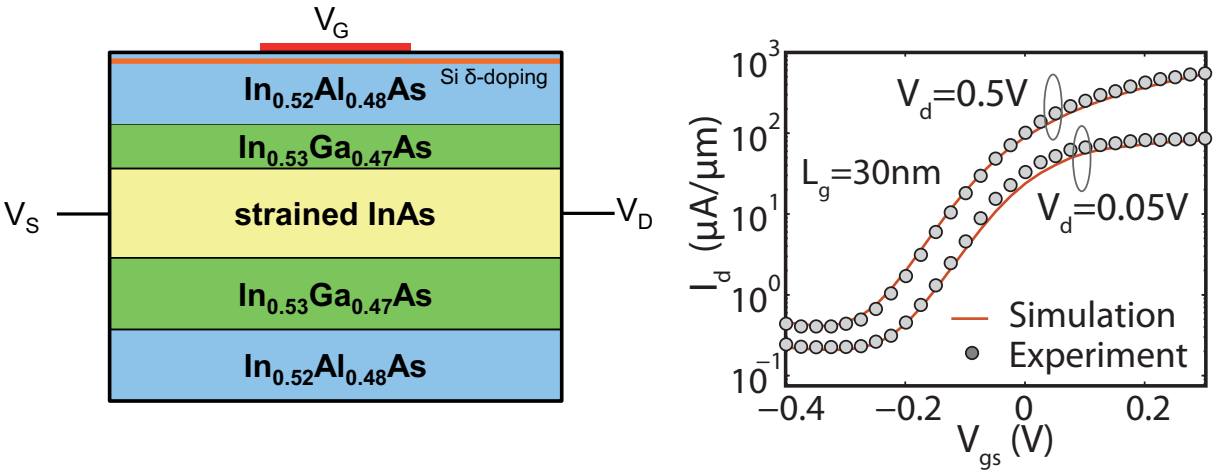


Figure 3: (left) Schematic view of a III-V multi-quantum well high electron mobility transistor (HEMT) composed of a 5 nm strained-InAs channel surrounded by $In_{0.53}Ga_{0.47}As$ and $In_{0.52}Al_{0.48}As$ barriers. The gate length of the experimental devices is as short as 30 nm [21]. (right) Comparison between experimental data (circles) and simulation results (solid lines) for the HEMT transfer characteristics $I_d$-$V_{gs}$ at different drain-to-source voltages $V_{ds}$.

overcome include a reduction of the source and drain contact resistances, the growth of high-$\kappa$ dielectric layers on III-V channels, and the design of devices with good $p$-type performance.

Despite not being candidates to replace Si transistors, III-V HEMTS represent a good testbed on the way towards competitive III-V MOSFETs, both from an experimental and modeling perspective. In effect, they allow for a deep investigation of the intrinsic transport properties of materials such as InGaAs or InGaSb without the difficulties arising from high-$\kappa$ dielectrics or contact dimensions. Furthermore, a lot of experimental data has been generated for HEMTs, that can be used to verify the accuracy of advanced simulation approaches. Hence, in Fig. 3, the results of OMEN are compared to the measurement from Ref. [21]. The comparison shows a good agreement in the OFF-state of the transistor, dominated by gate leakage currents, and in the ON-state where the contact series resistances have a strong influence.

## 3.2 Carbon nanotube field-effect transistor

In the second application, a carbon nanotube field-effect transistor (CNT FET) is considered. The motivation for studying such devices is the same as for III-V semiconductors: CNTs exhibit an electron and hole mobility that is much higher than Si, thus making them good candidates to become the next generation switch at the horizon of 2020. As additional benefit of CNT FETs, devices with a gate length of 9 nm only have already been fabricated and showed extremely good characteristics, especially an impressively small inverse subthreshold slope of 94 mV/decade [22]. A sketch of the device structure is given in Fig. 4.

This ultra-short CNT FET has been simulated with OMEN and the experimental and modeling results compared to each other. As for the III-V HEMT, very good agreement between them could be obtained, as reported in Fig. 4. It is important to realize that the current distribution in HEMTs and CNT FETs is relatively different, but the reproduction of experimental data very good in both cases. In HEMTs, electrons flow on the top of a potential barrier controlled by the

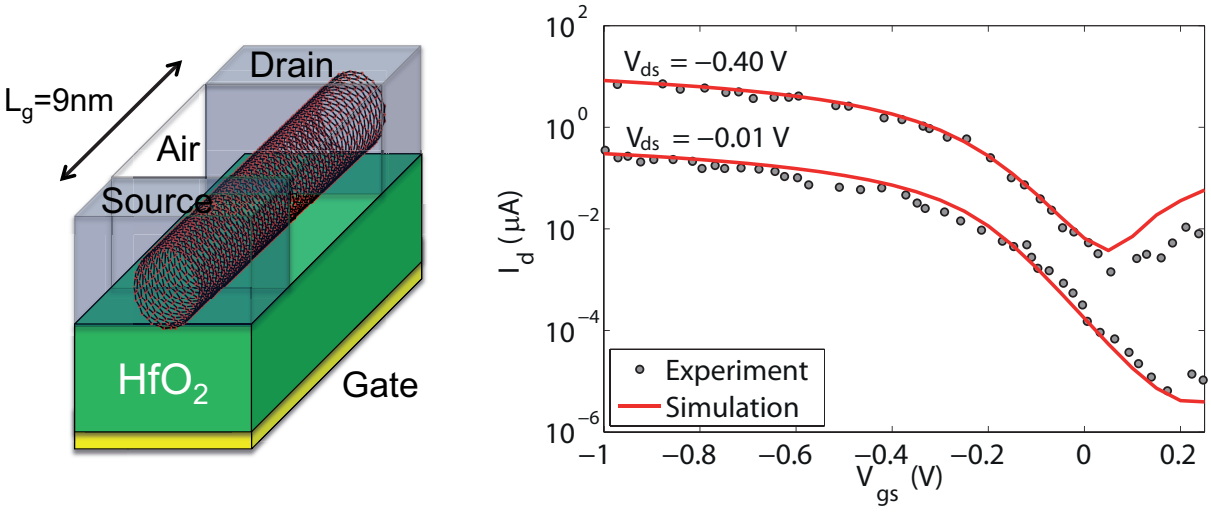


Figure 4: (left) Schematic view of a carbon nanotube (CNT) field-effect transistor deposed on a $HfO_2$ dielectric layer and having a gate length $L_g$=9 nm [22]. The red dots indicate carbon atoms. (right) Comparison between the experimental (circles) and simulated (solid lines) transfer characteristics of the CNT FET shown on the right.

gate contact. In CNT FETs both electrons an holes can flow through the device structure, leading to an ambipolar behavior where the drain current decreases till $V_{gs} \approx 0$ (hole contribution) and then starts to increase (electron contribution).

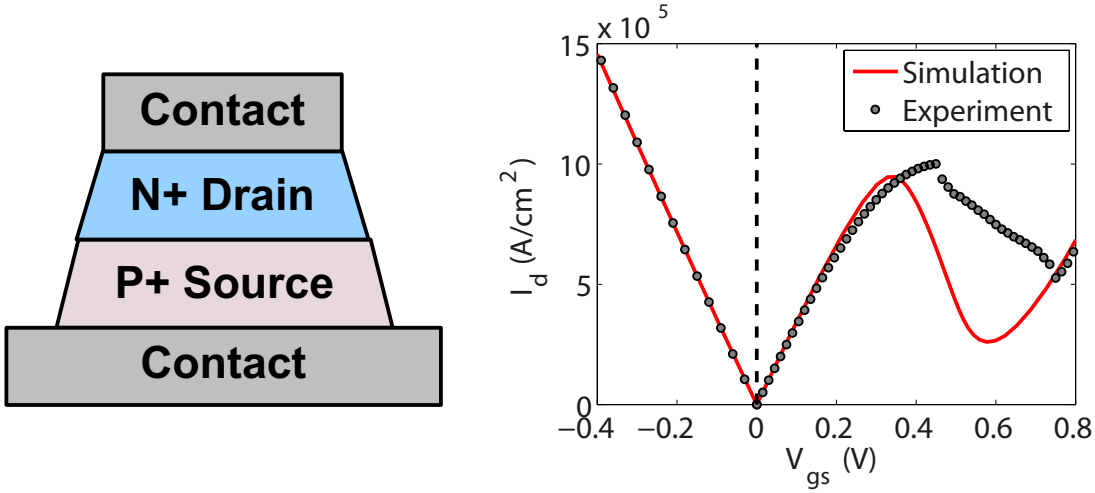


Figure 5: (left) Schematic view of $p$-$n$ $In_{0.53}Ga_{0.47}As$ band-to-band (Esaki) tunneling diode. (right) Comparison between the experimental data (circles) [23] and simulation results (solid lines) for different applied voltages.

## 3.3 III-V band-to-band tunneling diode

Reducing the power consumption and heat dissipation of integrated circuits has become a goal of utmost importance. In conventional Si transistors, this has been made difficult by the fact that the device dimensions have scaled much faster than the supply voltages, thus increasing

the local power density. Novel device concepts based on quantum mechanical tunneling instead of thermionic currents have started to emerge. They may eventually circumvent the power consumption problem of ICs. These band-to-band tunneling transistors (TFETs) rely on cold electrons and should be able to provide high ON-currents at lower supply voltages. The basic idea is to reduce the amount of voltage needed to increase the device current by one order of magnitude. In conventional transistors, at least 60 mV must be applied to reach this goal, but in TFETs, there is theoretically no lower limit.

So far, there have been very few successful demonstrations of properly working TFETs, mainly due to technical issues (source regrowth, high-$\kappa$ dielectric layers, electrostatic control). However, band-to-band tunneling (or Esaki) diodes have been manufactured in mass. Based on the characteristics of such devices, it is possible to estimate the maximum tunneling current that can be obtained from a single material or from an heterojunction once used in a TFET configuration. The $In_{0.53}Ga_{0.47}As$ tunneling diode idealized in Fig. 5 has therefore been simulated with OMEN and the results compared to experimental data. Again, a good agreement between them is obtained, at low and high voltages. There is only a small discrepancy in the valley current at around $V_{gs}$=0.55 V. The inclusion of electron-phonon scattering, which is thought to be the dominant effect in that region, did not help increase the simulation current.

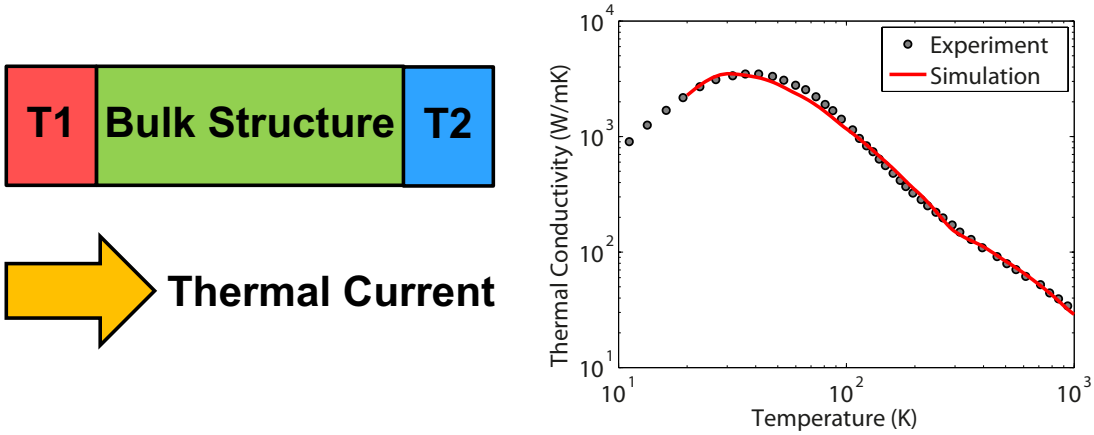


Figure 6: (left) Schematic view of Si bulk structure with different temperatures $T_1 > T_2$ applied to its left and right contact. (right) Comparison between the experimental (circles) and simulated (solid line) lattice thermal conductivity of bulk Si for temperatures ranging from 20 to 1000 K.

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## 3.4 Lattice thermal conductivity of bulk Si

The last application is centered around thermal rather than electronic transport. To better understand heat dissipation and self-heating effects in nanoscale transistors as well as to design more efficient thermo-generators based on the Seebeck effect, it is highly desirable to have a simulation tool that can precisely capture thermal current in nanostructures. The anharmonic phonon-phonon scattering model introduced in Section 2.2 has been developed in that spirit. To verify and validate its accuracy, the lattice thermal conductivity of bulk Si has been simulated with OMEN and compared to experimental data. The results are shown in Fig. 6. A good reproduction of the measurement data can be observed for temperatures up to 1000 K.

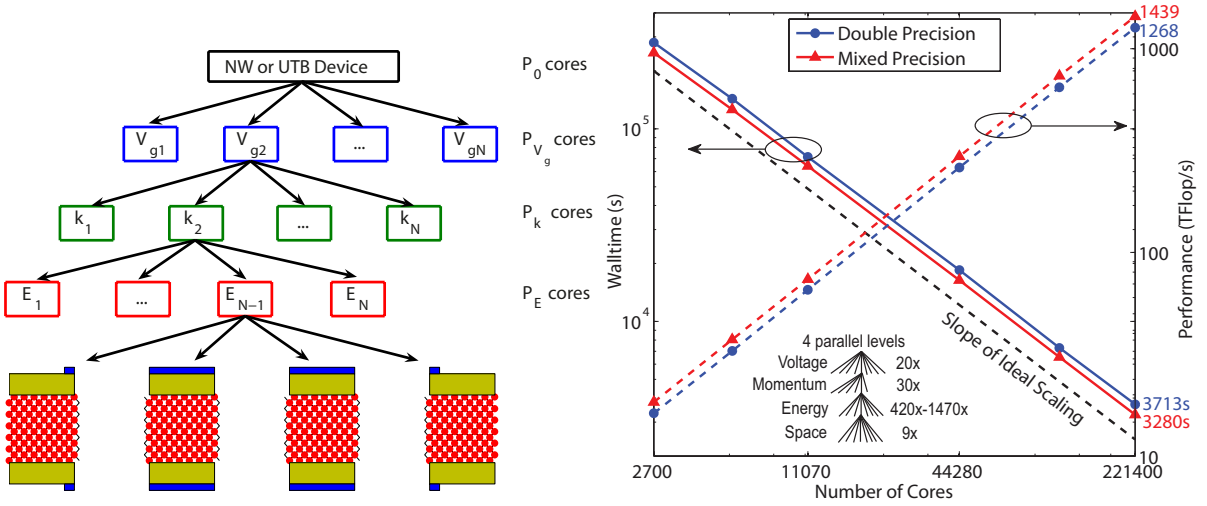


Figure 7: (left) Parallelization scheme of OMEN. The bias, the momentum, and the energy points are parallelized while a 1-D spatial domain decomposition is applied to form the fourth level of parallelism. (right) OMEN scaling performances on the former CRAY-XT5 Jaguar at Oak Ridge National Lab from 2,700 to 221,400 cores to simulate 20 bias points of the same InAs HEMT as in Fig. 3. A total of 30 momentum points are used, the number of energy points $N_E(k)$ varies from 420 to 1,470, and spatial domain decomposition is performed on 9 cores. Solid lines refer to the simulation time, dashed lines to the sustained performance. Two types of numerical experiments were conducted, in double (blue) and in mixed (red) precision [24].

To summarize, with one single computer aided design tool, OMEN, the current characteristics of existing structures cab be faithfully reproduced although their behavior rely on sometimes completely different transport mechanisms. These unprecedented modeling capabilities open new perspectives in the CAD of next generation nano-transistors. Being able to compare the performance of not-yet-fabricated devices and reliably identify the best design configuration is becoming a reality that will accelerate the innovation of novel types of logic switches, thermo-generators, and electro-optical converters.

# 4 Parallel Performance

All the applications in Section 3 require the utilization of sophisticated physical models that are computationally intensive and could not run on a single CPU. Hence, the distribution of the work load in OMEN is crucial to reduce the computational burden and allow for the simulation of larger device structures. Based on the algorithms presented in Section 2, four natural levels of parallelism have been identified, (i) the bias points, (ii) momentum points ($k$), (iii) energy points ($E$), and (iv) a 1-D spatial decomposition of the simulation domain, as depicted in Fig. 7 (left). The latter consists in solving the Schrödinger equation in parallel.

The number of cores attributed to each parallelization level is selected by the user at the beginning of the simulation. Starting from a total of $P_0$ cores, $N_{V_g}$ bias points are simultaneously treated on $P_{V_g}$=$P_0/N_{V_g}$ cores, where $P_{V_g}$ is an input parameter. The number of momentum points per bias point, $N_k$, is chosen by the user, but the number of cores dedicated to each $k$ group depends on the number of energy points, $N_E(k)$, and is dynamically allocated by OMEN.

An optimal balance of the work load results from this process. At the lowest parallel level, the spatial domain decomposition is accomplished on $P_E$ cores.

As an illustration of the quad-level parallel scheme described above, the same InAs HEMT structure as in Fig. 3 is considered. As shown in Fig. 7 (right), OMEN scales almost perfectly up to 221,400 cores on the former CRAY-XT5 Jaguar at ORNL to simulate this device in the ballistic limit of transport. A total of 20 bias points are calculated, for which the number of self-consistent Poisson iterations is limited to 5. The periodic $z$-axis is modeled via 30 momentum points, the number of energy points $N_E(k)$ is different for each momentum and is comprised between 420 and 1470. Finally, the spatial domain decomposition is accomplished on 9 cores using a home-made block cyclic reduction algorithm. In this specific simulation, the Schödinger equation has to be solved more than 2 millions times.

The parallelization of the work load reduces the simulation time from several years on a single CPU down to around 1 hour on 221,400 cores on Jaguar. At the same time, OMEN reaches a parallel efficiency of 90% in going from 2,700 up to 221,400 cores and a sustained performance of 1.44 PFlop/s on 221,400 cores in mixed precision and 1.27 PFlop/s in double precision. This corresponds to about 55% of the peak performance of the machine. When electron-phonon or anharmonic phonon-phonon scattering are turned on, the parallel performance of OMEN deteriorates due to a massive increase of inter-processor communication caused by the solution of Eq. (6) and (7). Nevertheless, the parallel efficiency remains above 70% for both scattering mechanisms when the number of cores increases from 2,000 up to 50,000.

# 5 Conclusion and Outlook

A physics-based simulation approach dedicated to nanoelectronic devices has been presented in this overview report. It is based on an accurate description of electron, hole, and phonon properties using tight-binding and valence-fore-field methods, includes quantum transport capabilities through the NEGF formalism, and rely on a massive parallelization of the work load. It has been demonstrated that the resulting CAD tool captures the physics and reproduces the experimental data of various types of nano-transistors. As next steps, close collaborations with experimental groups will be established to help them design next generation logic switches. On the modeling side, new physical models such as coupled electro-thermal transport will be added to the simulation environment, the parallel algorithms improved and ported to new hardware architectures, GPUs for example.

# Acknowledgments

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# 5

# CSE Research Projects

**Title:** Multi-level $\mu$-FE analysis for human bone structures

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

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

**Description:**

Micro-structural finite element ($\mu$FE) 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 $\mu$FE 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 $\mu$FE simulations.

**Web sites:** `http://people.inf.ethz.ch/arbenz/projects/bone.html`

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**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.

**Web sites:**
Project homepage: `http://people.inf.ethz.ch/arbenz/projects/maxwell.html`

**References:**

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.

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.

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)

**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.

**Web sites:**
Project homepage: `http://people.inf.ethz.ch/arbenz/projects/maxwell.html`

**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[⋆]
Benedikt Oswald[†]

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

**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.

**Web site:**
Project homepage: `http://people.inf.ethz.ch/arbenz/projects/lossy.html`

**References:**

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[⋆]
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:**

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).

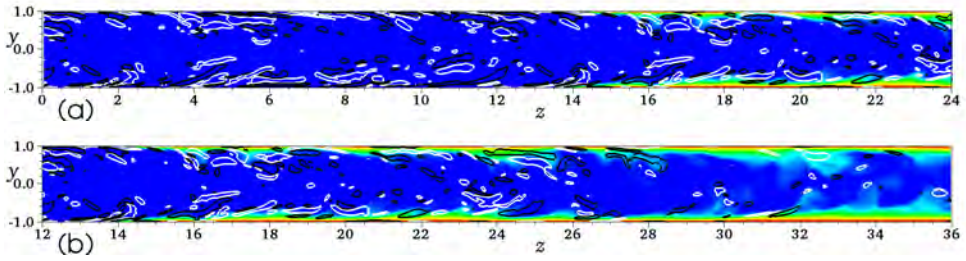
P. Arbenz, A. Hiltebrand, D. Obrist: *A parallel space-time finite difference solver for periodic solutions of the shallow-water equation.* In Parallel Processing and Applied Mathematics (PPAM 11) Part II. R. Wyrzykowski, J. Dongarra, K. Karczewski, J. Waśniewski (eds.). Lecture Notes in Computer Science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

**Title:** Three-dimensional direct numerical simulation of turbulent catalytic combustion

**Researchers:** F. Lucci[1,2], Christos E. Frouzakis[1], John Mantzaras[2]

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

The turbulent catalytic combustion of a fuel-lean hydrogen/air mixture (equivalence ratio $\phi$=0.24) was investigated by means of three-dimensional direct numerical simulation (DNS) in a platinum-coated plane channel with a prescribed wall temperature of 960 K and an incoming Reynolds number, based on the channel height, of 5700. Heat transfer from the hot catalytic walls laminarized the flow, as manifested by the progressive suppression of the high vorticity components of the flow aligned parallel to the channel walls at increasing streamwise distances. The impact of turbulence suppression on the mass transfer towards or away from the catalytic wall was subsequently assessed. Far upstream where high turbulence fluctuations persisted, the instantaneous local transverse gradient of the limiting hydrogen reactant (a quantity proportional to the catalytic reaction rate) as well as the instantaneous hydrogen concentration at the wall exhibited strong fluctuations by up to 300%, a result of finite-rate chemistry induced by the high inrush events towards the catalytic walls. Fourier analysis of the reaction rate fluctuations yielded peak frequencies of less than 1 kHz, values comparable to the thermal response frequencies of typical materials in commercial catalytic geometries. This has direct implications on the thermal stress of the reactor walls as well as on the decoupling between flow and solid thermal modeling currently used in practical catalytic reactors. Far downstream, the dampening of turbulence resulted in weaker hydrogen concentration fluctuations with nearly symmetric distributions. Finally, computed transverse turbulent species fluxes indicated inherent weaknesses of near-wall turbulence models in describing turbulent transport of species with disparate molecular diffusivities.




*Instantaneous temperature snapshot onto the $yz$-plane at $x = 1.5$ and of the quasi-streamwise streak vorticity structures demarcated by $\omega_z = -1$ (white lines) and $\omega_z = 1$ (black lines): (a) $0 \leq z \leq 24$, (b) $12 \leq z \leq 36$.*

**References:**

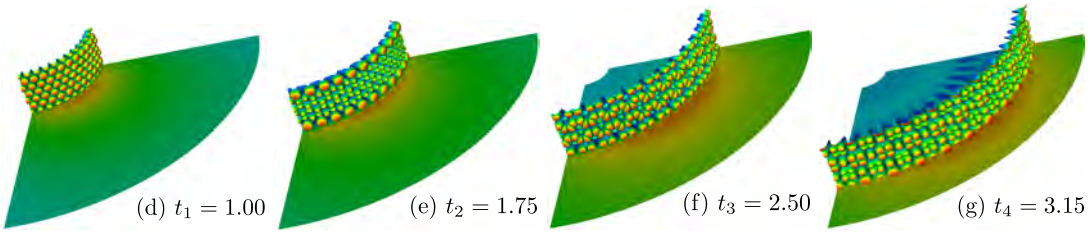
• F. Lucci, C.E. Frouzakis, J. Mantzaras, Three-dimensional direct numerical simulation of turbulent channel flow catalytic combustion of hydrogen over platinum, *Proc. Combust. Inst.*, 34, (in press)

**Title:** Instabilities of propagating circular and cylindrical lean premixed hydrogen/air flames

**Researchers:** C. Altantzis[1], C. E. Frouzakis[1], A. G. Tomboulides[2], K. Boulouchos[1]

**Institute/ Group:** [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]University of Western Macedonia, Kozani, Greece

The wrinkling of premixed flame fronts propagating in gravity-free, quiescent, diffusionally imbalanced mixtures results from the combined influence of hydrodynamic and thermodiffusive instabilities. In this paper, the evolution of expanding, lean (equivalence ratio $\phi$=0.6), premixed 2-D circular and 3-D cylindrical $H_2$/air flames is investigated numerically using a single-step reaction and detailed transport. The Lewis number of the deficient reactant is sufficiently low so that the flame is subjected to both instability mechanisms. Instead of following a monotonically accelerating behavior, the flame is found to switch between a self-accelerating fully wrinkled shape when the cellular structures are amplified and a decelerating flame when the cell amplification saturates and the flame surface becomes almost smooth. This behavior is more intense in the 3-D case. In order to elucidate the effect of the perturbation in the third direction, two 3-D cases with varying perturbation wavelength along the z-direction are considered. Finally, the effect of stretch rate on the local propagation characteristics of the flame is investigated for both 2-D and 3-D cases. It was observed that due to a wider range of curvatures, the 3-D flames experience negative displacement speeds relative to the flow along positively-curved flame segments.




*Cylindrical $H_2$-air flame: $T = 900$ K isosurface colored by the velocity magnitude at different time instants.*

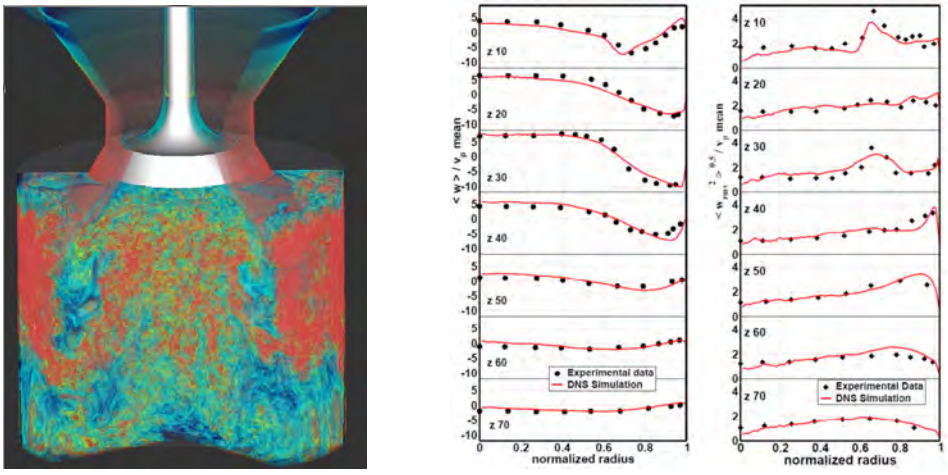
**References:**

• C. Altantzis, C.E. Frouzakis, A.G. Tomboulides, K. Boulouchos, Numerical simulation of propagating circular and cylindrical lean premixed hydrogen/air flames, *Proc. Combust. Inst.*, 34, (in press).

| | |
|---|---|
| **Title:** | Direct numerical simulation of engine-like flows |
| **Researchers:** | M. Schmitt[1], C. E. Frouzakis[1], A. G. Tomboulides[2], K. Boulouchos[1] |
| **Institute/ Group:** | [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ<br>[2]University of Western Macedonia, Kozani, Greece |

Internal combustion engine flows are turbulent, unsteady and exhibit high cycle-to-cycle variations. There are multiple turbulence generating mechanisms and their effects overlap in time and space, creating strong challenges for turbulence models currently used, at least for in-depth understanding of underlying mechanisms and predictive purposes. Even currently emerging LES-models for engine flows are subject to uncertainties with respect to sub-grid scale models, particularly for processes in the proximity of walls, which are prominent in engine combustion chambers.

In this work, a highly scalable parallel, spectral element low Mach number code based on the flow solver nek5000 is extented with an Arbitrary Lagrange/Eulerian (ALE) formulation to simulate an experimentally studied valve-piston assembly. The computed mean and r.m.s of the velocity profiles are in good agreement with the experimental findings, and the simulation data provide a detailed description of the flow which can be used to investigate cyclic variability and for model development and validation purposes.




(a) (b)

*(a) Volume rendering of instantaneous vorticity (visualization by J. Favre, CSCS) (b) Comparison of mean and r.m.s. of axial velocity from the experimental and simulation data at 144$^o$ crank angle degrees.*

**References:**

• M. Schmitt, C. E. Frouzakis, A. Tomboulides, Y. M. Wright, K. Boulouchos Direct numerical simulation of engine-like geometries, to be presented at LES4ICE, 28/29 Nov. 2012, IFP Rueil-Malmaison, Paris, France.

**Title:** Internal combustion engine related modeling activities

**Researchers:** Y. M. Wright[1], M. Bolla[1], M. Schmitt[1], K. Boulouchos[1]

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

Modeling activities in he field of internal combustion engines focused in on three areas:

1. Large Eddy Simulation (LES) of partially premixed spark ignited combustion in a methane direct injection passenger car engine. While classiscal Reynolds Averaged Navier Stokes (RANS) simulations return ensemble averaged quantities, LES has the potential to calculate cycle-to-cycle variability. As a consequence, a large number of engine cycles are required to provide statistically steady values. Findings reported in Schmitt et al. show much promise of the employed model to capture such effects and further provide a comparison with RANS as well as a sensitivity study with respect to mesh resolution and its influence on turbulent flame propagation as well as wall heat losses.

2. A soot model has been developed in the context of a high-fidelity combustion model for autoigniting n-heptane sprays at Diesel engine conditions. Two pressure/temperature levels at a range of ambient oxygen contents (representative of exhaust gas recirculation in engine operation, EGR) have been studied and compared to spatial distributions of soot from an optically accessible spray test rig. Excellent agreement is reported concerning the soot location and semi-quantitative values were found also with respect to the magnitudes (M. Bolla et al.). The study further features a conceptual analysis of the flame structures providing improved understanding on the respective governing processes at the different conditions.

3. LES simulations of auto-igniting fuel high pressure fuel sprays at conditions relevant to Diesel engines have been carried out with special focus on the stochasticity of individual ignition events. A large number of realizations have been computed in order to assess the spread in ignition delay and location. These are compared to experimental data from two different optically accessible high pressure/high temperature test rigs (Wright et al.) for which data is available at a wide range of different temperatures and pressures.

**References:**

• M. Schmitt, Y. M. Wright, C. E. Frouzakis and K. Boulouchos, Multiple cycle LES simulations of a direct injection methane engine, *Flow, Turbulence and Combustion* (submitted)

• M. Bolla , Y. M. Wright, K. Boulouchos, G. Borghesi and E. Mastorakos, Soot formation modelling of n-heptane sprays under diesel engine conditions using the Conditional Moment Closure approach, *Combustion Science Technology* (submitted)

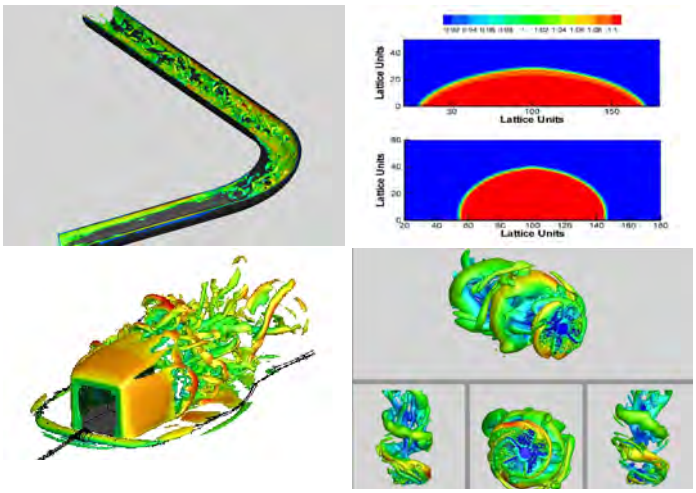
• Y. M. Wright, G. Borghesi, M. Bolla, E. Mastorakos and K. Boulouchos, Predicting the stochastic behaviour of autoignition in Diesel-like environments with LES-CMC, to be presented at LES4ICE, 28/29 Nov. 2012, IFP Rueil-Malmaison, Paris, France

**Title:** Entropic lattice Boltzmann methods for fluid mechanics

**Researchers:** I. Karlin, S. S. Chikatamarla, K. Boulouchos

**Institute/ Group:** 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 4.




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.* (submitted)

• 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* (submitted)

**Title:** Seismic sensitivity to boundary topography

**Researchers:** Andrea Colombi, Tarje Nissen-Meyer, Lapo Boschi

**Institute/Group:** Institute of Geophysics (ERDW) / Seismology and Geodynamics

**Description:**

In the PhD project I analyze and compute the sensitivity of body waves to Earth's global boundary perturbations and how they trade off with mantle structures surrounding the target area. I focus the investigation on the topography of the core-mantle boundary (CMB), very important region, yet not well known.
I use the full-waveform approach, implemented upon the adjoint method to compute sensitivity kernels used for the construction of the gradient operator that characterize this seismic inverse problem. I study how topography anomalies influence the energy partitioning at the interfaces of the CMB as a function of the frequency content, anomaly shape and mantle model. Exploiting an efficient axial-symmetric wave propagation solver we design a method to compute boundary kernels at unprecedented high frequency. Finally I propose some preliminary CMB maps derived by feeding our new algorithm with actual data collected by different authors.

**References:**

Efficient full-waveform inversion for CMB topography. Poster presentation during QUEST meeting, Tatranska Lomnica (SK).
Colombi, A., T. Nissen-Meyer, L. Boschi and D. Giardini, 2012. Seismic waveform sensitivity to global boundary topography. *Geophys. J. Int.*, doi 10.1111/j.1365-246X.2012.05660.x
Colombi, A., T. Nissen-Meyer, L. Boschi and D. Giardini, 2012 Efficient full-waveform inversion for CMB topography: validation, benchmarks and preliminary models. *Manuscript in preparation.*

**Title:** A 2D Spectral Element Method to Compute Spherical Earth Seismograms, Wavefields and Sensitivity Kernels

**Researchers:** M. van Driel, T. Nissen-Meyer

**Institute/Group:** Institute of Geophysics, Seismology and Geodynamics

**Description:**

We continue development of a method that enables the efficient computation of exact Frechet sensitivity kernels for a non-gravitating 3-D spherical earth. The crux of the method is a 2-D weak formulation for determining the 3-D elastodynamic response of the earth model to both a moment-tensor and a point-force source. The sources are decomposed into their monopole, dipole and quadrupole constituents, with known azimuthal radiation patterns. The full 3-D response and, therefore, the 3-D waveform sensitivity kernel for an arbitrary source–receiver geometry, can be reconstructed from a series of six independent 2-D solutions, which are obtained using a spectral-element method on a 2-D, planar, semicircular domain. Recent developments include parallelization for up to 256 CPUs for realistic problems, fully anisotropic media and parallel IO based on netcdf/hdf5. Benchmarks prove the physical accuracy of the method for periods down to 2 seconds on the global scale. In the near future, anelasticity/damping will be included in the code.

