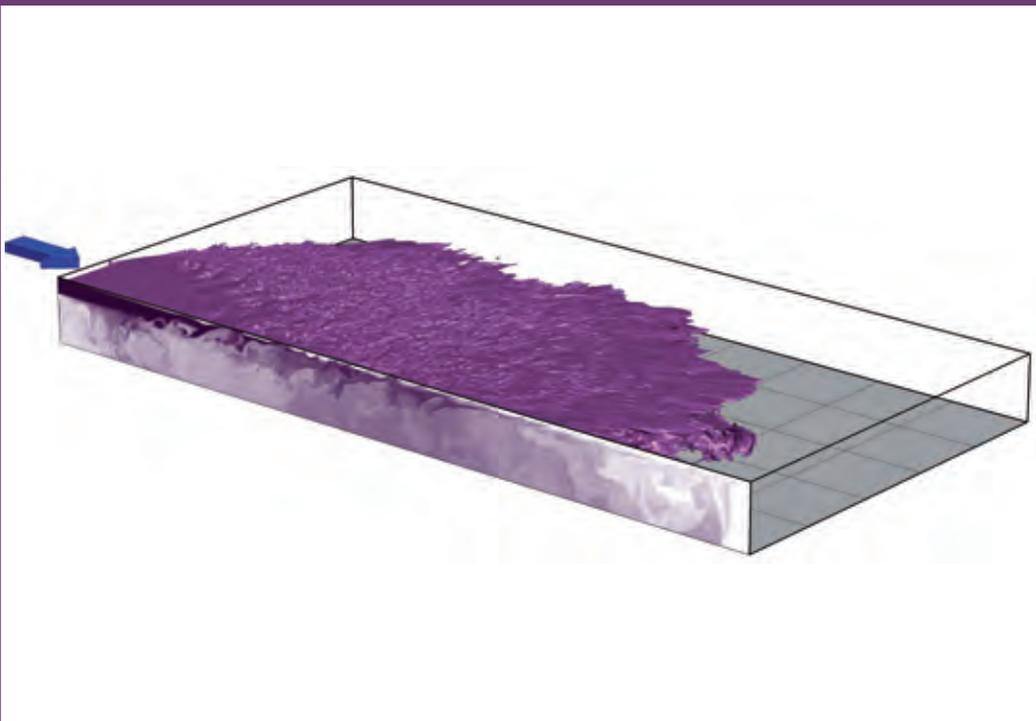


CSE

Computational Science and Engineering

Annual Report
2010 / 2011



CSE

Computational Science and Engineering

Annual Report 2010 / 2011

August 2010 to July 2011

Impressum:

© 2011
ETH Zürich

Editors:

Ralf Hiptmair, Kaspar Nipp, Wilfred van Gunsteren
ETH Zürich

PDF files of this report are available from:

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

or may be downloaded from:

www.rw.ethz.ch/dokumente/cse_annual_report_1011.pdf

CSE curricula at ETH Zürich on the internet:

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

Cover:

Snapshot of the particle sedimentation in a model estuary: the particle-laden fresh water of the river mixes with the heavier oceanic salt water. The particles (in magenta) separate gradually from the fresh water with increasing distance from the river mouth. The settling process is enhanced by turbulence.

Groups having contributed to this report

Research Group	Institute	Projects	Publs.
P. Arbenz	Computer Science	36 - 40	262
S. Bonhoeffer	Experimental and Theoretical Biology		263
K. Boulouchos	Engines and Combustion Laboratory	41 - 45	265
D. Giardini	Geophysics	46 - 64	266
M. Gross	Visual Computing	65 – 66	268
C. Hafner	Electromagnetic Fields	67	269
D. Helbing	Sociology	69	270
H. Herrmann	Building Materials	70 - 86	274
R. Hiptmair	Seminar for Applied Mathematics	87 - 88	
P. Hora	Virtual Manufacturing	89 - 90	
P. Hünenberger	Physical Chemistry	91 - 97	277
P. Jenny	Fluid Dynamics	98 - 110	280
H. Katzgraber	Theoretical Physics	111 - 118	284
L. Kleiser	Fluid Dynamics	119 - 122	285
M. Kröger	Polymer Physics	123	287
M. Luisier	Integrated Systems Laboratory	124	289
S. Mishra	Seminar for Applied Mathematics	125- 131	290
M. Parrinello	Computational Science & USI	132 - 148	292
R. Peikert	Visual Computing	149 - 150	
M. Quack	Physical Chemistry	151 - 171	294
M. Reiher	Physical Chemistry	172 - 189	297
I. Sbalzarini	Computational Biophysics	190 - 193	299
C. Schär	Atmospheric and Climate Science	194	300
C. Schwab	Seminar for Applied Mathematics	195 - 201	302
P. Tackley	Geophysics	202 - 215	305
M. Troyer	Theoretical Physics		310
W. van Gunsteren	Physical Chemistry	216 - 244	313
P. Werner	Theoretical Physics	245 - 256	321

Table of Contents

1	Introduction	9
2	Education	11
3	CSE Case Studies Seminar	17
4	Computational Highlight	21
5	CSE Research Projects	35
6	High-performance Hardware	257
	6.1 Competence Center for Computational Chemistry	
	6.2 Information Technology Services	
7	Publications in 2010/2011	261

1

Introduction

What do Art and Computational Science and Engineering have in common? Many aspects of course (challenge the human mind, require effort and creativity, are permanently evolving, etc.), but without doubt they both stubbornly defy attempts of a clear-cut definition.

What makes me address this are repeated requests that in my function as director of studies of the CSE curriculum I have to decide whether certain topics of student projects qualify as “genuinely CSE related”. Sometimes this leaves me in a quandary. Of course, when a student proposes a project that merely boils down to the implementation of a user interface for a finite element code it will draw an instant “No”. However, when a graphical tool for modeling complex regulatory networks is to be devised, the “CSE content” is no longer so clear. CSE traditionalists may reject it because there is next to no numerical simulation involved. Proponents of a wider notion will defend it as key component of a systems biology simulation code.

Many more modern developments entail such deliberations; generically, database programming is not regarded as CSE. Yet, more and more scientific simulations rely on massive amounts of data, which renders the efficient use of database technology a core issue for codes. Should I accept the design of database query strategies as a MSc thesis topic in CSE? Computer graphics is a similar borderline case, because many of its modern techniques to achieve realistic rendering heavily rely on physical models and numerical methods originally developed, for instance, for computational fluid dynamics.

The issue also arises with “discrete algorithms”, which were long considered outside CSE, but may soon be accepted as core CSE methods. Think of computational genomic research and its massive use of search and combinatorial pattern matching techniques. Researchers in this field would rightly be upset when told that they are not doing “real computational science”.

So, I am going to adopt a “political solution” to this dilemma, refrain from a definition, and pursue the very didactic policy of “definition by example”. This is also the purpose of this report: it is intended to define by example what is the concept of CSE at ETH Zürich. It demonstrates the very broad scope and diversity of CSE research. It strives to be comprehensive and to include everybody who considers his work related to CSE. All these researchers are invited to contribute and, unlike in the case of student projects, there is no screening, whether somebody “really does CSE”.

Zürich, November 9, 2011

Ralf Hiptmair,

Director of Studies CSE, member of the CSE Committee
SAM, ETH Zürich, CH-8092 Zürich, hiptmair@sam.math.ethz.ch

2

Education

In September 2010, 29 new students started their CSE Bachelor studies, 23 in the first semester and 6 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 2010/2011 was 120 (78 in the BSc program and 42 in the MSc program).

In the past academic year 32 students have successfully finished a CSE curriculum, 14 Bachelor students and 18 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, in parentheses, the name and the department of the advisor.

Bachelor Theses

R. Bourquin	Simulation of some non-adiabatic transitions (R. Hiptmair, D-MATH)
O. Brand	Modelling and simulation of learning from imperfect teachers (G. Tröster, D-ITET)
R. Casagrande	Composite finite element method for cellular solids (H. Herrmann, D-BAUG)
S. Deflorin	Explosive Percolation (H. Herrmann, D-BAUG)
A. Felder	Explosive Percolation (H. Herrmann, D-BAUG)
R. Gander	Level set in n Dimensions for C++ (J. Stelling, D-BSSE)
G. Härdi	Numerical Modelling and Comparison of Rigid-Body Swimming Micro-robots (B. Nelson, D-.MAVT)
D. Hupp	Comparison between BAMPS and relativistic lattice Boltzmann simulations of shock waves in quark-gluon plasma (H. Herrmann, D-BAUG)
U. Koch	Finite element computation of eigenvalues (C. Hafner, D-ITET)
N. Lardelli	Density profile analysis of 3D collapsing soil mode (H. Herrmann, D-BAUG)

- Y. Poltera Driven Ising Systems
(H. Herrmann, D-BAUG)
- M. Steinlechner A boundary element method for solving eigenvalue PDEs
(D. Kressner, D-MATH)
- S. Thöni Programming a Humanoid
(R. Riener, D-MAVT)
- P. Wyss Flexibility of Robust Risk Portfolios
(H. Lüthi, D-MATH)

Master Theses

- M. Amundadottir The demand pattern as driver of an optimal inventory policy
(H. Lüthi, D-MATH)
- N. Bedziuk Correlation skew modelling
(C. Schwab, D-MATH)
- S. Birri Continuous-Time Multivariate Asset Allocation
(H. Soner, D-MATH)
- R. Das Gupta Sparse Representations for SD objects
(M. Gross, D-INFK)
- R. Deb Modelling molecular mixing in spatially inhomogeneous turbulent flows
(P. Jenny, D-MAVT)
- A. Hildebrand Parallel solution of time-periodic problems
(L. Kleiser, D-MAVT)
- F. Imtiaz Emergence of Reflexive Behavior from Single Muscle Twitches
(F. Iida, D-MAVT)
- M. König Design and implementation of parallel island models for CMA-ES
(I. Sbalzarini, D-INFK)
- J. Lee Coarse-scale Moment Closure of Unstable Miscible Flow in Porous media
(P. Jenny, D-MAVT)
- P. Merz Molecular Dynamics Simulation in Artificial Ensembles
(W. van Gunsteren, D-CHAB)

G. Moll	Can measured residual dipolar couplings be sensibly used for structure refinement of proteins (W. van Gunsteren, D-CHAB)
M. Müller	Multi-linear face geometry modelling (L. van Gool, D-INFK)
S. Perez Saaibi	Risk diversification in portfolio optimization (K. Nipp, D-MATH)
E. Skopelitis	Towards a steady state spectral element solver for thermo-diffusive combustion models (K. Boulouchos, D-MAVT)
R. Vetter	Packing of elasto-plastic wires in three dimensional (H. Herrmann, D-BAUG)
S. Wettstein	Modified Invasion Percolation on Fracture Networks (H. Herrmann, D-BAUG)
Z. Zhu	Interaction Modelling for Online Social Networks (R. Wattenhofer, ITET)
M. Zollinger	Multilevel Monte Carlo for elliptic SPDEs (C. Schwab, D-MATH)

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

Term Papers

R. Das Gupta	Vectorized Random Number Generation for C++ (M. Troyer, D-PHYS)
S. Datye	Variability in Transport Micro-simulations Investigated for MATSim (K. Axhausen, D-BAUG)
R. Hellmüller	Checkpoint/Restart of massively parallel simulations (I. Sbalzarini, D-INFK)
A. Hildebrand	Fast Solvers for Eulerian Convection Schemes (R. Hiptmair, D-MATH)
S. Mani	On the fly re-meshing for cloth and thin shell animations (M. Gross, D-INFK)

- | | |
|-----------------|--|
| P. Merz | Basis Functions for an Infinite Potential Well with Constant Gradient Potential
(M. Troyer, D-PHYS) |
| M. Nescher | Krylov subspace recycling in the simulation of particle beams
(P. Arbenz, D-INFK) |
| T. Setz | Wavelet analysis of non-stationary time series
(D. Würtz, D-PHYS) |
| E. Skopelitis | Lagrangian particle modelling for heavy particles
(R. Hiptmair, D-MATH) |
| M. Steinlechner | Load balancing massively parallel Hartree-Fock calculations for large systems
(J. Hutter, Physikalisch Chemisches Institut, Uni Zürich) |

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 31, 2011

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 HS10

- | | |
|----------|---|
| 30.09.10 | G. Sartoris, ZHAW, Winterthur
2D+1D modeling of fuel cells |
| 07.10.10 | P. Jenny, Fluid Dynamics
A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion |
| 14.10.10 | M. Agio, Physical Chemistry
Light and photons in complex media: from classical to quantum computational electrodynamics |
| 21.10.10 | H.R. Künsch, Statistics
Climate models, uncertainty and statistics |
| 18.11.10 | D. Leuenberger, MeteoSwiss, Zürich
Forecasting the weather with supercomputers |
| 16.12.10 | A. Elsener, Informatik, Uni Zürich
An atomistic simulation method for oxygen impurities in aluminium based on variable charge molecular dynamics |

Case Studies Seminar FS11

- 03.03.11 Michael Spreng, AutoForm, Zürich
Simulation of sheet metal forming
- 17.03.11 Philipp Weis, Geochemie und Petrologie
Magmatic copper and gold deposits: Simulating compressible
multi-phase flow of hydrothermal fluids in the Earth's crust
- 24.03.11 Christine Bolliger, Clinical Research, Universität Bern
In vivo magnetic resonance spectroscopy: A non-invasive method
to quantify metabolite concentrations in human organs
- 07.04.11 Julian Engel, SENSIRION, Stäfa ZH
Gas flow sensor optimization
- 12.05.11 Merijn Schenk, Risk Modelling, SwissRe, Zürich
Modelling risk in reinsurance

4

Computational Highlight

Particle transport and settling in a model estuary

R. Henniger, L. Kleiser
Institute of Fluid Dynamics

Abstract

We examine the transport and settling of particles in a laboratory-scale model estuary using Direct Numerical Simulation (DNS). The configuration is a shallow saltwater-filled basin with large horizontal dimensions in which particle-laden freshwater enters over a relatively small inlet. Turbulence is generated by the collapse of Kelvin–Helmholtz (KH) vortices triggered in the freshwater/saltwater stratified mixing layer. The flow is computed until a statistically stationary solution is attained. Generally, the shape of the particle plume is characterized by a distinct near-surface plume, a zone of fast particle settling beneath this plume, and a nepheloid layer of slowly settling particles at the bottom of the basin. Our results demonstrate a significant increase of the particle settling speed compared to Stokes particle settling. This increase is attributed to sheet and finger convection for the beginning of the simulation. At later stages, the increased settling speed is a result of the turbulent mixing of the particle suspension with clear ambient fluid, the density differences between the different phases, and the Stokes settling.