**References:**

Nissen-Meyer, T., Dahlen, F. a., & Fournier, A. (2007). Spherical-earth Fréchet sensitivity kernels. *Geophysical Journal International*, **168**(3), 1051-1066. doi:10.1111/j.1365-246X.2006.03123.x

Nissen-Meyer, T., Fournier, A., & Dahlen, F. a. (2007). A two-dimensional spectral-element method for computing spherical-earth seismograms - I. Moment-tensor source. *Geophysical Journal International*, **168**(3), 1067-1092. doi:10.1111/j.1365-246X.2006.03121.x

Nissen-Meyer, T., Fournier, A., & Dahlen, F. a. (2008). A 2-D spectral-element method for computing spherical-earth seismograms-II. Waves in solid-fluid media. *Geophysical Journal International*, **174**(3), 873-888. doi:10.1111/j.1365-246X.2008.03813.x

**Title:** Faster Finite Elements for Computational Seismology and Wave Propagation

**Researchers:** Max Rietmann

**Institute/ Group:** Institute of Geophysics / Seismology and Geodynamics / ETH Zurich
Institute of Computational Science / Faculty of Informatics / USI Lugano

**Description:**

In computational seismology and acoustics, forward wave propagation, i.e., the solution of hyperbolic linear partial differential equations (PDEs) on heterogeneous domains is a well understood problem. In the last decade, scientists have been able to successfully simulate earthquakes and other phenomena on meshes with millions of elements and billions of degrees of freedom on top supercomputers, at very high efficiency. In seismology, these simulations are now limited by the underlying earth models that define the propagation velocity through the Earth's crust and mantle. The newest computational challenge is to improve the values and structure of the material properties defined in the physical model, called tomography in seismology, and generally framed as an inverse problem. Through the use of adjoint methods, we can harness the existing forward solvers, in order to build gradient-based, iterative methods, which converge to an improved earth model. The most challenging component of these methods are the computational costs requiring thousands of equivalent forward simulations.

Experiments and development involving profiling, optimization, and harnessing emergent computing architectures are critical to run these methods as efficiently as possible on current and next-generation supercomputing clusters. This research prospectus outlines existing work done extending the existing SPECFEM3D wave-propagation code to utilize GPU resources at the cluster level. Extending this work, we develop a Discontinuous Galerkin (DG) finite element solver, which will utilize higher-order, spatially adaptive time-stepping schemes such as local time stepping (LTS) to reduce the overall required time-steps on a spatially heterogeneous simulation domain. A further goal is to be able to use both tetrahedral elements where the domain is spatially irregular, and computationally efficient hexahedral elements where the domain is more regular. This will all be managed from a single software package that can run on both CPU and GPU clusters, at very high efficiency.

**References:**

M. Rietmann et al. Forward and Adjoint Simulations of Seismic Wave Propagation on Emerging Large-Scale GPU Architectures. Proceedings of the 2012 ACM/IEEE conference on Supercomputing (SC '12). ACM, New York, NY, USA. *Accepted for publication.*

**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 / 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 study 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 VSH ($\xi > 1$; horizontal flow) in the Central Pacific and an anomaly of faster VSV ($\xi < 1$; 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 (G3)*

**Title:** Development of Dynamic Rupture Models to Study the Physics of Earthquakes and Near-Source Ground Motion

**Researchers:** Dr. Luis Dalguer, (ETHZ), Prof. Domenico Guardini (ETHZ)

**Institute/Group:** Swiss Seismological Service (SED) / Earthquake Physics Group

**Description:**

This project is part of an ensemble of ongoing projects carried out by the Earthquake Physics group at the Swiss Seismological Service (SED) at ETH Zurich for which the use of High Performance Computation (HPC) is necessary, as such we have been awarded an allocation of 3 millions of CPU hrs per year during 3 years (from August 2010 to August 2013) to use in the Cray XT5 Rosa Super computer of the Swiss National Supercomputing Centre (CSCS)**.** Such projects are: PhD SNSF funded projects and European Commission funded projects that involve a number of excellence Institutions all over Europe: QUEST (Quantitative Estimation of Earth's Seismic Sources and Structure) Initial Training Network in Computational Seismology, and of NERA projects: Network of European Research Infrastructures for Earthquake Risk Assessment and Mitigation; Advanced Simulation of Coupled Earthquake and Tsunami Events" (ASCETE). The use of HPC to study earthquakes is gaining increasing importance in the Earth science & earthquake engineering community. Modern applied HPC offers an unprecedented opportunity to develop three-dimensional models at high resolution and large scale to accurately solve problems of earthquake source physics and capture details of the rupture process and near-field ground motion. Understanding these aspects will improve our capability to predict local ground motion, and therefore allows a more accurate assessment of the seismic hazard and risk. In the present project, we use modern HPC techniques to model the source rupture and near-source ground motion for basic and applied research of the earthquake phenomena.

**References:**

Dalguer, L. A. (2012), Numerical Algorithms for Earthquake Rupture Dynamic Modeling. *In "The mechanics of faulting: From Laboratory to Real Earthquakes"*, Research Signpost, 93-124, ISBN 978-81-308-0502-3, Editors A. Bizzarri and H Bath.

Mena, B.; L.A. Dalguer and P.M. Mai (2012), Pseudodynamic Source Characterization For Strike-Slip Faulting, Including Stress Heterogeneity and Super-shear Ruptures, *Bull. Seismol. Soc. Am,* **102**(4), pp. 1654–1680, August 2012, doi: 10.1785/0120110111.

Gabriel, A. A.; J. P. Ampuero; L. A. Dalguer and P. M. Mai (2012), The Transition of Dynamic Rupture Styles in Elastic Media Under Velocity-Weakening Friction. *J. Geophys. Res.,* **117**, B09311, doi:10.1029/2012JB009468.

Dalguer, L.A. and P.M. Mai (2012), Prediction of near-source ground motion exceeding 1g at low frequencies (<2Hz) from Mw~6.5 deterministic physics-based dynamic rupture simulations, *Proceedings of the 15th World Conference on Earthquake Engineering (15WCEE)*, Lisbon, Portugal, September 24-28, 2012.

Mai, P.M. and L.A. Dalguer (2012), Physics-based broadband ground motion simulations: rupture dynamics combined with seismic scattering in a heterogeneous earth crust, *Proceedings of the 15th World Conference on Earthquake Engineering (15WCEE)*, Lisbon, Portugal, September 24-28, 2012.

Causse, M.; L. Dalguer and P.M. Mai (2012) On Constraining Dynamic Source Properties from Finite-Source Rupture Models of Past Earthquakes, *Proceedings of the 15th World Conference on Earthquake Engineering (15WCEE)*, Lisbon, Portugal, September 24-28, 2012.

**Title:** Modeling Dynamic Source Rupture with Slip Reactivation and Near-Source Ground Motion of the 2012 Mw 9.0 Tohoku earthquake.

**Researchers:** PhD . Percy Galvez (ETHZ), Dr. Luis Dalguer (ETHZ), Prof. Jean Paul Ampuero (Caltech,USA), Dr. Tarje Nissen-Meyer(ETHZ).

**Institute/Group:** Swiss Seismological Service (SED) / Earthquake physics group, Seismology & Geodynamics Group.

**Description:**

The compilation of seismological, geodetic, bathymetric and tsunami observations as well as source inversion and back-projection studies of the 2011 Mw 9.0 Tohoku earthquake show that this earthquake is mainly characterized by three main features: 1) unusual large slip over 50m; 2) complex rupture patterns with multiple rupture fronts and slip reactivation; 3) distinct depth dependent frequency radiation patterns, in which the shallower part of the fault dominate the low frequency radiation and the deep part dominates the high frequency radiation.
In order to explain such observations we examine the complex rupture process of this event by means of dynamic rupture simulations. We employ the 3D spectral element code SPECFEM3D-SESAME, in which we recently implemented the capability of solving for dynamic fault rupture. Through the usage of a full-featured software toolkit CUBIT for robust unstructured mesh generation, our model can incorporate a non-planar geometry of the megathrust interface. Figure(a) shows the geometry of Japanese subuction zone done with CUBIT and Figure(b) shows a view of the megathurst interface and the bottom surface meshed with linear coarsening in the west-east direction.

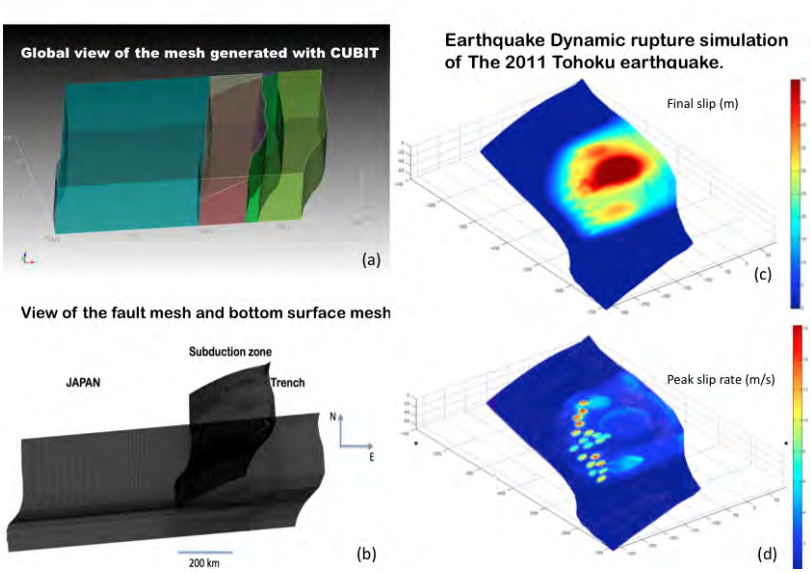



Figure 1. (a) y (b) Mesh of a realistic non-planar fault geometry of the Megathrust interface of the Mw9.0 2011 Tohoku earthquake in Japan. (c) Final slip from dynamic rupture simulation and (d) Peak slip rate obtained from dynamic rupture simulations.

**References:**

Modeling Dynamic Source Rupture with Slip Reactivation and Near-Source Ground Motion of the 2012 Mw 9.0 Tohoku earthquake. AGU-2012, Fall Meet. Suppl, Abstract **S33A-2516.**

**Title:** Developing a statistical framework for earthquake source process, consistent with statistical ground motion characterization

**Researchers:** Dr. Seok Goo Song (ETHZ), and Dr. Luis A. Dalguer (ETHZ)

**Institute/Group:** Swiss Seismological Service (SED) / Earthquake Physics (EP) group.

**Description:** We develop a statistical framework that controls physical earthquake rupture processes, consistent with the statistical framework used in ground motion characterization. Dynamic earthquake modeling with high performance computing (HPC) is an essential element in this study. As illustrated in the figures below, dynamic source parameters can be formulated within the framework of 1-point and 2-point statistics. And dynamic rupture modeling produces physically self-consistent kinematic source motions and ground motion. Analyzing produced kinematic source motions and ground motions in the same framework of 1-point and 2-point statistics, we develop a comprehensive statistical framework, in which we can investigate the effect of earthquake source on ground motions consistently.

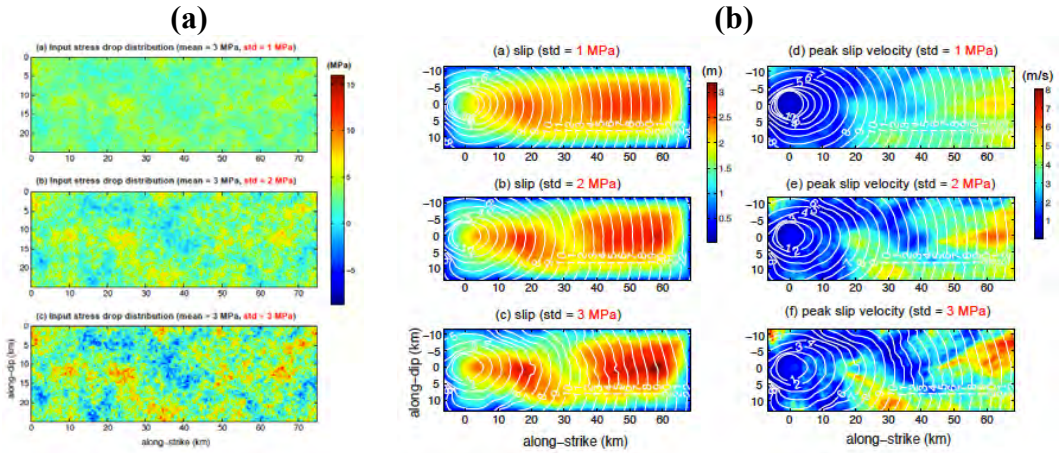



**Figure 1.** (a) Input stress drop distributions with different 1-point statistics, i.e., standard deviations from 1 MPa to 3 MPa, (b) Kinematic motions derived from dynamic modeling.

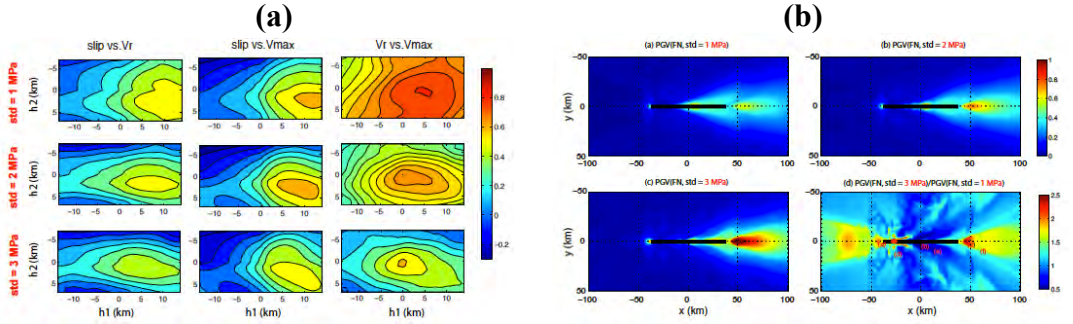



**Figure 2.** (a) Cross-correlation (2-point statistics) structure between kinematic source parameters, (b) Near-source ground motion distributions in peak ground velocity (PGV).

**References:**

Song, S., and L.A. Dalguer (2012). Importance of 1-point statistics in earthquake source modeling for ground motion simulation, *Geophys. J. Int.* (submitted)

Song, S., and L.A. Dalguer (2012). Propagation of 1-point and 2-point statistics from dynamic source through kinematic to ground motions, special session on "Toward improvement of GMPEs incorporating physics-based ground motion simulations," WCEE15, Lisbon, Portual.

**Title:** The seismic cycle at subduction thrusts: Dynamic implications of geodynamic simulations validated with laboratory models and extended to realistic geometries

**Researchers:** Ylona van Dinther, Taras Gerya, Luis Dalguer, Martin Mai, Fabio Corbi, Francesca Funiciello, and Gabriele Morra.

**Institute/Group:** Swiss Seismological Service (SED) / Earthquake Physics

**Description:**

The physics governing the seismic cycle at seismically active subduction zones remains poorly understood due to restricted direct observations in time and space. Realistic modeling of subduction zone physics can help to improve our understanding of the long-term, i.e. tens of thousands of years, seismic cycle in subduction zones.

To investigate subduction zone dynamics and associated interplate seismicity, we validated a continuum, visco-elasto-plastic numerical model with a new laboratory approach. The analogous laboratory setup includes a visco-elastic gelatin wedge underthrusted by a rigid plate with defined velocity-weakening and -strengthening regions.

Our geodynamic simulation approach includes velocity-weakening friction to spontaneously generate a series of fast frictional instabilities that correspond to analog earthquakes. A match between numerical and laboratory source parameters is obtained when velocity-strengthening is applied in the aseismic regions to stabilize the rupture. Spontaneous evolution of absolute stresses leads to nucleation by coalescence of neighboring patches, mainly occurring at evolving asperities near the seismogenic zone limits. Consequently, a crack-, or occasionally even pulse-like, rupture propagates toward the opposite side of the seismogenic zone by increasing stresses ahead of its rupture front, until it arrests on a barrier. The resulting surface displacements qualitatively agree with geodetic observations and show landward and, from near the downdip limit, upward interseismic motions. These are rebound and reversed coseismically. This slip produces stress shadows that are relaxed postseismically by afterslip and thereby produce persistent seaward motions. The wide range of observed physical phenomena, including back-propagation and repeated slip, and the agreement with laboratory results demonstrate that visco-elasto-plastic geodynamic models with rate-dependent friction represent a new tool that can greatly contribute to our understanding of the seismic cycle at subduction zones.

Subsequently, the lessons learned from this validation approach were implemented into a large-scale, complex, realistic geometry model, which now successfully produces seismic cycles as well. This is the first numerical model to include the three key components crucial to simulate the seismic cycles at convergent margins; a rate-dependent friction, b) visco-elastic mantle relaxation, and c) slow tectonic loading. Due to the large range of physical processes that need to be resolved in both space and time, the computational loads of this comprehensive model are especially high.

**References:**

Two manuscripts are under review in *Journal of Geophysical Research.*

**Title:** Simulation of wave propagation from subduction zone earthquakes for verification of regional long-period back projection methods

**Researchers:** Daniel Roten (ETHZ), Hiroe Miyake (ERI Tokyo), Kazuki Koketsu (ERI Tokyo)

**Institute/Group:** Swiss Seismological Service (SED), Engineering Seismology

**Description:**

The aim of this project was to study the rupture characteristics of the 2011 $M_w$ 9.1 Tohoku earthquake by back-projection of K-NET and KiK-net strong motion records. Because these networks are located at regional distance from the source, existing back-projection techniques based on P- or S-wave arrivals, which are routinely applied at teleseismic or local distance, are not suitable. Instead, we proposed an alternate approach based on surface waves. The method consists in isolating the signal at the period of interest with a continuous wavelet transform, and generating the stack using arrival times predicted from detailed fundamental mode Rayleigh wave group velocity maps. The method was validated by back-projecting acceleration time series from aftershocks with magnitudes between 6 and 6.5. Additionally, synthetic earthquake records representing sources off the coast of Tohoku proved valuable for verifying the method and for calibrating the amount of azimuthal weighting and distance-dependent tapering required for suppression of migration artifacts. These synthetic time series were obtained by running a 3D finite difference simulation of wave propagation (Fig. 1) using a 1575 x 2825 x 630 $km^3$ mesh based on the Japan Integrated Velocity Structure model.

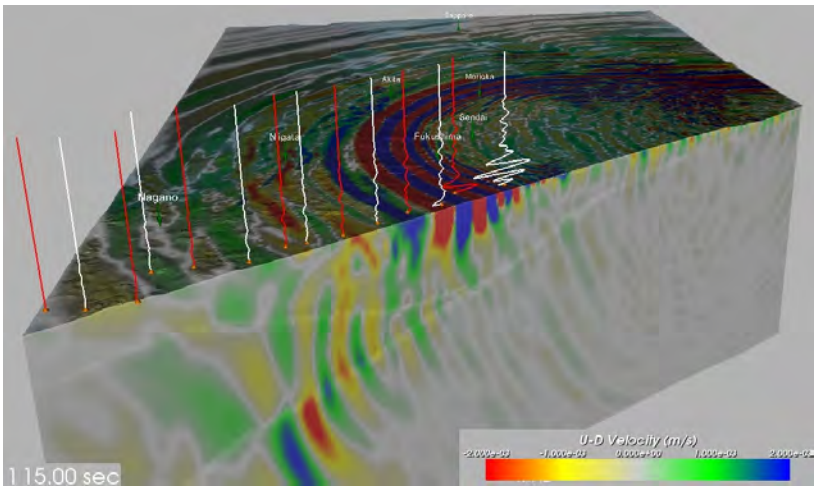



*Figure 1: Snapshot of surface velocity in up-down direction resulting from an $M_w$ 6.1 aftershock off the coast of Tohoku, including seismograms recorded along a NE-SW cross-section. The wave propagation simulations were performed on the Cray XT5 system "Monte Rosa" at CSCS.*

Application of the method to K-NET/KiK-net records of the $M_w$ 9.1 Tohoku earthquake revealed several Rayleigh wave emitters, which characterize the overall rupture progression with a weak initial stage, emission of energetic Rayleigh waves during stage II, and bilateral rupture towards the north and south during stage III.

**References:**

Roten, D., H. Miyake, and K. Koketsu (2012), A Rayleigh wave back-projection method applied to the 2011 Tohoku earthquake, *Geophys. Res. Lett.,* 39, L02302, doi:10.1029/2011GL050183.

**Title:** Earthquake Damage Scenario in Visp (Switzerland): From active fault to building damage

**Researchers:** Jan Burjánek[1], Donat Fäh[1], Luis Dalguer[1], Jan Laue[2],Pierrino Lestuzzi[3], Cyrill Baumann[1], Gabriela Gassner-Stamm[1], Armin Karbassi[3], Alexandru Marin[2], Clotaire Michel[1], Valerio Poggi[1],Daniel Roten[1]

**Institute/Group**: [1]Swiss Seismological Service, ETHZ, [2]Institute of Geotechnical Engineering, ETHZ, [3]Applied computing and Mechanics Laboratory,EPFL

**Description:**

The Valais is the area of greatest seismic hazard in Switzerland and has experienced a magnitude 6 or larger event every 100 years. The area of the city of Visp is of special interest, since damaging earthquakes occur on average every 40 years (Intensity VI-VIII). The significant earthquake damage was reported in the past resulting either directly from strong ground motion, or from different secondary phenomena including liquefaction and ground failure of the Rhone plain. As there are no available instrumental observations of these phenomena for the region, numerical modeling is the best method to improve predictions for future events. We present detailed damage scenarios based on multidisciplinary study which covers the key elements of the earthquake risk chain in Visp. These key elements are: (1) identification of the active faults in the area, (2) numerical simulation of the dynamic ruptures along these faults, (3) simulation of the seismic wave propagation in the 3D velocity model, and (4) quantitative estimation of the building damage resulting from simulated ground motions. Full dynamic rupture simulations are performed using heterogeneous initial and yielding stress fields constrained by the database of kinematic inversion results. The fault is embedded in the 3D velocity model, which is based on an extensive ambient noise measurement campaign.

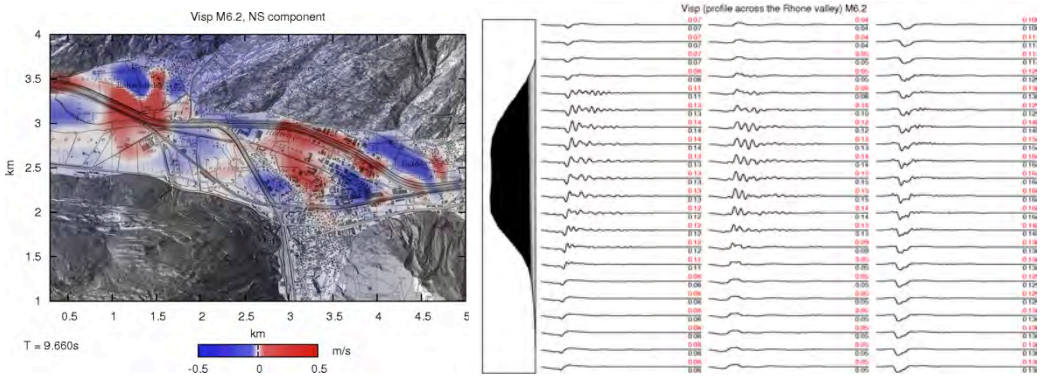



*Figure: Left: Snapshot of simulated ground velocity in Visp 9.66 seconds after earthquake origin time (~3 s after direct S wave arrival). Right: Simulated ground motion along a profile crossing Visp. The cross-section of the 3D model (left), velocity recordings (NS, EW, UP components respectively). The peak velocities are plotted on the right of each trace in meters per second.*

**References:** Burjánek, J., Fäh, D., Dalguer, L., Laue, J., Lestuzzi, P. , Baumann, C., Gassner-Stamm, G., Karbassi, A., Marin, A., Michel, C., Poggi, V., Roten D. (2012). Earthquake damage scenario in Visp (Switzerland): From active fault to building damage, Proceedings of the 15th World Conference on Earthquake Engineering, Lisbon, Portugal.

**Title:** Seismic waves estimation and wavefield decomposition: application to ambient vibrations

**Researchers:** Stefano Maranò[1], Christoph Reller[2], Hans-Andrea Loeliger[2], Donat Fäh[1]

**Institute/Group**: [1]Swiss Seismological Service, ETH Zurich
[2]Department of Information & Electrical Engineering, ETH Zurich

**Description:**

Passive seismic surveying methods represent a valuable tool in local seismic hazard assessment,oil and gas prospection, and in geotechnical investigations. Array processing techniques are used in order to estimate wavefield properties such as dispersion curves of surface waves and ellipticity of Rayleigh waves. However, techniques presently in use often fail to properly merge information from three-components sensors and do not account for the presence of multiple waves. In this paper, a technique for maximum likelihood estimation of wavefield parameters including direction of propagation, velocity of Love waves and Rayleigh waves, and ellipticity of Rayleigh waves is described. This technique models jointly all the measurements and all the wavefield parameters. Furthermore it is possible to model the simultaneous presence of multiple waves. The performance of this technique is evaluated on a high-fidelity synthetic data set and on real data. It is shown that the joint modeling of all the sensor components, decreases the variance of wavenumber estimates and allows the retrieval of the ellipticity value together with an estimate of the prograde/retrograde motion.

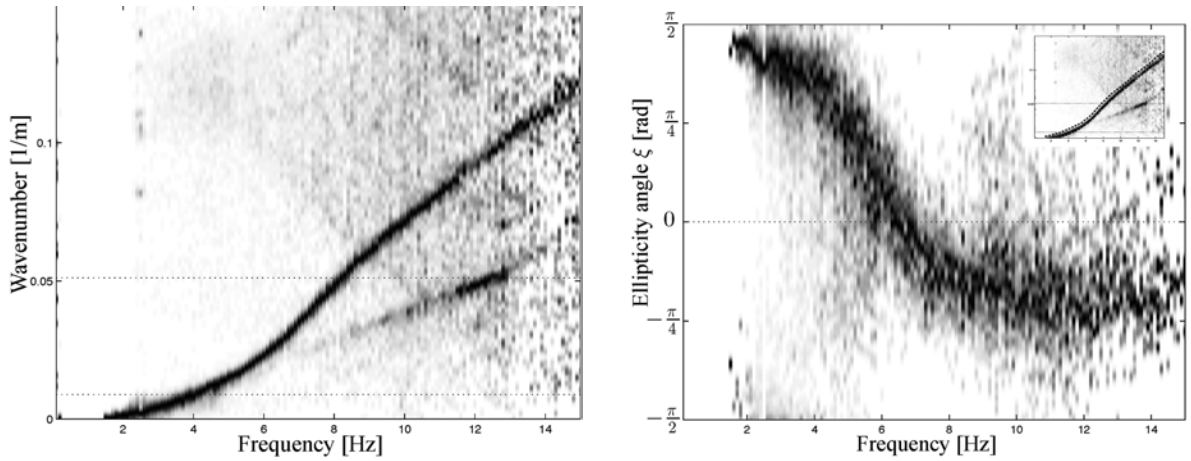



*Figure: Analysis of the site of Brigerbad, Wallis, using the proposed method. Left: Fundamental mode and first higher mode of Rayleigh wave. Right: Estimated Rayleigh wave ellipticity angle for the funamental mode.*

**References:**

Maranò S., Reller C., Loeliger H.-A., and Fäh D., 2012. Seismic waves estimation and wavefield decomposition: Application to ambient vibrations, Geophysical Journal International, **191**(1), 175-188.

**Title:** Inferring earthquake source properties from dynamic rupture models by means of non-linear kinematic source inversion

**Researchers:** Youbing Zhang (ETHZ), Seok Goo Song (ETHZ), Luis Dalguer (ETHZ), John Clinton (ETHZ)

**Institute/Group:** Swiss Seismological Service, Computational Seismology Group

**Description:**

One of the principal goals of earthquake seismology is to map the spatial and temporal evolution of source parameters from large earthquakes in detail. Spontaneous dynamic rupture modeling is capable of producing physically self-consistent kinematic descriptions of earthquake faulting and its associated seismic wave propagation, resulting in synthetic ground motions on the surface. Therefore, testing kinematic source inversion techniques by inverting these synthetic ground motions obtained from dynamic rupture simulations is a rigorous way of evaluating the suitability of different source inversion techniques for exploring the physics of the real earthquake source. It is important to investigate which mathematical form best represents the dynamic rupture slip velocity function (SVF) to image the kinematic rupture history on a finite fault. Besides, it is also interesting to address the question of how the number of stations or station coverage affects source inversion.

Three full dynamic source rupture processes (thrust, normal and strike slip), Mw 6.5~7.0, with normal stress depth-dependent and different source geometry were simulated using the method of Dalguer and Mai (2011). The Compsyn package (Spudich and Xu, 2002) was used to generate forward synthetic velocity waveforms. A non-linear kinematic inversion approach (Monelli and Mai 2008) was used for the inversion, and the Evolutionary Algorithm was used to search for the optimal source parameters on each sub-fault: peak slip velocity, rupture time, rise time and rake angle at low frequency (up to 1Hz). To quantify how different single window SVFs affect the source inversion result, we test three types of SVFs regularized Yoffe function (Tinti et al, 2005), and the widely used boxcar and isosceles triangular functions.

Our preliminary results show that the performance of a kinematic source inversion can be improved by using a kinematic SVF more compatible with earthquake dynamics (e.g. regularized Yoffe function), compared to other widely used mathematical forms (e.g. boxcar, triangular functions). However, details of slip velocity complexities, resulted from the dynamic rupture models, are not well captured by the kinematic source inversion, irrespective of SVF used. The seismograms used in the kinematic inversion constrain the model by means of waveform fitting, thus, given certain network geometry, there must be a minimum number of stations required in order to obtain a stable source inversion solution. Good waveform fitting is a necessary, but not sufficient condition for reliable inversion results.

**References:**

Zhang, Y., S. Song, L.A. Dalguer, and J. Clinton. Inferring earthquake source properties from dynamic rupture models by means of non-linear kinematic source inversion. ECGS Workshop, Luxembourg, 2012

**Title:** Development and application of numerical methods for computational electromagnetics

**Researchers:** Christian Hafner
Jürg Fröhlich
Aytac Alparslan
Christoph Böcklin
Nemat Dolatsha
Alexander Dorodnyy
Roman Kappeler
Nikolay Komarvesky
Patrick Leidenberger
Jens Niegemann
Sahar Sargheini
Sascha Schnepp
Pegah Souzanghar
Mengyu Wang

**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 low frequencies to microwaves and mm waves up to optical frequencies. These codes and commercial ones are applied to 1) metamaterials for 50 Hz magnetic field shielding, for radar absorption, microwave sealing, thermal protection, and efficient solar cells; 2) photonic crystals for optical frequencies as well as for fast interconnects in the mm wave range; 3) design of antenna structures ranging from radio frequencies up to optical frequencies, i.e., plasmonic nano antennas for bio sensing applications; 4) analysis and design of scanning probe tips for microwaves and for optics; 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), Finite Difference Time Domain (FDTD), etc. The semi-analytic MMP and MAS methods provide high accuracy, robustness, numerical efficiency for 2D applications and exhibit no problems with material dispersion and loss. For 3D simulations, TD-FEM and DG-FEM are favorable for the analysis of geometricall 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 2011 till fall 2012, a book chapter and 16 papers on various topics of computational electromagnetics were published in reviewed journals.

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| **Title:** | QLectives (Socially Intelligent ICT Systems for Quality) |
| **Researchers:** | Dirk Helbing |
| **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 *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

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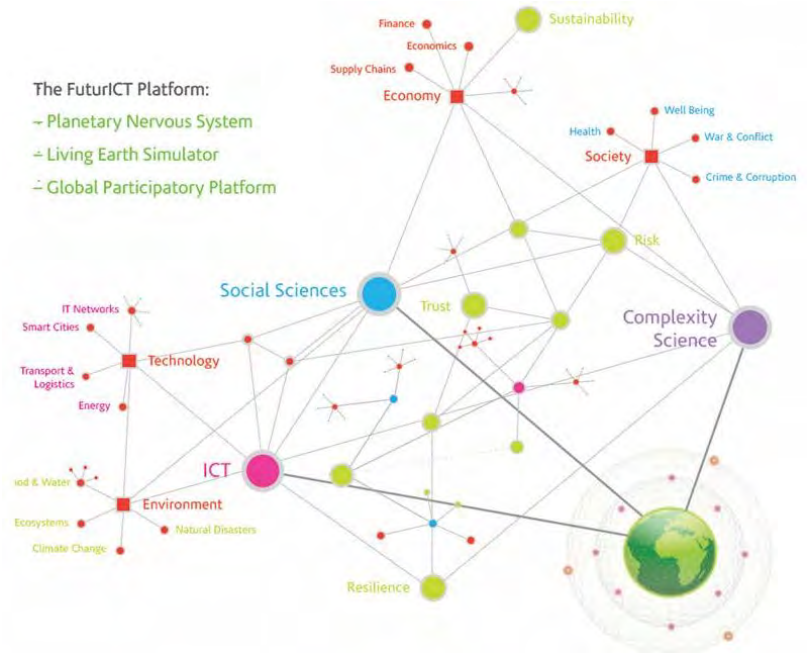
|---|---|
| **Title:** | FuturICT Knowledge Accelerator |
| **Researchers:** | Dirk Helbing |
| **Institute/ Group:** | Chair of Sociology, in particular of Modeling and Simulation, in cooperation with academic consortium (see www.futurict.eu for a full list of academic supporters) |

**Description:**

FuturICT is a visionary project that will deliver new science and technology to explore, understand and manage our connected world. This will inspire new information and communication technologies (ICT) that are socially adaptive and interactive, thus supporting collective awareness. Revealing the hidden laws and processes underlying our complex, global, socially interactive systems constitutes one of the most pressing scientific challenges of the 21st century. Integrating complexity science with ICT and the social sciences will allow us to design novel robust, trustworthy and adaptive technologies based on socially inspired paradigms. Data from a variety of sources will help us to develop models of techno-socioeconomic systems. In turn, insights from these models will inspire a new generation of socially adaptive, self-organised ICT systems. This will create a paradigm shift and facilitate a symbiotic co-evolution of ICT and society. In response to the European Commission's call for a "Big Science" project, FuturICT will build a large scale, Pan-European, integrated programme of research which will extend for 10 years and beyond.




**References:**


Conte, R., Gilbert, N., Bonelli, G. and Helbing, D. (2011) FuturICT and social Sciences: Big Data, Big Thinking. Zeitschrift Fur Soziologie, 40(5), pp. 412-413.

S. Bishop, D. Helbing, P. Lukowicz, and R. Conte (2011) FuturICT: FET Flagship Pilot Project. Procedia Computer Science 7, 34-38.

D. Helbing and S. Balietti (2011) How to create an innovation accelerator. Eur. Phys. J. Special Topics 195, 101-136.

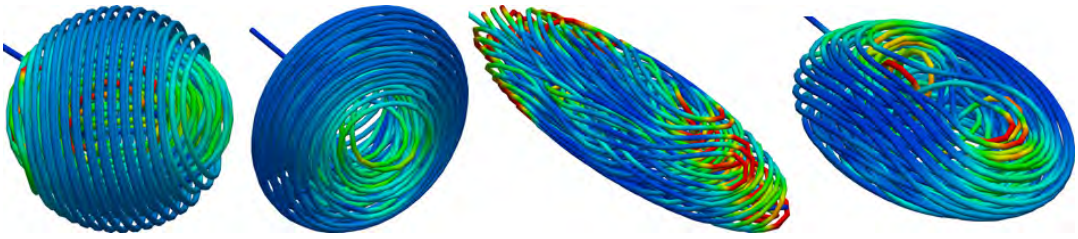
**Title:** Finite Element Simulation of Dense Wire Packings

**Researchers:** Roman Vetter
Dr. Falk K. Wittel
Dr. N. Stoop
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

We study the mutual mechanical interplay and of thin strands (wires, rods) and thin hollow surfaces (plates, shells, membranes) in the regime of very large deformations, using advanced finite element techniques. In particular, the process of packing elastic wires in three-dimensional confining cavities is studied. The wire is represented by third order beam elements and embedded into a corotational formulation to capture the geometric nonlinearity. The hyperbolic equations of motion are integrated in time using a Newmark predictor-corrector scheme with adaptive time stepping. The packing in hard ellipsoidal cavities is simulated, showing that packings in oblate spheroids and scalene ellipsoids are energetically preferred to spheres. It is thus expected that a wire inserted into a deformable, soft cavity will not naturally assume a spherically symmetric bulk shape. In order to numerically model flexible cavities, a Kirchhoff-Love-based thin shell finite element approach using highly efficient Loop subdivision surfaces is proposed, capable of dealing with large deformations and anisotropic growth.



Wires packed in different ellipsoidal cavities (color represents bending energy).

**References:**

[1] 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) 160–171

[2] R. Vetter, N. Stoop, F.K. Wittel, T. Jenni and H.J. Herrmann, Subdivision Shell Elements with Anisotropic Growth, *submitted*

**Title:** Multiscale analysis of coupled mechanical and moisture behavior of wood

**Researchers:** Dr. Stefan Hering
Francois Gaignat
Dr. Falk Wittel
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

Dimensional changes of clear wood during water ad- and desorption below the fiber saturation results in the poor durability of wood and wooden products in applications under alternating climatic conditions. The main problems are caused by the differential shrinkage in the three principal directions of a tree: longitudinal (L) along grain, radial (R) from the pith to the bark and tangential (T) to the growth rings.

The driving force behind the swelling is on the finest scale the hydrophilic nature of the cell wall components lignin, hemi-celluloses, and celluloses. Therefore, the hierarchical modeled cell wall consists of a laminate in which each layer is assumed to be a fiber reinforced composite formed by cellulose and are embedded in hemi-cellulose and lignin. The material is then imported in a FEM model for tissues.

After extrusion and partitioning the geometrical data, local coordinates are introduced and moisture-dependent material data is assigned. We investigate the driving forces behind swelling on different scales, swelling anisotropy and the mechanical behavior under climate variations. Results are validated on in-situ experiments on micro-samples of different tissue types (early/transition/late wood). The results of the hierarchical model are embedded in meso- and macroscopic models within the collaboration network.

**References:**

[1] A. Rafsanjani, D. Derome, F.K. Wittel, J. Carmeliet, *Computational up-scaling of anisotropic swelling and mechanical behavior of hierarchical cellular materials*, Composites Science and Technology 72 (6/2012) 744-751

**Title:** Bohman-Frieze-Wormald model on the lattice, yielding a discontinuous percolation transition

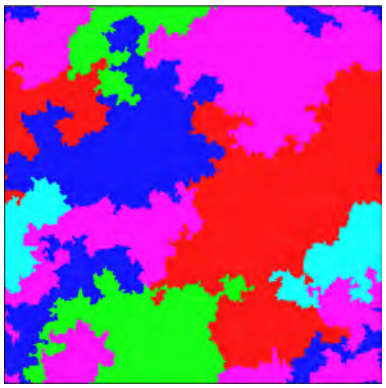
**Researchers:** K.J. Schrenk
Dr. N.A.M. Araújo
Prof. H.J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

In this project, the BFW model recently investigated in the framework of discontinuous percolation by Chen and D'Souza [1] is studied on the square and simple-cubic lattices [2]. Starting from a lattice without bonds, candidate bonds are sampled uniformly at random and occupied or rejected, while the fraction of accepted bonds cannot drop below a decreasing function, which eventually approaches a constant. We find numerical evidence for a strongly discontinuous transition. In two dimensions, the clusters at the threshold are compact with a fractal surface of fractal dimension $d_f = 1.49 \pm 0.02$.

Given that the percolation process studied here is not rejection-free and large lattice sizes need to be simulated to gain clarity on the nature of the transition, one faces a challenging computational task. The figure shows a snapshot of a system evolving according to the BFW model for a fraction of occupied bonds of 95%, close to the threshold.



**References:**

[1] W. Chen and R.M. D'Souza, *Explosive Percolation with Multiple Giant Components*, Phys. Rev. Lett. **106** (2011) 115701

[2] K.J. Schrenk, A. Felder, S. Deflorin, N.A.M. Araújo, R.M. D'Souza, and H.J. Herrmann, *Bohman-Frieze-Wormald model on the lattice, yielding a discontinuous percolation transition*, Phys. Rev. E **85** (2012) 031103

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

**Researchers:** Alessandro Leonardi
Dr. Falk Wittel
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

Landslides and debris flows are serious geo-hazards common to countries with mountainous landslides and terrains. The high speed and the enormity of debris mass make debris flows one of the most dangerous natural hazards. Debris flows are often triggered by landslides partially or completely mobilizing into debris flows.

The numerous devastating events worldwide have made us aware of the complexity of landslides and debris flows and our insufficient knowledge to make reliable predictions. The traditional tools for prediction and design are based on limit equilibrium analysis for landslides and single phase model for debris flows. These simple models are unable to account for the complex behaviour of landslides and debris flows.

Numerical simulations based on DEM will be carried out considering the complex interaction between solid and fluid. The results shall provide deep insight into numerous intricate phenomena in debris flow, e.g. segregation, transportation and sedimentation and shock wave propagation upon impact with obstacles. The aim is to develop a reliable tool for the prediction of runout dynamics, deposition pattern and impact forces for rational design of stabilization and protection structures.

**References:**

[1] H. Teufelsbauer, Y. Wang, S.P. Pudasaini, R.I. Borja and W. Wu, *DEM simulation of impact forces exerted by granular flow on rigid structures*, Acta Geotechnica **6** (2011) 199–133

[2] M.C. Chiou, Y. Wang and K. Hutter, *Influence of obstacles on rapid granular flows*, Acta Mechanica **175** (2005) 105–122

**Title:** Simulation of aeolian saltation

**Researchers:** Marcus Vinicius Carneiro Martins
Prof. Dr. Hans Jürgen Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

The transport of sand by wind commonly seen in dune motion reveals a complex interaction between granular media and a fluid. In saltation, the air lifts and accelerates sand grains that eject others as they impact back to the ground. We simulate this phenomenon in two and three dimensions using the Discrete Elements Method by considering a disoredered 3D particle bed below a logarithmic wind profile. The wind dynamically changes according to the momentum exchange between the grains and the wind. The saturated flux can be reasonably well fitted using the models of Owen (1964) and Sørensen (1991). Close to the threshold of saltation, we discovered a discontinuous transition in the saturated flux connected to the occurrence of the particle splash. Below this threshold, the impacting particles do not have the kinetic energy to eject others, and saltation is suspended. The jump of this first order transition is found at $u_{*t} = 0.18$ m/s for grains of the size $D_{mean} = 2 \times 10^{-4}$ with $\sigma = 0.15 D_{mean}$. The interval of coexistence of two metastable solutions located between the static and dynamic threshold is analyzed in the presence of perturbations and lift forces. Additionally, we show how the mid-air collisions between particles enhance the saturated flux. As a natural consequence of the mid-air collisions, particles play different roles that uniquely contribute to the saturated flux. We distinguish saltons, creepers and leapers. The last stage of our project is to introduce electrial charges in the sand grains and observe the behavior of saltation under the influence of long range forces.

**References:**

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

**Title:** Numerical modeling of liquid transport in wet granular matter

**Researchers:** Roman Mani
Dr. Dirk Kadau
Prof. Dani Or
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

Fluid transport and the interactions between particles in unsaturated granular materials are of broad interest and intensively studied. The main question addressed in this project is where liquid is migrating when shearing unsaturated granular materials and the influence on the mechanical and structural properties of the granular media. Here, we present a microscopic model for liquid transport at low liquid contents, where the volume of a ruptured bridge is redistributed to neighboring bridges and where liquid is allowed to be exchanged between individual liquid bridges due to Laplace pressure differences via the wetting layer coating the particle surfaces. We use contact dynamics to model spherical particles interacting via Coulombian friction as well as via cohesive capillary forces. The contact forces are determined by means of constraints and are computed iteratively in each time step. Using this model, we derived a modified diffusion equation describing the liquid transport in sheared granular matter. On the one hand, it predicts that liquid is driven out of shear bands despite the increased porosity due to dilatancy which was found in simulations as well as in experiments [1]. On the other hand, in plane shear which is of importance in industrial applications and powder technology, liquid is migrating in a diffusive manner [2]. It was found that liquid is migrating faster, i.e. mixing properties are enhanced at large applied shear stresses. Future plans include the refinement of the presented model by taking into account the contact angle hysteresis of the solid-liquid-gas interface and by allowing larger liquid contents beyond the capillary bridge regime.

**References:**

[1] R. Mani, D. Kadau, D. Or and H.J. Herrmann, *Fluid depletion in shear bands*, submitted

[2] R. Mani, D. Kadau, D. Or and H.J. Herrmann, *Liquid migration in sheared unsaturated granular media*, submitted

**Title:** Risk Analysis in Network of Oscillators

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

**Institute:** Computational Physics for Engineering Materials, IfB
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 [Phys. Rev. Lett. **105** (2010) 35701]. In this project we study the four typical dimensions of Risk Analysis (risk identification, mitigation [Sci. Rep. **2** (2012) 658], response, and recovery) 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 [Physica D **224** (2006) 27–34].

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, *How to suppres undesired synchronization*, Scientific Reports **2** (2012) 658

[3] A. Arenas, A. Diaz-Guilera and C.J. Pérez-Vicente, *Synchronization processes in complex networks*, Physica D **224** (2006) 27–34

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

**Researchers:** Fabrizio Lombardi
Prof. Hans J. Herrmann
Prof. Lucilla de Arcangelis

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

Neuronal avalanches, measured *in vitro* and *in vivo*, exhibit a robust critical behaviour with the absence of a charateristic size and duration. Experimental measurements of the waiting time distribution for spontaneous activity in the rat cortex *in vitro* show clearly that successive avalanches are correlated in time and exhibit a peculiar non monotonic behaviour, not usually found in any natural process. Numerical simulations provide evidence that this non monotonic behaviour is a consequence of alternation between states of high and low activity, named *up* and $down - states$. This alternation is the expression of an homeostatic regulation wich, during periods of high activity is activated to control the excitability of the system and avoid pathological behaviour. The critical state of the system then realizes the correct balance between excitation and inhibition via these self regulating system.

In order 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 needs to be performed.

**References:**

[1] 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** (2012) 228703

**Title:** Reliable timber and innovative wood products for structures:
Adhesive Bonding of Structural Hardwood Elements

**Researchers:** Mohammad Masoud Hassani
Dr. Falk K.Wittel
Prof. Hans J.Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

Engineered wood also called composite wood involves a broad range of wood products which are constructed by binding the timbers, lumbers, or veneers of wood together with adhesives to manufacture composite materials. Nowadays, employment of such layered composite woods because of their improved and enhanced structural integrity, high dimensional stability and load-bearing capacity, more homogenized properties in comparison with the solid wood, and their easy reproducibility has been significantly increased.

Glue-laminated hardwood beams and veneer based products out of hardwood that cannot be realized with softwood, are generally employed as building materials in residential or industrial constructions which provide great structural strength and integrity. For more accurate assessment and better prediction of mechanical behavior and probable failure modes of such layered configurations from hardwood specially the resistance of bond-line against delamination, numerical models comprising of moisture and time history dependent material constants by taking into account the wood orthotropy and hardwood intrinsic characteristics are required. For this purpose, in the current study adhesive bonding of structural hardwood elements (European Beech) in order to examine the evolution of moisture-induced stress and deformation fields under changing environmental conditions along with mechanical loading and predicting the failure processes particularly inside the bonding are investigated.

These residual stresses can lead to formation and development of cracks in particular in the bond-line which results in interfacial de-bonding and loss of integrity. To address the problem more efficiently, a sequentially three-dimensional moisture-displacement finite element approach is applied where all participating deformation mechanisms involving elastic, hygro-expansion, viscoelastic creep, mechano-sorption, and plastic along with moisture dependent material properties must be included. The current study establishes good insights into the evolution of residual stresses induced by change of moisture content of adherends and provides a useful criterion to the optimized design of laminated engineered hardwood to enhance their dimensional stability and bringing residual stresses down especially in the bond-line which is essential for attaining reliable bondings.

**References:**


[1] S. Hering, *Characterization and modeling of material properties of beech wood for the simulation of adhesive bondings*, PhD Thesis (2011)

[2] T. Gereke, *Moisture induced stresses in cross-laminated wood panels*, PhD Thesis (2009)

**Title:** Bursts and Flow in Fracture Networks

**Researchers:** Ali Nejad Ebrahimi
Dr. Falk K. Wittel
Dr. Nuno A.M. Araújo
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

The prediction of the penetration of an immiscible fluid into a fully saturated fracture network and its percolation is among the most challenging topics in sub-surface hydrology. The fluids can take several pathways, can be trapped, and exhibit path instabilities and scale dependencies, what makes the prediction of an effective permeability rather questionable. Detailed descriptions rarely are capable of capturing more than a handful of interconnected fractures and fail in representing the complex system dynamics that arises from the interaction of a large number of connected fractures entirely.

In the our previous work, we studied together with the NAGRA and Bill Lanyon from Fracture Systems Ltd. the breakthrough and flow of immiscible fluids in artificial fracture networks, mainly in the framework of student projects. Simplified discrete fracture networks (DFN), based on parallel plate models were synthesized and a classical invasion percolation scheme was modified to add simple physical behavior to inter- and intra-fracture flow. We demonstrated that invasion percolation with physical modifications is a useful numerical tool for the physical abstraction of the complicated situation of two-phase flow in fractured rock. The main advantage of our approach is the reduction of an immensely complicated system to a (maybe branched) percolation backbone that contains only a small fraction of invaded fractures where the flow is concentrated.

The rules for invasion through other fractures and penetration of fracture planes should be based on rules that are extracted from more detailed physics-based models. We propose volumetric calculations with computational fluid dynamics of flow in typical situations like fracture intersections with measured geometries to advance the inclination adjustments, or two-phase flow inside real fracture cavities in specific rock as such. Fractures have a complicated geometry with channel of preferred flow. These exhibit characteristic length scales that lead to size effects for fractures of different size. In our present approach fractures are scale-free. We propose to include these size dependencies on the path from in- to outflow inside a fracture plane, as well as the intersection lengths of fractures. This should add to a more realistic scaling of results. Since percolation features are strongly affected by correlations in the media, it would also be relevant to analyze the impact of spatially correlated distributions of apertures and fracture orientations on the flow properties.

**References:**

[1] S.J. Wettstein, F.K. Wittel, N.A.M. Araújo, B. Lanyon, H.J. Herrmann, *From invasion percolation to flow in rock fracture networks*, Physica A (Statistical Mechanics and its Applications) **391** (2012) 264–277

**Title:** Numerical and analytical studies of aeolian saltation

**Researchers:** Thomas Pähtz
Marcus Carneiro
Dr. Jasper Kok
Prof. Hans J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich
Department of Earth and Atmospheric Sciences
Cornell University

**Description:**

We present an analytical model of aeolian sand transport. The model quantifies the momentum transfer from the wind to the transported sand by providing expressions for the thickness of the saltation layer and the apparent surface roughness. These expressions are derived from basic physical principles and a small number of assumptions. The model further predicts the sand transport rate (mass flux) and the impact threshold (the smallest value of the wind shear velocity at which saltation can be sustained). We show that, in contrast to previous studies, the present model's predictions are in very good agreement with a range of experiments, as well as with numerical simulations of aeolian saltation. Because of its physical basis, we anticipate that our model will find application in studies of aeolian sand transport on both Earth and Mars.

Moreover, we reveal that the transition in the saturated flux for aeolian saltation is generically discontinuous by explicitly simulating particle motion in turbulent flow. This is the first time that a jump in the saturated flux has been observed. The discontinuity is followed by a coexistence interval with two metastable solutions. The modification of the wind profile due to momentum exchange exhibits a maximum at high shear strength.

**References:**

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

[2] T. Pähtz, J.F. Kok, H.J. Herrmann, *The apparent roughness of a sand surface blown by wind from an analytical model of saltation*, New J. Phys. **14** (2012) 043035

**Title:** Flow Through Randomly Curved Media

**Researchers:** M. Mendoza
Dr. S. Succi
Prof. H.J. Herrmann

**Institute:** Computational Physics for Engineering Materials, IfB
ETH Zürich

**Description:**

We present a computational study of the transport properties of campylotic (generally curved) media. It is found that the relation between the flow through a campylotic media, consisting of randomly located curvature perturbations, and the average Ricci scalar of the system, exhibits two distinct functional expressions, depending on whether the typical spatial extent of the curvature perturbation lies above or below the critical value maximizing the overall Ricci curvature. Furthermore, the flow through such systems as a function of the number of curvature perturbations, is found to present a sublinear behavior for large concentrations, due to the interference between curvature perturbations leading to an overall less curved space. We have also characterized the flux through such media as a function of the local Reynolds number and the scale of interaction between impurities. For the purpose of this study, we have developed and validated a new lattice kinetic model, capable of handling fluid flow in arbitrarily curved manifolds and highly complex spaces, in a very compact and efficient way.

**References:**

[1] M. Mendoza, S. Succi, and H.J. Herrmann, *Flow Through Randomly Curved Media*, Physical Review Letters (2012), submitted

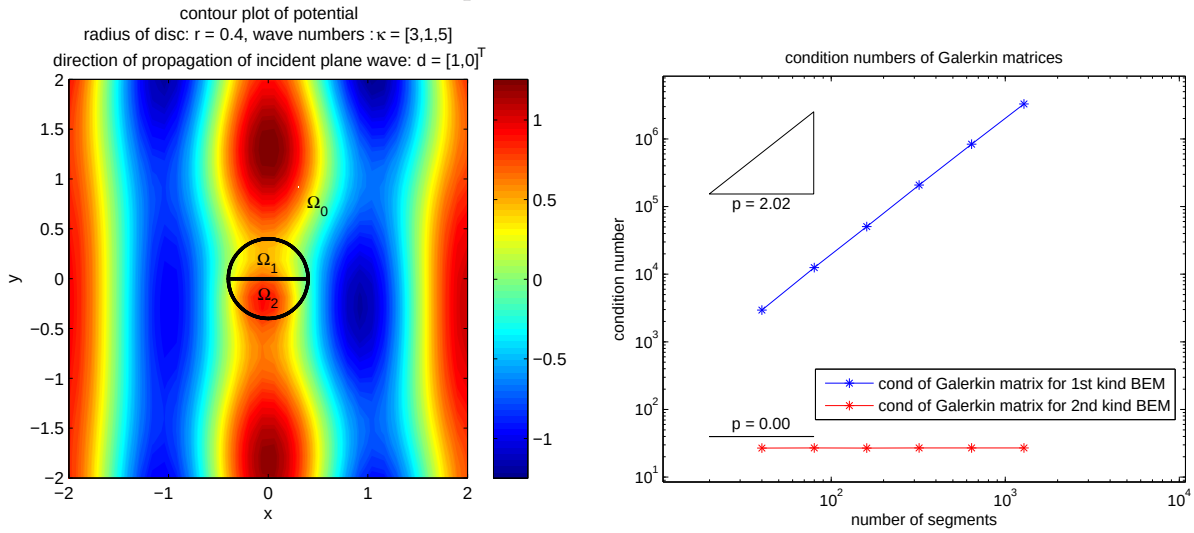
| | |
|---|---|
| **Title:** | Well-Conditioned Second Kind Single Trace BEM for Acoustic Scattering |
| **Researchers:** | Elke Spindler (SAM), Prof. Ralf Hiptmair (SAM) |
| **Institute:** | Seminar for Applied Mathematics, ETH Zürich |
| **Funding:** | SNF Grant 200021_137873 |

**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 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 fast convergence of GMRES. Several tests also indicate the absence of spurious modes in our new formulation.




# Publications:


[1] X. Claeys, *A single trace integral formulation of the second kind for acoustic scattering*, Technical Report, (2011).

[2] X. Claeys, R. Hiptmair, and E. Spindler, *Second kind Galerkin boundary element method for acoustic scattering at composite objects*, Technical Report, (2012, in preparation).

**Title:** BETL — A Boundary Element Template Library

**Researchers:** Dr. Lars Kielhorn
Prof. Dr. Ralf Hiptmair

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:**

The Boundary Element Template Library (BETL) is intended to provide building blocks for the Galerkin boundary element discretisation of boundary integral operators associated with important 2nd-order differential operators. Completely written in C++ and essentially a header-only library, it can be used for rapid prototyping as well as for the development of efficient boundary element solvers.

Here is a short but fully functional code example for the generation of the single layer matrix for the Laplace operator:

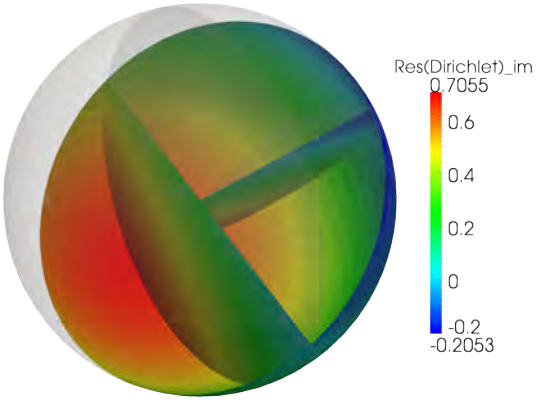
```
// based on an element type instantiate the mesh
Mesh< element_t > mesh( input );
// define the boundary element basis
typedef FEBasis< element_t, CONSTANT, Discontinuous, LagrangeTraits > basis_t;
// the dofhandler type and its instance
typedef DoFHandler< basis_t > dofhandler_t;
dofhandler_t dof_handler;
dof_handler.distributeDoFs( mesh.e_begin(), mesh.e_end() );
// typedefs for the fundamental solution, the kernel, and the integrator
typedef FundSol< LAPLACE, SLP > fs_t;
typedef GalerkinKernel< fs_t, dofhandler_t::FunctionType > kernel_t;
typedef GalerkinIntegrator< kernel_t, DefaultQuadrature > integrator_t;
// instances of the fundamental solution, the kernel, and the integrator
fs_t         fs;
kernel_t     kernel( fs );
integrator_t integrator( kernel );
// the type of the matrix generator and an instance
typedef BemOperator< integrator_t, dofhandler_t > bem_operator_t;
bem_operator_t bem_operator( integrator, dof_handler );
// finally, this computes the matrix A
bem_operator.compute( );
```

Other discrete boundary integral operators can obtained discretised alike. Currently, BETL supports polynomial boundary element functions up to degree three for Laplace/Helmholtz problems, as well as up to 3rd order geometry approximations. First order surface edge elements are implemented for operators related with Maxwell's equations.

Below is a result of a single trace formulation for the Helmholtz transmission problem.

$$\sum_{d=0}^{\#Domains} L_d^* A_d L_d \begin{bmatrix} \underline{u} \\ \underline{t} \end{bmatrix} = \begin{bmatrix} \underline{u}_{inc} \\ \underline{t}_{inc} \end{bmatrix}$$

$L_d$ : Localization operators $\Gamma \to \Gamma_d$
$A_d$ : Calderón operators for the Helmholtz eqn.

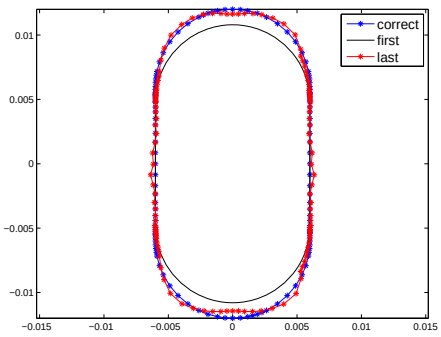


| | |
|---|---|
| **Title:** | Shape Calculus for Nano-Optics |
| **Researchers:** | Sahar Sargheini (SAM & IFH) , Alberto Paganini (SAM), Pegah Souzangar (SAM & IFH), Laura Scarabosio (SAM) Prof. Ralf Hiptmair (SAM) |
| **Institute:** | Seminar for Applied Mathematics, ETH Zürich |
| **Funding:** | ETH CHIRP project CH1-01 11-1 |

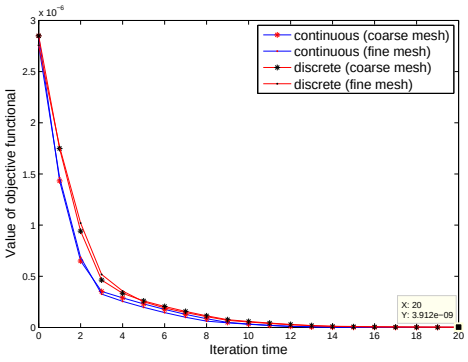
**Description:** Nano optics is the study of the interaction of light with sub-wavelength structures. There are different fabrication methods in this field, but all these methods introduce some perturbations to the initially designed structure. The sensitivity of the structure with respect to these variations can be evaluated by computing shape gradients.

On the other hand, different kinds of imaging methods, like SNOM, can be used to visualize the fabricated structure. Determining the shape of a structure starting from this information is an inverse problem which can be reformulated in terms of PDE constraint shape optimization. Shape gradients play also in this case a crucial role.

We have derived discrete and continuous shape gradients for 2D structures with PEC or dielectric scatterer. We have also implemented an algorithm based on a steepest descent method for solving the inverse problem. Some results of the experiment are shown in Figure (a) and (b). The implementation is written in MATLAB and is based on the library LehrFEM.




(a) Nodes position.




(b) Convergence history.

Figure (a) shows the position of the boundary nodes (red dots) after twenty iterations (based on the discrete shape gradient): starting from the initial shape (black line) they recover the reference shape (blue line). A similar result is obtained when using the continuous shape gradient. In (b) we see the convergence history of the algorithm. Discrete gradients (red line) and continous gradients (blue line) show a similar behaviour.

The next task is 3D implementation of the algorithm based on the C++ library NGSOLVE.

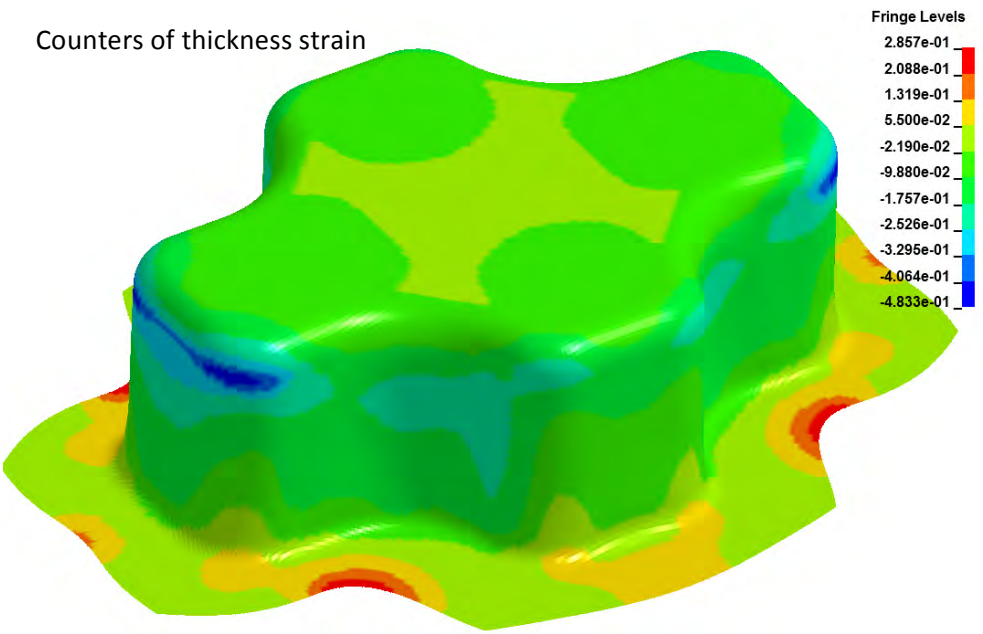
| | |
|---|---|
| Title | Advanced yield locus models taking into account anisotropic hardening effects for the simulation of sheet metal material |
| Researchers: | P.Peters, P. Hora |
| Institute / Group: | Institute of virtual manufacturing |

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.

For these reasons, advanced high strength materials are progressively used while at the same time, parts with more complex geometries have to be manufactured. Since nowadays, the numerical simulation of deep drawing processes during the development of car bodies is essential, ways must be found to describe the increasingly complex behavior of the materials used with an adequate accuracy.

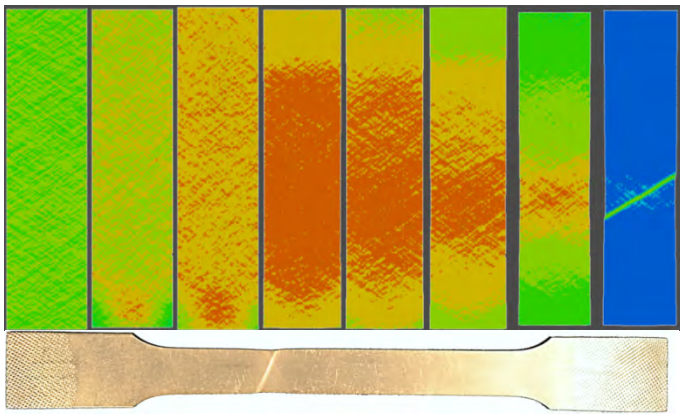
In the framework of this project, existing material models are enhanced to take into account not only a homogeneous expansion of yield surfaces (isotropic hardening), but also a change of their shape with ongoing deformation (anisotropic hardening). After the implementation of the new models in commercial FEM-Codes, the model parameters have to be identified by means of different mechanical tests. Finally, the models are validated by means of a comparison of the numerical results with measurements from real deep drawn parts.



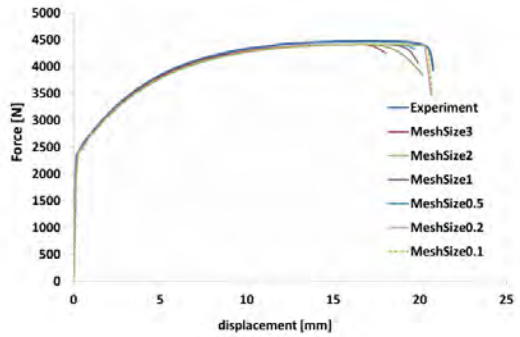
| | |
|---|---|
| Title | Numerical prediction of instabilities for ductile materials - Failure models and regularization methods |
| Researchers: | M. Gorji, P. Hora |
| Institute / Group: | Institute of virtual manufacturing |

Description:

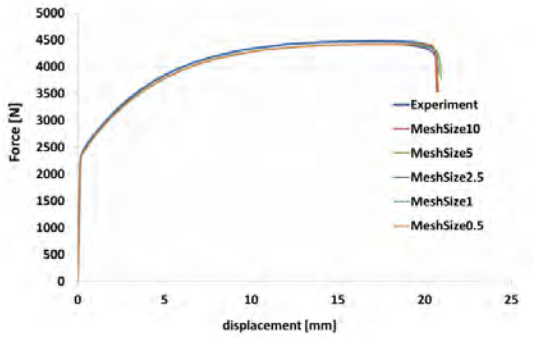
Over the past decade, various aspects of sheet metal forming have been studied extensively. In the beginning of the plastic process at low strain levels the state of strain is generally smooth. But after this initial stage the developing strain is often localized to a narrow area. This localization is called ***necking*** which is the prelude of fracture because a crack is ultimately formed in the necking region. Necking and consequently fracture are identified as major failure mechanisms of sheet metal forming. Therefore better understanding and more accurate simulation of the phenomenon of necking is important. On the other hand, through the simulation, mesh refinement in the presence of damage or failure can be problematic. One of the ways to enhance the efficiency in sheet metal forming analysis and to minimize this localization affect and consequently to reduce mesh size sensitivity is called ***mesh regularization method***. By compensate the amount of energy which has been dissipated with coarser element size, is allowed to regularize not only fracture strains but also the energy consumed during the post-critical deformation.



*[up] finite element results (plastic strain) of Aluminium alloy until one step before fracture in tensile test (shear bands during the test are observable) [down] tensile specimen of Aluminium alloy before the fracture*




*Mesh dependencies: Force-Displacement curves in tensile tests with different mesh sizes before implementing mesh regularization method*




*Force-Displacement curves in tensile tests with different mesh sizes after implementing mesh regularization method*

**Title:** Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: A molecular dynamics simulation study.

**Researchers:** S. Riniker*
B.A.C. Horta*
B. Thijssen*
S. Gupta*
W.F. van Gunsteren*
P.H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry

**Description :**

For most liquids, the static relative dielectric permittivity is a decreasing function of temperature, because enhanced thermal motion reduces the ability of the molecular dipoles to orient under the effect of an external electric field. Monocarboxylic fatty acids ranging from acetic to octanoic acid represent an exception to this general rule. Close to room temperature, their dielectric permittivity increases slightly with temperature. The causes for this anomaly are investigated here based on molecular dynamics simulations of acetic and propionic acids at different temperatures in the interval 283 - 363 K, using the GROMOS $53A6_{OXY}$ force field. The corresponding methyl esters are also considered for comparison. The dielectric permittivity is calculated using either the box-dipole fluctuation (BDF) or the external electric field (EEF) methods. The normal and anomalous temperature dependences of the permittivity for the esters and acids, respectively, are reproduced. Furthermore, in the EEF approach, the response of the acids to an applied field of increasing strength is found to present two successive linear regimes before reaching saturation. The low-field permittivity $\epsilon$, comparable to that obtained using the BDF approach, decreases with temperature. The higher-field permittivity $\epsilon'$ is slightly larger, and increases with temperature. Further analyses of the simulations in terms of radial distribution functions, hydrogen-bonded structures, and diffusion properties suggest that increasing the temperature or the applied field strength both promote a population shift from cyclic (mainly dimeric) to extended (chain-like) hydrogen-bonded structures. The lower effective dipole moment associated with the former structures compared to the latter ones provides an explanation for the peculiar dielectric properties of the two acids compared to their methyl esters.

**References:** S. Riniker, B.A.C. Horta, B. Thijssen, S. Gupta, W.F. van Gunsteren and P.H. Hünenberger
Chem. Phys. Chem. **13** (2012) 1182-1190.