1 Introduction

The fate of sedimentary particles on the continental shelves (figure 1) is controlled by many natural processes. One essential contribution is the particle supply by rivers which was estimated by Milliman and Syvitski [13] as approximately ten billion metric tons per year. Riverine particle-laden freshwater is often lighter than the surrounding saltwater, such that the river plumes are positively buoyant, i.e. the estuary is *hypopycnal*. The particles can be transported over relatively large distances with the surface freshwater current. However, the expansion of the particle plume is limited by the particle settling and the decreasing horizontal transport velocity.

Many of the processes involved are not fully understood, e.g. the mixing of freshwater with oceanic brine in the vicinity of river mouths [9] or the details of the particle transport with the buoyant freshwater currents [1, 11, 15]. Field measurements reveal that suspended particles typically settle with relatively large velocities from the freshwater plumes to the ground. These sediment fluxes cannot be explained by Stokes' law for disaggregated constituent grains [11].

The traditional explanation for the fast settling is the *flocculation* of individual particles to larger aggregates leading to correspondingly larger Stokes settling speeds [1, 5]. Another reason might be the influence of *turbulence* on the effective particle settling velocity [11, 15]. Turbulence is generated e.g. by the freshwater inflow, other ambient

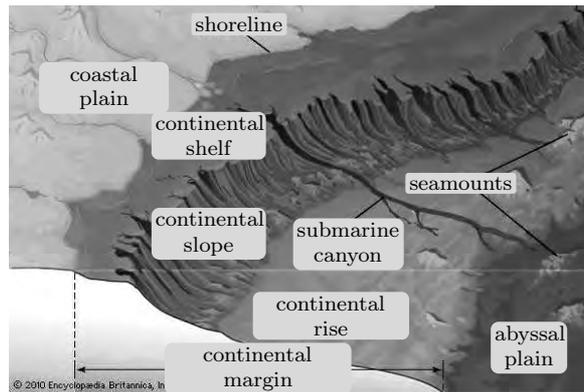


Figure 1: Sketch of a typical continental margin (with shelf, slope and rise) and adjacent abyssal plain (from Encyclopædia Britannica Online).

seawater currents, wind stresses, tides and/or waves. Also, the potential energy of the particle suspension in the buoyant freshwater current can contribute to an enhanced settling.

Other well-known settling-speed increasing mechanisms are the so-called *double-diffusive convection* [6] and the *settling-driven convection* (or *convective sedimentation*) [7], where the particles settle convectively out of an initially stably stratified surface particle plume. The convection is initiated either by diffusive transport and/or by Stokes particle settling. In either case, this mechanism can only explain an initial (i.e. transient) increase of the particle settling speed.

The main reason for the incomplete understanding of the particle settling in estuaries is the fact that a direct observation of such large-scale phenomena is almost impossible because they occur infrequently and unpredictably in remote and inaccessible environments [12] and tend to be destructive to submarine monitoring equipment [8]. As discussed by Meiburg and Kneller [12], the prediction of such flows must be based on an approach combining field observations/measurements, laboratory experiments, mathematical modeling and numerical simulations [12]. In the present work, we perform numerical simulations of particle-laden flows in laboratory-scale model problems to study the fate of the suspended particles.

2 Methodology

2.1 Configuration and characteristic parameters

In our simulations, we take into account only the most important physical effects, i.e. the density differences between particles, freshwater and saltwater, and the turbulent mixing of all species. Flocculation is not considered in order to avoid an interference with these effects. The same applies to other large-scale influences such as Coriolis forces due to earth rotation, tidal currents, wind-induced stresses, temperature gradients and ambient (alongshore) currents. The inertia of individual particles can be expected to have only a rather small impact on the results [3] such that we disregard this feature as well (see also section 2.2).

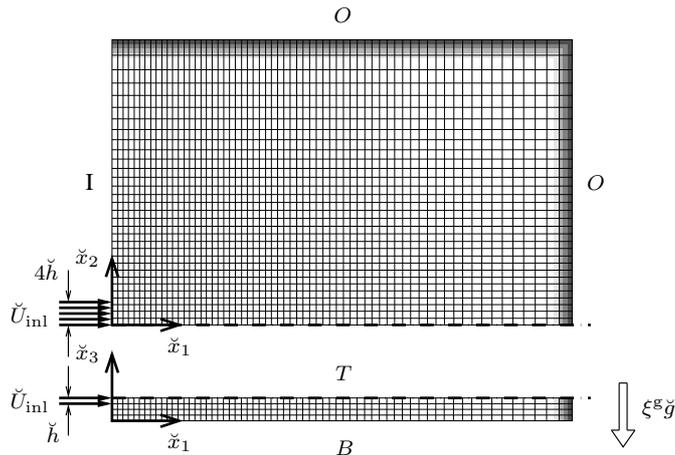


Figure 2: Simulation setup with coarsened computational grid and salinity sponge (gray). Freshwater (with suspended particles) enters the basins in a small portion (arrows) of the inflow planes I and abundant fluid leaves the domains via the outflow boundaries O .

The configuration used in the present work orients itself on the laboratory experiments of Maxworthy [10], Parsons et al. [15] and McCool and Parsons [11] such that qualitative comparisons between the results are feasible. However, these laboratory experiments were constricted by different practical limitations (mainly concerning the outflows and the attainment of proper statistically stationary states) which we can avoid in our numerical approach (cf. [3] for more details).

We use a laboratory-scale model basin with a relatively small (compared to the dimensions of the basin) inlet for the particle-laden freshwater (cf. figure 2). In our parameter range, pure freshwater as well as particle-laden freshwater are lighter than ambient saltwater. Therefore, the saltwater is typically located in the lower part of the domain and it is meaningful to establish the inlet directly at the water surface.

The basin is a rectangular box with dimensions $\check{L}_1 \times \check{L}_2 \times \check{L}_3$ ($\check{\cdot}$ indicates dimensional quantities) in which the flows are described in Cartesian coordinates $\check{x}_1, \check{x}_2, \check{x}_3$. The inflow boundary at $\check{x}_1 = 0$ is denoted as I , the outflow boundaries at $\check{x}_1 = \check{L}_1$ and $\check{x}_2 = \check{L}_2$ as O , the water surface at $\check{x}_3 = \check{L}_3$ as T , and the bottom at $\check{x}_3 = 0$ as B . To save computational effort, we introduce a symmetry plane at $\check{x}_2 = 0$ which halves the computational effort and does not seem to suppress any important effect. To ensure that we have at all times sufficiently large amounts of salinity inside the basin, we establish a salinity sponge [14] at the outflow O .

The reference length and velocity are given by the inlet depth \check{h} and the inflow velocity \check{U}_{inl} , respectively. Moreover, we use the gravitational acceleration \check{g} (acting in the direction $\xi^g = \{0, 0, -1\}^T$), the kinematic viscosity $\check{\nu}$, the freshwater density $\check{\rho}$, the particle density $\check{\rho}_{\text{grain}}$, the particle radius \check{r}_{grain} , the maximum particle volume fraction (observed at the inlet), ϕ_{part}^V , and the diffusivity \check{D}_{part} of the particle suspension as the reference quantities for our simulations. The maximum saltwater density $\check{\rho}_{\text{sal}}$ and salinity diffusivity \check{D}_{sal} are employed to characterize the salinity. With these quantities, the reduced gravitational accelerations of the particle suspension and the salinity read

$$\check{g}_{\text{part}}^r = \left[\frac{\check{\rho}_{\text{grain}}}{\check{\rho}} - 1 \right] \check{g} \phi_{\text{part}}^V \quad \text{and} \quad \check{g}_{\text{sal}}^r = \left[\frac{\check{\rho}_{\text{sal}}}{\check{\rho}} - 1 \right] \check{g}, \quad (1)$$

respectively, with which we define the Reynolds and Richardson numbers

$$Re = \frac{\check{U}_{\text{inl}}\check{h}}{\check{\nu}}, \quad Ri_i = \frac{\check{g}_i^r\check{h}}{\check{U}_{\text{inl}}^2}, \quad i = \{\text{part}, \text{sal}\}, \quad (2)$$

respectively. Throughout this work, ‘part’ refers to the particle suspension and ‘sal’ to the salinity. The corresponding Schmidt numbers are defined as

$$Sc_i = \frac{\check{\nu}}{\check{D}_i}, \quad i = \{\text{part}, \text{sal}\}, \quad (3)$$

and the nondimensional Stokes particle settling velocity U_{part}^s (scalar, in gravity direction ξ^g) with which individual particles settle in fluid at rest as

$$U_{\text{part}}^s = \frac{\check{U}_{\text{part}}^s}{\check{U}_{\text{inl}}} = \frac{2}{9} \frac{\check{r}_{\text{grain}}^2 \check{g}_{\text{part}}^r}{\check{\nu} \check{U}_{\text{inl}} \phi_{\text{part}}^V} \quad (4)$$

for the present configuration.

Most of the values of the characteristic parameters used in this work are about the same as in the simulations performed by Henniger et al. [3] and in the experiments of McCool and Parsons [11]. They refer to realistic scenarios except for the values of the Reynolds number and the Schmidt numbers which are restricted by the available computing resources. We perform DNS such that all length and time scales of the flow are resolved. The DNS approach minimizes the degree of modeling; however, it also limits us to at most laboratory-scale configurations due to the high numerical costs connected to larger configurations (nevertheless, the results of Henniger [2] indicate that even relatively small flow configurations might be sufficient to study and predict fundamental mechanisms at a high level of accuracy).

We set the Schmidt numbers to $Sc_{\text{sal}} = 1$ and $Sc_{\text{part}} = 2$ in order to avoid very fine grids which would be necessary to resolve steep gradients for $Sc_i \gg 1$. These Schmidt numbers are smaller than realistic values; however, they do usually not affect the overall numerical solution significantly and allow us to set the Reynolds number to a value of $Re = 4000$. Moreover, we employ particles with a settling speed of $U_{\text{part}}^s = 0.015$. The Richardson numbers are set to $Ri_{\text{sal}} = 0.5$ and $Ri_{\text{part}} = 0.05$ to obtain a slightly supercritical and hypopycnal [15] inflow. These are ‘typical’ values observed in genuine estuaries [5]. The width of the inlet as well as the total basin depth are set to 4, cf. figure 2. The spatial domain has the dimensions $L_1 \times L_2 \times L_3 = 65 \times 40 \times 4$ and the solution is advanced in time until $t = t_{\text{end}} = 1350$.

2.2 Governing equations

Since typical riverine sediment consists mainly of relatively small and not too heavy particles [11] we can describe the particles as a continuous concentration field. Such an Eulerian approach is also well suited for the salinity such that the nondimensional transport equations for the concentrations $c_{\text{part}} \geq 0$ and $c_{\text{sal}} \geq 0$ read

$$\frac{\partial c_{\text{part}}}{\partial t} + (u + U_{\text{part}}^s \xi^g) \cdot \nabla c_{\text{part}} = \frac{1}{Re Sc_{\text{part}}} \Delta c_{\text{part}}, \quad (5)$$

$$\frac{\partial c_{\text{sal}}}{\partial t} + u \cdot \nabla c_{\text{sal}} = \frac{1}{Re Sc_{\text{sal}}} \Delta c_{\text{sal}} + f_{\text{sal}}^c \quad (6)$$

with u as the fluid velocity and the salinity sponge f_{sal}^c .