**Title:** New interaction parameters for charged amino acid side chains in the GROMOS force field.

**Researchers:** M.M. Reif**
P.H. Hünenberger*
C. Oostenbrink**

**Institute/ Group:**
* Laboratory of Physical Chemistry
** Institute for Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria

**Description :**

A GROMOS force-field parameter set 54A8 is developed, which is based on the latest 54A7 set [Schmid *et al.*, Eur. Biophys. J. 40, 843-856 (2011)] and involves a recalibration of the non-bonded interaction parameters for the charged amino acid side chains, based on ionic side chain analogs. After a thorough analysis of the available experimental data, conventional hydration free energies for the ammonium, mono-, di-, tri- and tetramethyl-ammonium, formate, acetate, propanoate, imidazolium and guanidinium ions are combined with a standard absolute intrinsic proton hydration free energy $\Delta G^{\ominus}_{\mathrm{hyd}}[\mathrm{H}^{+}_{g}] = -1100$ kJ·mol$^{-1}$ to yield absolute intrinsic single-ion hydration free energies serving as experimental target data. The raw hydration free energies calculated from atomistic simulations are affected by electrostatic and finite-size artifacts, and corrections are applied to reach methodological independence prior to comparison with these experimental values. Except for monomethyl-ammonium, ions with parameters derived directly from the 54A7 force field considerably underestimate (ammonium, formate, acetate, propanoate, guanidinium) or overestimate (di-, tri- and tetramethyl-ammonium, imidazolium) the magnitude of the intrinsic hydration free energy, the largest deviation affecting the acetate ion (40.0 kJ·mol$^{-1}$). After reparameterization into 54A8, the mean and maximal absolute deviations between simulated and experimental data over the set of ten ions are reduced from 23.1 and 40.0 kJ·mol$^{-1}$, respectively, to 1.8 and 6.3 kJ·mol$^{-1}$, respectively. Although the 54A7 and 54A8 parameter sets differ significantly in terms of the hydration free energies of the ions considered, other properties such as ion-water radial distribution functions and ion-ion potentials of mean force appear to be only moderately sensitive to this change. These properties are similar for the two sets and, in the case of the ion-water radial distribution functions, in good agreement with available experimental data.

**References:** M.M. Reif, P.H. Hünenberger and C. Oostenbrink
J. Chem. Theory Comput. (2012) in press.

**Title:** Calculation of derivative thermodynamic hydration and aqueous partial molar properties of ions based on atomistic simulations.

**Researchers:** B. Dahlgren*
M.M. Reif**
P.H. Hünenberger*
N. Hansen*

**Institute/ Group:**
* Laboratory of Physical Chemistry
** Institute for Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria

**Description :**

The raw ionic solvation free energies calculated based on atomistic (explicit-solvent) simulations are extremely sensitive to the boundary conditions and treatment of electrostatic interactions used during these simulations. However, as shown recently [Kastenholz & Hünenberger, J. Chem. Phys. 124, 224501 (2006); Reif & Hünenberger, J. Chem. Phys. 134, 144104 (2011)], the application of an appropriate correction scheme permits to convert the methodology-dependent raw data into methodology-independent results. In this work, methodology-independent derivative thermodynamic hydration and aqueous partial molar properties are calculated for the $Na^+$ and $Cl^-$ ions at $P^\circ = 1$ bad and $T^- = 298.15$ K, based on the SPC water model and on ion-solvent Lennard-Jones interaction coefficients previously reoptimized against experimental hydration free energies. The hydration parameters considered are the hydration free energy and enthalpy. The aqueous partial molar parameters considered are the partial molar entropy, volume, heat capacity, volume-compressibility and volume-expansivity. Two alternative calculation methods are employed to access these properties. Method I relies on the difference in average volume and energy between two aqueous systems involving the same number of water molecules, either in the absence or in the presence of the ion, along with variations of these differences corresponding to finite pressure or/and temperature changes. Method II relies on the calculation of the hydration free energy of the ion, along with variations of this free energy corresponding to finite pressure or/and temperature changes. Both methods are used considering two distinct variants in the application of the correction scheme. In Variant A, the raw values from the simulations are corrected after application of finite difference in pressure or/and temperature, based on correction terms specifically designed for derivative parameters at $P^\circ$ and $T^-$. In Variant B, these raw values are corrected prior to differentiation, based on corresponding correction terms appropriate for the different simulation pressures $P$ and temperatures $T$. The results corresponding to the different calculation schemes show that, except for the hydration free energy itself, accurate methodological independence and quantitative agreement with even the most reliable experimental parameters (ion-pair properties) are not yet reached. Nevertheless, approximate internal consistency and qualitative agreement with experiment can be achieved, but only when an appropriate correction scheme is applied, along with a careful consideration of standard-state issues.

**References:** B. Dahlgren, M.M. Reif, P.H. Hünenberger and N. Hansen
J. Chem. Theory Comput. (2012) in press.

**Title:** A GROMOS parameter set for vicinal diether functions: properties of polyethyleneoxide and polyethyleneglycol.

**Researchers:** P.F.J. Fuchs**
H.S. Hansen*
P.H. Hünenberger*
B.A.C. Horta*

**Institute/ Group:**
* Laboratory of Physical Chemistry
** Université Paris Diderot, Sorbonne Paris Cité, Paris, France

**Description :**

An extension 53A6$_{OXY+D}$ to the GROMOS 53A6$_{OXY}$ force field is reported that includes an accurate description of the vicinal diether function. The calibration is based on the model compound 1,2-dimethoxyethane (DXE) and involves a fitting of the relevant torsional-energy parameters against quantum-mechanical (QM) rotational energy profiles for the OCCO and CCOC dihedral angles in vacuum, followed by a validation against experimental conformer populations in the pure liquid and in aqueous mixtures. A systematic comparison between the 53A6, 56A6$_{CARBO}$, 53A6$_{OXY}$, and 53A6$_{OXY+D}$ parameter sets is also performed in terms of these properties, as well as in terms of the thermodynamic properties of dimethylether (DME), diethylether (DEE), 1-methoxypropane (MPH), and DXE. Finally, the new parameter set is further validated in the context of polyethers, namely polyethyleneoxide (PEO) and polyethylenegycol (PEG). The 53A6$_{OXY+D}$ set reproduces well the QM rotational profiles of DXE in vacuum (by calibration), the conformational populations of DXE in the pure liquid and in aqueous mixtures, and the experimental thermodynamic pure-liquid and (polar and nonpolar) solvation properties of DME, DEE, MPH, and DXE. In particular, it accounts appropriately for the gauche-effect, both in its solvent-independent stereoelectronic component and in its solvent-dependent dielectric-screening component. In contrast to 53A6$_{OXY}$, it also suggests a higher affinity of DXE for water compared to octanol, in agreement with the experimental partition coefficient. In the context of aqueous polyethers, the calculated size (Flory) exponent ($\tau_g = 0.61$) for the molecular-weight dependence of the radius of gyration and persistence length ($L_p = 0.39 \pm 0.04$ nm) agree well with estimates based on experiment or previous simulations with other force fields. The simulations also suggest a picture of aqueous polyethers as "water sponges", in which the diether function "adsorbs" an essentially constant number of water molecules corresponding to first-shell hydrogen-bonded saturation of its oxygen atoms, with a tendency to include other ether oxygen atoms along the chain in the second shell, resulting in "water bridging".

**References:** P.J.F. Fuchs, H.S. Hansen, P.H. Hünenberger and B.A.C. Horta J. Chem. Theory Comput. (2012) in press.

**Title:** Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: Influence of the system size and force-field parameters.

**Researchers:** M. Laner*
B.A.C. Horta*
P.H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry

**Description :**

Phase-transition properties of glycerol-1-monopalmitate (GMP) bilayers are investigated using explicit-solvent molecular dynamics (MD) simulations, initiated from structures appropriate for the gel (GL) or liquid crystal (LC) phases, and carried out at different hydration levels and temperatures. Building up on a previous study and based on 600 ns simulations, the influence of the system size and of the force field on the equilibrium thermodynamic and dynamic parameters of the bilayers in the GL and LC phases, as well as on the temperature $T_m$ and properties of the GL $\leftrightarrow$ LC phase transition, are analysed. Qualitatively speaking, the results agree with the available experimental data for the area per lipid in the two phases and for the phase-transition temperatures at the three hydration levels irrespective of the selected model parameters. They also suggest that the total number of hydrogen bonds formed between a lipid headgroup and its environment is essentially constant, amounting to about four in both the LC and the GL phases. Quantitatively speaking, the dependence of $T_m$ on the hydration level is found to be non-systematic across the different combinations of model parameters. This results in part from a sensivity of the results on the system size and force-field parameters, but also from the limited accuracy of the bracketing approach employed here to estimate $T_m$. Finally, a simple kinetic model is proposed to account for the timescales of the transitions. This model involves enthalpy and entropy increases of about 26 $\mathrm{kJ\,mol^{-1}}$ and 83 $\mathrm{J\,mol^{-1}\,K^{-1}}$ per lipid, upon going from the GL to the LC phase. The transition state is associated with activation parameters corresponding to 13 and 11%, of these values along the GL $\rightarrow$ LC transition, resulting in an activation free energy of about 0.3 $\mathrm{kJ\,mol^{-1}}$ per lipid at $T_m$.

**References:** M. Laner, B.A.C. Horta and P.H. Hünenberger
Mol. Simul. (2012) submitted.

**Title:** Turbulent reactive flow

**Researchers:** Michael Wild
Benjamin Zoller
Daniel Meyer
Patrick Jenny

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

**General description:**
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 probability density function (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 Reynolds-averaged Navier-Stokes (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.

**References:** [1] [7] [14] [15] [20] [21] [32] [33] [34] [36] [40] [45]

**Title:** Hybrid LES/RANS modeling framework

**Researchers:** Heng Xiao
Patrick Jenny

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

**Description:**
While large eddy simulation (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:** [30] [31] [44] [45]

**Title:** Flow and transport in porous and fractured media

**Researchers:** Dimitrios Karvounis
Florian Müller
Karim Khayrat
Davide Cortinovis
Manav Tyagi (now ALSTOM)
Hadi Hajibeygi (now AP TT at TU Delft)
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 the 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 Arbenz (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.
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.

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

| | |
|---|---|
| **Title:** | Fluid dynamics in biological systems and biomedical optics |
| **Researchers:** | Adrien Lücker<br>Franca Schmid<br>Milos Sormaz (now ALSTOM)<br>Patrick Jenny |
| **Institute/ Group:** | Institute of Fluid Dynamics<br>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] [48]

**Title:** Fokker-Planck model for non-equilibrium gas flow

**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]

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|---|---|
| **Title:** | Development of numerical schemes and solution algorithms |
| **Researchers:** | Florian Müller<br>Halvor Lund<br>Jinfen Kang<br>Giuseppe Bonfigli (now Andritz Hydro AG)<br>Patrick Jenny |
| **Institute/**<br>**Group:** | Institute of Fluid Dynamics<br>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]

**Title:** Error thresholds for topological quantum computing proposals

**Researchers:** H. G. Katzgraber*
R. Andrist*
H. Bombin**
M.-A. Martin Delgado***

**Institute/Group:** *Theoretische Physik, ETH Zürich
**Perimeter Institute for Theoretical Physics, Canada
***Universidad Complutense de Madrid, Spain

**Description:**

Sensitivity to noise makes most of the current quantum computing schemes prone to error and nonscalable, allowing only for small proof-of-principle devices. Topologically-protected quantum computing aims at solving this problem by encoding quantum bits and gates in topological properties of the hardware medium that are immune to noise that does not impact the entire medium at once. There are different approaches to achieve topological stability or active error correction, ranging from quasiparticle braidings to spin models and topological color codes that use brane-net condensates in 3-colexes. The stability of these proposals against noise can be quantified by the error threshold. This figure of merit can be computed by mapping the problem onto complex statistical mechanical spin models with local disorder on nontrival lattices that can have many-body interactions or are described by lattice gauge theories. The error threshold then represents the point in the temperature-disorder phase diagram where a stable ferromagnetic phase vanishes. Using large-scale Monte Carlo simulations the stability of topological quantum computing proposals (topological color codes, Kitaev model, topological subsystem codes) against different kinds of errors is studied. The results illustrate the generic robustness of topologically-protected quantum computing proposals, thus paving the road towards stable and scalable systems.

**References:**

H. Bombin, Ruben S. Andrist, Masayuki Ohzeki, Helmut G. Katzgraber, and M.-A. Martin-Delgado, Phys. Rev. X **2**, 021004 (2012)

R. S. Andrist, H. Bombin, Helmut G. Katzgraber, and .-A. Martin-Delgado, Phys. Rev A **85**, 050302(R) (2012)

**Title:** Boolean decision problems with competing interactions on scale-free networks: Critical thermodynamics.

**Researchers:** Helmut Katzgraber*
Katharina Janzen**
Creighton K. Thomas***

**Institute/Group:** * Theoretische Physik, ETH Zürich
** Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, DE
***Department of Physics, Texas A&M University, USA

**Description:**

We study the critical behavior of Boolean variables on scale-free networks with competing interactions (Ising spin glasses). Our analytical results for the disorder–network-decay-exponent phase diagram are verified using large-scale Monte Carlo simulations. When the probability of positive (ferromagnetic) and negative (antiferromagnetic) interactions is the same, the system undergoes a finite-temperature spin-glass transition if the exponent that describes the decay of the interaction degree in the scale-free graph is strictly larger than 3. However, when the exponent is equal to or less than 3, a spin-glass phase is stable for all temperatures. The robustness of both the ferromagnetic and spin-glass phases suggest that Boolean decision problems on scale-free networks are quite stable to local perturbations.

**References:**

H. G. Katzgraber, Katharina Janzen and Creighton K. Thomas, Phys. Rev. E , in press (arXiv:cond-mat/1202:1153)

**Title:** Novel disordering mechanism in ferromagnetic systems with competing interactions

**Researchers:** Juan Carlos Andresen*
Helmut Katzgraber*
Creighton K. Thomas**
Moshe Schechter***

**Institute/Group:** * Theoretische Physik, ETH Zürich
** Department of Physics, Texas A&M University, USA
***Physics Department, Ben Gurion University, IL

**Description:**

We study the interplay between ferromagnetic and spin-glass phases in magnetic systems such as LiHoxY1−xF4 theoretically, as well as using numerical simulations of a three-dimensional diluted long-range dipolar Ising model with competing interactions in the presence of a random field. Our results suggest the ex- istence of a novel disordering mechanism of the ferromagnetic phase due to the underlying spin-glass phase when a random field is applied. We numerically compute the zero-temperature phase boundary between the quasi-spin-glass and ferromagnetic phases as a function of the Ho concentration and random-field strength, and explain the peculiar linear dependence of the critical temperature on the strength of the random field found in recent experiments by Silevitch *et al*. [Nature **448**, 567 (2007)] on the LiHoxY1−xF4 compound.

**References:**

Juan Carlos Andresen, Creighton K. Thomas, H. G. Katzgraber and Moshe Schechter, Phys. Rev. Lett., submitted, (arXiv:cond-mat/1205.1572)

**Title:** Ultrametric of the spin-glass state in a field

**Researchers:** Helmut Katzgraber*
Thomas Jörg**
Florent Krzakala**
Alexander K. Hartmann***

**Institute/Group:** * Theoretische Physik, ETH Zürich
** Laboratoire PCT, UMR Gulliver CNRS-ESPCI 7083, FR
*** Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, DE

**Description:**

We study the ultrametric structure of phase space of one-dimensional Ising spin glasses with random power-law interaction in an external random field. Although in zero field the model in both the mean-field and non-mean-field universality classes shows an ultrametric signature [Phys. Rev. Lett. **102**, 037207 (2009)], when a field is applied ultrametricity seems only present in the mean-field regime. The results for the non-mean field case in an external field agree with data for spin glasses studied within the Migdal-Kadanoff approximation. Our results therefore suggest that the spin-glass state might be fragile to external fields below the upper critical dimension.

**References:**

H. G. Katzgraber, Thomas Jorg, Florent Krzakala, Alexander K. Hartmann, Phys. Rev. B, submitted, (arXiv:cond-mat/1205.4200)

**Title:** The low-temperature phase of the Edwards-Anderson spin glass seems not mean-field-like

**Researchers:** Burcu Yucesoy*
Helmut Katzgraber**
Jonathan Machta*

**Institute/Group:** * Department of Physics, Univ. Massachussets Amherst, USA
** Theoretische Physik, ETH Zürich

**Description:**

The three-dimensional Edwards-Anderson Ising spin glass and the fully-connected mean-field Sherrington-Kirkpatrick Ising spin glass are studied via large-scale Monte Carlo simulations at low temperatures, deep within the spin-glass phase. Performing a careful statistical analysis of several thousand independent disorder realizations and using an observable that detects peaks in the overlap distribution, we show that the Sherrington-Kirkpatrick and Edwards-Anderson models have a distinctly different low-temperature behavior. The structure of the spin-glass overlap distribution for the Edwards-Anderson model suggests that its low-temperature phase has only a single pair of pure states.

**References:**

B. Yucesoy, H. G. Katzgraber, J. Machta, Phys. Rev. Lett., submitted, (arXiv:cond-mat/1206.0783)

**Title:** Bond disorder induced criticality of the three-color Ashkin-Teller model

**Researchers:** Arash Bellafard*
Helmut Katzgraber**
Matthias Troyer**
Sudip Chakravarty*

**Institute/Group:** * Department of Physics and Astronomy, University of California, Los Angeles, USA
** Theoretische Physik, ETH Zürich

**Description:**

An intriguing result of statistical mechanics is that a first-order phase transition can be rounded by disorder coupled to energy-like variables. In fact, even more intriguing is that the rounding may manifest itself as a critical point, quantum or classical. In general, it is not known, however, what universality classes, if any, such criticalities belong to. In order to shed light on this question we examine in detail the disordered three- color Ashkin-Teller model by Monte Carlo methods. Extensive analyses indicate that the critical exponents define a new universality class. We show that the rounding of the first-order transition of the pure model due to the impurities is manifested as criticality. However, the magnetization critical exponent, $\beta$, and the correlation length critical exponent, $\nu$, are found to vary with disorder and the four-spin coupling strength, and we conclusively rule out that the model belongs to the universality class of the two-dimensional Ising model.

**References:**

Arash Bellafard, Helmut G. Katzgraber, Matthias Troyer, and Sudip Chakravarty, Phys. Rev. Lett., submitted, (arXiv:cond-mat/1207.1080)

**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 sensors for head movements (semicircular canals and otolith organs) as well as the sensory hearing organ (cochlea). We study the (patho-)physiology of the semicircular canals (SCC) and the cochlea by numerical simulations.

The transduction of SCC is mediated by the interaction of sensory structures with a fluid called endolymph. We compute the endolymph flow by the method of fundamental solutions (MFS). The numerical stability and the accuracy of the MFS strongly depend on the position of the source points of the fundamental solutions. Standard implementations of the MFS rely on an arbitrary positioning of the source points such that numerical instabilities are often observed. To overcome this problem, we proposed an efficient and accurate version of the MFS, the multilayer MFS, which employs an optimization algorithm to position the source points. The multilayer MFS was applied to realistic three-dimensional SCC to compute the endolymph flow during head rotations. These simulations revealed a vortical flow which maximizes the fluid shear stress in the proximity of the sensory tissues. Multilayer MFS was also extended to flows with particles by coupling it with the Force Coupling Method which is a convenient model for finite-size particles. This coupling has allowed us to study a pathological condition of the SCC 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 are also investigating a nonlinear effect of the fluid motion, the steady streaming, and the influence of different stimulation modes on the hearing.

Finally, there are pathological conditions where the separation of the organs of hearing and balance breaks down such that there exists sensory cross-talk. In Tullio's phenomenon, the stimulation of the inner ear with sound results in a misleading flow inside the SCCs which leads to vertigo. We perform numerical investigations of this phenomenon with the open source software OpenFOAM. Our simulations include pulse propagation and strongly coupled fluid-structure interaction on a finite-volume grid of the SCCs.

**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:**

Aerodynamically generated noise plays a significant role in the development of jet engines. The high unsteadiness of the flow during the turbulent breakdown of the jet is the major source of sound pressure waves emitted to the far field. Time-dependent flow simulations using high-order numerical schemes are able to accurately predict this jet noise without empiricism and to obtain insight in the underlying noise generation mechanism.

Of particular current interest is the investigation of jet flows with an initially turbulent shear layer. In order to investigate this type of flow, the nozzle was included into the simulation domain. After the validation of the numerical setup, simulations of jet flows have been performed with a turbulent nozzle exit boundary layer while maintaining a potential flow core. Sound pressure spectra obtained in the acoustic near-field agree well with experimental data for the downstream direction. In order to shed light on the noise generation mechanism, nozzle exit flow conditions were varied and the comparison of simulation results is in progress.

In addition to the isothermal single jet invesigations, a new project has been started which investigates the noise radiation originating from flow disturbances in heated coaxial jet flows. This configuration leads to a more realistic representation of the flow conditions observed in current commercial jet engines. A focus is on the hydrodynamic stability of the jet shear layer and the noise associated with the streamwise development of flow instabilities.

Furthermore, we investigate the stability and transitional behaviour of swirling jets at medium to high swirl numbers. At sufficiently high azimuthal velocity the jets break down and a recirculation zone around the centreline 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 behaviour 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 behaviour is additionally investigated.

**References:** See separate list.

**Title:** Instability of the Leading Edge Boundary Layer

**Researchers:** Michael John, Dominik Obrist and Leonhard Kleiser

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

**Description:**

The instability of laminar flows, which leads to transitional and fully turbulent flows, is one of the canonical yet unclosed problems of fluid dynamics. Theoretical results for many situations were obtained by linear stability analysis of the laminar base flow, but nonlinear or secondary mechanisms often play a dominant role. Typically, these mechanisms cannot be described analytically and need experimental or numerical treatment.
The boundary layer along the leading-edge of swept airplane wings (swept Hiemenz boundary layer) is inherently three-dimensional and its instability is of the so-called subcritical type, rendering it particularly challenging. This flow has been thoroughly investigated experimentally since the 1940s, nevertheless no concise theoretical explanation for the subcritical instability is available to date.
Results from an investigation of this problem have potentially a high value both for scientific as well as industrial applications. Also, an investigation of subcritical instability of differential equations is of high academic value. Moreover, there exist practical trials in the airplane industry with boundary layer suction to optimize the flow at the leading-edge of swept wings. Our work might be able to contribute to the theoretical basis for such devices.

Recently, direct numerical simulations carried out by our group have uncovered a nonlinear transition mechanism which resembles a bypass transition mechanism for flat plate boundary layers known from the literature. Furthermore, we succeeded in formally demonstrating the similarity of this flow to a substantially simpler configuration, namely an asympototic suction boundary layer, for which the occurrence and properties of bypass transition have been investigated. Together, these two observations lead to the assumption that the instability of this complicated three-dimensional flow configuration is closely related to the known mechanisms for two-dimensional boundary layers. Our goal is to develop a theory for the subcritical instability mechanism observed in the simulations based on known theories for two-dimensional boundary layers.
Our primary tools of investigation are direct numerical simulations with our existing high-fidelity simulation code IMPACT. Furthermore, stability solvers will be applied in order to analyze the linear stability of the flow field at different stages of the transition process.

**References:** None

**Title:** Simulation of Particle-Laden Flows

**Researchers:** R. Henniger, Y. Reinhardt, T. Chadha, and L. Kleiser

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

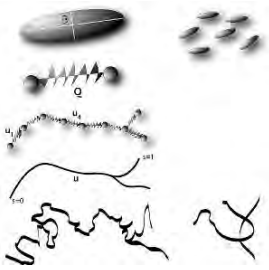
**Description:**

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. An appropriate simulation code must allow for high accuracy at relatively little computational cost and for a high scalability with the problem size on massively-parallel computers. To this end, a high order (typically $4^{\text{th}}$ or $6^{\text{th}}$ order) simulation code for incompressible flows has been developed, employing compact finite differences on staggered grids in space and a semi-implicit time integration scheme. This approach permits an iterative solution for the pressure and an efficient three-dimensional data decomposition. The scalability with the problem size has been demonstrated for a channel flow in a weak scaling test with up to 100 billion grid points and 400 billion unknowns. To further increase the Reynolds number range, we added 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. 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 in oceanic environments, 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.

In a second project we are developing methods for computations of abrasive water jet cutting. In recent years the use of abrasive water jet technology has become increasingly popular for material cutting applications. The aim of this project is to model the abrasive water jet, more precisely 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 code OpenFOAM is used. High Reynolds numbers and 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. 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:** Hairy pores, nanotube buckypaper & protein adsorption



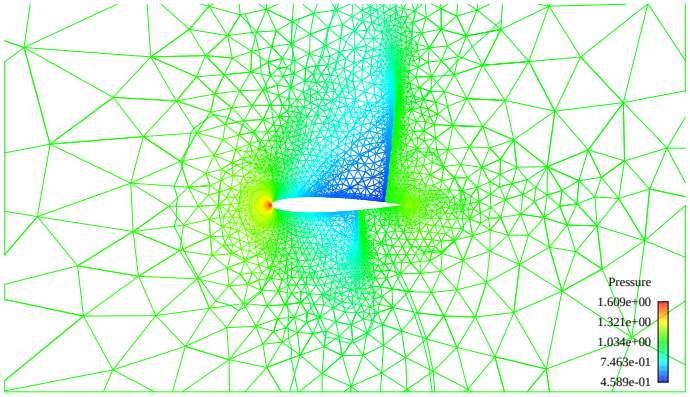
**Researchers:** Prof. Martin Kröger [1]
Prof. Avraham Halperin [2]
Prof. Igal Szleifer & Ying Li [3]
Prof. Manuel Laso [4]
Prof. Juan J. de Pablo [5]

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

**Description:**

We recently focused our attention on the viscoelasticity of carbon nanotube buckypaper [1], as well on its entanglement length and pore size [2], the effect of nanoparticle geometry on the structure, dynamics and anisotropic viscosities of polyethylene nanocomposites [3], the effects of carbon nanotube entanglement and bundling on structural and mechanical properties of buckypaper [4], the evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings [5], the mechanisms of harvesting cells cultured on thermoresponsive polymer brushes [6], the influence of nanorod inclusions on structure and primitive path network of polymer nanocomposites at equilibrium and under deformation [7], the design of strong and tough biomimetic polymer networks [8], the morphology control of hairy nanopores [9], primitive chain networks of uncrosslinked and crosslinked cis-polyisoprene polymers [10], the adsorption of core-shell nanoparticles at liquid-liquid interfaces [11]. We presented a molecularly derived constitutive equation for low-molecular polymer melts from thermodynamically guided simulation [12] and studied the collapse of thermoresponsive brushes and the tuning of protein adsorption [13]. Details available at http://www.complexfluids.ethz.ch

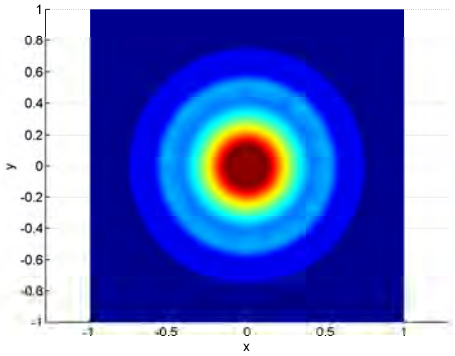
[1] Y. Li, M. Kröger, Soft Matter **8** (2012) 7822-7830.
[2] Y. Li, M. Kröger, Appl. Phys. Lett. **100** (2012) 021907.
[3] Y. Li, M. Kröger, W.K. Liu, Macromolecules **45** (2012) 2099-2112.
[4] Y. Li, M. Kröger, Carbon **50** (2012) 1793-1806.
[5] N.C. Karayiannis, R. Malshe, M. Kröger, J.J. de Pablo, M. Laso, Soft Matter **8** (2012) 844-858.
[6] A. Halperin, M. Kröger, Biomaterials **33** (2012) 4975-4987.
[7] G.N. Toepperwein, N.C. Karayiannis, R.A. Riggleman, M. Kröger, J.J. de Pablo, Macromolecules **44** (2011) 1034-1045.
[8] I.G. Salib, G.V. Kolmakov, B.J. Bucior, O. Peleg, T. Savin, M. Kröger, V. Vogel, K. Matyjaszewski, A.C. Balazs, Langmuir **27** (2011) 13796-13805.
[9] O. Peleg, M. Tagliazucchi, M. Kröger, Y. Rabin, I. Szleifer, ACS Nano **5** (2011) 4737-4747.
[10] Y. Li, M. Kröger, W.K. Liu, Polymer **52** (2011) 5867-5878.
[11] L. Isa, *et al.*, E. del Gado, P. Ilg, M. Kröger, E. Reimhult, Soft Matter **7** (2011) 7663-7675.
[12] P. Ilg, M. Kröger, J. Rheol. **55** (2011) 69-93.
[13] A. Halperin, M. Kröger, Macromolecules **44** (2011) 6986-7005.




**Title:** High-resolution entropy stable finite volume schemes for systems of conservation laws on unstructured grids

**Researchers:** S. Mishra, U.S. Fjordholm, A. Madrane (Bombardier Aerospace, Canada), E. Tadmor (U. Maryland).
**Institute:** Seminar for Applied Mathematics (SAM), ETH Zürich.
**Description:** Systems of conservation laws modelling physical and engineering systems are equipped with an entropy formulation that provides stability estimates and selects the physically meaningful. We design high-resolution finite volume numerical schemes that satisfy a discrete version of the entropy inequality. The novel feature of the schemes is the fact that are implemented on unstructured grids that allow for the treatment of general geometries, for instance for the Euler equations in aerodynamics.
**Publications:**

1. A. Madrane, U.S. Fjordholm, S. Mishra and E. Tadmor, Entropy conservative and entropy stable numerical schemes for multi-dimensional conservation laws on unstructured meshes *Research Report 2012-31,* SAM, ETH Zürich, to appear in Proc. ECCOMASS, 2012.




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

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

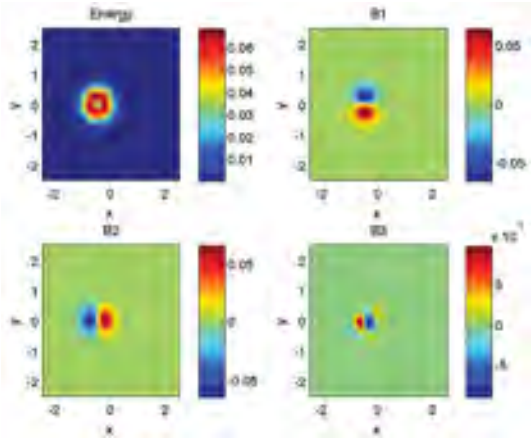
**Institute:** Seminar for Applied Mathematics (SAM), ETH Zürich.

**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 is a particular highlight. Future work is focused on the design of efficient preconditioners for improving the efficiency of the solution of resulting non-linear systems at every time step.

**Publications:**

1. Entropy stable shock capturing streamline diffusion space-time discontinuous Galerkin (DG) methods for systems of conservation laws, A. Hiltebrand and S. Mishra, *Research Report 2012-07,* SAM, ETH Zürich.

2. A convergent shock capturing streamline diffusion space-time discontinuous Galerkin (DG) methods for multidimensional scalar conservation laws, A. Hiltebrand, U. Koley and S. Mishra, In preparation, 2012.



**Title:** Stable numerical schemes for the Hall-MHD equations.

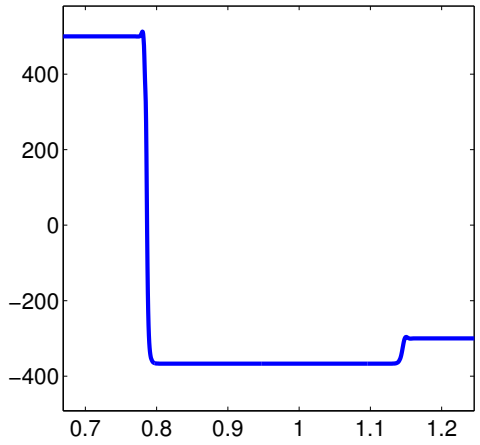
**Researchers:** S. Mishra, P. Corti.

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

**Description:** . Hall-MHD equations can model finite Larmor radius effects like magnetic reconnection. In this model, the MHD equations are augmented with a Ohm's law that includes magnetic resistivity, electron inertia and the Hall effect. The first phase of the project considers the Hall induction equations and designs stable high-order finite difference schemes to approximate them. In the second phase, we aim to develop robust preconditioners for a DG discretization of the Hall induction equations. These methods are coupled with standard MHD solvers to simulate the full Hall-MHD equations in an efficient manner.

**Publications:**


1. Stable numerical schemes for the Hall induction equations, P. Corti, PhD thesis, ETH Zurich, in preparation, 2012.



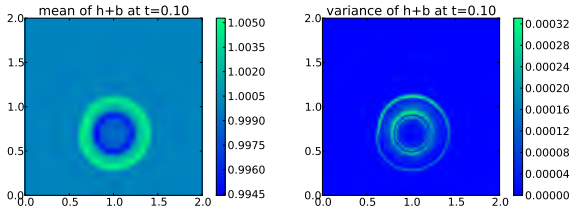

**Title:** Robust numerical approximation of small-scale dependent shock waves.

**Researchers:** S. Mishra, J. Ernest and P. G. LeFloch (U. Paris VI).
**Institute:** Seminar for Applied Mathematics (SAM), ETH Zürich.

**Description:** Small scale dependent shock waves arise in a number of interesting hyperbolic systems where the solution depends explicitly on the underlying small scale behavior. Prototypical examples are non-classical shocks that arise in non-strictly convex hyperbolic systems such as systems of nonlinear elasticity and MHD. Standard numerical schemes add implicit numerical diffusion and are unable to approximate these shock waves. We design a new class of schemes, the so-called Well Controlled Dissipation (WCD) schemes that use very high-order diffusion operators to approximate these shock waves, even of arbitrarily high shock strength.
**Publications:**

1. J. Ernest, P. G. LeFloch and S. Mishra, Numerical schemes with well-controlled dissipation (I): Non-classical shock waves, in preparation, 2012.

2. G.M. Coclite, L. Di Ruvo, J. Ernest and S. Mishra, Convergence of vanishing capillarity approximations for scalar conservation laws with discontinuous fluxes, *research report 2012-30*, SAM ETH Zürich.




**Title:** Efficient numerical methods for quantifying uncertainty in hyperbolic PDEs

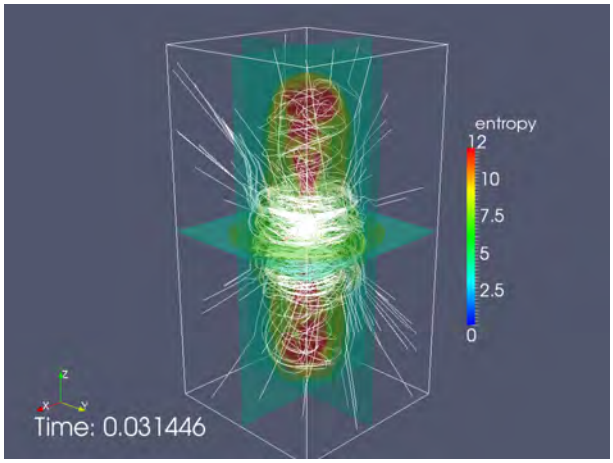
**Researchers:** S. Mishra, C. Schwab, J. Sukys, S. Tokareva and N . H. Risebro (U. Oslo)
**Institute:** Seminar for Applied Mathematics (SAM), ETH Zürich.
**Description:** Uncertainty quantification (UQ) is a grand challenge in numerical computation of conservation laws. We develop novel MLMC and stochastic 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, Ch. Schwab and J. Sukys, Multi-level Monte Carlo finite volume methods for shallow water equations with uncertain topography in multi-dimensions, *Research report 2011-70*, SAM ETH Zürich, SIAM J. Sci. Comput, to appear.

2. 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.

3. 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.

4. 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.




**Title:** Simulation of core collapse supernovas (CCSN)

**Researchers:** S. Mishra, R. Käppeli and Basel Supernova group
**Institute:** Seminar for Applied Mathematics (SAM), ETH Zürich.
**Description:** Explosions of Core collapse supernovas (CCSNs) are modeled in terms of the equations of MHD, together with the equations of neutrino transport. An efficient code, FISH, developed by the Basel Supernova group is further enhanced by adding well-balancing of the gravity source terms using high-resolving finite volume schemes, that preserve a discrete hydrostatic equilibrium. Very large massively parallel implementation is able to resolve interesting physical phenomena associated with core collapse supernovas.
**Publications:**

1. C. Winteler, R. Kppeli, A. Perego, A. Arcones, N. Vasset, N. Nishimura, M. Liebendrfer and F.-K. Thielemann Magneto-rotationally driven Supernovae as the origin of early galaxy r-process elements, *Research report 2012-05*, SAM ETH Zürich.

2. R. Käppeli and S. Mishra, Well-balanced schemes for general hydrostatic equilibria, in preparation, 2012.

**Title:** Metadynamics

**Researchers:** A. Barducci
M. Bonomi*
M. Parrinello

**Institute/Group:** Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
*University of California, San Francisco, School of Pharmacy, Department of Bioengineering and Therapeutic Sciences, San Francisco, CA, USA

**Description:**

Metadynamics is a powerful technique for enhancing sampling in molecular dynamics simulations and reconstructing the free-energy surface as a function of few selected degrees of freedom, often referred to as collective variables (CVs). In metadynamics, sampling is accelerated by a history-dependent bias potential, which is adaptively constructed in the space of the CVs. Since its first appearance, significant improvements have been made to the original algorithm, leading to an efficient, flexible, and accurate method that has found many successful applications in several domains of science. Here, we discuss first the theory underlying metadynamics and its recent developments. In particular, we focus on the crucial issue of choosing an appropriate set of CVs and on the possible strategies to alleviate this difficulty. Later in the second part, we present a few recent representative applications, which we have classified into three main classes: solid-state physics, chemical reactions, and biomolecules.

**References:** *Comp. Mol. Sci.*,1 (5), 826-843, 2011, DOI: 10.1002/wcms.31

**Title:** Exploring the free energy surfaces of clusters using reconnaissance metadynamics

**Researchers:** G. A. Tribello
J. Cuny
H. Eshet
M. Parrinello

**Institute/Group:** Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

**Description:**

A new approach is proposed for exploring the low-energy structures of small to medium-sized aggregates of atoms and molecules. This approach uses the recently proposed reconnaissance metadynamics method [G. A. Tribello, M. Ceriotti, and M. Parrinello. Proc. Natl. Acad. Sci. U.S.A. 107(41), 17509 (2010)] in tandem with collective variables that describe the average structure of the coordination sphere around the atoms/molecules. We demonstrate this method on both Lennard-Jones and water clusters and show how it is able to quickly find the global minimum in the potential energy surface, while exploring the finite temperature free energy surface.

**References:** *J. Chem. Phys.*, 135 (11), 114109, 2011, DOI: 10.1063/1.3628676

**Title:** Effect of Urea on the beta-Hairpin Conformational Ensemble and Protein Denaturation Mechanism

**Researchers:** A. Berteotti
A. Barducci*
M. Parrinello*

**Institute/Group:** Italian Institute of Technology, Department of Drug Discovery & Devices, I-16163 Genoa, Italy
*Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

**Description:**

Despite the daily use of urea to influence protein folding and stability, the molecular mechanism with which urea acts is still not well understood. Here the use of combined parallel tempering and metadynamics simulation allows us to study the free-energy landscape associated with the folding/unfolding 0f beta-hairpin GB1 equilibrium in 8 M urea and pure water. The nature of the unfolded state in both solutions has been analyzed: in urea solution the addition of denaturants acts to expand the denatured state, while in pure water solution the unfolded state is noticeably more compact. For what concerns the mechanism by which urea acts as a denaturant, a preferential direct interaction between urea molecules and protein backbone has been found. However, the bias toward urea solvation is largest at intermediate values of the gyration radius.

**References:** *J. Am. Chem. Soc.* 133 (43), 17200-17206, 2011, DOI: 10.1021/ja202849a

**Title:** Hydrogen Oxidation Reaction at the Ni/YSZ Anode of Solid Oxide Fuel Cells from First Principles

**Researchers:** C. S. Cucinotta
M. Bernasconi*
M. Parrinello**

**Institute/Group:** College Green, Dublin 2, Sch Phys, Dublin, Ireland and College Green Dublin 2, CRANN, Dublin, Ireland
*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, 20125 Milano, Italy
**Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

**Description:**

By means of ab initio simulations we here provide a comprehensive scenario for hydrogen oxidation reactions at the Ni/zirconia anode of solid oxide fuel cells. The simulations have also revealed that in the presence of water chemisorbed at the oxide surface, the active region for H oxidation actually extends beyond the metal/zirconia interface unraveling the role of water partial pressure in the decrease of the polarization resistance observed experimentally.

**References:** *Phys. Rev. Lett.*,107 (20), 206103, 2011,
DOI: 10.1103/PhysRevLett.107.206103

**Title:** On the recombination of hydronium and hydroxide ions in water

**Researchers:** A. Hassanali
M. K. Prakash
H. Eshet
M. Parrinello

**Institute/Group:** Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

**Description:**

The recombination of hydronium and hydroxide ions following water ionization is one of the most fundamental processes determining the pH of water. The neutralization step once the solvated ions are in close proximity is phenomenologically understood to be fast, but the molecular mechanism has not been directly probed by experiments. We elucidate the mechanism of recombination in liquid water with ab initio molecular dynamics simulations, and it emerges as quite different from the conventional view of the Grotthuss mechanism. The neutralization event involves a collective compression of the water-wire bridging the ions, which occurs in approximately 0.5 ps, triggering a concerted triple jump of the protons. This process leaves the neutralized hydroxide in a hypercoordinated state, with the implications that enhanced collective compressions of several water molecules around similarly hypercoordinated states are likely to serve as nucleation events for the autoionization of liquid water.

**References:** *PNAS*, 108 (51), 20410-20415, 2011, DOI: 10.1073/pnas.1112486108

**Title:** Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt/Ph) through Metadynamics Simulations

**Researchers:** G. Grazioso, V. Limongelli*
D. Branduardi**, E. Novellino*
C. De Micheli, A. Cavalli***
M. Parrinello****

**Institute/Group:** University of Milan, Dipartimento Scienze e Farmaceut., Pietro Prates, I-20133 Milan, Italy
*University of Naples Federico 2, Dipartimento Chimica, Farmaceutica e Tossicologia, I-80131 Naples, Italy
**Italian Institute of Technology, Department of Drug Discovery & Devices, I-16163 Genoa, Italy
***University of Bologna, Department of Pharmaceutical Science, I-40126 Bologna, Italy
****Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland

**Description:**

A homeostatic concentration of glutamate in the synaptic cleft ensures a correct signal transduction along the neuronal network. An unbalance in this concentration can lead to neuronal death and to severe neurodegenerative diseases such as Alzheimer's or Parkinson's. Glutamate transporters play a crucial role in this respect because they are responsible for the reuptake of the neurotransmitter from the synaptic cleft, thus controlling the glutamate concentration. Understanding the molecular mechanism of this transporter can provide the possibility of an exogenous control. Structural studies have shown that this transporter can assume at least three conformations, thus suggesting a pronounced dynamical behavior. However, some intermediate states that lead to the substrate internalization have not been characterized and many aspects of the transporter mechanism still remain unclear. Here, using metadynamics simulations, we investigate the substrate uptake from the synaptic cleft and its release in the intracellular medium. In addition, we focus on the role of ions and substrate during these processes and on the stability of the different conformations assumed by the transporter. The present dynamical results can complement available X-ray data and provide a thorough description of the entire process of substrate uptake, internalization, and release.

**References:** *J. Am. Chem. Soc.* 134 (1), 453-463, 2012, DOI: 10.1021/ja208485w

**Title:** Sampling protein motion and solvent effect during ligand binding

**Researchers:** V. Limongelli
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**Description:**

An exhaustive description of the molecular recognition mechanism between a ligand and its biological target is of great value because it provides the opportunity for an exogenous control of the related process. Very often this aim can be pursued using high resolution structures of the complex in combination with inexpensive computational protocols such as docking algorithms. Unfortunately, in many other cases a number of factors, like protein flexibility or solvent effects, increase the degree of complexity of ligand/protein interaction and these standard techniques are no longer sufficient to describe the binding event. We have experienced and tested these limits in the present study in which we have developed and revealed the mechanism of binding of a new series of potent inhibitors of Adenosine Deaminase. We have first performed a large number of docking calculations, which unfortunately failed to yield reliable results due to the dynamical character of the enzyme and the complex role of the solvent. Thus, we have stepped up the computational strategy using a protocol based on metadynamics. Our approach has allowed dealing with protein motion and solvation during ligand binding and finally identifying the lowest energy binding modes of the most potent compound of the series, 4-decyl-pyrazolo[1,5-a]pyrimidin-7-one.

**References:** *PNAS*, 109 (5), 1467-1472, 2012, DOI: 10.1073/pnas.1112181108

**Title:** Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure

**Researchers:** H. Eshet
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**Description:**

X-ray diffraction experiments have shown that sodium exhibits a dramatic pressure-induced drop in melting temperature, which extends from 1000 K at similar to 30 GPa to as low as room temperature at similar to 120 GPa. Despite significant theoretical effort to understand the anomalous melting, its origins are still debated. In this work, we reconstruct the sodium phase diagram by using an ab initio quality neural-network potential. Furthermore, we demonstrate that the reentrant behavior results from the screening of interionic interactions by conduction electrons, which at high pressure induces a softening in the short-range repulsion.

**References:** *Phys. Rev. Lett.*, 108 (11), 115701, 2012,
DOI: 10.1103/PhysRevLett.108.115701

**Title:** Using sketch-map coordinates to analyze and bias molecular dynamics simulations

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**Description:**

When examining complex problems, such as the folding of proteins, coarse grained descriptions of the system drive our investigation and help us to rationalize the results. Oftentimes collective variables (CVs), derived through some chemical intuition about the process of interest, serve this purpose. Because finding these CVs is the most difficult part of any investigation, we recently developed a dimensionality reduction algorithm, sketch-map, that can be used to build a low-dimensional map of a phase space of high-dimensionality. In this paper we discuss how these machine-generated CVs can be used to accelerate the exploration of phase space and to reconstruct free-energy landscapes. To do so, we develop a formalism in which high-dimensional configurations are no longer represented by low-dimensional position vectors. Instead, for each configuration we calculate a probability distribution, which has a domain that encompasses the entirety of the low-dimensional space. To construct a biasing potential, we exploit an analogy with metadynamics and use the trajectory to adaptively construct a repulsive, history-dependent bias from the distributions that correspond to the previously visited configurations. This potential forces the system to explore more of phase space by making it desirable to adopt configurations whose distributions do not overlap with the bias. We apply this algorithm to a small model protein and succeed in reproducing the free-energy surface that we obtain from a parallel tempering calculation.

**References:** *PNAS*, 109 (14), 5196-5201, 2012, DOI: 10.1073/pnas.1201152109

**Title:** Locating binding poses in protein-ligand systems using reconnaissance metadynamics

**Researchers:** P. Soederhjelm
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**Description:**

A molecular dynamics-based protocol is proposed for finding and scoring protein-ligand binding poses. This protocol uses the recently developed reconnaissance metadynamics method, which employs a self-learning algorithm to construct a bias that pushes the system away from the kinetic traps where it would otherwise remain. The exploration of phase space with this algorithm is shown to be roughly six to eight times faster than unbiased molecular dynamics and is only limited by the time taken to diffuse about the surface of the protein. We apply this method to the well-studied trypsin-benzamidine system and show that we are able to refind all the poses obtained from a reference EADock blind docking calculation. These poses can be scored based on the length of time the system remains trapped in the pose. Alternatively, one can perform dimensionality reduction on the output trajectory and obtain a map of phase space that can be used in more expensive free-energy calculations.

**References:** *PNAS*, 109 (14), 5170-5175, 2012, DOI: 10.1073/pnas.1201940109

**Title:** The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates

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**Description:**

The motion of the excess proton is understood as a process involving interconversion between two limiting states, namely, the Eigen and Zundel cations. Nuclear quantum effects (NQE) and the organization of the surrounding solvent play a significant role in this process. However, little is known about how these factors can change the limiting state in molecular systems and the physicochemical properties of its surrounding hydrogen-bond environment. In this work we use state of the art ab initio molecular dynamics simulations to examine the role of NQE on the nature of the proton in four hydrogen chloride hydrates. We demonstrate that NQE significantly alter the phase space properties of the proton and that the local electronic structure of the proton is an exquisitely sensitive indicator of the limiting state in each of the crystals. We evaluate both the proton momentum distribution and the proton chemical shifts and demonstrate that deep inelastic neutron scattering and solid-state nuclear magnetic resonance experiments can serve as complementary techniques for probing the quantum nature of the proton in hydrogen-bonding systems. We believe that the rich and insightful information we obtain for these acid hydrates provides a motivation for new experimental studies.

**References:** *J. Am. Chem. Soc.*, 134 (20), 8557-8569, 2012, DOI: 10.1021/ja3014727

**Title:** Ab Initio Molecular Dynamics Study of the Dehydroxylation Reaction in a Smectite Model

**Researchers:** D. Munoz-Santiburcio
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**Description:**

We have studied the dehydroxylation reaction in a smectite model, with the purpose of determining the influence of the octahedral layer composition and the possible role of the interlayer cations. Employing ab initio molecular dynamics and with the help of metadynamics for accelerating the reaction, we study the two possible mechanisms for the formation of the first water molecule. In the first mechanism, the migration of the proton across the octahedral vacancy takes place by means of a stable intermediate in which the proton is coordinated with an apical oxygen. The formation of this intermediate is not possible without a local deformation of the tetrahedral sheet, in which a Si-O basal bond is broken so that the Si coordinates with the O that releases the H, stabilizing its residual charge. In turn, the basal oxygen that loses the Si is stabilized by the nearest interlayer Na atoms. This tetrahedral deformation is permanent at this step of the reaction. In the second mechanism the proton migrates to the neighboring OH group in the same octahedral units. This takes place without reaction intermediates and it does not imply any permanent distortion in the structure, though it is observed that the environment of a tetrahedral Si spontaneously fluctuates between a tetrahedral and a ditrigonal bipyramidal arrangement.

**References:** *J. Phys. Chem. C,* 116 (22), 12203-12211, 2012, DOI: 10.1021/jp301366r

**Title:** Metadynamics with Adaptive Gaussians

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**Description:**

Metadynamics is an established sampling method aimed at reconstructing the free-energy surface relative to a set of appropriately chosen collective variables. In standard metadynamics, the free-energy surface is filled by the addition of Gaussian potentials of preassigned and typically diagonal covariance. Asymptotically the free-energy surface is proportional to the bias deposited. Here, we consider the possibility of using Gaussians whose variance is adjusted on the fly to the local properties of the free-energy surface. We suggest two different prescriptions: one is based on the local diffusivity and the other on the local geometrical properties. We further examine the problem of extracting the free-energy surface when using adaptive Gaussians. We show that the standard relation between the bias and the free energy does not hold. In the limit of narrow Gaussians an explicit correction can be evaluated. In the general case, we propose to use instead a relation between bias and free energy borrowed from umbrella sampling. This relation holds for all kinds of incrementally deposited bias. We illustrate on the case of alanine dipeptide the advantage of using adaptive Gaussians in conjunction with the new free-energy estimator both in terms of accuracy and speed of convergence.

**References:** *J. Chem. Theory Comput.*, 8 (7), 2247-2254, 2012,
DOI: 10.1021/ct3002464

**Title:** Energy-scale aware feature extraction for unsteady flow visualization

**Researchers**: A. Pobitzer, M. Tutkun, Ø. Andreassen, R. Fuchs, R. Peikert and H. Hauser

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

**Description:**

In the visualization of flow simulation data, feature detectors often tend to result in overly rich response, making some sort of filtering or simplification necessary to convey meaningful images. In this paper we present an approach that builds upon a decomposition of the flow field according to dynamical importance of different scales of motion energy. Focusing on the high-energy scales leads to a reduction of the flow field while retaining the underlying physical process. The presented method acknowledges the intrinsic structures of the flow according to its energy and therefore allows focusing on the energetically most interesting aspects of the flow. Our analysis shows that this approach can be used for methods based on both local feature extraction and particle integration and we provide a discussion of the error caused by the approximation. Finally, we illustrate the use of the proposed approach for both a local and a global feature detector and in the context of numerical flow simulations.

**References:** Computer Graphics Forum 30(3), pp. 771-780, 2011.

**Title:** The State of the Art in Topology-based Visualization of Unsteady Flow

**Researchers**: A. Pobitzer, R. Peikert, R. Fuchs, B. Schindler, A. Kuhn, H. Theisel, K. Matkovic, and H. Hauser

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

**Description:**

Vector fields are a common concept for the representation of many different kinds of flow phenomena in science and engineering. Methods based on vector field topology are known for their convenience for visualizing and analyzing steady flows, but a counterpart for unsteady flows is still missing. However, a lot of good and relevant work aiming at such a solution is available. We give an overview of previous research leading towards topology-based and topology-inspired visualization of unsteady flow, pointing out the different approaches and methodologies involved as well as their relation to each other, taking classical (i.e. steady) vector field topology as our starting point. Particularly, we focus on Lagrangian methods, space–time domain approaches, local methods and stochastic and multifield approaches. Furthermore, we illustrate our review with practical examples for the different approaches.

**References:** Computer Graphics Forum, 30(6), pp. 1789-1811, 2011.

**Title:** Multi-layer illustrative dense flow visualization

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

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

**Description:**

We present a dense visualization of vector fields on multi-layered surfaces. The method is based on the illustration buffer, which provides a screen space representation of the surface, where each pixel stores a list of all surface layers. This representation is implemented on the GPU using shaders and leads to a fast output sensitive technique. In our approach, we first use procedural noise to create an initial spot pattern on the surface that has both an almost constant screen space frequency and is view independent. Then, we perform anisotropic diffusion simultaneously on all surface layers using a discretization scheme that maintains second order convergence while only accessing the four neighboring pixels. Finally, we enhance this result with illustrative techniques and composite the final image. Our method works with time-evolving surfaces, time-dependent vector fields, and moving cameras. We apply our method to CFD data sets from engineering and astronomy as well as synthetic velocity fields.

**References:** Computer Graphics Forum 31(3), pp. 895-904, 2012.

**Title:** Highest resolution Fourier transform infrared (FTIR) spectroscopy of polyatomic molecules with and without synchrotron radiation

**Researchers**: S. Albert*
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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 discuss the analysis of the high resolution FTIR spectra of the bicyclic compounds naphthalene, azulene and indole measured with synchrotron radiation in the context of the identification of the unidentified infrared bands (UIB). The FTIR spectra of phenol and aniline have been analysed to get a deeper insight into the torsional dynamics of the OH and $NH_2$ groups. The analysis of the spectra of the chiral compounds CDBrClF and CHBrIF might be the starting point to conduct line shifts experiments using ultra-high resolution devices for the experimental detection of parity violation. Extensive computational simulations support the analyses of the experiments.

**References:**
1. S. Albert, K. Keppler Albert, P. Lerch, M. Quack in “Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012)”, Alpe d’Huez, France, 22 to 27 January 2012, pages 86 – 89, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds., Innsbruck University Press (IUP), Innsbruck, 2012), ISBN 978-3-902811-42-4
2. S. Albert, K. Keppler Albert, M. Quack, “High Resolution Fourier Transform Infrared Spectroscopy”, in “Handbook of High-Resolution Spectroscopy”, Vol. 2, chapter 26, pages 965–1019, M. Quack and F. Merkt, Eds., Wiley, Chichester, 2011, ISBN-13: 978-0-470-06653-9.

**Title:** Inversion tunneling in normal and substituted anilines from infrared spectroscopy and quasiadiabatic channel reaction path Hamiltonian calculations

**Researchers**: E. Miloglyadov
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**Institute/Group:** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

**Description:**

We report the spectra and assignment of the NH-stretching modes up to the second overtone in the room temperature FTIR spectra of ortho-$C_6H_4FNHD$ and $C_6F_5NHD$ as well as the direct measurement of ground state tunneling splittings in the both molecules. The decrease of the tunneling splitting in ortho-$C_6H_4FNHD$ and $C_6F_5NHD$ with higher NH-stretching excitation demonstrates the inhibiting nature of the NH-stretching mode in these substituted anilines. Results of theoretical investigations on the basis of DFT calculations with B3LYP/6-31G** and the quasi-adiabatic channel Reaction Path Hamiltonian (RPH) model showed a good agreement with the experimental results.

**References:**

1. E. Miloglyadov, R. Prentner, G. Seyfang, and M. Quack in “Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012)”, Alpe d’Huez, France, 22 to 27 January 2012, pages 234 – 237, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds., Innsbruck University Press (IUP), Innsbruck, 2012), ISBN 978-3-902811-42-4.
2. M. Hippler, E. Miloglyadov, M. Quack, and G. Seyfang, “Mass and Isotope Selective Infrared Spectroscopy” in “Handbook of High-Resolution Spectroscopy”, Vol. 2, chapter 28, pages 1069–1118, M. Quack and F. Merkt, Eds., Wiley, Chichester, 2011, ISBN-13: 978-0-470-06653-9

**Title:** IR-laser induced population transfer from highly populated rotational levels of $NH_3$ in a molecular beam

**Researchers**: P. Dietiker
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**Institute/Group:** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

**Description:**

Although the theoretical calculation of the parity violating energy difference in molecules is now well established its experimental verification is still missing. In principle this energy difference can be measured in sophisticated high-resolution spectroscopic experiments or alternatively in a well defined time resolved experiment. In the paper we present an experimental scheme and the first experimental results towards the detection of the parity violating energy difference in molecules by the proposed time resolved technique. We discuss the comparison with theoretical calculations.

**References:**

1. P. Dietiker, M. Quack, A. Schneider, G. Seyfang, and F. Ünlü, in "Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012)", Alpe d'Huez, France, 22 to 27 January 2012, pages 263 – 267, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds., Innsbruck University Press (IUP), Innsbruck, 2012), ISBN 978-3-902811-42-4
2. M. Quack, "Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy" in "Handbook of High-Resolution Spectroscopy", Vol. 1, chapter 18, pages 659–722, M. Quack, and F. Merkt, Eds. Wiley Chichester, 2011, ISBN-13: 978-0-470-06653-9.

**Title:** Assessing noise sources at synchrotron infrared ports

**Researchers**: Ph. Lerch*
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J.-C. Denard**
L. Stingelin*
L. Nadolski**
T. Garvey*
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**Description:**
Today, the vast majority of electron storage rings delivering synchrotron radiation for general user operation offer a dedicated infrared port. There is growing interest expressed by various scientific communities to exploit the mid-IR emission in microspectroscopy, as well as the far infrared (also called THz) range for spectroscopy. Compared with a thermal (laboratory-based source), IR synchrotron radiation sources offer enhanced brilliance of about two to three orders of magnitude in the mid-IR energy range, and enhanced flux and brilliance in the far-IR energy range. Synchrotron radiation also has a unique combination of a broad wavelength band together with a well defined time structure. Thermal sources (globar, mercury filament) have excellent stability. Because the sampling rate of a typical IR Fourier-transform spectroscopy experiment is in the kHz range (depending on the bandwidth of the detector), instabilities of various origins present in synchrotron radiation sources play a crucial role. Noise recordings at two different IR ports located at the Swiss Light Source and SOLEIL (France), under conditions relevant to real experiments, are discussed. The lowest electron beam fluctuations detectable in IR spectra have been quantified and are shown to be much smaller than what is routinely recorded by beam-position monitors.

**References:**
Ph. Lerch, P. Dumas, T. Schilcher, A. Nadji, A. Luedeke, N. Hubert, L. Cassinari, M. Boege, J.-C. Denard, L. Stingelin, L. Nadolski, T. Garvey, S. Albert, C. Gough, M. Quack, J. Wambach, M. Dehler and J. M. Filhol, J. Synchrotron Rad. **19**, 1 – 9 (2012).

**Title:** Reinvestigation of the $\nu_2 + 2\nu_3$ subband in the overtone icosad of $^{12}CH_4$ using cavity ring-down (CRD) spectroscopy of a supersonic jet expansion

**Researchers**: C. Manca Tanner, M. Quack

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

**Description:**

We report a detailed reinvestigation of the $\nu_2 + 2\nu_3$ combination band of methane $^{12}CH_4$ centred at (7510.3378±0.003) $cm^{-1}$ ((225.154263±0.0001) THz) within the icosad of the overtone absorption. A new experimental setup is described, allowing us to carry out cw-laser cavity ring-down spectroscopy (cw-CRDS) at instrumental resolution in the MHz range in seeded supersonic jet expansions down to rotational temperature of 7 K compared to previous cw-CRDS measurements in our group achieving about 50K in expansions of neat $CH_4$. We provide a careful re-analysis on the basis of our new experimental results for the Q and R branch transitions including data obtained between about 7 and 300 K under various conditions. We resolve previously observed discrepancies of assignments and are able to present a definitive assignment for lines involving angular momentum quantum numbers up to $J$=4. The analysis of relative intensities in spectra taken at rotational and effective translational temperatures between about 50 K and less than 10 K indicate conservation of nuclear spin symmetry upon supersonic jet expansion, in agreement with previous results using other techniques and covering other spectral ranges. Numerical simulations of the experiments support the analyses of the experiments.

**References:**

1. C. Manca Tanner, M. Quack, Mol. Phys. **110**, 2111 – 2135 (2012).
2. C. Manca Tanner, M. Quack, in "Proceedings of the 22nd Colloquium on High-Resolution Spectroscopy", Université de Bourgogne, Dijon, August 29 - September 2, 2011, p. 355, (Ed.: V. Boudon), (2011)
3. S. Albert, K. Keppler Albert, H. Hollenstein, C. Manca Tanner, M. Quack, "Fundamentals of Rotation-Vibration Spectra", in "Handbook of High-Resolution Spectroscopy", Vol. 1, chapter 3, pages 117–173, M. Quack, and F. Merkt, Eds. Wiley Chichester, 2011, ISBN-13: 978-0-470-06653-9.
4. M. Snels, V. Horká-Zelenková, H. Hollenstein, M. Quack, "High Resolution FTIR and Diode Laser Spectroscopy of Supersonic Jets", in "Handbook of High-Resolution Spectroscopy", Vol. 2, chapter 27, pages 1021–1067, M. Quack and F. Merkt, Eds., Wiley, Chichester, 2011, ISBN-13: 978-0-470-06653-9.

**Title:** Molecular Parity Violation and Chirality: The Asymmetry of Life and the Symmetry Violations of Physics

**Researchers**: M. Quack

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

**Description:**

After a brief introduction into some basic asymmetries observed in nature, such as the biomolecular homochirality in living species on earth, the dominance of matter over antimatter in the observable universe, and irreversibility in physical-chemical processes providing a preferred arrow of time, we provide a discussion of the concepts of fundamental symmetries in physics and of the three different kinds of symmetry breakings, spontaneous, de facto, and de lege, by means of the example of the dynamics of chiral molecules. We then give a brief review of the current status of the theory and experiments on molecular parity violation. We discuss the various hypotheses on the origin of biomolecular homochirality and conclude with some cosmological speculations related to the fundamental symmetry breakings. These include possibilities of observing CPT violation in future experiments providing a possible fundamental basis for irreversibility, as well as possibilities for observing heavy "right handed" neutrinos as one possible basis for "dark matter" in the universe.

**References:**

1. M. Quack, "Molecular Parity Violation and Chirality: The Asymmetry of Life and the Symmetry Violations of Physics", in "Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Proceedings of QSCP XVI, Kanazawa 11 to 17 September 2011", Chapter 3, pages 47-76, Series Title: "Progress in Theoretical Chemistry and Physics", (Kiyoshi Nishikawa; Jean Maruani; Erkki Brändas; Gerardo Delgado-Barrio; Piotr Piecuch Eds., Springer Verlag 2012).
2. M. Quack, „Die Asymmetrie des Lebens und die Symmetrieverletzungen der Physik: Molekulare Paritätsverletzung und Chiralität", in „Moleküle aus dem All?", Kapitel 12, pages 277 – 310, Katharina Al-Shamery Hrsg., Wiley VCH, Weinheim (2011), ISBN 978-3-527-32877-2.
3. M. Quack, "Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy", in "Handbook of High-Resolution Spectroscopy", Vol. 1, chapter 18, pages 659–722, M. Quack, and F. Merkt, Eds. Wiley Chichester, 2011, ISBN-13: 978-0-470-06653-9.

**Title:** Regioselectivity of H-Cluster Oxidation

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**Description:**

The $H_2$ evolving potential of [FeFe] hydrogenases is severely limited by the oxygen sensitivity of this class of enzymes. Recent experimental studies on hydrogenase from *C. reinhardtii* point to $O_2$ induced structural changes in the $[Fe_4S_4]$ subsite of the H-cluster. Here, we investigate the mechanistic basis of this observation by means of density functional theory. Unexpectedly, we find that the isolated H-cluster shows a pathological catalytic activity for the formation of reactive oxygen species like $O_2^-$ and $HO_2^-$. After protonation of $O_2^-$, a OOH radical may coordinate to the Fe atoms of the cubane whereas $H_2O_2$ specifically reacts with the S atoms of the cubane-coordinating cysteine residues. Both pathways are accompanied by significant structural distortions that compromise cluster integrity and thus catalytic activity. These results explain the experimental observation that $O_2$ induced inhibition is accompanied by distortions of the $[Fe_4S_4]$ moiety and account for the irreversibility of this process.

**References:** M. K. Bruska, M. T. Stiebritz, M. Reiher, *J. Am. Chem. Soc.*, **2011**, *133*, 20588.

**Title:** Extracting Elements of Molecular Structure From the All-Particle Wave Function

**Researchers:** Edit Mátyus[1]
Jürg Hutter[2]
Ulrich Müller-Herold[3]
Markus Reiher[1]

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**Description:**

Structural information is extracted from the all-particle (non-BornOppenheimer) wave function by calculating radial and angular densities derived from n-particle densities. As a result, one- and two-dimensional motifs of classical molecular structure can be recognized in quantum mechanics. Numerical examples are presented for three- ($H^-$, $Ps^-$, $H_2^+$), four- ($Ps_2$, $H_2$), and five-particle ($H_2D^+$) systems.

**References:** E. Mátyus, J. Hutter, U. Müller-Herold, M. Reiher, *J. Chem. Phys.*, **2011**, *135*, 204302.

**Title:** Exact Decoupling of the Relativistic Fock Operator

**Researchers:** Daoling Peng
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**Institute/Group:** Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

**Description:**

It is generally acknowledged that the inclusion of relativistic effects is crucial for the theoretical description of heavy-element-containing molecules. Four-component Dirac-operator-based methods serve as the relativistic reference for molecules and highly accurate results can be obtained — provided that a suitable approximation for the electronic wave function is employed. However, four-component methods applied in a straightforward manner suffer from high computational cost and the presence of pathologic negative-energy solutions. To remove these drawbacks, a relativistic electron-only theory is desirable for which the relativistic Fock operator needs to be exactly decoupled. Recent developments in the field of relativistic two-component methods demonstrated that exact decoupling can be achieved following different strategies. The theoretical formalism of these exact-decoupling approaches is reviewed and followed by a comparison of efficiency and results.

**References:** D. Peng, M. Reiher, *Theor. Chem. Acc.*, **2012**, *131*, 1081.

**Title:** Local Relativistic Exact Decoupling

**Researchers:** Daoling Peng
Markus Reiher

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

**Description:**

We present a systematic hierarchy of approximations for *local* exact-decoupling of four-component quantum chemical Hamiltonians based on the Dirac equation. Our ansatz reaches beyond the trivial local approximation that is based on a unitary transformation of only the atomic block-diagonal part of the Hamiltonian. Systematically, off-diagonal Hamiltonian matrix blocks can be subjected to a unitary transformation to yield relativistically corrected matrix elements. The full hierarchy is investigated with respect to the accuracy reached for the electronic energy and for selected molecular properties on a balanced test molecule set that comprises molecules with heavy elements in different bonding situations. Our atomic (local) assembly of the unitary exact-decoupling transformation — called local approximation to the unitary decoupling transformation DLU — provides an excellent local approximation for any relativistic exact-decoupling approach. Its order-$N^2$ scaling can be further reduced to linear scaling by employing a neighboring-atomic-blocks approximation. Therefore, it is an efficient relativistic method perfectly well suited for relativistic calculations on large molecules. If a large molecule contains many light atoms (typically hydrogen atoms), the computational costs can be further reduced by employing a well-defined nonrelativistic approximation for these light atoms without significant loss of accuracy. We also demonstrate that the standard and straightforward transformation of only the atomic block-diagonal entries in the Hamiltonian — denoted DLH in this paper — introduces an error that is on the order of the error of second-order Douglas–Kroll–Hess (i.e., DKH2) when compared with exact-decoupling results. Hence, the local DLH approximation would be pointless in an exact-decoupling framework, but can be efficiently employed together with the fast to evaluate DKH2 Hamiltonian in order to speed up calculations for which accuracy is not the major concern.

**References:** D. Peng, M. Reiher, *J. Chem. Phys.*, **2012**, *136*, 244108.

**Title:** How many Chiral Centers can Raman Optical Activity Spectroscopy Distinguish in a Molecule?

**Researchers:** Benjamin Simmen
Thomas Weymuth
Markus Reiher

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

**Description:**

To study the capabilities and limitations of Raman Optical Activity, (−)-($M$)$\sigma$-[10]Helicene and (−)-($M$)$\sigma$-[4]Helicene serve as scaffold molecules on which new chiral centers are introduced by substitution of hydrogen atoms with other functional groups. These functional groups are deuterium atoms, fluorine atoms, and methyl groups. Multiply deuterated species are compared. Then, results of singly deuterated derivatives are compared against results obtained from singly fluorinated and methylated derivatives. The analysis required the calculation of a total of 2433 Raman Optical Activity spectra. The method we propose for the comparison of the various Raman Optical Activity spectra is based on the total intensity of squared difference spectra. This allows a qualitative comparison of pairs of Raman Optical Activity spectra and the extraction of the pair of most similar Raman Optical Activity spectra for each group of stereoisomers. Different factors were accounted for, such as the spectral resolution (modeled by line broadening) and the range of vibrational frequencies considered. In the case of $\sigma$-[4]Helicene all generated stereoisomers in each group can be distinguished from one another by Raman Optical Activity spectroscopy. For $\sigma$-[10]Helicene this holds except for the lower one of the two resolutions considered. Here, the group consisting of stereoisomers with five chiral centers contains at least one pair of derivatives whose Raman Optical Activity spectra cannot be distinguished from one another. This indicates that an increased molecular size has a negative effect on the number of chiral centers which can be distinguished by Raman Optical Activity spectroscopy. Regarding the different substituents, stereoisomers are distinguishable in Raman Optical Activity spectroscopy the better, the more distinct the signals of the substituent are from the rest of the spectrum.