Generally, we can assume that the carrier fluid is incompressible and that all density variations due to salinity and suspended particles are very small compared to the mean density [3]. Therefore, we can apply the Boussinesq approximation with which the Navier–Stokes equations for incompressible flows read (in nondimensional form)

$$\frac{\partial u}{\partial t} + (u \cdot \nabla) u = -\nabla p + \frac{1}{Re} \Delta u + f^u, \quad (7a)$$

$$\nabla \cdot u = 0, \quad (7b)$$

where the pressure p is normalized by the mean density. Nevertheless, the density differences due to suspended particles and/or salinity lead to additional volumetric forces f^u on the carrier fluid,

$$f^u = \xi^g (Ri_{\text{part}} c_{\text{part}} + Ri_{\text{sal}} c_{\text{sal}}). \quad (8)$$

In order to obtain a well-posed problem, we need to specify also appropriate initial conditions $u(x, t = 0)$ and boundary conditions $u(x \in \partial\Omega, t)$ for the velocity u ($\partial\Omega = B \cup I \cup O \cup T$ is the entire boundary of the spatial domain Ω). For simplicity, we assume a non-deformable water surface T which is best described by a free-slip boundary for the fluid velocity u ,

$$u \cdot \xi^n = 0, \quad (\xi^n \cdot \nabla)(u - (u \cdot \xi^n) \xi^n) = 0 \quad \text{at } x \in T. \quad (9)$$

Furthermore, we employ Dirichlet boundary conditions for the concentrations c_i , $i = \{\text{part}, \text{sal}\}$, and for the velocity u ,

$$c_{\text{part}} = F \quad \text{at } x \in I, \quad (10a)$$

$$c_{\text{sal}} = 1 - F \quad \text{at } x \in I, \quad (10b)$$

$$u = \{F, 0, 0\}^T \quad \text{at } x \in I, \quad (10c)$$

$$u = \{0, 0, 0\}^T \quad \text{at } x \in B, \quad (10d)$$

with a suitable function F for the definition of the inlet. To trigger disturbances in the inflow, we excite the shear flow instability by moving the vertical position of the interface randomly about the average position. Moreover, we use no-flux and advective boundary conditions, respectively,

$$\xi^n \cdot \left\{ c_i u_i^{\text{b,c}} - \frac{1}{Re Sc_i} \nabla c_i \right\} = 0 \quad \text{at } x \in \partial\Omega \setminus I \quad \text{for } \xi^n \cdot u_i^{\text{b,c}} \leq 0, \quad (11a)$$

$$\frac{\partial c_i}{\partial t} + u_i^{\text{b,c}} \cdot \nabla c_i = 0 \quad \text{at } x \in B \cup O \quad \text{for } \xi^n \cdot u_i^{\text{b,c}} > 0, \quad (11b)$$

$$\frac{\partial u}{\partial t} + (u^{\text{b,u}} \cdot \nabla) u = 0 \quad \text{at } x \in O, \quad (11c)$$

where $u_i^{\text{b,c}} = u + U_i^s \xi^g$ denotes the advection velocity of the concentration c_i (note that $U_{\text{sal}}^s \equiv 0$) and

$$u^{\text{b,u}} = u + (U^{\text{b,n}} - u \cdot \xi^n) \xi^n \quad \text{with } U^{\text{b,n}} > \max_{x \in O, t} \{u \cdot \xi^n, 0\} \quad (12)$$

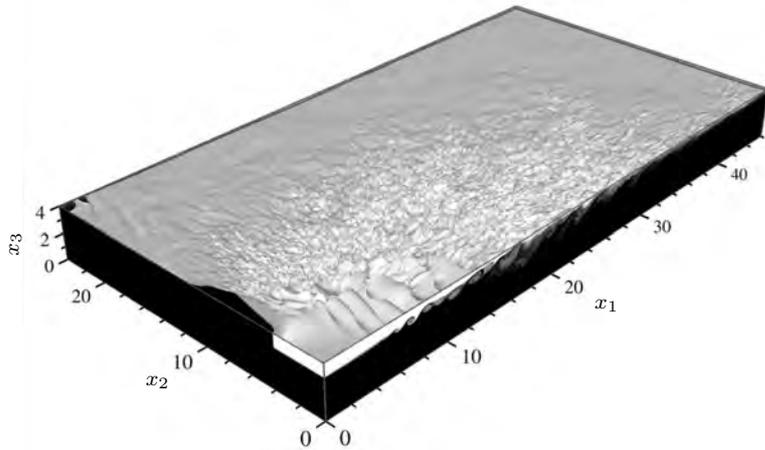


Figure 3: Salt concentration c_{sal} around the freshwater inflow region at $t = 0$. Isosurfaces (gray): $c_{\text{sal}} = 0.75$. Lateral faces: white: $c_{\text{sal}} = 0$ (freshwater); black: $c_{\text{sal}} = 1$ (saltwater).

is the advection velocity of the fluid at the boundary. The parameter $U^{b,n}$ is the fluid advection velocity in the boundary-normal direction ξ^n . It needs to be specified appropriately.

The advective boundary conditions (11b) & (11c) are well suited to mimic an ‘indefinitely’ large basin reminiscent of an ocean. Since the outflow boundary conditions in the present form would successively wash the salt concentration out of the domain, we replace equation (11a) by $c_{\text{sal}} = 1$ at $x \in O$ for $u_{\text{sal}}^{b,c} \leq 0$. This measure ensures that an appropriate and unique statistically stationary state exists at later times.

We initiate the simulation without particles and compute the flow until the freshwater/saltwater mixture has attained a statistically stationary state. Then, at a time denoted as $t = 0$, the freshwater/saltwater base flow has fully developed and we start adding the particles to the freshwater inflow. Generally, time-averages for the analysis of the statistically stationary state are indicated by the operation

$$\langle \cdot \rangle = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} (\cdot) dt^* \quad (13)$$

with $t_1 = 1\,000$ and $t_2 = 1\,350$.

The numerical method used in this work is described by Henniger [2] and Henniger et al. [4] in detail. It is based on a finite-difference approach of at least 5-th order in space and a three-step third-order Runge–Kutta time integration scheme. The pressure is computed iteratively using a multigrid-preconditioned BiCGstab solver. We use an equidistant grid in the vertical direction and stretched grids in the horizontal directions with $N_1 \times N_2 \times N_3 = 4\,609 \times 3\,073 \times 513$ grid points and compute the solution over 580 000 time steps.

3 Interaction of freshwater and ambient saltwater

We begin with a brief study of the freshwater/saltwater mixing. A snapshot of the statistically stationary state is depicted in figure 3 (yet without particles). The picture reveals

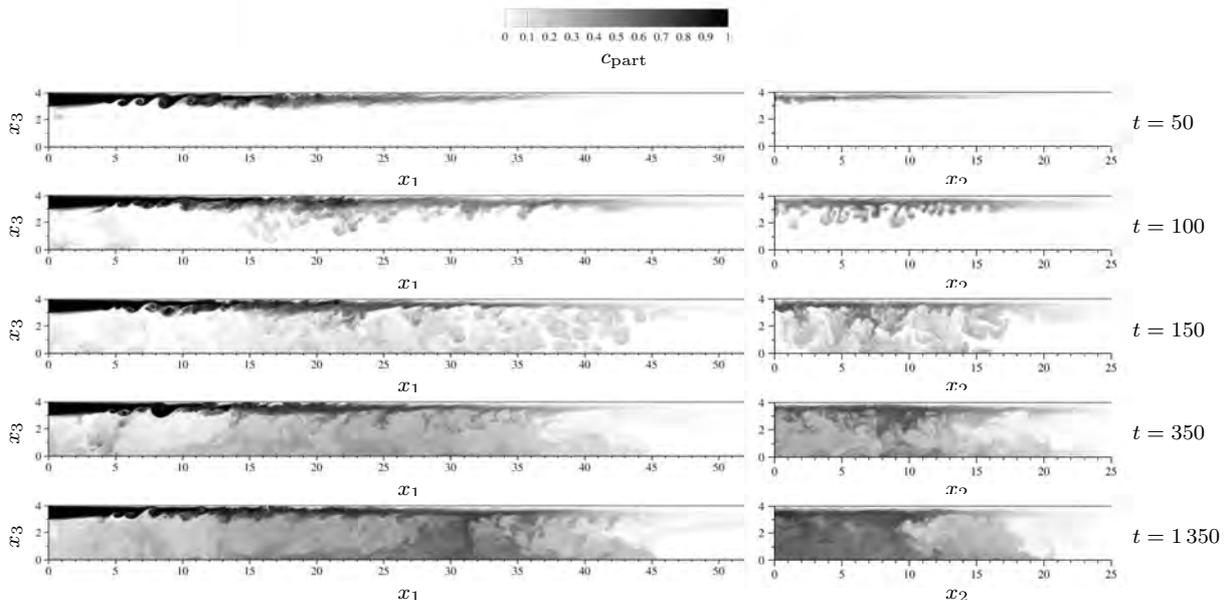


Figure 4: Particle concentration c_{part} in the planes $x_2 = 3$ (left column) and $x_1 = 30$ (right column) at different times in the transient ($t \lesssim 1000$) and statistically stationary ($t \gtrsim 1000$) stages. White: $c_{\text{part}} = 0$ (clear fluid); black: $c_{\text{part}} = 1$ (maximum particle concentration).

that two-dimensional KH waves evolve quickly at the interface and travel downstream up to $x_1 \approx 15 \dots 20$. The billows expand laterally with growing distance to the inflow as a result of the horizontal spreading of the freshwater plume. The limited inlet width triggers strong secondary instabilities in the lateral direction which contribute to the collapse of the KH billows. Before they collapse, they plunge deeper below the water surface such that the resulting more unstable stratification contributes to the breakdown. The collapse strongly enhances the mixing of the freshwater with the ambient saltwater. The mixing in all other areas beyond the turbulent zone is dominated by diffusion.

4 Particle transport and settling

4.1 Particle distribution

The following results for the particle transport and settling are *qualitatively* not very sensitive with respect to variations of the characteristic parameters, except for large values of the Richardson number of the particle suspension, Ri_{part} . Therefore, our observations turn out to be more or less ‘unique’ for small Ri_{part} . To examine the evolution of the particle plume, we visualize two representative slices through the plume at $x_2 = 3$ and $x_1 = 30$ at different times $t = 50, 100, 150, 350, 1350$ (figure 4). Additionally, an isosurface of the particle concentration is depicted from below in figure 5 at the same instances.

In the vicinity of the inflow, the particles are transported rather passively with the surface freshwater current because the inertia of the particle-laden freshwater dominates over other forces acting on the particles. Because the thickness of the freshwater layer

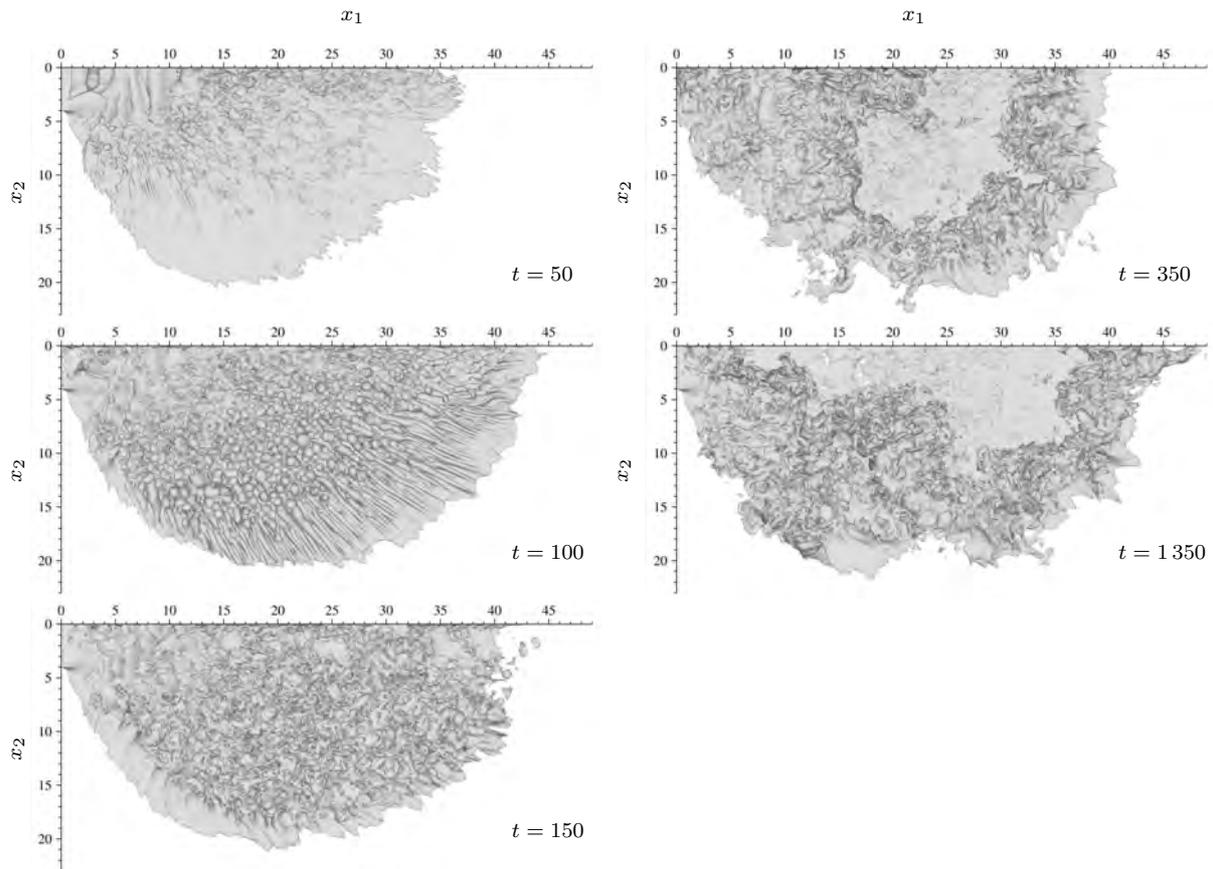


Figure 5: Isosurface ($c_{\text{part}} = 0.25$, seen from below) of the particle concentration c_{part} at different times.

decreases with increasing distance to the inlet, the particles are slightly lifted, especially in the vicinity of the inlet. Moreover, the transport velocity decelerates farther away from the inlet due to the spreading in both horizontal directions such that the impact of the inertial forces diminishes. Correspondingly, the density differences, viscous/diffusive effects and also the Stokes settling velocity of the particle concentration play a more important role. The particles form a *near-surface particle plume* [10, 11, 15] in the freshwater/saltwater interface.

Around $t \approx 100$, we observe so-called *sheet settling convection* [15] close to the near-surface particle plume, followed by *finger settling convection* [15] closer to the ground. The sheets are approximately aligned with the surface streamlines (not shown). We suspect that the shear stresses caused by the transversal freshwater current at the surface and the saltwater backflow beneath are responsible for this phenomenon, see also [3]. It is quite obvious that the sheet/finger convection is related to so-called *double-diffusive (particle) convection* and *settling-driven convection/convective sedimentation* [6, 7].

Beyond $t \approx 100$, the shape and horizontal expansion of the particle plume remain about the same and only the particle concentration beneath the near-surface plume in the freshwater/saltwater interface gradually increases. However, the average concentration is still lower than in the near-surface plume. Additionally, the particle motion is more disordered and isotropic than during the initial transient because the flow is now fully

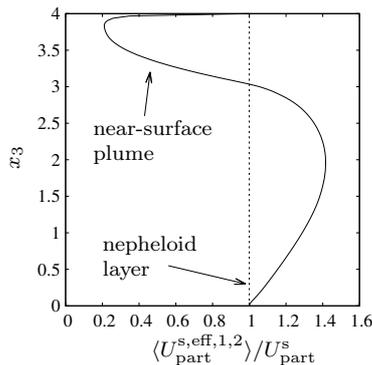


Figure 6: Horizontally and temporally averaged particle settling velocity, $\langle U_{\text{part}}^{\text{s,eff},1,2}(x_3) \rangle$, for the statistically stationary state. A value of unity indicates an average settling with the Stokes value.

turbulent in these areas. We also observe a so-called *nepheloid layer* close to the bottom formed by slower settling particles. Such layers were also reported by McCool and Parsons [11]. Around $t \approx 1000$, the flow has attained a statistically stationary state indicated e.g. by the total mass of suspended particles (not shown here).

4.2 Vertical mass flux, particle distribution and effective particle settling velocity

In the present case, the so-called *effective* particle settling speed [5] considers both the advective transport with $u \cdot \xi^g$ in the gravity direction and the Stokes drift U_{part}^s . We can assess it by averaging both contributions over space and/or time (using a meaningful control volume and/or time interval). For the statistically stationary state, we average the vertical advection velocity over each horizontal plane independently,

$$U_{\text{part}}^{\text{s,eff},1,2}(x_3, t) = \int_0^{L_2} \int_0^{L_1} c_{\text{part}}(u + U_{\text{part}}^s \xi^g) \cdot \xi^g dx_1^* dx_2^* / \int_0^{L_2} \int_0^{L_1} c_{\text{part}} dx_1^* dx_2^*. \quad (14)$$

The time-average of this expression, $\langle U_{\text{part}}^{\text{s,eff},1,2} \rangle$, is depicted in figure 6. Obviously, the particles attain their maximum effective settling speed slightly below the basin half-height ($x_3 \approx 2$), whereas the particles in the near-surface particle plume settle only very slowly on average, even slower than the Stokes settling velocity. The latter observation is attributed to the lift (cf. section 4.1) and the horizontal spreading of the particles near the inflow. The effective settling velocity at the bottom B equals the Stokes settling velocity corresponding to the boundary condition (10).

To illustrate the evolution of the effective particle settling speed over time, we average $(u + U_{\text{part}}^s \xi^g) \cdot \xi^g$ over a meaningful subvolume Ω^{sd} , i.e. we compute

$$U_{\text{part}}^{\text{s,eff}} = \int_{\Omega^{\text{sd}}} c_{\text{part}}(u + U_{\text{part}}^s \xi^g) \cdot \xi^g dV / \int_{\Omega^{\text{sd}}} c_{\text{part}} dV. \quad (15)$$

The result of this expression strongly depends on the choice of Ω^{sd} . We choose $\Omega^{\text{sd}} = \{1 \leq x_3 \leq 2\}$ because we observed the largest values of $\langle U_{\text{part}}^{\text{s,eff},1,2} \rangle / U_{\text{part}}^s$ for this interval, cf. figure 6. The result is plotted in figure 7. Obviously, the effective particle settling

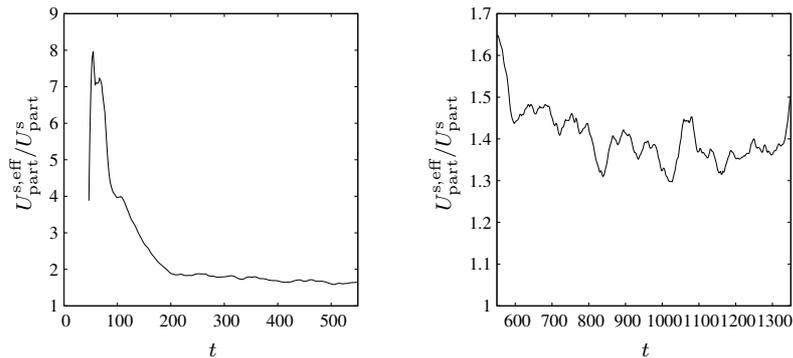


Figure 7: Temporal evolution of the spatially averaged particle settling velocity, $U_{\text{part}}^{\text{s,eff}}$, during the initial transient and the later statistically stationary state.

velocity reaches its maximum in the interval $t \approx 50 \dots 100$, i.e. during the period of intense sheet/finger convection (cf. section 4.1 and figures 4 & 5). The *relative* increase of the spatially averaged settling velocity, $(U_{\text{part}}^{\text{s,eff}}/U_{\text{part}}^{\text{s}} - 1)$, attains a value of up to 700% and drops to about 40% on average for the statistically stationary state. Generally, the results for the transient phase roughly agree with the laboratory experiments of McCool and Parsons [11], although a serious comparison between the numerical simulations and the laboratory experiments is not feasible because the values of the characteristic parameters as well as the configurations are not identical, cf. also Henniger et al. [3].

5 Summary and discussion

The main objective of this study was to predict and understand the shape and temporal evolution of particle plumes in estuaries. In the areas where the inertia of the carrying freshwater is dominant, the particles are transported rather passively. Farther away from the inflow, the particles settle out of the freshwater plume and deposit on the ground. Our simulation is able to reproduce basic particle settling mechanisms such as sheet/finger settling convection and turbulence-enhanced particle settling. These phenomena can be observed within a certain transient period of time after adding the particles to the inflow. Later, a statistically stationary state is attained, i.e. the particle supply and the deposition rate are balanced on average. The flow is fully turbulent at this stage.

The sheet/finger settling state is connected to a strong transient increase of the effective particle settling speed (expressed by the velocities $U_{\text{part}}^{\text{s,eff}}$ and $U_{\text{part}}^{\text{s,eff},1,2}$, cf. section 4.2) of up to about 700%. These numbers drop to smaller values on the order of 40% as soon as the flow has reached the statistically stationary state. Especially the latter numbers cannot be compared directly with laboratory experiments, because such states were not attained in any comparable experimental study (at least to our knowledge).

As explained in Henniger et al. [3], local concentration gradients in the particle plume are required to achieve an increase of the effective settling speed. This is quite obvious for the sheet/finger convection state. For the statistically stationary state, such gradients can be established by convectively mixing the particle suspension with clear ambient fluid. The convective motion can be provided by turbulence. The inertia of individual particles suspended in turbulent fluid usually leads to concentration gradients as well; however,

this effect was assumed to be negligible for the present study [3].

We found that a distinct near-surface particle plume establishes in the beginning of the simulations and persists in a less distinct form also during the statistically stationary states. Its shape is governed by the surface freshwater current and the (relatively weak) backflow beneath. The backflow results from the entrainment of ambient fluid with the freshwater plume. Moreover, a nepheloid layer (cf. section 4.1) can be observed close to the ground. This feature is a consequence of the fast particle settling directly beneath the near-surface plume and the rather low particle deposition rate on the ground.

Acknowledgements

We thank Eckart Meiburg for stimulating this research project and for giving precious input and advice. The work has been supported through the ETH research grant TH-23/05-2. The presented simulation was conducted as a 'high-impact project' at the Swiss National Supercomputing Centre (CSCS) consuming about 8 Mio. CPU hours on a Cray XT5.

References

- [1] W. R. Geyer, P. S. Hill, and G. C. Kineke. The transport, transformation and dispersal of sediment by buoyant coastal flows. *Cont. Shelf Res.*, 24:927–949, 2004.
- [2] R. Henniger. *Direct and large-eddy simulation of particle transport processes in estuarine environments*. PhD thesis, ETH Zürich, Zürich, Switzerland, 2011. Diss. ETH No. 19656, available online at <http://e-collection.library.ethz.ch/view/eth:2996>.
- [3] R. Henniger, L. Kleiser, and E. Meiburg. Direct numerical simulations of particle transport in a model estuary. *J. Turbulence*, 11:N 39, 2010.
- [4] R. Henniger, D. Obrist, and L. Kleiser. High-order accurate solution of the incompressible Navier–Stokes equations on massively parallel computers. *J. Comput. Phys.*, 229(10):3543–3572, 2010.
- [5] P. S. Hill, T. G. Milligan, and W. R. Geyer. Controls on effective settling velocity of suspended sediment in the Eel River flood plume. *Cont. Shelf Res.*, 20:2095–2111, 2000.
- [6] D. C. J. D. Hoyal, M. I. Bursik, and J. F. Atkinson. The influence of diffusive convection on sedimentation from buoyant plumes. *Mar. Geol.*, 159(1–4):205–220, 1999.
- [7] D. C. J. D. Hoyal, M. I. Bursik, and J. F. Atkinson. Settling-driven convection: A mechanism of sedimentation from stratified fluids. *J. Geophys. Res.*, 104(C4):7953–7966, 1999.
- [8] D. L. Inman, C. E. Nordstrom, and R. E. Flick. Currents in submarine canyons: an air-sea-land interaction. *Annu. Rev. Fluid Mech.*, 8:275–310, 1976.
- [9] D. A. Luketina and J. Imberger. Characteristics of a surface buoyant jet. *J. Geophys. Res.*, 92(C5):5435–5447, 1987.
- [10] T. Maxworthy. The dynamics of sedimenting surface gravity currents. *J. Fluid Mech.*, 392:27–44, 1999.

- [11] W. W. McCool and J. D. Parsons. Sedimentation from buoyant fine-grained suspensions. *Cont. Shelf Res.*, 24:1129–1142, 2004.
- [12] E. Meiburg and B. Kneller. Turbidity currents and their deposits. *Annu. Rev. Fluid Mech.*, 42:135–156, 2010.
- [13] J. D. Milliman and J. P. M. Syvitski. Geomorphic tectonic control of sediment discharge to the ocean—the importance of small mountainous rivers. *J. Geol.*, 100:525–544, 1992.
- [14] J. Nordström, N. Nordin, and D. Henningson. The fringe region technique and the Fourier method used in the direct numerical simulation of spatially evolving viscous flows. *SIAM J. Sci. Comp.*, 20(4):1365–1393, 1998.
- [15] J. D. Parsons, J. W. M. Bush, and J. P. M. Syvitski. Hyperpycnal plume formation from riverine outflows with small sediment concentrations. *Sedimentology*, 48:465–478, 2001.

5

CSE Research Projects

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

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

Institute/ *Chair of Computational Science, ETH Zürich
Group: †Institute for Biomechanics, ETH Zürich

Description:

Micro-structural finite element (μ 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 μ 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 μ FE simulations.

Web sites: <http://people.inf.ethz.ch/arbenz/projects/bone.html>

References:

C. Flaig, P. Arbenz: *A scalable memory efficient multigrid solver for micro-finite element analyses based on CT images*. Parallel Computing (2011), doi:10.1016/j.parco.2011.08.001.

C. Flaig, P. Arbenz: *A highly scalable matrix-free multigrid solver for μ FE analysis based on a pointer-less octree*. Accepted for publication in the proceedings of LSSC 2011.

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.

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

Researchers: Peter Arbenz*
 Andreas Adelman†
 Yves Ineichen*,†

Institute/ *Chair of Computational Science, ETH Zürich
Group: †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:

A. Adelman, P. Arbenz, Y. Ineichen: "Improvements of a fast parallel Poisson solver on irregular domains". Accepted for publication in the proceedings of PARA2010: Workshop on the State-of-the-Art in Scientific and Parallel Computing, Reykjavik, Iceland, June 6-9, 2010.

A. Adelman, P. Arbenz, and 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 Adelman†
 Christof Kraus*

Institute/ *Chair of Computational Science, ETH Zürich
Group: †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. Adelman, 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/ *Chair of Computational Science, ETH Zürich
Group: †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, A. Adelman, P. Arbenz, A. Falone, C. Kraus, and B. Oswald: *Computation of Electromagnetic Modes in the Transverse Deflecting Cavity*. Proceedings of the 2010 International Particle Accelerator Conference, Kyoto, Japan, 2010.

H. Guo, B. Oswald, P. Arbenz: *3-dimensional eigenmodal analysis of plasmonic nanostructures*. 2011. Submitted for publication.

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

Researchers: Peter Arbenz*
Dominik Obrist†

Institute/ *Chair of Computational Science, ETH Zürich
Group: †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. Hildebrand, D. Obrist: *A parallel space-time finite difference solver for periodic solutions of the shallow-water equation*. Accepted for publication in the proceedings of PPAM 2011, Torun, Poland, September 11-14, 2011.

Title: Chaotic dynamics in premixed hydrogen/air channel flow combustion

Researchers: Gianmarco Pizza^{1,2}, Christos E. Frouzakis¹, John Mantzaras²

**Institute/
Group:** ¹Aerothermochemistry and Combustion Systems Laboratory, ETH Zurich

²Combustion Research Laboratory, Paul Scherrer Institute, Villigen

The complex oscillatory behavior observed in fuel-lean premixed hydrogen/air atmospheric pressure flames in an open planar channel with prescribed wall temperature is investigated by means of direct numerical simulations, employing detailed chemistry descriptions and species transport, and nonlinear dynamics analysis. As the inflow velocity is varied, the sequence of transitions includes harmonic single frequency oscillations, intermittency, mixed mode oscillations, and finally a period-doubling cascade leading to chaotic dynamics. The observed modes are described and characterized by means of phase-space portraits and next amplitude maps. It is shown that the interplay of chemistry, transport, and wall-bounded developing flow leads to considerably richer dynamics compared to fuel-lean hydrogen/air continuously stirred tank reactor studies.