**References:** B. Simmen, T. Weymuth, M. Reiher, *J. Phys. Chem. A*, **2012**, *116*, 5410.

**Title:** Hydrogenases and Oxygen

**Researchers:** Martin T. Stiebritz
Markus Reiher

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

**Description:**

Hydrogenases represent a heterogeneous group of enzymes consisting of three evolutionary unrelated classes, i.e. [NiFe], [FeFe] and [Fe] hydrogenases. They allow the unicellular organisms in which they are expressed to use hydrogen as energy source or to reduce protons as a sink for excess reduction equivalents. Because of this capability there is growing interest in exploiting these enzymes in the field of sustainable energy generation. However, most hydrogenases which are appealing in this context are reversibly or irreversibly inhibited by dioxygen. In this work we summarized the current picture of oxygen-induced inhibition of the different classes of hydrogenases and discussed possible avenues that might lead to tailored oxygen-robust enzyme variants.

**References:** M. T. Stiebritz, M. Reiher, *Chem. Sci.*, **2012**, *3*, 1739.

**Title:** Accurate Ab Initio Spin Densities

**Researchers:** Katharina Boguslawski[1]
Konrad H. Marti[1]
Örs Legeza[2]
Markus Reiher[1]

**Institute/Group:** [1]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
[2]Wigner Research Centre, H-1525 Budapest

**Description:**

We present an approach for the calculation of spin density distributions for molecules that require very large active spaces for a qualitatively correct description of their electronic structure. Our approach is based on the density-matrix renormalization group (DMRG) algorithm to calculate the spin density matrix elements as a basic quantity for the spatially resolved spin density distribution. The spin density matrix elements are directly determined from the second-quantized elementary operators optimized by the DMRG algorithm. As an analytic convergence criterion for the spin density distribution, we employ our recently developed sampling-reconstruction scheme [*J. Chem. Phys.* **2011**, *134*, 224101] to build an accurate complete-active-space configuration-interaction (CASCI) wave function from the optimized matrix product states. The spin density matrix elements can then also be determined as an expectation value employing the reconstructed wave function expansion. Furthermore, the explicit reconstruction of a CASCI-type wave function provides insight into chemically interesting features of the molecule under study such as the distribution of  and  electrons in terms of Slater determinants, CI coefficients, and natural orbitals. The methodology is applied to an iron nitrosyl complex which we have identified as a challenging system for standard approaches [*J. Chem. Theory Comput.* **2011**, *7*, 2740].

**References:** K. Boguslawski, K. H. Marti, Ö. Legeza, M. Reiher, *J. Chem. Theory Comput.*, **2012**, *8*, 1970.

**Title:** MoViPac: Vibrational Spectroscopy with a Robust Meta-Program for Massively Parallel Standard and Inverse Calculations

**Researchers:** Thomas Weymuth[1]
Moritz P. Haag[1]
Karin Kiewisch[1,2]
Sandra Luber[1,3]
Stephan Schenk[1,4]
Christoph R. Jacob[5]
Carmen Herrmann[6]
Johannes Neugebauer[7]
Markus Reiher[1]

**Institute/Group:** [1]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
[2]present address: Amsterdam Center for Multiscale Modeling, VU University Amsterdam, 1081 HV Amsterdam
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[6]Institut fr Anorganische und Angewandte Chemie, University of Hamburg, 20146 Hamburg
[7]Institute for Physical and Theoretical Chemistry, Technical University Braunschweig, 38106 Braunschweig

**Description:**

We present the software package MoViPac for calculations of vibrational spectra, namely infrared, Raman, and Raman Optical Activity (ROA) spectra, in a massively parallelized fashion. MoViPac unites the latest versions of the programs Snf and Akira alongside with a range of helpful add-ons to analyze and interpret the data obtained in the calculations. With its efficient parallelization and meta-program design, MoViPac focuses in particular on the calculation of vibrational spectra of very large molecules containing on the order of a hundred atoms. For this purpose, it also offers different subsystem approaches such as Mode- and Intensity-Tracking to selectively calculate specific features of the full spectrum. Furthermore, an approximation to the entire spectrum can be obtained using the Cartesian Tensor Transfer Method. We illustrate these capabilities using the example of a large $\pi$-helix consisting of 20 (S)-alanine residues. In particular, we investigate the ROA spectrum of this structure and compare it to the spectra of $\alpha$- and $3_{10}$-helical analogs.

**References:** T. Weymuth, M. P. Haag, K. Kiewisch, S. Luber, S. Schenk, Ch. R. Jacob, C. Herrmann, J. Neugebauer, M. Reiher, *J. Comput. Chem.*, **2012**, *33*, 2186.

**Title:** Molecular Structure Calculations: A Unified Quantum Mechanical Description of Electrons and Nuclei Using Explicitly Correlated Gaussian Functions and the Global Vector Representation

**Researchers:** Edit Mátyus
Markus Reiher

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

**Description:**

We elaborate on the theory for the variational solution of the Schrdinger equation of small atomic and molecular systems without relying on the Born-Oppenheimer paradigm. The all-particle Schrdinger equation is solved in a numerical procedure using the variational principle, Cartesian coordinates, parameterized explicitly correlated Gaussian functions with polynomial prefactors, and the global vector representation. As a result, non-relativistic energy levels and wave functions of few-particle systems can be obtained for various angular momentum, parity, and spin quantum numbers. A stochastic variational optimization of the basis function parameters facilitates the calculation of accurate energies and wave functions for the ground and some excited rotational-(vibrational-)electronic states of $H_2^+$ and $H_2$, three bound states of the positronium molecule, $Ps_2$, and the ground and two excited states of the $^7$Li atom.

**References:** E. Mátyus, M. Reiher, *J. Chem. Phys.*, **2012**, *137*, 024104.

**Title:** Electron Density in Quantum Theory

**Researchers:** Samuel Fux
Markus Reiher

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

**Description:**

In this work, we review the theory of the electron density in quantum chemistry and discuss to which extent relativistic effects are recovered by approximate relativistic Hamiltonians. For this purpose, we give an overview on different approximations to the fully relativistic many-electron Hamiltonian. In addition, we present new results, considering correlation effects on the electron density of a transition metal complex.

**References:** S. Fux, M. Reiher, *Struct. Bonding*, **2012**, *147*, 99.

**Title:** Relativistic Douglas-Kroll-Hess Theory

**Researchers:** Markus Reiher

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

**Description:**

Relativistic effects on molecular properties and energies are ubiquitous in chemistry. Their consideration in quantum chemical calculations requires Dirac's theory of the electron, whose application is not without obstacles. DouglasKrollHess theory accomplishes a decoupling of positive- and negative-energy eigenstates of the Dirac one-electron Hamiltonian by an expansion in the external potential. At low orders, this expansion already converges and provides efficient relativistic Hamiltonians to be used in routine quantum chemical calculations. The basic principles of the approach are reviewed, and most recent developments are discussed.

**References:** M. Reiher, *Wiley Interdisciplinary Reviews — Computational Molecular Science*, **2012**, *2*, 139.

**Title:** Hydrogen Spillover to Nonreducible Supports

**Researchers:** R. Prins
V. K. Palfi
Markus Reiher

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

**Description:**

Density functional theory (DFT) calculations show that the interaction between a hydrogen atom and the surface of MgO is weak, the interaction between a hydrogen atom and the surface of $SiO_2$ is repulsive, and the migration of H atoms from a metal particle to a nonreducible support is endothermic. As a consequence, transition-state theory estimates that the migration of a hydrogen atom from a metal particle to the surface of a nonreducible support is too slow to explain the observed hydrogenation of molecules adsorbed on the support by spillover of H atoms. On the other hand, H atoms bind strongly to the surface of $WO_3$, because the H atoms decompose into electrons, which reduce the $W^{6+}$ cations, and protons, which bind strongly to the oxygen anions. Hydrogen spillover to defect-free surfaces of nonreducible metal oxides cannot take place, but spillover to defects is possible, as is spillover from a metal particle to an oxygen-containing group on a carbon surface. Defects and carbonaceous deposits may therefore be responsible for observations that have been ascribed to hydrogen spillover.

**References:** R. Prins, V. K. Palfi, M. Reiher, *J. Phys. Chem. C*, **2012**, *116*, 14274.

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

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

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

**Description:**

The main objective of our group is to improve the understanding of the climate system and its interactions with the water cycle on time-scales from 1 day to 100 years. Our mission is to better understand the underlying mechanisms, trends, variations and extremes; and to improve the predictive capabilities and exploitation of weather and climate models. To this end we are using global and regional atmospheric models on a wide range of temporal and spatial scales.

The high-resolution modeling uses the COSMO-CLM limited-area atmospheric model. The main thrust of this work is dedicated to the understanding and simulation of the European and Alpine climate. Comprehensive European-scale climate-change scenario simulations are conducted in the framework of the COordinated Regional climate Downscaling Experiment (CORDEX) at a horizontal resolution of 12 km covering the period 1950-2100. Current work is addressing the calibration of the model, the analysis of potential changes in heat-wave and heavy precipitation events, snow cover, the height dependence of the change signals and the representation of aerosol effects. 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 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). The use of the COSMO-CLM is coordinated by Drs. Daniel Lüthi, Jürg Schmidli and Sven 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.

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

[2] A. Barth and A. Lang, *$L^p$ and almost sure convergence of a Milstein scheme for stochastic partial differential equations*. SAM report 2011-15, June 2009.

[3] ——, *Milstein Approximation for Advection-Diffusion Equations Driven by Multiplicative Noncontinuous Martingale Noises*, Appl. Math. Opt., (2012). SAM report 2011-36.

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

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

[6] A. Barth, A. Lang, and C. Schwab, *Multilevel Monte Carlo Finite Element method for parabolic stochastic partial differential equations*, BIT Num. Math., (2012).

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

[8] ——, *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.

[9] ——, *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.

[10] 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.

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

**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.

[1] M. Hansen, C. Schillings, and C. Schwab, *Sparse approximation algorithms for high dimensional parametric initial value problems*, tech. rep., 2012. Proceedings.

[2] M. Hansen and C. Schwab, *Analytic regularity and best n-term approximation of high dimensional parametric initial value problems*, Tech. Rep. 2011/64, Seminar for Applied Mathematics, ETH Zürich, 2011.

[3] ——, *Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic pdes*, Tech. Rep. 2011/29, Seminar for Applied Mathematics, ETH Zürich, 2011.

[4] C. Schillings and C. Schwab, *Smolyak quadrature for inverse problems*, tech. rep., 2012. in preparation.

**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 Boltzmann equation, the fastest solvers have been designed using Fourier series representations in velocity space, as this allows a reasonably fast evaluation of the collision operator. We have generalized this to a hyperbolic cross representation for the spatially homogeneous case in two dimensions, which gains all the known advantages of sparse grids. Future work could focus on three dimensions, adaptivity, and the addition of a physical space solver for the inhomogeneous case.

For the radiative transfer problem, we have laid the theoretical foundations for two sparse tensor versions of popular solution approaches, i. e. the discrete ordinates method and the spherical harmonics method. These sparse tensor versions converge equally fast as the full tensor methods up to logarithmic factors, while the number of degrees of freedom is reduced to that of a purely spatial transport problem, again up to logarithms.

Work on a flexible and efficient parallelized C++ implementation of the sparse methods to solve real-world 3D/2D problems is ongoing.

**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.

**Title:** Generalized and Fast hp-FEM for High Frequency Wave Propagation in Locally Periodic Media

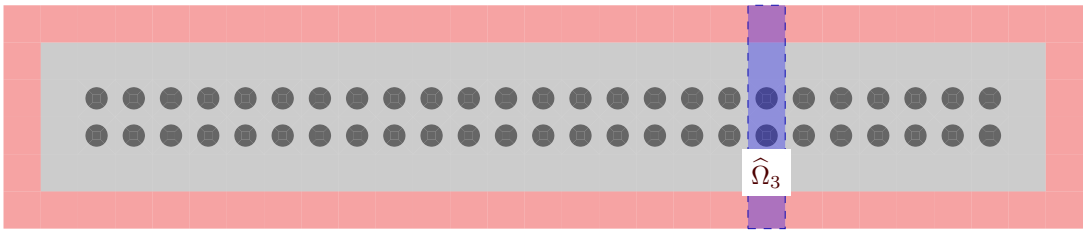
**Researchers:** Prof. C. Schwab
Holger Brandsmeier

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:** Wave propagation in locally periodic media is difficult when both the wave length and the microscopic periodicity length are much smaller than the macroscopic size of the domain. This high variation makes numerical simulations of realistic locally periodic structures with many replications of the periodic pattern infeasible with standard discretization techniques such as FDTD or h-, p- and hp-FEM.

In particular we study Photonic Crystals (PhC) structures, which is a locally periodic dielectric metamaterial used in optical signal processing to mold the flow of light. The macroscopic PhC device, e.g. a PhC waveguide, is many times larger than the size of the elementary cell of the crystal. When the frequency is about the same size as the elementary cell, an instance of *high frequency scattering*, interesting physical phenomena appear. The PhC structure can guide an electromagnetic wave with minimal losses around bends and sharp corners, slow its group velocity and reflect or transmit the wave depending on slight variations in its frequency.

The project aims at developing fast accurate simulation techniques for this class of problems. One such methods is a generalized FEM with non-polynomial, problem-adapted basis functions which can efficiently simulate large PhC structures. Those problem adapted basis functions have a multiscale nature, where the microscopic part comes from solving the limit problem of an infinitely replicated PhC, the so called *Bloch modes*. Another approach is, to apply a standard *hp*-FEM discretization with an identical mesh on each replication of the pattern. Then the matrices for each pattern are identical, and using recursive static condensation a fast solver can be obtained.




PhC waveguide with pattern $\hat{\Omega}_3$, 25 replications and PML boundary condition.

[1] H. Brandsmeier, K. Schmidt, and C. Schwab, *A multiscale hp-FEM for 2D photonic crystal bands*, Journal of Computational Physics, 230 (2011), pp. 349–374.

**Title:** Multi-level Monte Carlo Finite Volume methods for stochastic non-linear systems of conservation laws

**Researchers:** Jonas Šukys, Siddhartha Mishra, Christoph Schwab

**Institute:** Seminar for Applied Mathematics (SAM)

**Description:** The main interest of this research project is the solution to the *linear and nonlinear systems of stochastic hyperbolic conservation laws in multi-dimensions.* Examples of such systems include the shallow water equations of oceanography, the Euler equations of gas dynamics, the Magnetohydrodynamics (MHD) equations of plasma physics and the equations of linear elasticity. Since there are no global well-posedness results even for the deterministic case of such systems of hyperbolic PDEs, various numerical methods need to be used to obtain approximations of the solutions.

The most straightforward approach would be to combine the well-established deterministic solvers such as finite volume methods (FVM) with sampling algorithms of Monte Carlo (MC) type. Unfortunately, due to slow converge of MC type methods, such combination is computationally unfeasible in multiple dimensions of the physical space.

Our alternative approach is to use the Multi-Level Monte Carlo Finite Volume Method (MLMC-FVM), which (in other contexts) was proved to have the asymptotic computational complexity equivalent of a *deterministic* solution of the conservation law.

The main aim of this research project is error convergence analysis, highly scalable parallel implementation and extensive testing of MLMC-FVM for *uncertainty* quantification in the solutions of multi-dimensional hyperbolic *systems* of conservation laws with *uncertain initial data*, *uncertain sources* and *uncertain fluxes.*

[1] S. Mishra, C. Schwab, and J. Šukys, *Multi-level monte carlo finite volume methods for shallow water equations with uncertain topography in multi-dimensions.*, SIAM Journal of Scientific Computing, (submitted), (2011).

[2] ——, *Monte carlo and multi-level monte carlo finite volume methods for uncertainty quantification in nonlinear systems of balance laws*, Submitted, (2012).

[3] ——, *Multi-level monte carlo finite volume methods for nonlinear systems of conservation laws in multi-dimensions*, J. Comp. Phys., 231(8):3365–3388, (2012).

[4] J. Šukys, S. Mishra, and C. Schwab, *Static load balancing for multi-level monte carlo finite volume solvers.*, PPAM 2011, Part I, LNCS 7203, pp. 245–254. Springer, Heidelberg., (2012).

[5] J. Šukys, C. Schwab, and S. Mishra, *Multi-level monte carlo finite difference and finite volume methods for stochastic linear hyperbolic systems*, Submitted, (2012).

**Title:** Space-time discretization of parabolic evolution equations

**Researchers:** Roman Andreev, Christoph Schwab

**Institute:** Seminar for Applied Mathematics (SAM)

**Description:** In [2] we presented compressive algorithms for the linear parabolic equations which compute the solutions in space and time simultaneously. The discretization procedure is novel and non-standard, as it is based on a minimal residual Petrov-Galerkin formulation and an a priori stable choice of space-time finite element spaces. Space-time adaptivity in form of sparse tensor product trial subspaces is possible. Convergence of the solution with optimal a priori convergence rates follows, if suitable equivalent norm generating operators are available. Such norm generating operators may be obtained using suitable wavelet bases; novel parabolic BPX preconditioners [1] provides a computationally more accessible alternative. Further, the extension to nonlinear parabolic evolution equations (with small data) was addressed in [1]. The numerical experiments in [2, 1] fully support the theory, e.g. mesh-independent convergence rates of the employed fixed point iteration. In a colloborative effort [3] with Christine Tobler[1] the parabolic BPX preconditioners for space-time Petrov-Galerkin discretizations of parabolic evolution equations were shown to be compatible with adaptive hierarchical tensor formats, leading to space-time adaptive solution algorithms.

First space-time variational saddle point formulations of the Stokes and Navier-Stokes equations were developed in [4].

[1] R. Andreev, *Stability of space-time Petrov-Galerkin discretizations for parabolic evolution equations*, PhD thesis, ETH Zürich, 2012. To appear.

[2] ——, *Stability of sparse space-time finite element discretizations of linear parabolic evolution equations*, IMA Journal of Numerical Analysis, (2012).

[3] R. Andreev and C. Tobler, *Multilevel preconditioning and low rank tensor iteration for space-time simultaneous discretizations of parabolic PDEs*, tech. rep., ETH Zürich, 2012. In review. Preprint at `http://www.sam.math.ethz.ch/reports/2012/16`.

[4] R. Guberovic, C. Schwab, and R. Stevenson, *Space-time variational saddle point formulations of Stokes and Navier-Stokes equations*, tech. rep., ETH Zürich, 2011. In review. Preprint at `http://www.sam.math.ethz.ch/reports/2011/66`.

[1] MATHICSE, EPF Lausanne, Switzerland

**Title:** Intrinsic Fault Tolerance of Multi Level Monte Carlo Methods

**Researchers:** Stefan Pauli, Peter Arbenz, Christoph Schwab

**Institute:** Computer Science Department
& Seminar for Applied Mathematics (SAM)

**Description:**

In [1] we analyze the performance of both Monte Carlo (MC) and Mulit Level Monte Carlo (MLMC) stochastic partial differential equation solvers in the presence of hardware failures at runtime. In particular, we investigate the convergence behavior of these methods if processors fail with a certain probability. In our analysis, we do not distinguish the reasons of failure. So, we do not distinguish between node, program, network, or any other type of failure. We assume that the complete MC sample is lost if one of the (maybe multiple) processors fails that are used for its simulation. We disregard all samples affected by a failure and compute the results with the 'surviving' ones.

While in MC all samples are from the (single) finest level (or grid), MLMC gets its statistics also from samples corresponding to coarser grids. (The resolution of the finest level is determined by the required discretization error.) By using information on multiple levels MLMC needs much fewer samples on the finest level than ordinary MC to attain the same quality of answer. MLMC turns out to be much more efficient than MC. To get the optimal MLMC convergence rate (wrt. work), it is crucial to choose properly the numbers $M_\ell$ of samples on level $\ell$.

In the presence of failures samples on all levels are lost. The larger samples of the finer levels are more vulnerable than the smaller samples on the coarser levels. On finer levels large enough $M_\ell$ may not be sustainable. The error components of faulty levels increase and the overall convergence rate is reduced. In particular, with a sufficiently high failure rate a whole level may get lost such that the attainable error is bounded by the discretization error of that level.

We prove convergence of MC and MLMC for the first moment (mean) provided that sufficiently many samples survive on average. We compute the effect of failures according to existing failure models. Numerical experiments of MLMC for hyperbolic PDE's coupled with the Weibull failure model validate our theory. We further investigate the failure resilience of one and three dimensional time-dependent grid applications, like finite elements, finite differences, or finite volumes. These results are obtained by MC simulations treating the sample sizes $M_\ell$ as random variables.

[1] S. Pauli, P. Arbenz, and C. Schwab, *Intrinsic fault tolerance of Multi Level Monte Carlo methods*, in SAM-Reports, http://www.sam.math.ethz.ch/reports/2012/24, Aug 2012.

**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 coefficients, 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.

Numerical analysis as well as implementation, parallelization and testing of the proposed algorithms form the major part of this project.

# References

[1] Ch. Schwab and S. Tokareva. High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data. *Under revision in M2AN*, 2012. http://www.sam.math.ethz.ch/reports/2011/53.

**Title:** Tensor-structured solution of high-dimensional PDEs

**Researchers:** Vladimir Kazeev, Oleg Reichmann, Christoph Schwab

**Institute:** Seminar for Applied Mathematics (SAM)

**Description:**

The project focuses on the numerical solution of high-dimensional 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 robust 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 so-called *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 QTT structure of the operators and solutions; investigation of appropriate discretizations in time (for parabolic problems); solution of linear systems in the TT format; high-performance implementation of the TT arithmetics.

[1] 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.

[2] ——, *Low-rank tensor structure of linear diffusion operators in the TT and QTT formats*, Report 13, Seminar for Applied Mathematics, ETH Zürich, 2012.

**Title:** Simulating the thermo-chemical magmatic and tectonic evolution of Venus' mantle and lithosphere

**Researchers:** M. Armann
P. J. Tackley

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

**Description:**

Numerical convection models of the thermo-chemical evolution of Venus are compared to present-day topography and geoid and recent resurfacing history. The models include melting, magmatism, decaying heat-producing-elements, core cooling, realistic temperature-dependent viscosity and either stagnant lid or episodic lithospheric overturn. In stagnant lid convection the dominant mode of heat loss is magmatic heat pipe, which requires massive magmatism and produces very thick crust, inconsistent with observations. Episodic lid overturn interspersed by periods of quiescence effectively loses Venus' heat while giving lower rates of volcanism and a thinner crust. Crustal recycling occurs by entrainment in stagnant lid convection, and by lid overturn in episodic mode. Venus-like amplitudes of topography and geoid can be produced in either stagnant or episodic modes, with a viscosity profile that is Earth-like but shifted to higher values. The basalt density inversion below the olivine-perovskite transition causes compositional stratification around 730km; breakdown of this layering increases episodicity but far less than episodic lid overturn. The classical stagnant lid mode with interior temperature ~rheological temperature scale lower than $T_{CMB}$ is not reached because mantle temperature is controlled by magmatism while the core cools slowly from a superheated start. Core heat flow decreases with time, possibly shutting off the dynamo, particularly in episodic cases.

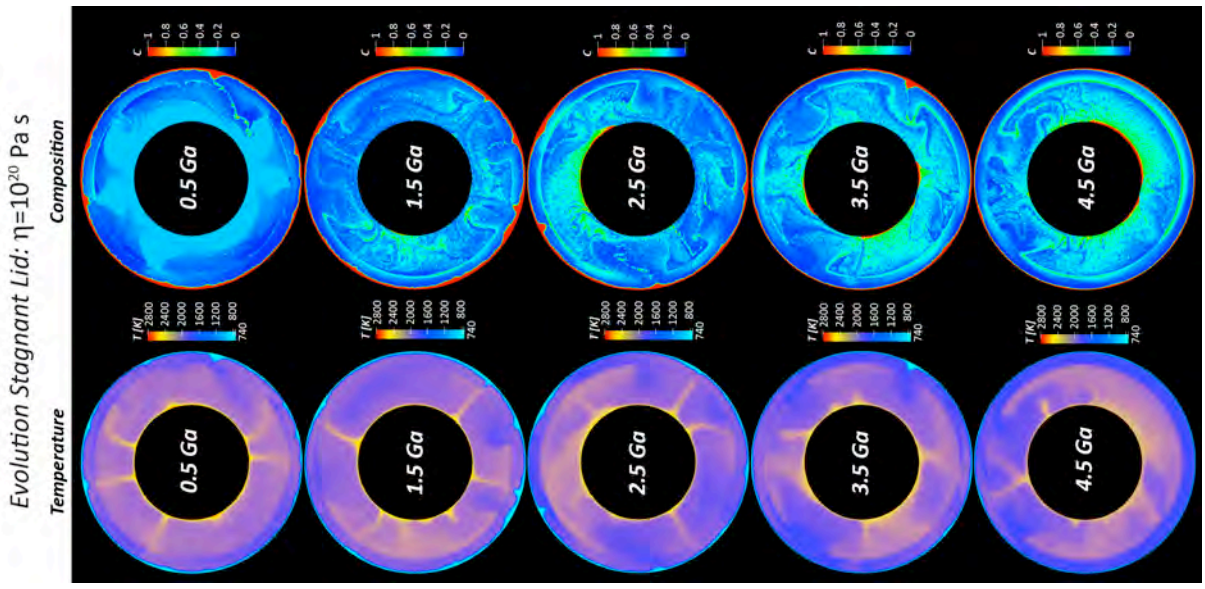



**Figure**. Evolution of compositional (top) and thermal (bottom) fields in a 4.5 billion year simulation of Venus.

**References:** Manuscript submitted to *Journal of Geophysical Research*.

**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 an Earth-like planet the viscosity is strongly dependent on temperature, such that the cold upper boundary layer of the convecting system becomes completely stagnant, if no other complexity is accounted for. On Earth, however, this cold, stiff layer, named the lithosphere, is broken into several different 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.

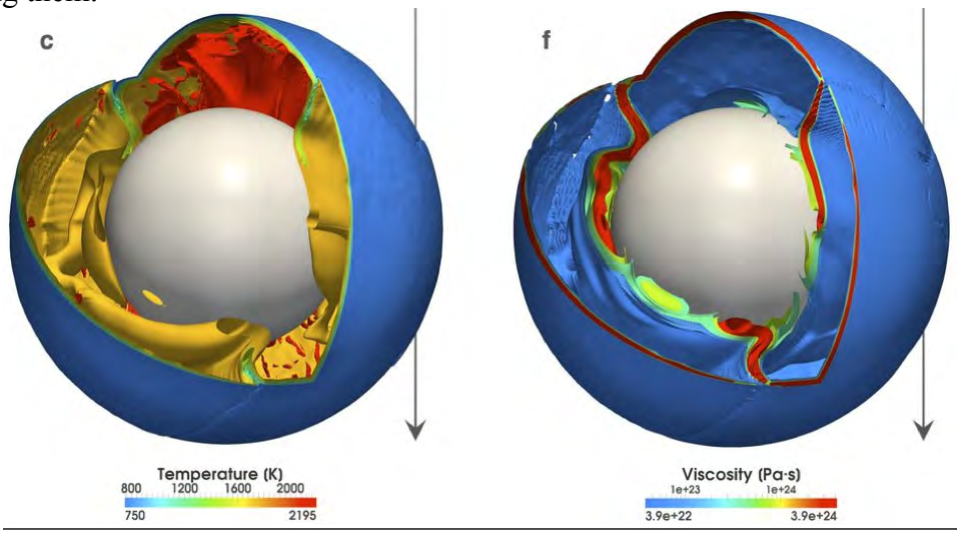



**Figure**. Convection with strongly temperature- and yield stress-dependent viscosity and a free outer surface. Earth-like single-sided subduction is obtained.

**References:** 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

**Title:** Numerical modelling of continental collision zones

**Researchers:** Taras Gerya
Thibault Duretz

**Institute/ Group:** Institute of Geophysics, D-ERDW, ETH-Zurich
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:

- Exhumation of ultrahigh-pressure rocks during collision (Li et al., 2012; Sizova et al., 2012) (Fig.1)
- Dynamics of delamination in collision zones (Ueda et al., 2012)
- Dynamics of slab breakoff and eduction (Duretz et al., 2012)

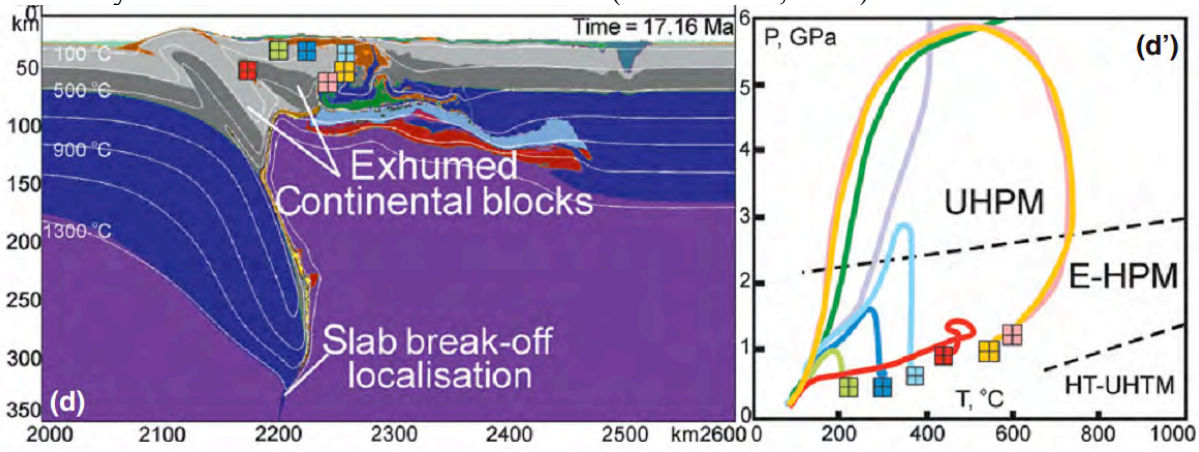



**Fig. 2.** Exhumation of ultrahigh-pressure rocks by crustal-scale stacking (Sizova et al., 2012).

**References:**

Duretz, T., Gerya, T.V., Kaus, B.J.P., Andersen, T.B. (2012a) Thermomechanical modeling of slab eduction. Journal of Geophysical Research, 117, Article Number: B08411.

Duretz T., Schmalholz, S.M., Gerya T.V. (2012b) Dynamics of slab detachment. Geochemistry, Geophysics, Geosystems, 13, Article Number: Q03020.

Li, Z., Xu, Z., Gerya, T. (2012) Numerical geodynamic modeling of continental convergent margins. In: Earth Sciences, Ed. Imran Ahmad Dar, Pub. InTech, pp. 273-296.

Sizova, E., Gerya, T., Brown M.(2012) Exhumation mechanisms of melt-bearing ultrahigh pressure crustal rocks during collision of spontaneously moving plates. Journal of Metamorphic Geology, doi:10.1111/j.1525-1314.2012.01004.x

Ueda, K., Gerya, T.V., Burg, J.-P. (2012) Delamination in collisional orogens: Thermomechanical modelling. Journal of Geophysical Research, 117, Article Number: B08202.

**Title:** Numerical modelling of lithospheric extension and faulting processes

**Researchers:** Taras Gerya
Filippo Schenker
Jie Liao
Christoph Puthe

**Institute/ Group:** Institute of Geophysics, D-ERDW, ETH-Zurich
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:

- Lithospheric extension and associated crustal doming (Schenker et al., 2012)(Fig.3)
- Continental breakup and transition to oceanic spreading
- Development of spreading patterns at mid-ocean ridges
- Lithospheric Rayleigh–Taylor instabilities in intra-cratonic settings (Gorczyk et al., 2012)

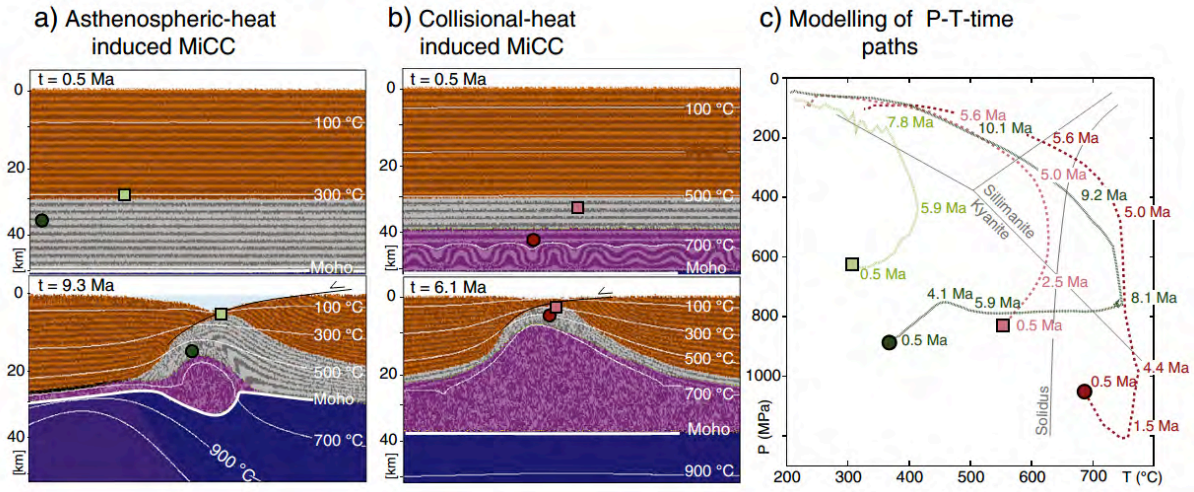



**Fig. 3.** Extensional doming in the continental crust (Schenker et al., 2012)

**References:**

Gorczyk, W., Hobbs, B., Gerya, T. (2012) Initiation of Rayleigh–Taylor instabilities in intra-cratonic settings. Tectonophysics, 514-517, 146-155.

Schenker, F.L., Gerya, T., Burg, J.-P. (2012) Bimodal behavior of extended continental lithosphere: Modeling insight and application to thermal history of migmatitic core complexes. Tectonophysics, http://dx.doi.org/10.1016/j.tecto.2012.07.002

**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

**Description:**

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:** 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

**Description:**

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.

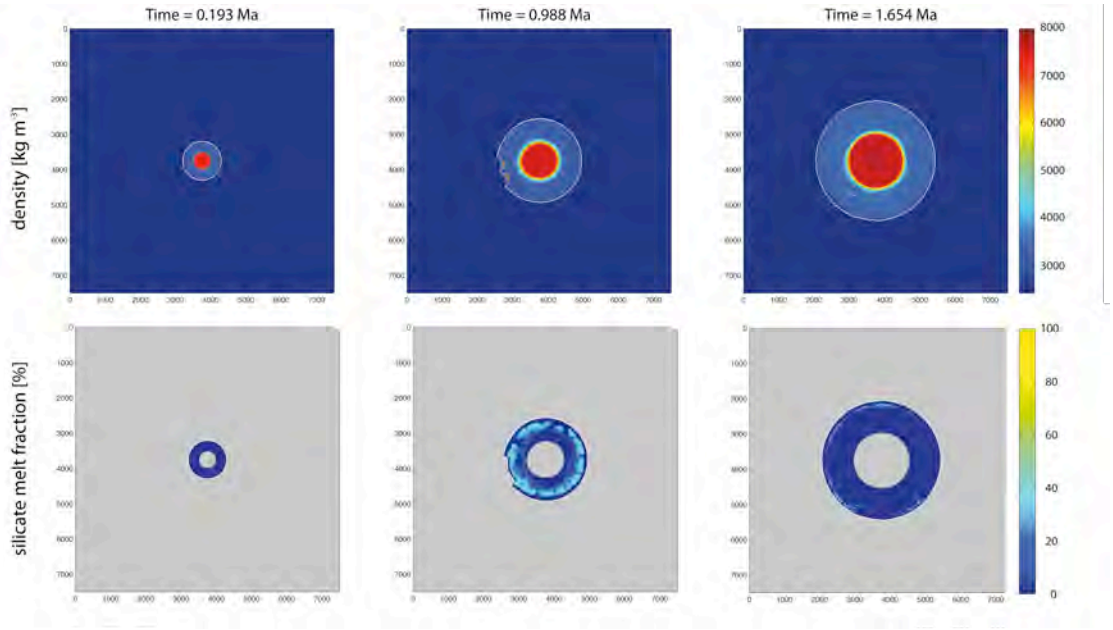



Figure: Thermochemical evolution of an accreting protoplanet.