References:

- G. Pizza, C.E. Frouzakis, J. Mantzaras, Chaotic dynamics in premixed hydrogen/air channel flow combustion, *Combust. Theory Modeling*, (in press)

Title: Hydrodynamic and thermal-diffusive instability effects on the evolution of laminar planar lean premixed hydrogen flames

Researchers: C. Altantzis¹, C. E. Frouzakis¹, A. G. Tomboulides², M. Matalon³, K. Boulouchos¹

Institute/ Group: ¹Aerothermochemistry and Combustion Systems Laboratory, ETH, Zurich

²University of Western Macedonia, Kozani, Greece

³Dept. of Mechanical Engineering, U. Illinois at Urbana-Champaign, U.S.A.

The instabilities of premixed hydrogen/air flames propagating in 2D channel-like domains are investigated numerically to study the initial linear growth of perturbations superimposed on the planar flame front and long term non-linear evolution. Unity Lewis number, where only hydrodynamic instability appears, as well as subunity Lewis number, where the flame propagation is strongly affected by the combined effect of hydrodynamic and thermal-diffusive instabilities are considered. The dispersion relation between the growth rate and the wavelength of the perturbation characterizing the linear regime is extracted from the simulations and compared with linear stability theory. As predicted by the theory, unity Lewis number flames are found to form a single cusp structure which propagates unchanged with constant speed. The long-term dynamics of the subunity Lewis number flames include steady cell propagation, lateral flame movement, oscillations and regular as well as chaotic cell splitting and merging.

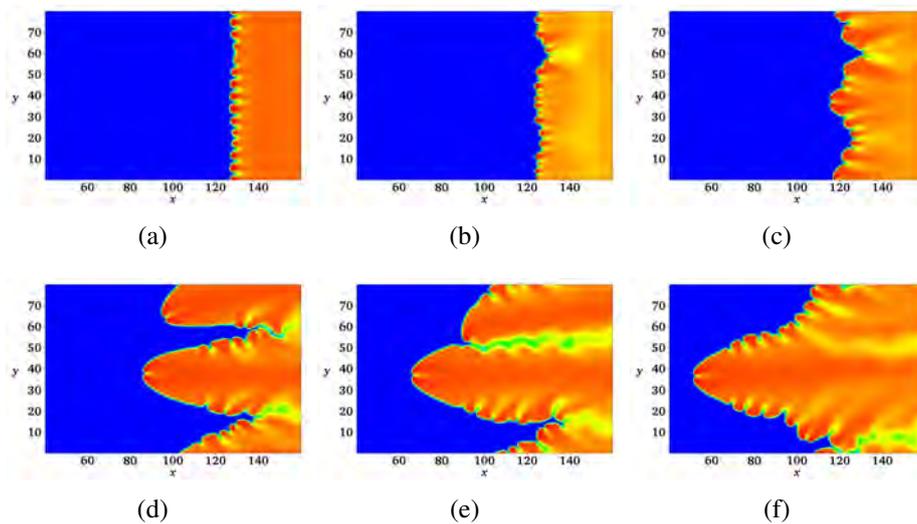


Figure 1: Isocontours of temperature of the $Le_{\text{eff}} = 0.404$ flame propagating in a domain of height equal to 80 planar premixed flame thicknesses.

References:

- 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.*, (submitted).

Title: Adaptive simplification of complex multiscale systems

Researchers: E. Chiavazzo¹ and I. Karlin²

**Institute/
Group:** ¹ Department of Energetics, Politecnico di Torino, 10129 Torino,
Italy
² Aerothermochemistry and Combustion Systems Laboratory, ETH
Zurich

A fully adaptive methodology is developed for reducing the complexity of large dissipative systems. This represents a significant step toward extracting essential physical knowledge from complex systems, by addressing the challenging problem of a minimal number of variables needed to exactly capture the system dynamics. Accurate reduced description is achieved, by construction of a hierarchy of slow invariant manifolds, with an embarrassingly simple implementation in any dimension. The method is validated with the autoignition of the hydrogen-air mixture where a reduction to a cascade of slow invariant manifolds is observed.

References:

E. Chiavazzo and I. Karlin, Adaptive simplification of complex multiscale systems, *Phys. Rev. E* 83, 036706 (2011).

Title: Droplet Collision Simulation by a Multi-Speed Lattice Boltzmann Method

Researchers: Daniel Lycett-Brown¹, Ilya Karlin² and Kai H. Luo¹

Institute/ ¹University of Southampton, UK
Group: ²Aerothermochemistry and Combustion Systems Laboratory, IET, D-MAVT, ETH Zurich

Realization of the Shan-Chen multi-phase flow lattice Boltzmann model is considered in the framework of the higher-order Galilean invariant lattices. The present multi-phase lattice Boltzmann model is used in two-dimensional simulation of droplet collisions at high Weber numbers. Results are found to be in a good agreement with experimental findings.

References:

D. Lycett-Brown, I. Karlin and K. H. Luo, Droplet Collision Simulation by a Multi-Speed Lattice Boltzmann Method, *Commun. Comput. Phys.* 9, 1219-1234 (2011).

Title: Matrix lattice Boltzmann reloaded

Researchers: I. Karlin¹, P. Asinari² and S. Succi³

**Institute/
Group:** ¹ Aerothermochemistry and Combustion Systems Laboratory, ETH
Zurich

² Department of Energetics, Politecnico di Torino, 10129 Torino,
Italy

³ Istituto Applicazioni Calcolo CNR, Via dei Taurini 19, 00185
Roma, Italy

The lattice Boltzmann equation was introduced about 20 years ago as a new paradigm for computational fluid dynamics. In this paper, we revisit the main formulation of the lattice Boltzmann collision integral (matrix model) and introduce a new two-parametric family of collision operators, which permits us to combine enhanced stability and accuracy of matrix models with the outstanding simplicity of the most popular single-relaxation time schemes. The option of the revised lattice Boltzmann equation is demonstrated through numerical simulations of a three-dimensional lid-driven cavity.

References:

I.V. Karlin, P. Asinari and S. Succi, Matrix lattice Boltzmann reloaded, *Phil. Trans. R. Soc. A* 369, 2202-2210 (2011).

Title: Seismic sensitivity to global boundary topography

Researchers: PhD student Andrea Colombi, Dr. Tarje Nissen-Meyer, Dr. Lapo Boschi (all ETHZ)

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

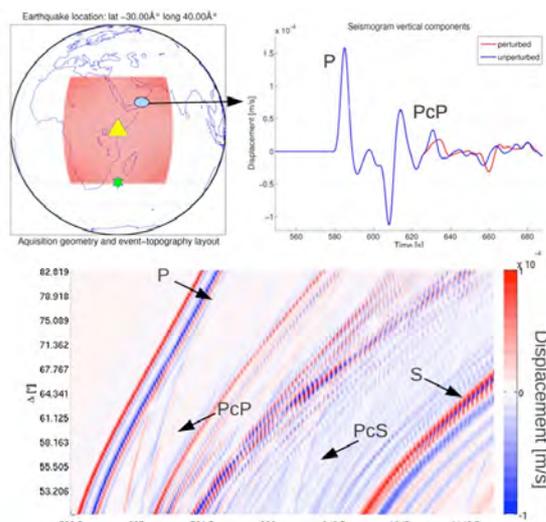
Description: The modern approach to seismic tomography can exploit all the information contained in seismograms, account for the finite-frequency character of the propagating waves and provide models that seem consistent with geodynamics or observations from mineral physics, geology and Earth magnetism. Yet, it fails to provide quantitative uncertainty estimations.

The rigorous mathematic approach of the adjoint method employed to calculate the model derivatives for a 3-D Earth already requires an immense computational power. An uncertainty analysis based on the exploration of the model-parameters space is therefore not yet feasible.

We set up a synthetic experiment to investigate, quantify and potentially improve the resolving power of this tomographic technique. The classical approach to seismic tomography investigates volumetric properties (velocity, density, impedance) of the Earth, disregarding other unknowns such as, for example, boundary perturbations. We include the effect of weak boundary perturbations with respect to the reference model in the synthetic experiment and inversion. Such perturbations, besides their effects being not well known, have not been included as free parameter in a joint full-wave inversion. We investigate the feasibility to resolve a trade off between these two contributions to the observations.

Starting from a known Earth model, slightly modified to embed a topography perturbation to the core mantle boundary, we are computing a collection of synthetic data varying the important parameters (frequency content, source-receiver geometry, structure dimensions...). The reference model being in our hands allows us to quickly evaluate at what extent unknown features has been recovered.

Computational challenges inside the project are several. Filling the database with synthetic seismograms up to 0.2 Hz accurate requires several large scale computations with the spectral element software SPECFEM3D GLOBE for nearly 2 billions degrees of freedom and 2 Tbyte of data. For this phase we have an active allocation at the Swiss Supercomputing Center (CSCS) of 0.5 Millions CPU hours. The application of the full waveform technique for the database inversions is under development using the efficient spectral element solver AXISEM optimized to face the massive I/O that this inversion requires on a reduced number of processors. The software exploits parallel netcdf I/O and is designed to give results up to 0.2 Hz, a frontier in seismology. The vtk visualization is embedded in the code for large dataset on Paraview. This code is currently running on Brutus and Palu.



Records from different sources (stars) & CMB topography (triangle). The topography effect can be observed on seismograms. The database covers a variety of configurations (3D models, topography, source-receiver configurations).

Publications: A. Colombi, T. Nissen-Meyer, L. Boschi, D. Giardini, 2011: Seismic sensitivity to boundary topography, to be submitted to Geoph. J. Int.

Title: Ambient-noise tomography of the European lithosphere

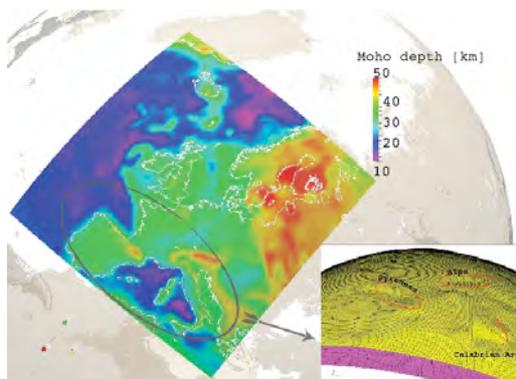
Researchers: Dr. Piero Basini, Dr. Tarje Nissen-Meyer, Dr. Lapo Boschi (all ETHZ)

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

Description: Europe is covered nonuniformly by both seismic instruments and earthquakes. To enhance seismic resolution, it is essential to exploit the information coming from cross-correlation of stacked seismic ambient noise. We compiled a dense regional database of European station-station surface-wave dispersion between 8-35 seconds using noise-interferometry, resulting in a dramatic growth in seismic coverage with respect to earthquake-based tomography. It has recently been shown how adjoint techniques can be applied to ambient-noise data, overcoming the often severe nonuniformity in the geographic distribution of noise "sources", and the subsequent discrepancies between the recorded noise cross-correlation and the theoretical Green's function. We focus on using seismic ambient noise generated in oceans as data to map 3D structure beneath Europe. While earlier "noise-tomography" studies have relied on ray-theory (the infinite-frequency approximation), we apply an iterative, gradient-based inversion where Fréchet derivatives are computed using a spectral-element wave propagation (SPECFEM3D) and adjoint method. The most computationally challenging task consists of constructing surface-wave sensitivity kernels: we proceed by constructing a flexible mesh of the upper mantle, honouring all discontinuities. Restricting ourselves to the shallowest few hundred km of the Earth reduces computational costs significantly, and is perfectly adequate to the data we are interested in. We mesh an initial Earth model which is composed of two contributions:

(1) EPcrust, a new crustal model for the European plate, derived from collection of numerous independent previous studies of multiple scale lengths; (2) a new adaptive-grid surface-wave tomography of the uppermost mantle down to periods of 35 seconds.

The sensitivity kernels we obtain are at the core of an iterative, nonlinear, gradient-based inversion scheme that will ultimately provide a new tomographic image with a resolution much higher than is currently possible. A better understanding of shallow structure in this region will help us map the lithosphere-asthenosphere boundary region, and the upper mantle with increasing accuracy. This is crucial to understand the dynamics of this tectonically complex region. Our parallel simulations run at CSCS. Our model of Europe contains $3 \cdot 10^6$ hexahedral elements in 324 processors, simulations take 1.5 hours at 0.5 Gb per process.



A 3D crustal model, where the crust/mantle interface ("Moho") and surface topography are honored by the hexahedral mesh. The model, based on ballistic sources, is the starting point for iterative inversions with higher-frequency ambient noise.

References:

Basini, P., Nissen-Meyer, T., Boschi, L., Verbeke, J. (2011), Ambient noise correlations for non-linear inversion for upper-mantle structure beneath Europe, *Geoph. J. Int.*, in prep.

Basini, P., et al. (2010), Towards Multi-resolution adjoint Tomography of the European Crust and Upper Mantle, S31A-2005, Fall Meeting, AGU, San Francisco, Calif., 13-17 Dec.

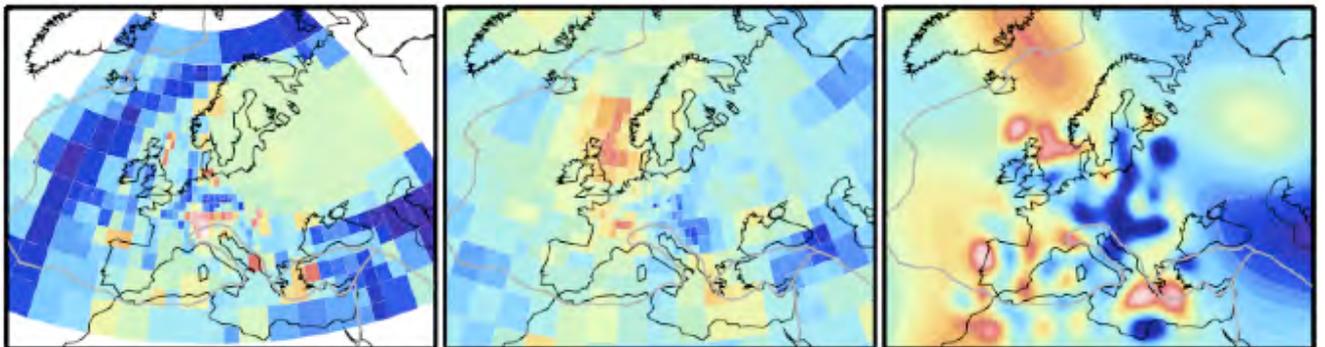
Basini, P., Nissen-Meyer, T., Boschi, L., Schenk, O., Verbeke, J., Giardini, D., Ambient-noise tomography of the European lithosphere: numerical calculation of sensitivity kernels for nonuniform noise-source distributions. *Geoph. Res. Abstr.* Vol. 13, EGU2011-11554, 2011, EGU assembly.

Title: Adaptively Anisotropic Tomography of the European Upper Mantle

Researchers: PhD Student Julia Schäfer, Dr. Lapo Boschi, Prof. Edi Kissling (all ETHZ)

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

Description: Observations of seismic surface waves are a very powerful tool to constrain the 3D structure of the Earth's upper mantle, including its anisotropy, because they sample this volume efficiently due to their sensitivity over a wide depth range along the raypath. On a global scale, surface-wave tomography models are often parameterized uniformly, without accounting for inhomogeneities in data coverage and, as a result, in resolution, that are caused by effective under- or over-parameterization in many areas. If the local resolving power of seismic data is not taken into account when parameterizing the model, features will be smeared and distorted in tomographic maps, with subsequent misinterpretation. Parameterization density has to change locally, for models to be robustly constrained without losing any accurate information available in the best sampled regions. We have implemented a new algorithm for upper mantle surface-wave tomography, based on adaptive-voxel parameterization: high image resolution is achieved in regions with dense data coverage, while lower image resolution is kept in regions where data coverage is poorer. This way, parameterization is everywhere tuned to optimal resolution, minimizing both the computational costs, and the non-uniqueness of the solution. The spacing of our global grid is locally as small as ~50 km. We apply our method to identify a new global model of vertically and horizontally polarized shear velocity, with resolution particularly enhanced in the European lithosphere and upper mantle. We find our new model to resolve lithospheric thickness and radial anisotropy better than earlier results based on the same data.



Radial anisotropy defined as the squared ratio of horizontally vs. vertically polarized shear velocity, obtained from (left) geodynamical modeling, (center) adaptive-resolution tomography and (right) uniform-resolution tomography. Our adaptive approach improves the correlation between tomography and geodynamics.

References:

Schäfer, J., L. Boschi and E. Kissling (2010), Adaptively parameterized 3D models of the European upper mantle from surface wave tomography, QUEST workshop on 'Seismic Wave Propagation'.

Schäfer, J., L. Boschi, and E. Kissling (2010), Adaptively parameterized surface wave tomography: Methodology and a global model of the upper mantle, AGU fall meeting.

Schäfer, J. F., Boschi, L. and Kissling, E. (2011), Adaptively parametrized surface wave tomography: methodology and a new model of the European upper mantle. *Geophysical Journal International*, 186: 1431–1453. doi: 10.1111/j.1365-246X.2011.05135.x.

Schäfer, J. F., Boschi, L., Becker, T., & Kissling, E. (2011), Radial Anisotropy in the European Mantle: Tomographic Studies Explored in Terms of Mantle Flow, submitted to *Geophysical Research Letters*.

Title: Harmonic Earth spectrum inversion of global travel-time data

Researchers: Steve Della Mora (Ph.D. student), Dr. Lapo Boschi (ETHZ), Prof. D. Giardini (ETHZ)

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

Description:

The variance of a set of seismic observations associated with nearby sources and nearby receivers should reflect the degree of complexity of the medium between sources and receivers. We group sources and receivers in geographic bins of varying spatial extent, and measure the dependence of seismic travel-time variance on bin size and mean epicentral distance. We attempt to relate variance, averaged over the whole globe, to a statistical measure of the Earth's complexity: its spherical- harmonic spectrum. We first follow an earlier study by Gudmundsson et al. (1990) and find an approximate analytical relationship between averaged variance and harmonic spectrum: we can then determine the latter from a measurement of the former via a linear least-squares inversion. We next solve the same problem through a massive set of forward calculations, using a genetic algorithm to identify a best-fitting spectrum. The high computational costs require that the genetic algorithm be parallel, and we run on the Brutus cluster the parallel version of the genetic-algorithm package PIKAIA (Metcalf and Charbonneau 2003). This strategy allows us to drop most of the approximations of Gudmundsson et al. (1990). Yet, the resulting resolution of the Earth's spectrum is inferior to that achieved by classical tomography.

References:

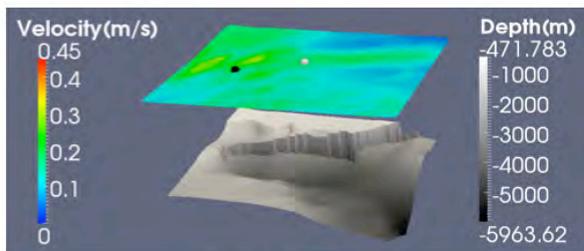
Della Mora, S., L. Boschi, T. W. Becker and D. Giardini, 2011. Can the Earth's harmonic spectrum be derived directly from the stochastic inversion of global travel-time data? *Geophys. J. Int.*, submitted.

Title: 3D elastic wave focusing effects in the Los Angeles basin upon the Northridge earthquake

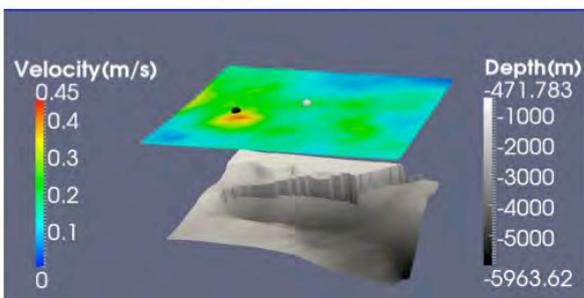
Researchers: Andrea Tesoniero (M.Sc), Dr. Tarje Nissen-Meyer (ETHZ), Dr. Piero Basini (ETHZ)

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

Description: As a consequence of the Mw 6.7 1994 Northridge earthquake, the area of Santa Monica in the Los Angeles basin experienced concentrated and unexpectedly high values of ground shaking. Elastic focusing wave effects have been proposed by several authors as a cause for the enhanced ground shaking. We use a 3D spectral element method to simulate a kinematic point source and finite source models for the Northridge mainshock in a Southern California hexahedral mesh model with the 3D tomographic velocity model CVM-H, including external and internal interface topography. We show how amplification effects of relatively low frequencies (0-0.4Hz) are observed in a limited area in the Santa Monica region when a smoothed representation of the Santa Monica overthrust, that acts as a focusing lens, is specifically honored by the numerical mesh. We present 3 different models of the overthrust, accounting both for the geometrical extent of the smoothed area and for the velocity structures. We modify the velocity model with a distinctive but physically acceptable velocity jump in order to honor the overthrust geometry. This increases the PGV by 40% with respect to the original CVM-H model, matching also the actual amplitudes recorded at the Santa Monica City Hall seismic station. We also show that the geometric extent of the modified area has a higher contribution to the enhanced ground motion than a stronger velocity contrast at the overthrust edge. We conclude that in regions of complex 3D subsurface settings, where complex wave phenomena such as elastic focusing might happen, honoring these structures both numerically (by the mesh model) and physically (by the velocity model) is important for a proper representation of the seismic ground shaking.



(a) Original tomographic model



(b) Sharpened 1 tomographic model

Detailed shakemaps in the Santa Monica region. The geometry and the topographic altitude of the Santa Monica overthrust are also represented in the maps. In the original tomographic model (a) the highest value of PGV was experienced in two zones and it is around 30 cm/s. In the sharpened 1 tomographic model (b), the maximum ground shaking converges to a limited small area just below the seismic station Santa Monica City Hall (black sphere), and it is characterized by a value which is 15% higher than (a).

Conferences:

A. Tesoniero, T. Nissen-Meyer, P. Basini, E. Casarotti, 2012. 3D elastic wave focusing effects in the Los Angeles basin upon the Northridge earthquake. Swiss Geoscience Master Congress.

Publications:

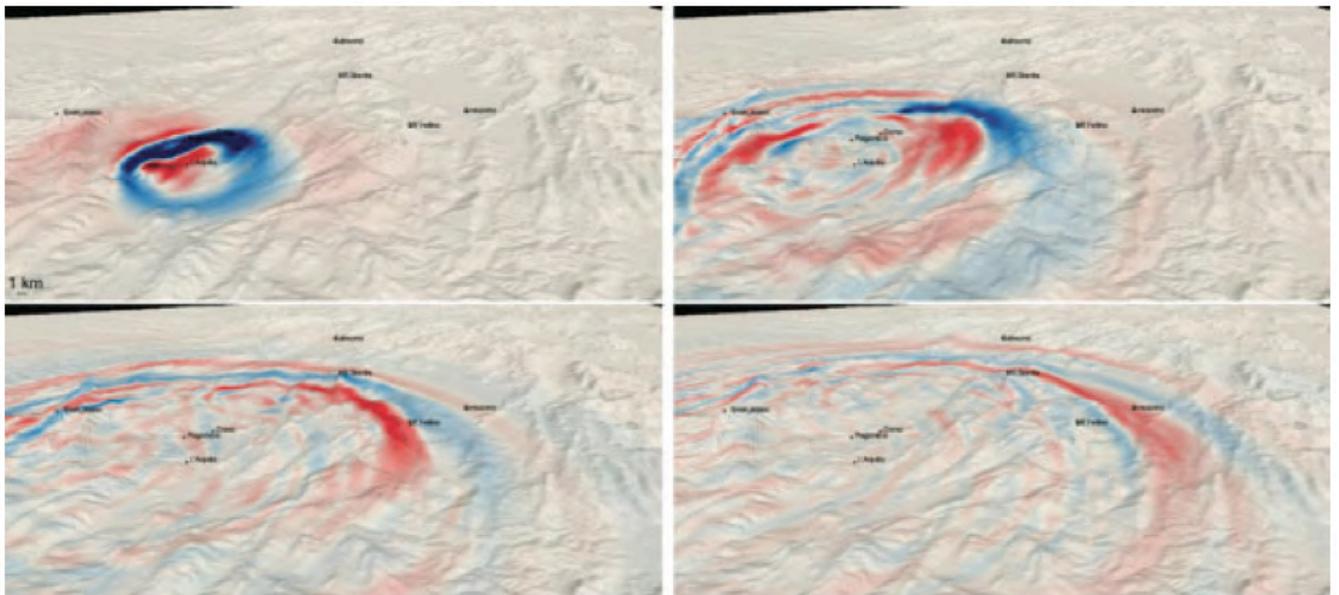
A. Tesoniero, T. Nissen-Meyer, P. Basini, E. Casarotti, 2012. 3D elastic wave focusing effects in the Los Angeles basin upon the Northridge earthquake, in preparation.

Title: Spectral-element simulations of seismic wave propagation on unstructured hexahedral meshes

Researchers: Dr. D. Peter (Princeton University), P. Le Loyer (Universite de Pau), Dr. E. Cassarotti (INGV Rome), Dr. Tarje Nissen-Meyer (ETHZ), Dr. Piero Basini (ETHZ), PhD student Y. Luo (Princeton University), Prof. J. Tromp (Princeton University)

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

Description: We present forward and adjoint spectral-element simulations of acoustic and (an)elastic seismic wave propagation on unstructured hexahedral meshes. Simulations benefit from recent advances in hexahedral meshing, load balancing, and software optimization. Meshing may be accomplished using a mesh generation tool kit such as CUBIT, and load balancing is facilitated by graph partitioning based on the SCOTCH library. Coupling between fluid and solid regions is incorporated using domain decomposition. Topography, bathymetry and Moho undulations are readily included in the mesh, and physical dispersion and attenuation associated with anelasticity are accounted for using a series of standard linear solids. The software is benchmarked against a discrete wavenumber method for a layer-cake model. Finite-frequency Fréchet derivatives are calculated using adjoint methods in both fluid and solid domains. We present various examples of hexahedral meshes, snapshots of wavefields, and finite-frequency kernels generated by the new ‘Sesame’ version of the widely used open source spectral-element package SPECFEM3D.



Wavefield snapshots for the 2009 April 6, L'Aquila earthquake, taken after 6 s, 11 s, 16 s and 21 s. Plotted are vertical displacements (up/down as red/blue).