**Title:** Towards quantifying the strength of coupling between deep mantle dynamics and surface processes using adjoint based sensitivity analysis

**Researchers**: Dave A. May
Anna FitzMaurice

**Institute/ Group:** Geophysical Fluid Dynamics
Department of Earth Sciences

**Description:**

Due to the inherently long time scales associated with geological processes, in order to develop insight into the geodynamic setting, researchers typically resort to using analogue or numerical models. One of the biggest advantages of the numerical modeling over traditional laboratory experiments is the strong control we have on the input rheology, boundary conditions and that fact that we can readily "inspect" the velocity, pressure and temperature fields obtained from the output of such models.

The development of numerical models suitable to describe a geological setting (even in 2D) will frequently require a numerous material lithologies. Each lithology possesses a particular geometry and a set of constants which define the rheological behaviour of the material. So whilst it is true that we have a strong control on the model input in numerical simulations, it is often difficult to disentangle the relative importance each of these parameters may have on a given output quantity (e.g. surface uplift). Traditionally such a question is answered by performing a "brute force" search of the parameter space, however such an approach is not possible when each input parameter is a continuous variables and there are many inputs.

Here we exploit an adjoint based sensitivity analysis which has been extensively developed in the aeronautics industry for the optimal design of airfoils. The adjoint sensitivity analysis is an extremely efficient technique to understand the response of an objective function with respect to all input parameters. In practice, to obtain the sensitivities we require one solve of the forward model, and for each input parameter one adjoint solve.

Presently we are applying this technique to examine the sensitivity of the surface uplift in response to mantle dynamics with the intent to assess the strength of coupling between the surface dynamics and the mantle. This idea will be extended to 3D and applied to quasi-instantaneous geodynamic models which are now a popular technique to constrain the effective present-day rheology of the system.

**Title:** Scalable, parallel, matrix-free multi-level preconditioners for variable viscosity Stokes flow in 3D

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

**Institute/ Group:** Geophysical Fluid Dynamics
Department of Earth Sciences

**Description:**

The use of a mixed finite element formulation to discretise Stokes equations, coupled with a particle based Lagrangian representation of the material lithology is a common numerical technique employed within geodynamics to study large deformation processes. The extension of this methodology to enable high-resolution, three-dimensional simulations still represents a number of significant computational challenges. Of most concern are the high computational memory requirements of the favoured Q2-P1 element, and the development of efficient, 'light-weight' and robust linear and non-linear solvers, which are performant on multi-core, massively parallel computational hardware.

Our objective is to develop a 'cheap' and efficient methodology utilizing the mixed element Q2-P1, to study 3D geodynamic processes including subduction, rifting and folding with the inclusion of visco-plastic materials. For this class of problems, careful treatment of all of the aforementioned technical challenges is essential to achieve high resolution simulations.

I have developed flexible methodology which aims to rectify all of these issues. The key to the approach is 1) always pose the discrete problem in defect-correction form and 2) utilise a mixture of assembled and matrix-free operations to evaluate the non-linear residual and apply the operators and smoothers required to define the multi-level preconditioner for the Jacobian.

The performance characteristics of the matrix-free, multi-level preconditioning strategy is currently being investigated by considering several 3D visco-plastic models. The robustness of the preconditioner and non-linear solver with respect to the viscosity contrast and the topology of the viscosity field, together with the parallel scalability are focuses of this research.

**References:**

D. A. May, A scalable, matrix-free finite element based Stokes discretisation for geodynamic applications, Computer Methods in Applied Mechanics and Engineering (2012) [in preparation]

**Title:** Volume reconstruction of point cloud data sets derived from computational geodynamic simulations

**Researchers:** Dave A. May

**Institute/ Group:** Geophysical Fluid Dynamics
Department of Earth Sciences

**Description:**

One of the most widely used numerical modeling techniques in geodynamics to study the evolution of geomaterials is the "marker-and-cell" technique. In such methods the material lithology is represented by Lagrangian particles (markers), while the continuum equations are solved on a background mesh. Significant research has been devoted to improving the efficiency and scalability of these numerical methods to enable high-resolution simulations to be performed on modest computational resources. In contrast, little attention has been given to developing visualization techniques suitable for interrogation high-resolution 3D particle data sets. We describe an efficient algorithm for performing a volume reconstruction of the lithology field defined via particles (code available upon request from the author). The algorithm generates an Approximate Voronoi Diagram (AVD) which transforms particle data sets into a cell-based, volumetric data set. The volumetric representation enables cross sections of the material configuration to be constructed efficiently and unambiguously, thereby enabling the interior material structure of the simulation results to be analyzed. Examples from geodynamic simulations are used to demonstrate visual results possible using this visualization technique. Performance comparisons are made between existing implementations of exact and approximate Voronoi diagrams. Overall, the AVD developed herein is found to be extremely competitive as a visualizing tool for massive particle data sets as it is extremely efficient, has low memory requirements and can be trivially used in a distributed memory computing environment.

**References:**

D. A. May, Volume reconstruction of point cloud data sets derived from computational geodynamic simulations, Geochem. Geophys. Geosyst., 13, (2012), Q05019, DOI:10.1029/2012GC004170.

**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

**Description:**

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.

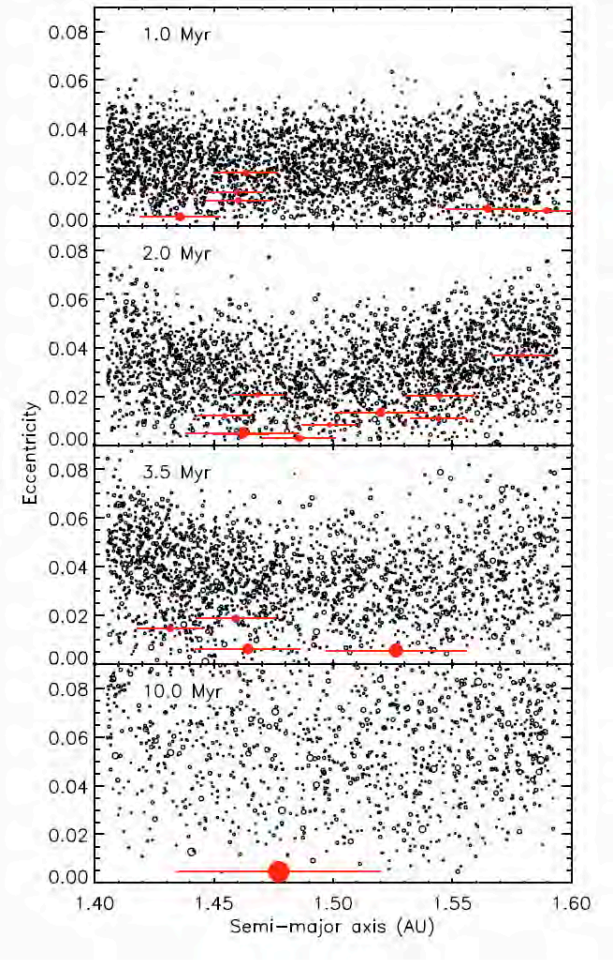



Figure: N-body results on the growth of planetary embryos from an anullus of planetesimals.

References: A manuscript is submitted to Earth and Planetary Science Letters.

**Title:** Influence of magmatism on mantle cooling, surface heat flow and Urey ratio

**Researchers:** T. Nakagawa, P. J. Tackley

**Institute/Group:** Institute of Geophysics/Geophysical Fluid Dynamics

**Description:**

Two-dimensional thermo-chemical mantle convection simulations are used to investigate the influence of melting-inducted differentiation on the thermal evolution of Earth's mantle, focussing in particular on matching the present-day surface heat flow and the 'Urey ratio'. High initial mantle temperatures, which are expected following Earth's accretion, cause major differences in early mantle thermo-chemical structures, but by the present-day surface heat flux and internal structures are indistinguishable from cases with a low initial temperature. All of the investigated cases, regardless of exact parameters, have approximately Earth's present-day heat flow, with substantial fractions coming from the core and from mantle cooling. The range of present-day Urey ratio observed in simulations here is about 0.3 to 0.5, which is consistent with observational and geochemical constraints (Jaupart et al., 2007). Magmatic heat transport contributes an upper bound of 9% to Earth's present-day heat loss but a much higher fraction at earlier times —often more than convective heat loss—so neglecting this causes an overestimation of the Urey ratio. Magmatic heat transport also plays an important role in mantle cooling. Considering these points, it is important to include magmatic effects when attempting to understand the thermal evolution of the Earth.

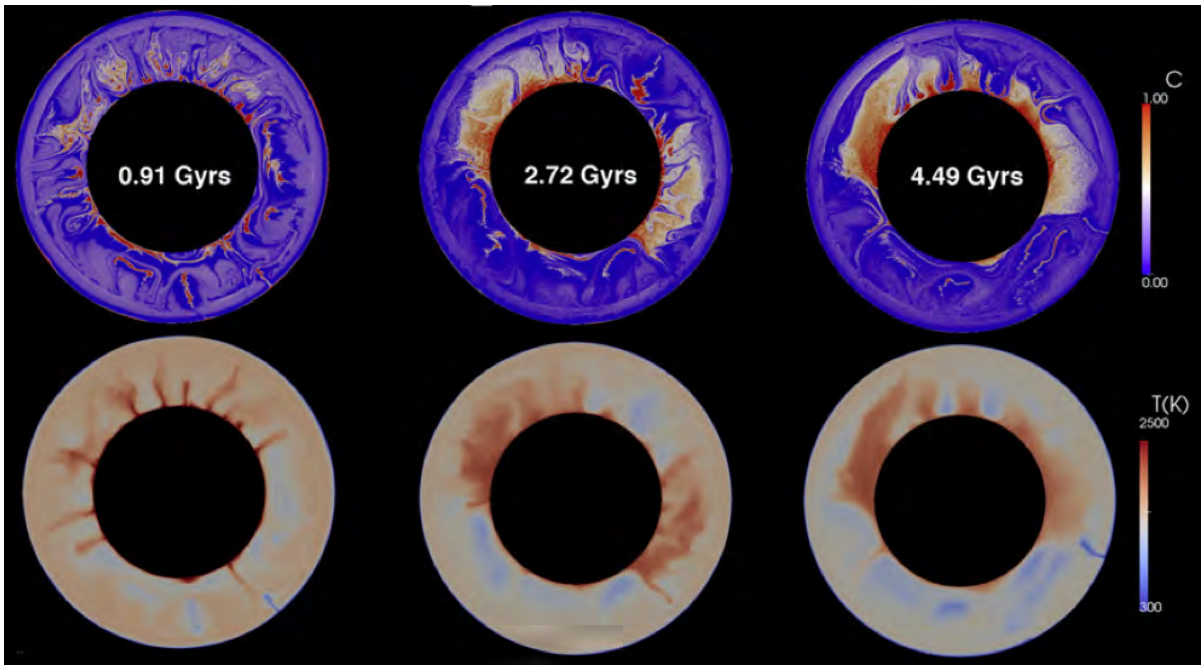



**Figure**. Thermo-chemical evolution of the model mantle over 4.5 billion years.

**References**: 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.

**Title:** Modelling the Influence of Continents on Plate Tectonics

**Researchers:** T. Rolf
P. J. Tackley

**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. Long-term stability of a continents can only exist if their viscosity and yield strength are sufficiently higher than for oceanic lithosphere. 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. Depending on the lateral extent of the craton the critical strength can be increased by a factor of 2 compared to results with a homogeneous lithosphere. Thus, continents make plate tectonics easier. Important parameters are the lateral extent of the continent and the thickness ratio of continental and oceanic plate.

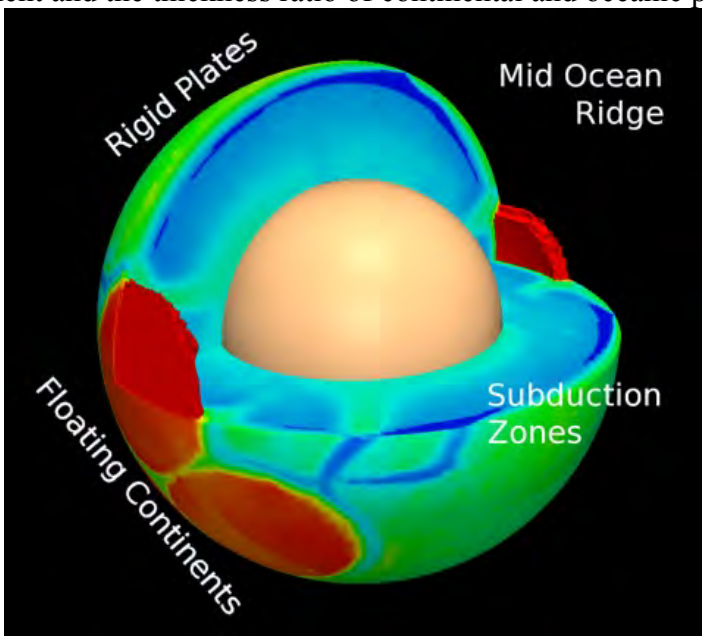



**Figure**. Numerical simulation of plate tectonics with buoyant continents in 3-D spherical geometry. Plotted is effective viscosity (red=high to blue=low).

**References:** (i) 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.; (ii) Coltice, N., T. Rolf, P. J. Tackley and S. Labrosse, Dynamic causes of the relation between area and age of the ocean floor, Science 336, 6079, 335-338, DOI:10.1126/science.1219120.

**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

**Description:**

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.

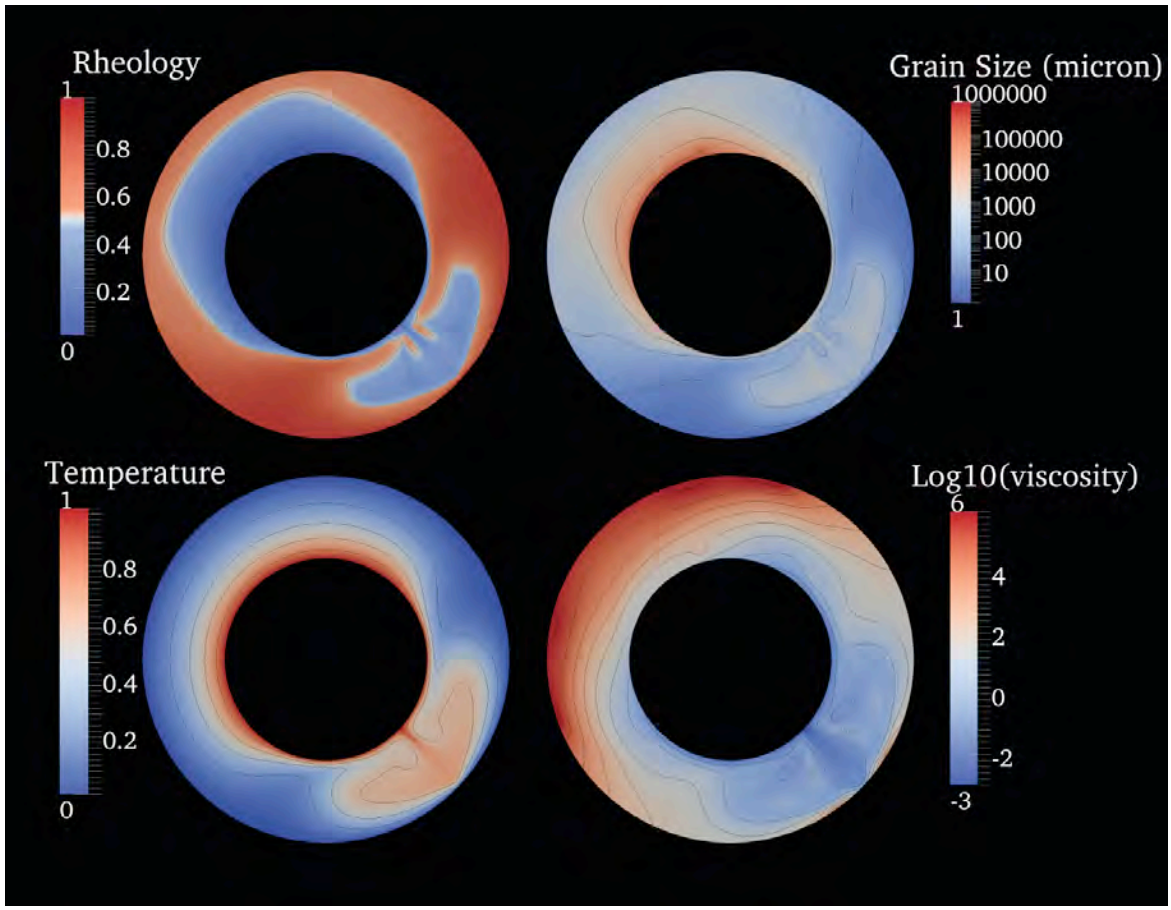



Figure: Long-term evolution of mantle convection considering the infleunce of grain size evolution.

**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

**Description:**

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.

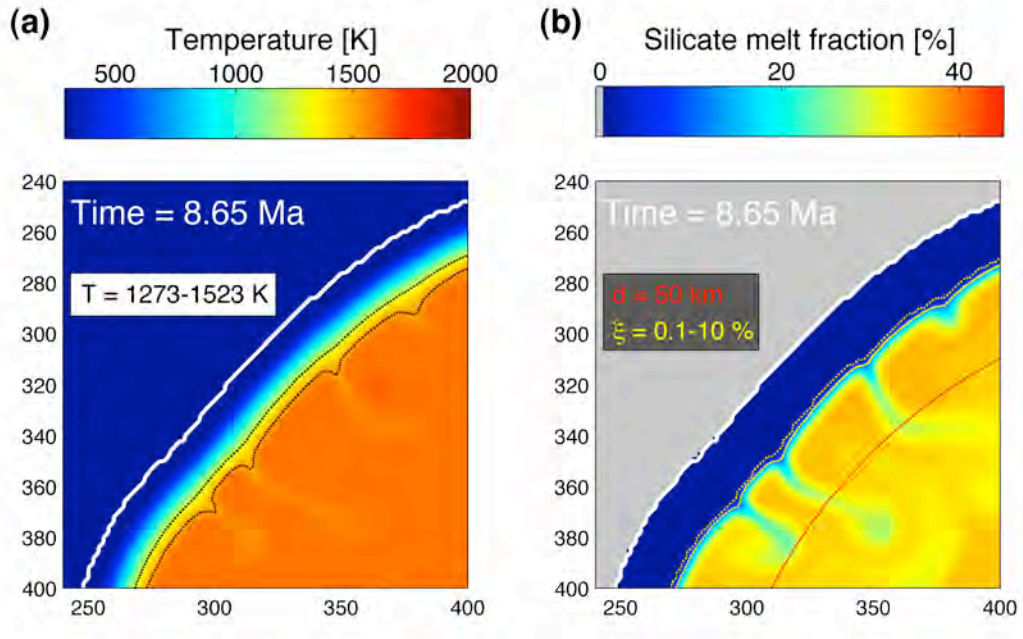



Figure: Early thermochemical evolution of a Vesta-like body displaying regions from which meteorite NWA 5480 could be derived from.

References: A manuscript is submitted to Nature Geoscience.

**Title:** Numerical modelling of subduction zones

**Researchers:** Guizhi Zhu, Katharina Vogt, Taras Gerya, Diana Dymkova, Thibault Duretz, Bettina Baitsch-Ghirardello

**Institute/ Group:** Institute of Geophysics, D-ERDW, ETH-Zurich
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:

- Origin of double seismic zones in subducting slabs (Faccenda et al., 2012) (Fig.1)
- Crustal growth at active continental margins: (Vogt et al., 2012)
- Subduction of narrow oceanic basins (Malatesta et al., 2012)
- Defining future directions in subduction modeling (Gerya, 2011)

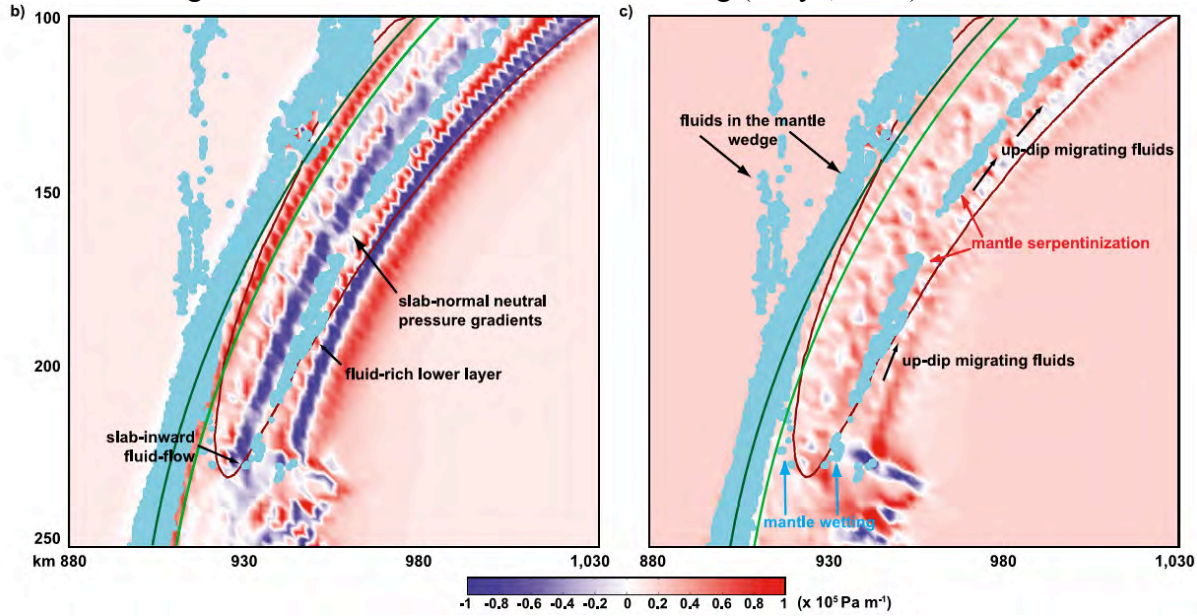



**Fig. 1.** Dynamics of fluid percolation inside the subducting slab (Faccenda et al., 2012).

**References:**

Faccenda, M., Gerya, T.V., Mancktelow, N.S., Moresi, L. (2012) Fluid flow during slab unbending and dehydration: Implications for intermediate-depth seismicity, slab weakening and deep water recycling. Geochemistry, Geophysics, Geosystems, 13, Article Number: Q01010.

Malatesta, C., Gerya, T., Scambelluri, M., Federico, L., Crispini, L., Capponi, G. (2012) Intraoceanic subduction of "heterogeneous" oceanic lithosphere in narrow basins: 2D numerical modeling. Lithos, 140–141, 234–251.

Vogt, K., Gerya, T.V., Castro, A. (2012) Crustal growth at active continental margins: Numerical modeling. Phys. Earth Planet. Interiors, 192-193, 1-20.

**Title:** An improved structural characterisation of reduced french bean plastocyanin based on NMR data and local-elevation molecular dynamics simulation

**Researchers:** D. Steiner
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** Computer-aided chemistry

**Description:**

Deriving structural information about a protein from NMR experimental data is still a non-trivial challenge to computational biochemistry. This is because of the low ratio of the number of independent observables to the number of molecular degrees of freedom, the approximations involved in the different relationships between particular observable quantities and molecular conformation, and the averaged character of the experimental data. For example, protein $^{3}J$-coupling data are seldom used for structure refinement because of the multiple-valuedness and limited accuracy of the Karplus relationship linking a $^{3}J$-coupling to a torsional angle. Moreover, sampling of the large conformational space is still problematic. Using the 99-residue protein plastocyanin as an example we investigated whether use of a thermodynamically calibrated force field, inclusion of solvent degrees of freedom, and application of adaptive local-elevation sampling that accounts for conformational averaging produces a more realistic representation of the ensemble of protein conformations than standard single-structure refinement in a non-explicit solvent using restraints that do not account for averaging and are partly based on non-observed data. Yielding better agreement with observed experimental data, the protein conformational ensemble is less restricted than when using standard single-structure refinement techniques, which are likely to yield a picture of the protein which is too rigid.

**References:** *Eur. Biophys. J.* ***41*** *(2012) 579-595*

**Title:** On the calculation of $^3J_{\alpha\beta}$-coupling constants for side chains in proteins

**Researchers:** D. Steiner
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**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology,
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**Group:** computer aided chemistry

**Description:**

Structural knowledge about proteins is mainly derived from values of observables, measurable in NMR spectroscopic or X-ray diffraction experiments, i.e. absorbed or scattered intensities, through theoretically derived relationships between structural quantities such as atom positions or torsional angles on the one hand and observable quantities such as squared structure factor amplitudes, NOE intensities or $^3J$-coupling constants on the other. The standardly used relation connecting $^3J$-couplings to torsional angles is the Karplus relation, which is used in protein structure refinement as well as in the evaluation of simulated properties of proteins. The accuracy of the simple and generalized Karplus relations is investigated using side-chain structural and $^3J_{\alpha\beta}$ -coupling data for three different proteins, Plastocyanin, Lysozyme, and FKBP, for which such data are available. The results show that the widely used Karplus relations are only a rough estimate for the relation between 3Jab-couplings and the corresponding $\chi_1$-angle in proteins.

**References:** *J. Biomol. NMR* ***53*** *(2012) 223-246*

**Title:** Mixing coarse-grained and fine-grained water in molecular dynamics simulations of a single system

**Researchers:** S. Riniker
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The use of a supra-molecular coarse-grained (CG) model for liquid water as solvent in molecular dynamics simulations of biomolecules represented at the fine-grained (FG) atomic level of modelling may reduce the computational effort by one or two orders of magnitude. However, even if the pure FG model and the pure CG model represent the properties of the particular substance of interest rather well, their application in a hybrid FG/CG system containing varying ratios of FG versus CG particles is highly non-trivial, because it requires an appropriate balance between FG-FG, FG-CG, and CG-CG energies, and FG and CG entropies. Here, the properties of liquid water are used to calibrate the FG-CG interactions for the simple-point-charge water model at the FG level and a recently proposed supra-molecular water model at the CG level that represents five water molecules by one CG bead containing two interaction sites. Only two parameters are needed to reproduce different thermodynamic and dielectric properties of liquid water at physiological temperature and pressure for various mole fractions of CG water in FG water. The parametrisation strategy for the FG-CG interactions is simple and can be easily transferred to interactions between atomistic biomolecules and CG water.

**References:** *J. Chem. Phys.* ***137*** *(2012) 044120*

**Title:** Structural effects of an atomic-level layer of water molecules around proteins solvated in supra-molecular coarse-grained water

**Researchers:** S. Riniker
A. P. Eichenberger
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Atomistic molecular dynamics simulations of proteins in aqueous solution are still limited to the multinanosecond time scale and multinanometer 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. A recent comparison of the properties of four proteins in CG water versus FG water showed the preservation of the secondary and tertiary structure with a computational speed-up of at least an order of magnitude. However, an increased occurrence of hydrogen bonds between side chains was observed due to a lack of hydrogen-bonding partners in the supra-molecular solvent. Here, the introduction of a FG water layer around the protein to recover the hydrogen-bonding pattern of the atomistic simulations is studied. Three layer thicknesses of 0.2, 0.4, and 0.8 nm are considered. A layer thickness of 0.8 nm is found sufficient to recover the behavior of the proteins in the atomistic simulations, whereas the hybrid simulation is still three times more efficient than the atomistic one and the cutoff radius for nonbonded interactions could be increased from 1.4 to 2.0 nm.

**References:** *J. Phys. Chem.* ***B 116*** *(2012) 8873-8879*

**Title:** Using enveloping distribution sampling (EDS) to compute the free enthalpy difference between right- and left-handed helices of a $\beta$-peptide in solution

**Researchers:** Z. Lin
T. A. Timmerscheidt
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Recently, the method of enveloping distribution sampling (EDS) to efficiently obtain free enthalpy differences between different molecular systems from a single simulation has been generalized to compute free enthalpy differences between different conformations of a system [Z. X. Lin, H. Y. Liu, S. Riniker, and W. F. van Gunsteren, J. Chem. Theory Comput. **7**, 3884 (2011)]. However, the efficiency of EDS in this case is hampered if the parts of the conformational space relevant to the two end states or conformations are far apart and the conformational diffusion from one state to the other is slow. This leads to slow convergence of the EDS parameter values and free enthalpy differences. In the present work, we apply the EDS methodology to a challenging case, i.e., to calculate the free enthalpy difference between a right-handed $2.7_{10/12}$-helix and a left-handed $3_{14}$-helix of a hexa-$\beta$-peptide in solution from a single simulation. No transition between the two helices was detected in a standard EDS parameter update simulation, thus enhanced sampling techniques had to be applied, which included adiabatic decoupling (AD) of solute and solvent motions in combination with increasing the solute temperature, and lowering the shear viscosity of the solvent. AD was found to be unsuitable to enhance the sampling of the solute conformations in the EDS parameter update simulations. Lowering the solvent shear viscosity turned out to be useful during EDS parameter update simulations, i.e., it did speed up the conformational diffusion of the solute, more transitions between the two helices were observed. This came at the cost of more CPU time spent due to the shorter time step needed for simulations with the lower solvent shear viscosity. Using an improved EDS parameter update scheme, parameter convergence was five-fold enhanced. The resulting free enthalpy difference between the two helices calculated from EDS agrees well with the result obtained through direct counting from a long MD simulation, while the EDS technique significantly enhances the sampling of both helices over non-helical conformations.

**References:** *J. Chem. Phys.* ***137*** *(2012) 064108*

**Title:** Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations

**Researchers:** S. Riniker
A. P. Eichenberger
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Simulation of the dynamics of a protein in aqueous solution using an atomic model for both the protein and the many water molecules is still computationally extremely demanding considering the time scale of protein motions. The use of supra-atomic or supra-molecular coarse-grained (CG) models may enhance the computational efficiency, but inevitably at the cost of reduced accuracy. Coarse-graining solvent degrees of freedom is likely to yield a favourable balance between reduced accuracy and enhanced computational speed. Here, the use of a supra-molecular coarse-grained water model that largely preserves the thermodynamic and dielectric properties of atomic level fine-grained (FG) water in molecular dynamics simulations of an atomic model for four proteins is investigated. The results of using an FG, a CG, an implicit, or a vacuum solvent environment of the four proteins are compared, and for hen egg-white lysozyme a comparison to NMR data is made. The mixed-grained simulations do not show large differences compared to the FG atomic level simulations, apart from an increased tendency to form hydrogen bonds between long side chains, which is due to the reduced ability of the supra-molecular CG beads that represent five FG water molecules to make solvent-protein hydrogen bonds. But, the mixed-grained simulations are at least an order of magnitude faster than the atomic level ones

**References:** *Eur. Biophys. J.* ***41*** *(2012) 647-661*

**Title:** Recent advances in computational actinoid chemistry

**Researchers:** D. Wang[†,‡]
W. F. van Gunsteren[‡]
Z. Chai[†]

**Institute/** [†]Multidisciplinary Initiative Center, Institute of High Energy Physics, Chinese Academy of Sciences, 100049, Beijing, P.R. China
[‡]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

We briey review advances in computational actinoid (An) chemistry during the past ten years in regard to two issues: the geometrical and electronic structures, and reactions. The former addresses the An-O, An-C, and M-An (M is a metal atom including An) bonds in the actinoid molecular systems, including actinoid oxo and oxide species, actinoid carbenoid, dinuclear and diatomic systems, and the latter the hydration and ligand exchange, the disproportionation, the oxidation, the reduction of uranyl, hydroamination, and the photolysis of uranium azide. Concerning their relevance to the electronic structures and reactions of actinoids and their importance in the development of an advanced nuclear fuel cycle, we also mentioned the work on actinoid carbide and nitride, which have been proposed to be candidates of next generation of nuclear fuel, and the oxidation of $PuO_{\chi}$, which is important to understand the speciation of actinoids in the environment, followed by a brief discussion on the urgent need for a heavier involvement of computational actinoid chemistry in developing advanced reprocessing protocols of spent nuclear fuel. The paper is concluded with an outlook.

**References:** *Chem. Soc. Rev. (2012) accepted*

**Title:** On the use of advanced modelling techniques to investigate the conformational discrepancy between two X-ray structures of the AppA BLUF domain

**Researchers:** K. Meier
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The conformation of the BLUF domain of the signalling protein AppA in the dark state is a matter of intensive research, both, experimental and theoretical, and has not yet unambiguously been determined. Two contradicting X-ray structures of the dark state have been published previously. We aim at resolving this seeming contradiction by exploring conformational pathways between the two X-ray structures using advanced modelling techniques, such as local-elevation searching and sampling, soft-core non-bonded interactions and protocols of successively biasing the sampling of sets of torsional angles which adopt different values in the two alternative X-ray structures. The results suggest a high energetic barrier for a change of the Trp104 side chain from a ”Trp-in” to a ”Trp-out” conformation or vice versa and illustrate the complexity to model conformational transitions involving a large number of degrees of freedom.

**References:** *Phys. Chem. Chem. Phys. (2012) submitted*

**Title:** Molecular dynamics simulation of thionated hen egg white lysozyme

**Researchers:** W. Huang
A. P. Eichenberger
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Understanding of the driving forces of protein folding is a complex challenge because different types of interactions play a varying role. To investigate the role of hydrogen bonding involving the backbone, the effect of thio substitutions in a protein, hen egg white lysozyme (HEWL), was investigated through molecular dynamics simulations of native as well as partly (only residues in loops) and fully thionated HEWL using the GROMOS 54A7 force field. The results of the three simulations show that the structural properties of fully thionated HEWL clearly differ from those of the native protein, while for partly thionated HEWL they only changed slightly compared with native HEWL. The analysis of the torsional-angle distributions and hydrogen bonds in the backbone suggests that the α-helical segments of native HEWL tend to show a propensity to convert to $3_{10}$- helical geometry in fully thionated HEWL. A comparison of the simulated quantities with experimental NMR data such as nuclear overhauser effect (NOE) atom–atom distance bounds and $^{3}J_{HNH\alpha}$ - couplings measured for native HEWL illustrates that the information content of these quantities with respect to the structural changes induced by thionation of the protein backbone is rather limited.

**References:** *Prot. Sci.* ***21*** *(2012) 1153-1161*

**Title:** On developing coarse-grained models for biomolecular simulation: a review

**Researchers:** S. Riniker
J. R. Allison
W. F. van Gunsteren

**Institute/** [a]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[b]Centre for Theoretical Chemistry and Physics, Institute of Natural Sciences, Massey University Albany, New Zealand
**Group:** computer aided chemistry

**Description:**

So-called coarse-grained models are a popular type of model for accessing long time scales in simulations of biomolecular processes. Such models are coarse-grained with respect to atomic models. But any modelling of processes or substances involves coarse-graining, i.e. the elimination of non-essential degrees of freedom and interactions from a more fine-grained level of modelling. The basic ingredients of developing coarse-grained models based on the properties of fine-grained models are reviewed, together with the conditions that must be satisfied in order to preserve the correct physical mechanisms in the coarse-graining process. This overview should help the reader to determine how realistic a coarse-grained model of a biomolecular system is, i.e. whether it reflects the underlying physical mechanisms or merely provides a set of pretty pictures of the process or substances of interest.