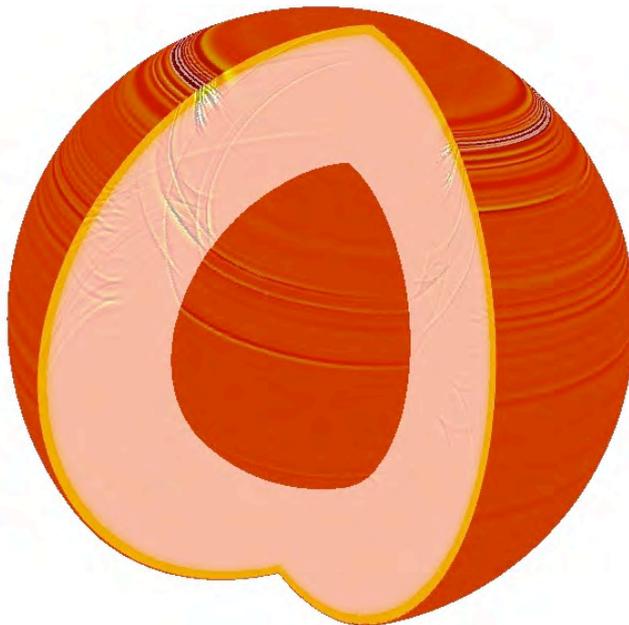
References: D. Peter, D. Komatitsch, Y. Luo, R. Martin, N. Le Goff, E. Casarotti, P. Le Loher, F. Magnoni, Q. Liu, C. Blitz, T. Nissen-Meyer, P. Basini, J. Tromp, 2011. *Forward and adjoint simulations of seismic wave propagation on fully unstructured hexahedral meshes*, Geophysical Journal International, doi: 10.1111/j.1365-246X.2011.05044.x

Title: A community-available database of seismograms at the global scale

Researchers: Dr. T. Nissen-Meyer (ETHZ), Dr. C. Trabant & Dr. D. Simpson (IRIS consortium, USA)

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

Description: The aim of this project is to compute, store and make available a complete database of waveforms that constitute a primitive yet complete basis for instantaneous computation of seismograms of any configuration type at the scale of the globe, i.e. a once-and-for-all solution to the forward problem upon spherically symmetric earth models. This is done in collaboration with the IRIS consortium in the USA, the prime source for data collection in seismology. The numerical database will be made available through IRIS' web services along with interfaces and scripts that conduct convolutions with any desired source time function at any frequency, any source-receiver configuration and freely chosen source radiation patterns. This extremely efficient concept is based upon our own axisymmetric spectral-element method that allows for a dimensional reduction in the calculation of full 3D seismograms in a reference coordinate system such that all of the above operations can be conducted a posteriori. The same concept is planned for waveforms throughout the earth that constitute the basis for seismic sensitivity kernels, but as this requires many tens Terabytes of permanent storage, can be seen as a longer-term effort.



Snapshot of the propagating global wavefield as simulation using our method AXISEM, in which the computationally intensive numerical operations are confined to a 2D disk embedded within this sphere. This allows for extremely efficient computation of arbitrary earthquake-seismometer configurations once-and-for-all.

Title: Born and Neumann scattering in deep-earth tomography

Researchers: Dr. Tarje Nissen-Meyer (ETHZ), PhD student Martin van Driel (ETHZ), Dr. Eric Beucler (Universite de Nantes), Dr. Alexandre Fournier (IPG Paris), Dr. Yann Capdeville (Universite de Nantes)

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

Description: The three-dimensional effects of heterogeneities located in the D" layer on the traveltimes of core-diffracted phases can be large (several seconds). In an attempt to quantify them, we compute synthetic seismograms for various models in the core-mantle boundary region under- and overlaid by a spherical symmetric Earth. Based on a catalog of deep (> 100km) and $M_W > 6$ earthquakes, the seismograms are computed using a coupled spectral-element-modal method (Capdeville et al., 2003), for periods down to 10s. The statistics of traveltime anomalies are computed using the reference comprehensive symmetric spherical Earth model. We emphasize the impact of three-dimensional propagation on these statistics, and discuss the validity range of the Born approximation when trying to recover the structure and the amplitude of the various anomalies. Partly computed on ETH workstations and Brutus.

This study is being continued in a larger framework of conducting Born modeling of realistic Earth models derived from tomography, and eventually amended using a modified Neumann series approach together with our axisymmetric spectral-element method to extremely efficient wave propagation through 3D models.

References: Eric Beucler, Yann Capdeville, Alexandre Fournier, Tarje Nissen-Meyer, 2010. Impact of deep mantle structural heterogeneities on core-diffracted traveltimes: constraints on full-wave Born sensitivity kernel tomography, AGU fall meeting.

T. Nissen-Meyer, A. Fournier, 2011. Time-frequency sensitivity in global tomography, submitted to Geoph. J. Int.

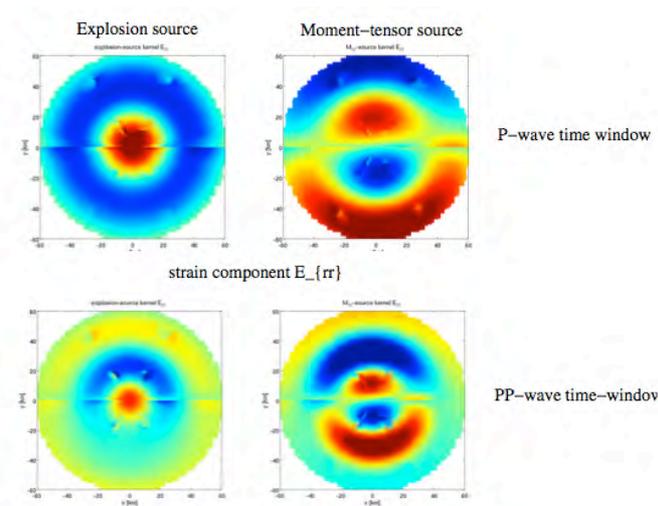
T. Nissen-Meyer, A. Fournier, 2011. Subjective imprints on inverse global wave propagation, to be submitted to Geoph. J. Int.

Title: Real-time global seismic wave propagation and waveform inversion for source and structure

Researchers: Dr. Tarje Nissen-Meyer (ETHZ), Dr. Alexandre Fournier (IPG Paris), Prof. Martin Mai (KAUST), Dr. Florian Haslinger (ETHZ), Prof. Domenico Giardini (ETHZ)

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

Description: The last two decades have witnessed rapid progress in computational infrastructures (supercomputers, GPU, cloud computing) and sophisticated numerical techniques. This has enabled seismologists to tackle geophysical scales of interest by solving realistic 3D wave propagation and seismic inversion for Earth-model and excitation-source parameters. We present highly accurate spectral-element techniques for an efficient and rapid determination of these parameters within the framework of adjoint-based non-linear and linearized matrix optimization. Full waveforms are used while allowing for any desired complexity within the misfit function (traveltimes, amplitudes, waveforms, phase/envelope decomposition), source (source time function, radiation pattern, location, magnitude, finite kinematic rupture) and model parameters (wavespeeds, anisotropy, seismic discontinuities, attenuation). In particular, we focus on our own axisymmetric method which solves 3D global wave propagation in a 2D-computational domain for spherically symmetric background structure. This significant drop in computational cost allows for real-time global wave propagation and non-linear adjoint or probabilistic inversions for all of the above-mentioned source properties. It is computationally trivial to reach the highest desirable frequencies (e.g. Hz-range for global distances), which may help in discriminating nuclear explosions from earthquakes within a full-wave teleseismic inversion framework. Moreover, this method relies on a separate treatment of moment-tensor elements and can therefore be an efficient tool in discriminating indigenous (i.e. traceless, shear-dominated radiation) from volumetric, explosive wavefield characteristics. We show several examples for wave propagation, source complexities, and sensitivity kernels to underline the flexibility and applicability of such approaches.



Backprojection of teleseismic wavefields, i.e. "sending back the data" to determine and discriminate the radiation pattern of seismic signals. All of these operations are conducted in one simulation at dominant source period 3 seconds, using a dense receivers ring at 90° distance.

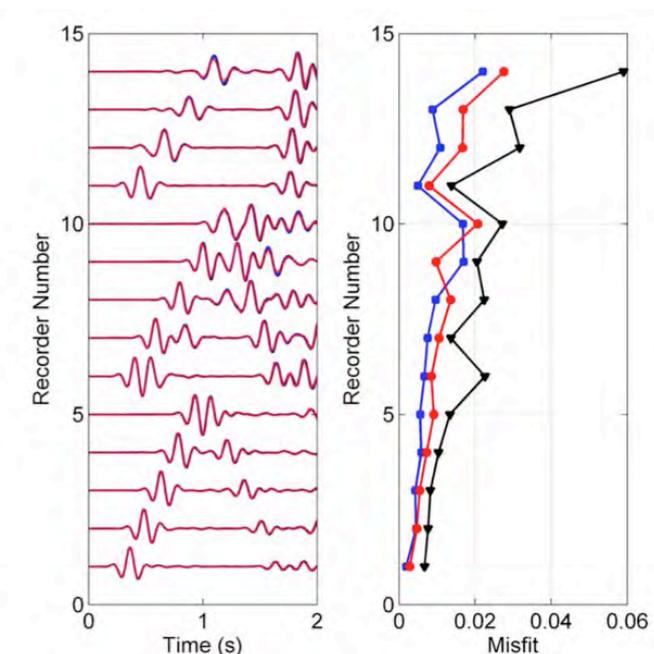
References: Tarje Nissen-Meyer, Alexandre Fournier, Martin Mai, Florian Haslinger, Domenico Giardini, 2011. Real-time global seismic wave propagation and waveform inversion for source and structure, 2011 CTBT Science & Technology meeting, Vienna, Austria.

Title: A lattice Boltzmann method for elastic wave propagation

Researchers: Dr. G.S. O'Brien (UC Dublin), Dr. Tarje Nissen-Meyer (ETHZ), Prof. C. Bean (UC Dublin)

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

Description: The lattice Boltzmann (LB) method is a numerical method which has its origins in discrete mechanics. The method is based on propagating discrete density distributions across a fixed lattice and implementing conservation laws between the density distributions at lattice intersections. The method has been successfully applied to a wide variety of problems in fluid dynamics but has yet to be applied to elastic wave propagation. In this article we outline a new 2D and 3D lattice Boltzmann solution to the elastic wave equation in a Poisson solid using a regular lattice, in 2D a square geometry and in 3D a cubic geometry. We outline the theory behind the method and derive the elastic wave equation from a Chapman-Enskog expansion about the Knudsen number. The scheme is shown to give rise to the elastic wave equation with a fixed Poisson's ratio of 0.25 with a Knudsen number truncation error of order two. We have performed a Von Neumann plane wave analysis and found that the numerical dispersion is comparable to other discrete methods for modeling wave propagation. We have compared the numerical method to two problems, a 3D infinite homogeneous medium and a 2D heterogeneous layered model. In both cases we found the solutions agreed showing that the Lattice Boltzmann method can be used to model elastic wave propagation. The scheme is implemented for a Poisson solid and is computationally in the same order of magnitude as traditional finite-difference methods and other discrete schemes but the Courant condition is more restrictive. However, it offers the potential to model the interaction of several continuum equations within one solver as the continuum equation is solely dependent on the equilibrium distribution.



Vertical seismograms from three numerical methods calculated with a heterogeneous model. The left panel shows the three numerical solutions which are identical at this scale. The right hand shows the misfits between the numerical methods with the LB and EL methods shown as triangles, the misfit between the LB and FD as squares and the FD and EL methods as circles. It can be clearly seen the LB provides a good solution when compared with the other two numerical solutions.

References: G. S. O'Brien, T. Nissen-Meyer, C. Bean, 2011. *A lattice Boltzmann method for elastic wave propagation*, subject to minor revision, Bull. Seis. Soc. America.

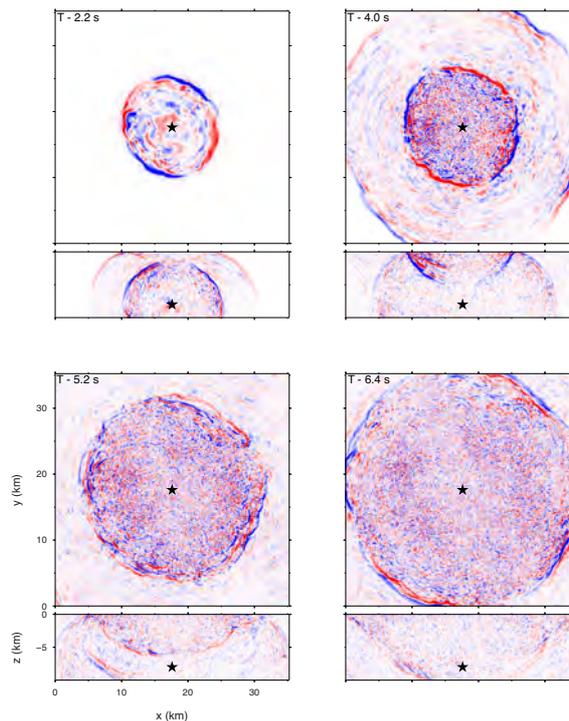
Title: High-Frequency Finite Differences Simulations of Seismic Scattering in Heterogeneous Three-Dimensional Crustal Media

Researchers: PhD student Walter Imperatori (ETHZ), Prof. Martin P. Mai (Kaust, King Abdullah University of Science and Technology)

Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: Deterministic simulations of wave propagation in highly heterogeneous media at high frequencies have been always limited to 2D structures or 3D acoustic approximations. Here we study seismic scattering and wavefield characteristics between 0 and 10 Hz in complex heterogeneous 3D media, using finite differences method to solve the elastic equations of motion. Exploring and understanding the behavior of travelling high-frequency perturbations is an essential step to improve our knowledge on scattering-related effects especially close to the seismic source. Other aspects we try to address are connected to the hybrid broad-band synthetics computation and the nature of the high-frequencies present in recorded ground motions. Debate amongst scientists on these topics is still completely open. Due to the high frequencies involved, our simulations require noticeable computational resources and the most advanced cluster-computers nowadays available.