**References:** *Phys. Chem. Chem. Phys.* ***14*** *(2012) 12423-12430*

**Title:** Interfacing the GROMOS (bio)molecular simulation software to quantum-chemical program packages

**Researchers:** K. Meier
N. Schmid
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The newly implemented quantum-chemical/molecularmechanical (QM/MM) functionality of the Groningen molecular simulation (GROMOS) software for (bio)molecular simulation is described. The implementation scheme is based on direct coupling of the GROMOS C++ software to executables of the quantum-chemical program packages MNDO and TURBOMOLE, allowing for an independent further development of these packages. The new functions are validated for different test systems using program and model testing techniques. The effect of truncating the QM/MM electrostatic interactions at various QM/MM cutoff radii is discussed and the application of semiempirical versus density-functional Hamiltonians for a solute molecule in aqueous solution is compared.

**References:** *J. Comput. Chem.* ***33*** *(2012) 2108-2117*

**Title:** Exploration of swapping enzymatic function between two proteins: a simulation study of chorismate mutase and isochorismate pyruvate lyase

**Researchers:** A. Choutko
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The enzyme chorismate mutase EcCM from Escherichia coli catalyzes one of the few pericyclic reactions in biology, the transformation of chorismate to prephenate. The isochorismate pyruvate lyase PchB from Pseudomonas aeroginosa catalyzes another pericyclic reaction, the isochorismate to salicylate transformation. Interestingly, PchB possesses weak chorismate mutase activity as well thus being able to catalyze two distinct pericyclic reactions in a single active site. EcCM and PchB possess very similar folds, despite their low sequence identity. Using molecular dynamics simulations of four combinations of the two enzymes (EcCM and PchB) with the two substrates (chorismate and isochorismate) we show that EcCM influences the forces on and the conformations adopted by chorismate in a way which favors the chorismate to prephenate transition and that, analogously, PchB influences the forces on and the conformations adopted by isochorismate in a way which favors the isochorismate to salicylate transition. However, EcCM and to a lower extent PchB fail in influencing the forces and conformations of the substrate such as to favor the other chemical reaction (isochorismate pyruvate lyase (IPL) activity for EcCM and chorismate mutase activity for PchB). Additionally, we show that motions of some residues far from the active site are correlated with those of residues in the active site, while for PchB such correlations are not observed. This might explain the impossibility of engineering IPL activity in EcCM by solely mutating active site residues.

**References:** *ChemBioChem (2012) submitted*

**Title:** 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

**Researchers:** A. Choutko
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The protein chorismate mutase MtCM from Mycobacterium Tuberculosis catalyzes one of the few pericyclic reactions known in biology: the transformation of chorismate to prephenate. Chorismate mutases have been widely studied experimentally and computationally to elucidate the transition state of the enzyme catalyzed reaction and the origin of the high catalytic rate. However, studies about substrate entry and product exit to and from the highly occluded active site of the enzyme have to our knowledge not been performed on this enzyme. Crystallographic data suggest a possible substrate entry gate, which involves a slight opening of the enzyme for the substrate to access the active site. Using multiple molecular dynamics simulations, we investigate the natural dynamic process
of the product exiting from the binding pocket of MtCM. We identify a dominant exit pathway, which is in agreement with the gate proposed from the available crystallographic data. Helices H2 and H4 move apart from each other which enables the product to exit from the active site. Interestingly, in almost all exit trajectories, two residues arginine 30 and arginine 134, which participate in the burying of the active site, are accompanying the product on its exit journey from the catalytic site.

**References:** *Prot. Sci. (2012) accepted*

**Title:** Conformational preferences of a β-octapeptide as function of solvent and force-field parameters

**Researchers:** A. Choutko
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

The ability to design properly folded β-peptides with a specific biological activity requires detailed insight into the relationship between the amino acid sequence and the secondary and/or tertiary structure of the peptide. One of the most used spectroscopic techniques for resolving the structure of a biomolecule is Nuclear Magnetic Resonance (NMR) spectroscopy. Because only signal intensities and frequencies are measured in the experiment, a conformational interpretation of the measured data is not straightforward, especially for flexible molecules. The occurrence of conformational and/or time-averaging and the limited number and accuracy of experimental data hampers the precise conformational determination of a biomolecule. In addition the relation between experimental observables with the underlying conformational ensemble is often only approximately known thereby aggravating the difficulty of structure determination of biomolecules. The problematic aspects of structure refinement based on NMR nuclear Overhauser effect (NOE) intensities and $^{3}J$-coupling data are illustrated by simulating a β-octapeptide in explicit methanol and water as solvents using three different force fields. NMR measurements indicated that this peptide would fold into a $3_{14}$- helix in methanol and into a hairpin in water. Our analysis focused on the conformational space visited by the peptide, on structural properties of the peptide and on agreement of the MD trajectories with available NMR data. We conclude that (1) although the $3_{14}$-helical structure is present when the peptide is solvated in methanol, it is not the only relevant conformation and that (2) the NMR data set available for the peptide when solvated in water is not providing enough information to derive a single secondary structure, but rather a multitude of folds that fulfill the NOE data set.

**References:** *Helv. Chim. Acta (2012) accepted*

**Title:** Thirty-five years of biomolecular simulation: development of methodology, force fields, and software

**Researchers:** W. F. van Gunsteren
J. Dolenc

**Institute/** Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Computer simulation of biomolecular systems has become a standard research instrument for the investigation of biomolecular processes at the atomic level of modelling and interpretation. A bird's eye view of the development of simulation methodology, of biomolecular interaction functions and simulation software is presented, together with the challenges in regard to these three aspects of biomolecular simulation.

**References:** *Mol. Sim. (2012) accepted*

**Title:** On the choice of a reference state for one-step perturbation calculations between polar and non-polar molecules in a polar environment

**Researchers:** Z. Lin
W. F. van Gunsteren

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**Group:** computer aided chemistry

**Description:**

One-step perturbation is an efficient method to estimate free energy differences in molecular dynamics simulations, but its accuracy depends critically on the choice of an appropriate, possibly unphysical, reference state that optimizes the sampling of the physical end states. In particular the perturbation from a polar moiety to a non-polar one and vice versa in a polar environment such as water poses a challenge which is of importance when estimating free energy differences that involve entropy changes and the hydrophobic effect. We systematically study the performance of the one-step perturbation method in the calculation of the free enthalpy difference between a polar water solute and a non-polar "water" solute molecule solvated in a box of 999 polar water molecules. Both these polar and non-polar physical reference states fail to predict the free enthalpy difference as obtained by thermodynamic integration (TI), but the result is worse using the non-polar physical reference state, because both a properly sized cavity and a favorable orientation of the polar solute in a polar environment are rarely, if ever, sampled in a simulation of the non-polar solute in such an environment. Use of non-physical soft-core reference states helps to sample properly sized cavities, and post-MD simulation rotational and translational sampling of the solute to be perturbed leads to much improved free enthalpy estimates from one-step perturbation.

**References:** *J. Comput. Chem. (2012) accepted*

**Title:** Free enthalpies of replacing water molecules in protein binding pockets

**Researchers:** S. Riniker
L. J. Barandun
F. Diederich
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W. F. van Gunsteren

**Institute/** Laboratory of Organic Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
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**Group:** computer aided chemistry

**Description:**

Water molecules in the binding pocket of a protein and their role in ligand binding have increasingly raised interest in recent years. Displacement of such water molecules by ligand atoms can be either favourable or unfavourable for ligand binding depending on the change in free enthalpy. In this study, we investigate the displacement of water molecules by an apolar probe in the binding pocket of two proteins, cyclin-dependent kinase 2 (CDK2) and tRNA-guanine transglycosylase (TGT), using the method of enveloping distribution sampling (EDS) to obtain free enthalpy differences. In both cases, a ligand core is placed inside the respective pocket and the remaining water molecules are converted to apolar probes, both individually and in pairs. The free enthalpy difference between a water molecule and a CH3 group at the same location in the pocket in comparison to their presence in bulk solution calculated from EDS molecular dynamics (MD) simulations corresponds to the binding free
enthalpy of CH3 at this location. From the free enthalpy difference and the enthalpy difference, the entropic contribution of the displacement can be obtained too. The overlay of the resulting occupancy volumes of the water molecules with crystal structures of analogous ligands shows qualitive correlation between experimentally measured inhibition constants and the calculated free enthalpy differences. Thus, such an EDS analysis of the water molecules in the binding pocket may give valuable insight for potency optimization in drug design.

**References:** *J. Comput. Aided Mol. Des. (2012) submitted*

**Title:** Rapid sampling of folding equilibria of β-peptides in methanol using a supra-molecular solvent model

**Researchers:** W. Huang
S. Riniker
W. F. van Gunsteren

**Institute/** Laboratory of Organic Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Molecular dynamics simulation of bio-molecules in solvent using an atomic model for both the bio-molecules and the solvent molecules is still computationally rather demanding considering the time scale of the bio-molecular motions. The use of a supra-molecular coarse-grained (CG) model can speed up the simulation considerably, but it also reduces the accuracy inevitably. Combining an atomic fine-grained (FG) level of modeling for the bio-molecules and a supra-molecular CG level for the solvent into a hybrid system, the increased computational efficiency may outweigh the loss of accuracy with respect to the bio-molecular properties in the hybrid FG/CG simulation. Here, a 1:1 mixture of FG and CG methanol is used to calibrate the FG-CG interactions using thermodynamic and dielectric screening data for liquid methanol. Three promising FG-CG interaction parameter sets are found and applied in hybrid FG/CG solute/solvent simulations of the folding equilibria of three β-peptides that adapt different folds. The properties of the peptides are compared with those obtained in pure FG simulations and with experimental NMR data. The comparison shows that the folding equilibria in the mixed-grained simulations are similar to those in the FG simulations, while the use of the supra-molecular CG model of methanol reduces the computational effort by at least a factor 6.

**References:** *J. Chemt. Theory Comput. (2012) submitted*

**Title:** Influence of 63Ser phosphorylation and dephosphorylation on the structure of the stathmin helical nucleation sequence: A molecular dynamics study

**Researchers:** J. H. Missimer[1]
M. O. Steinmetz[1]
W. F. van Gunsteren[2]
J. Dolenc[2,3]

**Institute/** [1]Biomolecular Research, Paul Scherrer Institute, 5232 Villigen, Switzerland
[2]Laboratory of Physical Chemistry, ETH, Swiss Federal Institute of Technology, 8093 Zürich, Switzerland
[3]Faculty of Chemistry and Chemical Technology, University of Ljubljana, 1000 Ljubljana, Slovenia
**Group:** computer aided chemistry

**Description:**

Phosphorylation is an important mechanism regulating protein-protein interactions involving intrinsically disordered protein regions. Stathmin, an archetypical example of an intrinsically disordered protein is a key regulator of microtubule dynamics in which phosphorylation of 63Ser within the helical nucleation sequence strongly down-regulates the tubulin-binding and microtubule destabilizing activities of the protein. Experimental studies on a peptide encompassing the 19-residue helical nucleation sequence of stathmin (residues 55-73) indicate that phosphorylation of 63Ser destabilizes the peptide's secondary structure by disrupting the salt bridges supporting its helical conformation. In order to investigate this hypothesis at atomic resolution, we performed molecular dynamics simulations of nonphosphorylated and phosphorylated stathmin-[55-73] at room temperature and pressure, neutral pH and explicit solvation using the recently released GROMOS force field 54A7. In the simulations of nonphosphorylated stathmin-[55-73] emerged salt bridges associated with helical configurations. In the simulations of 63Ser phosphorylated stathmin-[55-73] these configurations dispersed and were replaced by a proliferation of salt bridges yielding disordered configurations. The transformation of the salt bridges was accompanied by emergence of numerous interactions between main and side chains, involving notably the oxygen atoms of the phosphorylated 63Ser. The loss of helical structure induced by phosphorylation is reversible, however, as a final simulation showed. The results extend the hypothesis of salt bridge derangement suggested by experimental observations of the stathmin nucleation sequence, providing new insights into regulation of intrinsically disordered protein systems mediated by phosphorylation.

**References:** *Biochemistry (2012) accepted*

**Title:** Multi-resolution simulation in chemistry: methodological issues and exploration of the origins of differential catalysis observed between two structurally similar enzymes

**Researchers:** K. Meier
A. Choutko
S. Riniker
W. F. van Gunsteren

**Institute/** Laboratory of Physical Chemistry, ETH, Swiss Federal Institute of Technology, 8093 Zürich, Switzerland
**Group:** computer aided chemistry

**Description:**

Theoretical-computational modelling with an eye to explaining experimental observations in regard to a particular chemical phenomenon or process requires choices concerning essential degrees of freedom and types of interactions and the generation of a Boltzmann ensemble or trajectories of configurations. Depending on the degrees of freedom that are essential to the process of interest, e.g. electronic or nuclear versus atomic, molecular or supra-molecular, quantumor classical-mechanical equations of motion are to be used. In multi-resolution simulation, various levels of resolution, e.g. electronic, atomic, supra-atomic or supra-molecular, are combined in one model. This allows an enhancement of the computational efficiency, while maintaining sufficient detail with respect to particular degrees of freedom. The basic challenges and choices with respect to multi-resolution modelling are reviewed and as an illustration the differential catalytic properties of two enzymes with similar folds but different substrates with respect to these substrates are explored using multi-resolution simulation at the electronic, atomic and supra-molecular levels of resolution.

**References:** *Angew. Chem. 2012 (submitted)*

# 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 community, and to serve as a platform for the interaction with partners from other areas of science or from outside academia. C4 was launched twenty years ago as a scientific collaboration between the IBM Research Laboratory and ETH Zürich, and has grown considerably since. Today, the C4 network covers a broad spectrum of research activities involving fifteen research groups from ten different institutes.

The network and its activities are presented in the C4 Annual Report (see www.c4.ethz.ch for more detail)

*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), Wilfred F. van Gunsteren, and PD Dr. Hans P. Lüthi (both ETH Zürich).

*C4 Seminar*
The actual "backbone" of C4 is its Seminar Program. During the 2011 Fall- and 2012 Spring-Term the C4 Seminar Program covered 14 lectures, again some of them presented by leaders in the field of computational chemistry. The seminar, which takes place every second Thursday during the semester, enjoys a remarkable popularity bringing together between forty and sixty students and researchers each time. One C4 seminar was hosted by the IBM Research Laboratory.

*Compute Resource*
In May 2011, after five years of nearly uninterrupted service, the C4 compute-cluster Obélix, a 32 node quadcore IBM Opteron cluster operated by the ETH Informatikdienste, was decommissioned. At the same time the existing C4 Brutus share was extended by 10 standard and 5 fat nodes, i.e. a total of 720 cores, based on an infrastructure-grant of ETH and a financial contribution of the ETH Department of Chemistry.

Many of the members of the C4 community have their own computing facilities, or have access to central compute clusters. In addition, some are users of the resources of the Centro Svizzero die Calcolo Scientifico (CSCS), *i.e.* were awarded computing time based on proposals they had submitted. These resources respond to a specific demand, and the results and achievements reported in the C4 Annual Report typically involve "machine cycles" drawn from more than just one of these resources.

*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. However, in order to respond to the demand of the local community, C4 will offer tutorials again.

*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 jointly to equal parts to Marco Schweizer (D-MATL; Group of Prof. Ch. Oettinger) and Thomas Weymuth (D-CHAB; Group of Prof. M. Reiher) for their MSc theses entitled "*Simulation of Dissipative Quantum Systems* " and "*Identifying Protein beta-Turns with Vibrational Raman Optical Activity"*
"

The 2011 Award Ceremony, for the second time, took place at the ETH Tag with the Rector, Prof. Heidi Wunderli-Allenspach, handing out the award to the winner. The two laureates also presented their research at the occasion of a special C4 Seminar held on May 31, 2012, at the IBM Research Laboratory in Rüschlikon. For more detail please refer to the respective section in this report.

*IBM Shared University Research (SUR) Grant Awarded to C4*
Based on their grant proposal, Alessandro Curioni and Hans P. Lüthi were awarded an IBM Power 755 server with 32 POWER7 cores and 256 GBytes of (shared) memory. The server is dedicated to method development projects in the area of density functional theory.

*Outlook*
Computational chemistry "made in Zurich" is still growing, and a network such as C4 plays an important role when it comes to the exchange of information and know-how within the field or with similar organizations such as the CS&E community. Also in the next year we will make sure that C4 is a valuable platform for its stakeholders.

Hans P. Lüthi, Leiter C4
October 12, 2012

### 6.2 Information Technology Services

The following resource is available:

The Information Technology Services operates a Linux Cluster co-owned with the departments of Chemistry (D-CHEM), 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).

This cluster consists of the following node types:

**Standard nodes**
104 nodes with four 12-core AMD Opteron 6174 CPUs and 64 GB of RAM (4'992 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**
64 nodes with four 12-core AMD Opteron 6174 CPUs and 256 GB of RAM (3'072 cores)
6 nodes with two 12-core AMD Opteron 6174 CPUs and 128 GB of RAM (144 cores)
10 nodes with four quad-core AMD Opteron 8380 CPUs and 128 GB of RAM (160 cores)
7 nodes with eight dual-core AMD Opteron 8220 CPUs and 64–128 GB of RAM (112 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 6 Nvidia Tesla C1060 GPUs (24 cores + 12 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 18'400 cores.
All nodes are connected to the cluster's internal Gigabit Ethernet backbone.
All nodes (except the legacy nodes) are connected to a high speed/low latency InfiniBand QDR network.

The peak performance of the cluster is more than 190 teraflops.

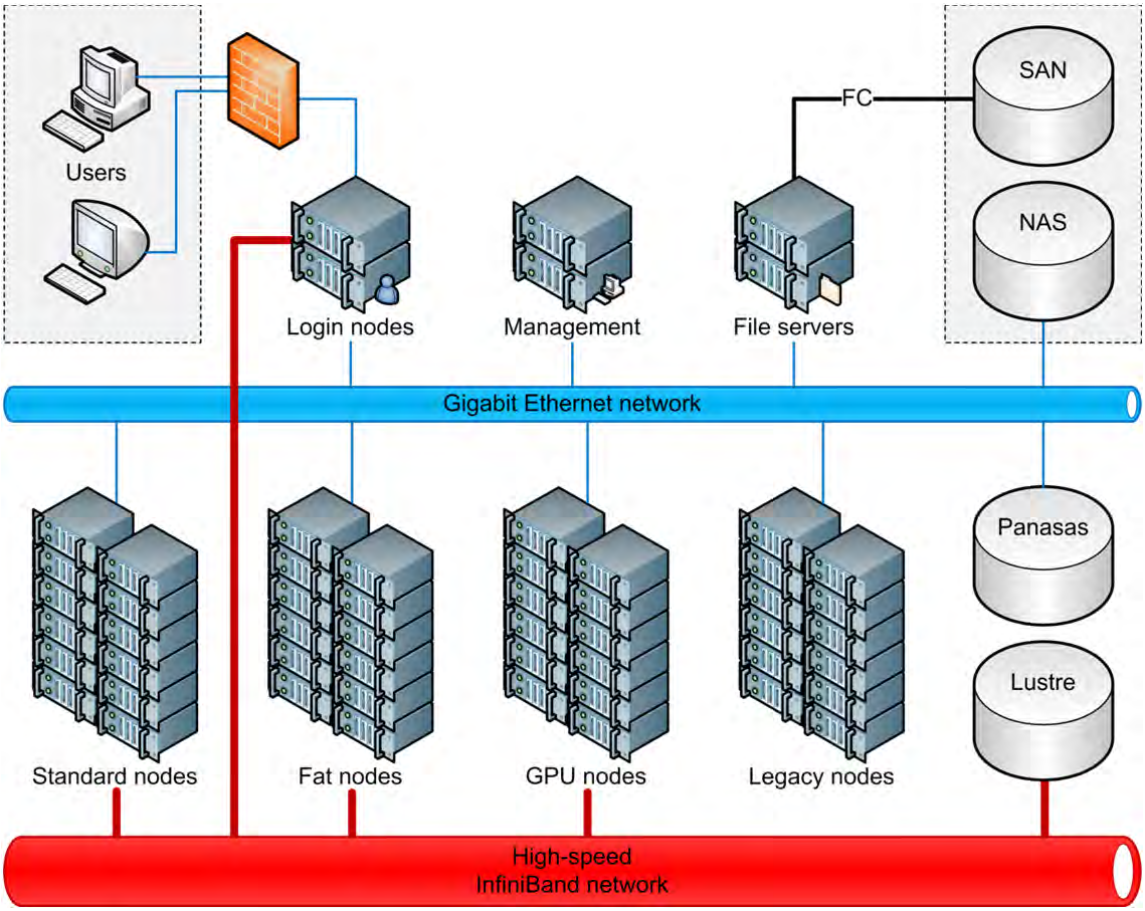
A high performance Lustre parallel filesystem with a capacity of more than 400 TB is available as work storage for data and I/O intensive computations with large files. A Panasas parallel filesystem with more than 70 TB of capacity is available for medium and large files.

Parts of the cluster are operated as a central resource, which can be used on a fair share base by the ETH community without being co-owner of the cluster.

The cluster nodes connected through the InfiniBand network are intended for parallel code (typically MPI based) needing high bandwidth and low latency communications, but not a globally shared memory. The Ethernet connected part (legacy nodes) of the cluster is intended for single node throughput computing and not communication intensive parallel jobs.

All login nodes, management nodes, fileservers and some network switches have been replaced during the past year with new hardware for better performance, higher availability and/or higher network throughput (10GbE / cluster internal and external ETH network).

**Schematic view of the Brutus cluster:**



# 7

# Publications* in 2011/2012

*only CSE-related articles
in refereed journals

# Group of P. Arbenz

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).

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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.

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. 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.

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: *A Fast Parallel Poisson Solver on Irregular Domains Applied to Beam Dynamic Simulations*, J. Comp. Phys. 229 (12): 4554–4566 (2010)

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.

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.

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.

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).

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.

# Group of S. Bonhoeffer

**2012**

Moslonka-Lefebvre, M, Bonhoeffer, S, Alizon, S
Weighting for sex acts to understand the spread of STI on networks
JOURNAL OF THEORETICAL BIOLOGY (2012) 311:46-53

Cadosch, D, Bonhoeffer, S, Kouyos, R
Assessing the impact of adherence to anti-retroviral therapy on treatment failure and resistance evolution in HIV
JOURNAL OF THE ROYAL SOCIETY INTERFACE (2012) 9:2309-2320

Arnoldini, M, Mostowy, R, Bonhoeffer, S, Ackermann, M
Evolution of Stress Response in the Face of Unreliable Environmental Signals
PLOS COMPUTATIONAL BIOLOGY (2012)

Mostowy, R, Kouyos, RD, Hoof, I, Hinkley, T, Haddad, M, Whitcomb, JM, Petropoulos, CJ, Kesmir, C, Bonhoeffer, S
Estimating the Fitness Cost of Escape from HLA Presentation in HIV-1 Protease and Reverse Transcriptase
PLOS COMPUTATIONAL BIOLOGY (2012)

Kouyos, RD, Leventhal, GE, Hinkley, T, Haddad, M, Whitcomb, JM, Petropoulos, CJ, Bonhoeffer, S
Exploring the Complexity of the HIV-1 Fitness Landscape
PLOS GENETICS (2012)

Leventhal, GE, Kouyos, R, Stadler, T, von Wyl, V, Yerly, S, Boni, J, Cellerai, C, Klimkait, T, Gunthard, HF, Bonhoeffer, S
Inferring Epidemic Contact Structure from Phylogenetic Trees
PLOS COMPUTATIONAL BIOLOGY (2012)

Stadler, T, Kouyos, R, von Wyl, V, Yerly, S, Boni, J, Burgisser, P, Klimkait, T, Joos, B, Rieder, P, Xie, D, Gunthard, HF, Drummond, AJ, Bonhoeffer, S
Estimating the Basic Reproductive Number from Viral Sequence Data
MOLECULAR BIOLOGY AND EVOLUTION (2012) 29:347-357

**2011**

Kouyos, RD, von Wyl, V, Hinkley, T, Petropoulos, CJ, Haddad, M, Whitcomb, JM, Boni, J, Yerly, S, Cellerai, C, Klimkait, T, Gunthard, HF, Bonhoeffer, S
Assessing Predicted HIV-1 Replicative Capacity in a Clinical Setting
PLOS PATHOGENS (2011)

von Wyl, V, Kouyos, RD, Yerly, S, Boni, J, Shah, C, Burgisser, P, Klimkait, T, Weber, R, Hirschel, B, Cavassini, M, Staehelin, C, Battegay, M, Vernazza, PL, Bernasconi, E, Ledergerber, B, Bonhoeffer, S, Gunthard, HF
The Role of Migration and Domestic Transmission in the Spread of HIV-1 Non-B Subtypes in Switzerland
JOURNAL OF INFECTIOUS DISEASES (2011) 204:1095-1103

Hinkley, T, Martins, J, Chappey, C, Haddad, M, Stawiski, E, Whitcomb, JM, Petropoulos, CJ, Bonhoeffer, S
A systems analysis of mutational effects in HIV-1 protease and reverse transcriptase
NATURE GENETICS (2011) 43:487-+

**Supplementary Material**

zur Wiesch, PA, Kouyos, R, Engelstadter, J, Regoes, RR, Bonhoeffer, S
Population biological principles of drug-resistance evolution in infectious diseases
LANCET INFECTIOUS DISEASES (2011) 11:236-247

Kouyos, RD, zur Wiesch, PA, Bonhoeffer, S
Informed Switching Strongly Decreases the Prevalence of Antibiotic Resistance in Hospital Wards
PLOS COMPUTATIONAL BIOLOGY (2011)

Mostowy, R, Kouyos, RD, Fouchet, D, Bonhoeffer, S
The Role of Recombination for the Coevolutionary Dynamics of HIV and the Immune Response
PLOS ONE (2011)

Takizawa, H, Regoes, RR, Boddupalli, CS, Bonhoeffer, S, Manz, MG
Dynamic variation in cycling of hematopoietic stem cells in steady state and inflammation
JOURNAL OF EXPERIMENTAL MEDICINE (2011) 208:273-284

Kouyos, RD, von Wyl, V, Yerly, S, Boni, J, Rieder, P, Joos, B, Taffe, P, Shah, C, Burgisser, P, Klimkait, T, Weber, R, Hirschel, B, Cavassini, M, Rauch, A, Battegay, M, Vernazza, PL, Bernasconi, E, Ledergerber, B, Bonhoeffer, S, Gunthard, HF
Ambiguous Nucleotide Calls From Population-based Sequencing of HIV-1 are a Marker for Viral Diversity and the Age of Infection
CLINICAL INFECTIOUS DISEASES (2011) 52:532-539

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1. C. Altantzis, C.E. Frouzakis, A.G. Tomboulides, M. Matalon, K. Boulouchos, Hydrodynamic and thermal-diffusive instability effects on the evolution of laminar planar lean premixed hydrogen flames, *J. Fluid Mech.*, 700, 329–361, (2012).

2. G. Pizza, C. E. Frouzakis, J. Mantzaras, Chaotic dynamics in premixed hydrogen/air channel flow combustion, *Combust. Theory Model.*, 16(2), 275–299, (2012)

3. C. Altantzis, C.E. Frouzakis, A.G. Tomboulides, K. Boulouchos, Numerical simulation of propagating circular and cylindrical lean premixed hydrogen/air flames, *Proc. Combust. Inst.* 34, (in press).

4. 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, (in press).

5. S. G. Kerkemeier, C. N. Markides, C.E. Frouzakis, K. Boulouchos, Direct Numerical Simulation of the Autoignition of a Hydrogen Plume in a Turbul ent Co-flow of Hot Air, *J. Fluid Mech.*, (submitted).

6. M. Schmitt, Y. M. Wright, C. E. Frouzakis and K. Boulouchos, Multiple cycle LES simulations of a direct injection methane engine, *Flow, Turbulence and Combustion* (submitted).

7. M. Bolla , Y. M. Wright, K. Boulouchos, G. Borghesi and E. Mastorakos, Soot formation modelling of n-heptane sprays under diesel engine conditions using the Conditional Moment Closure approach, *Combustion Science Technology* (submitted).

8. Chikatamarla S. and Karlin I., Entropic lattice Boltzmann method for turbulence: Wall boundary conditions. *Physica A.* (submitted)

9. 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* (submitted)

# Group of Domenico Giardini

## Seismology and Geodynamics

A. Colombi, , T. Nissen-Meyer, L. Boschi, D. Giardini.
Seismic waveform sensitivity to global boundary topography
*Geophys. J. Int.* (2012), doi 10.1111/j.1365-246X.2012.05660.x

R.A. Harris, M. Barall, D.J. Andrews, B. Duan, S. Ma, E. Dunham, A. Gabriel, Y. Kaneko, Y. Kase, B. Aagaard, D.D. Oglesby, T.C. Hanks, N. Abrahamson
Verifying a computational method for predicting extreme groundmotion at the proposed Yucca Mountain repository
*Seism. Res. Lett.* (2011); 82: 638-644

D. Peter, D. Komatitsch, Y. Luo, R. Martin, N. Le Goff, E. Casarotti, P. Le Loher, F. Magnoni, Q. Liu, C. Blitz, T. Nissen-Meyer, P. Basini, J. Tromp
Forward and adjoint simulations of seismic wave propagation on fully unstructured hexahedral meshes
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*Bull. Seism. Soc. Am.* (2012), 102(3), 1224-1234.

J.F. Schaefer, L. Boschi, T. W. Becker, E. Kissling
Radial anisotropy in the European mantle: Tomographic studies explored in terms of mantle flow
*Geophys. Res. Lett.*, (2011); 38 L23304, doi:10.1029/2011GL049687

J. F. Schaefer, L. Boschi, E. Kissling.
Adaptively parametrized surface wave tomography: methodology and a new model of the European upper mantle.
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Numerical Algorithms for Earthquake Rupture Dynamic Modeling. In "The mechanics of faulting: From Laboratory to Real Earthquakes"
Research Signpost (2012), 93-124, ISBN 978-81-308-0502-3, Editors A. Bizzarri and H Bath

S. M. Day, D. Roten, K. B. Olsen
Calculating the Source and Path Sensitivies of Basin Guided Waves by Adjoint Simulations
*Geopys. J. Int.* (2012), **189**, 1103-1124, doi:10.1111/j.1365-246X.2012.05416.x

A. A. Gabriel; J. P. Ampuero; L. A. Dalguer, P. M. Mai
The Transition of Dynamic Rupture Styles in Elastic Media Under Velocity-Weakening Friction.
*J. Geophys. Res. (2012),* **117**, B09311, doi:10.1029/2012JB009468

S. Maranò, C. Reller, H.-A. Loeliger, D. Fäh
Seismic waves estimation and wavefield decomposition: Application to ambient vibrations,
*Geophys. J. Int* (2012), **191**(1), 175-188

B. Mena; L.A. Dalguer and P.M. Mai
Pseudodynamic Source Characterization For Strike-Slip Faulting, Including Stress Heterogeneity and Super-shear Ruptures
*Bull. Seismol. Soc. Am* (2012)*,* **102**(4), pp. 1654–1680, August 2012, doi: 10.1785/0120110111

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A Rayleigh wave back-projection method applied to the 2011 Tohoku earthquake
*Geophys. Res. Lett.* (2012)*,* **39**, L02302, doi:10.1029/2011GL050183

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Exhumation and subduction erosion in orogenic wedges: insights from numerical models
*Geochem. Geophys. Geosyst.* (2012) **13**, Q06003, http://dx.doi.org/10.1029/2011GC004011

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The seismic cycle at subduction thrusts: 1. Insights from laboratory models
Submitted to *J. Geophys. Res.* (2012)

D. Fäh, J. Moore, J. Burjanek, I. Iosifescu, L. Dalguer, F. Dupray, C. Michel, J. Woessner, A. Villiger, J. Laue, I. Marschall, V. Gischig, S. Loew, A. Marin, G. Gassner, S. Alvarez, W. Balderer, P. Kästli, D. Giardini, C. Iosifesu, L. Hurni, P. Lestuzzi, A. Karbassi, C. Baumann, A. Geiger, A. Ferrari, L. Laloui, J. Clinton, N. Deichmann
Coupled seismogenic geohazards in alpine regions
*Bolletino di Geofisica Teorica ed Applicata* (2012) in press. doi: 10.4430/bgt0048

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Submitted to *Geophys. Res. Lett.* (2012)

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Importance of 1-point statistics in earthquake source modeling for ground motion simulation
Submitted to *Geophys. J. Int.* (2012)

Y. van Dinther, T. Gerya, L. Dalguer, F. Corbi, F. Funiciello, P. Mai
The seismic cycle at subduction thrusts: 2. Dynamic implications of geodynamic simulations benchmarked with laboratory models
Submitted to *J. Geophys. Res.* (2012)

# Group of Ch. Hafner

**Book Chapter**

**Ch. Hafner, J. Smajic, R. Vogelgesang**, Computational Techniques for Plasmonic Antennas and Waveguides, *Nanoscience and Technology, vol. 4, Plasmonics and Plasmonic Metamaterials: Analysis and Applications, pp. 389-448, Ed. G. Shvets; I. Tsukerman, World Scientific Publishing Co., New Jersey, USA. 2012.*

**Reviewed Journals**

1. **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*
2. **P. Kaspar, R. Kappeler, H. Jäckel, Ch. Hafner**, Toward low-loss photonic crystal waveguides in InP/InGaAsP heterostructures, *Optics Letters, Vol. 37, Issue 17, pp.3717-3719, Sept. 2012.*
3. **M. Naderi-Boldaji, R. Alimardani, A. Hemmat, A. Sharifi, A. Keyhani, N. Dolatsha, T. Keller**, Improvement and field testing of a combined horizontal penetrometer for on-the-go measurement of soil water content and mechanical resistance, *Elsevier, Soil & Tillage Research,, Vol. 123, pp.1-10, July 2012.*
4. **L. Colella, C. Beyer, J. Fröhlich, M. Talary, P. Renaud**, Microelectrode-based dielectric spectroscopy of glucose effect on erythrocytes, *Bioelectrochemistry, Vol. 85, pp.14-20, June 2012.*
5. **E. Mohler, P. Frei, J. Fröhlich, C. Braun-Fahrländer, M. Röösli, the QUALIFEX-team**, Exposure to Radiofrequency Electromagnetic Fields and Sleep Quality: A Prospective Cohort Study, *PLoS ONE 7(5): e37455, doi:10.1371/journal.pone.0037455, Vol. 7, Issue 5, May 2012.*
6. **N. Dolatsha, J. Hesselbarth**, Millimeter-wave chip-to-chip transmission using an insulated image guide excited by an on-chip dipole antenna at 90 GHz, *IEEE Microw. Wireless Comp. Lett., Vol. 22, Issue 5, pp.266-268, May 2012.*
7. **A. Fallahi, B. Oswald, P. Leidenberger**, The element level time domain (ELTD) method for the analysis of nano-optical systems: I. Nondispersive media, *Photonic. Nanostruct., Vol. 10, Issue 2, pp.207-222, April 2012.*
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Computational Science and Engineering

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