Figure: Ground motion snapshots for a double-couple point source



Publications/References:

Imperatori, W., and Mai, P. M. (2011) Near-Field Ground-Motion Simulation Including 3D Scattering. SSA meeting, 13th-15th April 2011, Memphis.

P M Mai, W Imperatori and K B Olsen (2010). Hybrid Broadband Ground-Motion Simulations: Combining Long-Period Deterministic Synthetics with High-Frequency Multiple S-to-S Backscattering. Bulletin of the Seismological Society of America, Vol. 100, No. 5A, pp. 2124–2142, October 2010, doi: 10.1785/0120080194

Title: The Transition of Dynamic Rupture Styles in Elastic Media Under Velocity-Weakening Friction

Researchers: PhD student Alice-Agnes Gabriel (ETHZ), Dr. Jean-Paul Ampuero (Caltech, USA), Dr. Luis Dalguer, (ETHZ), Prof. Martin P. Mai (King Abdullah University of Science and Technology)

Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: We study dynamic rupture styles and their transitions in 2D in-plane rupture on faults governed by velocity-and-state-dependent friction with dramatic velocity-weakening. Our study is based on numerical simulations that employ the 2D spectral element method (SEM2DPAK of Ampuero, 2008). Our results demonstrate the general existence of sub- and super-shear ruptures in pulses and cracks and their systematic transitions as a function of initial fault stress and nucleation conditions. We find the asymptotic behavior of sustained ruptures to be independent of nucleation details, unlike the transient approach to that asymptotic behavior. Transitional rupture styles correspond to previous analytical work and are determined by competing critical propagation distances. Interestingly, the pulse-crack transition involves re-activation of the previously healed rupture due to gradual stress build-up near the hypocenter. These results lead to the conjecture that heterogeneities present in nature over a broad range of scales can trigger any of the dynamically stable rupture regimes described above.

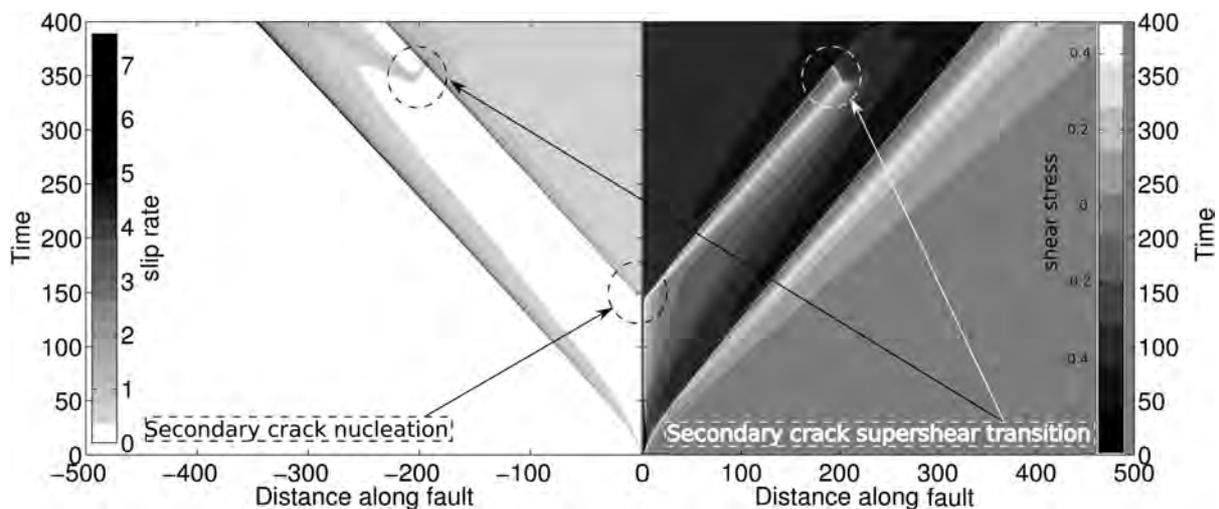


Figure: Nucleation of a supershear front by a secondary crack. Spatio-temporal evolution of slip rate (left) and shear stress (left) for a superposition of a primary pulse and a secondary subshear crack (triggered near $t = 150$) which in turn nucleates a supershear crack (near $t = 350$).

Reference:

Gabriel, A. A.; J. P. Ampuero; L. A. Dalguer and P. M. Mai (2011), The Transition of Dynamic Rupture Styles in Elastic Media Under Velocity-Weakening Friction. To be submitted to J. Geophys. Res.

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, and N. Abrahamson (2011) "Verifying a computational method for predicting extreme groundmotion at the proposed Yucca Mountain repository" Seismological Research Letters.2011; 82: 638-644.

Title: The long-term seismic cycle at subduction thrusts: Benchmarking numerical to analogue models and applying them to realistic geometry large-scale models

Researchers: Ylona van Dinther, Taras Gerya, Luis Dalguer, Martin Mai, Gabriele Morra, Francesca Funicciello, Fabio Corbi

Institute/Group: Swiss Seismological Service (SED) / Computational seismology

Description: The main objective of this project year was to benchmark our fluid-dynamic visco-elastic-plastic code that includes many natural complexities to more simple and understandable analogue experiments, which demonstrated the occurrence of regular seismic events. The ultimate goal is to increase our understanding of the physics governing the long-term seismic cycle, which so far remains illusive due to a subduction zone's inaccessibility and a too short of observational time span. Our benchmarking results showed that a static friction coefficient leads to a series of irregular, rather slowly slipping events in which yielding of the seismogenic zone, represented by sand paper, leads to a short duration reversal of gelatine wedge velocities. These rather long and slow events are, however, sensitive to a range of numerical parameters. In order to achieve an analogue-like, regular periodicity, the implementation of a velocity-weakening friction coefficient was required. Using a carefully selected range of material and frictional properties, inter- and co-seismic duration, and co-seismic slip can be matched to within a standard deviation of the analogue models. On the side the methodology on how to analyze seismicity in large-scale, more realistic geometry models continued, together with an implementation of the new friction model, as was evident from our analogue modeling benchmark. The high computational load results from resolving a wide range in both time and space, as well as from a large set of parameters that needed to be tested in order to fit the results of the analogue models.

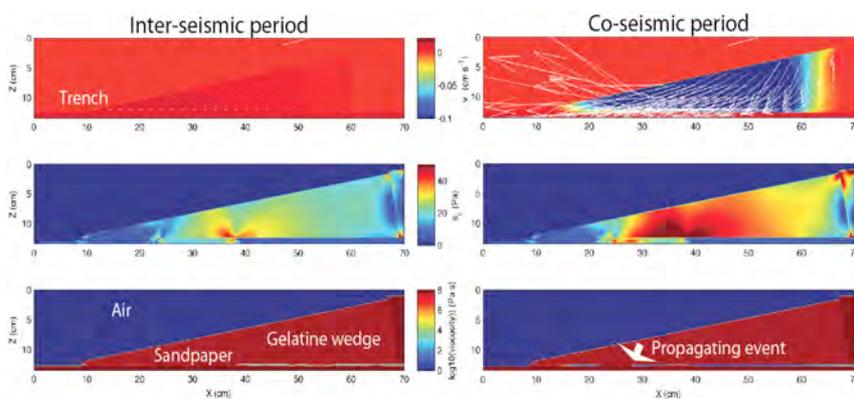


Figure 1: Snap shots during the inter-seismic (left) and co-seismic period (right) of a triangular wedge, which is underlain by a rightward subducting slab containing a velocity-weakening seismogenic zone (sandpaper).

Physical properties from

top to bottom show horizontal velocity, second invariant of deviatoric stress, and viscosity.

Publications:

van Dinther, Y., Gerya, T.V., Corbi, F., Funicciello, F., Dalguer, L.A., and Mai, P.M. (2011). The long-term seismic cycle at a subduction thrust in geodynamic numerical simulations compared to analogue gelatin models. Geophys. Res. Abs. 13, EGU2011- 9891.

van Dinther, Y., Gerya, T.V., Mai, P. M., Dalguer, L. A., and Morra, G. (2011). The long-term seismic cycle in geodynamic, numerical simulations of a subduction zone. Geophys. Res. Abs. 13, EGU2011-10001.

van Dinther, Y., Gerya, T.V., Corbi, F., Funicciello, F., Dalguer, L.A., and Mai, P.M. (2011). The long-term seismic cycle at a subduction thrust in geodynamic numerical simulations compared to analogue gelatin models, IUGG, Melbourne, 2011.

Title: Development of Earthquake Source Physics Models for the seismological assessment of future earthquakes and ground motion prediction in the Alpine regions

Researchers: PhD student Cyrill Baumann (ETHZ), Dr. Luis Dalguer, (ETHZ)

Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: In the present project we propose to develop suite of earthquake source physics-based numerical models to study rupture dynamic complexity and the resulted near-source ground motion, implementing laboratory-based constitutive friction models for different geological structures in the Alpine regions, for the seismological assessment of past and future earthquakes and ground motion prediction in the Alpine regions.

The Swiss Alps, specifically the Valais area which shows the largest seismic hazard in Switzerland, has experienced a magnitude 6 or larger event every 100 years, with the least magnitude 6.1 earthquake in 1946 close to Sion and Siere. Considering that the probability of observing a major earthquake (up to magnitude 6.5) in the next 40 years in the region is high. The earthquake physics models developed for this project, will provide a better physical understanding of how earthquakes operate in this area, and consequently it will help to improve our capability for ground motion prediction for the assessment of seismic hazard and to mitigate the seismic risk in the area. Furthermore this site-specific study will contribute to the evaluation of the critical facilities installed in this area, contributing to improved seismic safety of future and existing structures.

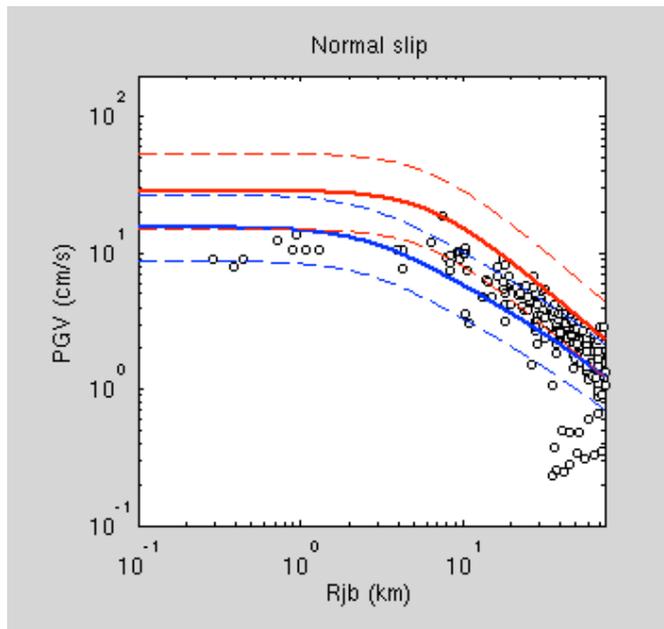


Figure: Synthetic PGV for a $M_w=6.52$ of a normal fault compared with Ground Motion Predicting Equations (blue: Boore & Atkinson 2008, red: Akkar & Bommar, 2010)

Publications:

Baumann C., Dalguer L.A., Burjanek J., Clotaire M., Fäh D., (2011). Modelling $M_w=6.5$ earthquakes ground motions in the Valais area, Switzerland, using dynamic rupture approach. SSA 2011 Annual Meeting, Memphis, Tennessee (USA). Abstract in Seismological Research Letters, Vol. 82, Nr. 2.

Donat Fäh, Jeffrey R. Moore, Jan Burjanek, Ionuț Iosifescu, Luis Dalguer, et al (2011), Coupled seismogenic geohazards in alpine regions, Bollettino di Geofisica Teorica e Applicada, in press.

Title: Dynamic rupture modelling of the 2011 M9 Tohoku earthquake with unstructured 3D spectral element method

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

Institute/Group: Swiss Seismological Service, Computational Seismology Group, Seismology & Geodynamics Group

Description: On March 11th 2011, a Mw 9 earthquake struck Japan causing 28000 victims and triggering a devastating tsunami that caused severe damage along the Japanese coast. The exceptional amount of data recorded by this earthquake, with thousands of sensors located all over Japan, provides a great opportunity for seismologist and engineers to investigate in detail the rupture process in order to better understand the physics of this type of earthquakes and their associated effects, like tsunamis. In this project we investigate, by means of dynamic rupture simulations, a plausible mechanism to explain key observations about the rupture process of the 2011 M9 Tohoku earthquake, including the spatial complementarity between high and low frequency aspects of slip (e.g, Simons et al, Science 2011, Meng et al, GRL 2011).

To model the dynamic rupture of this event, we use a realistic non-planar fault geometry of the megathrust interface, using the unstructured 3D spectral element open source code SPEC-FEM3D-SESAME, in which we recently implemented the dynamic fault boundary conditions. This implementation follows the principles introduced by Ampuero (2002) and Kaneko et al. (2008) and involves encapsulated modules plugged into the code. Our current implementation provides the possibility of modeling dynamic rupture for multiple, non-planar faults governed by slip-weakening friction. We successfully verified the code in several SCEC benchmarks, including a 3D problem with branched faults, as well as modeling the rupture of subduction megathrust with a splay fault, finding results comparable to published results.

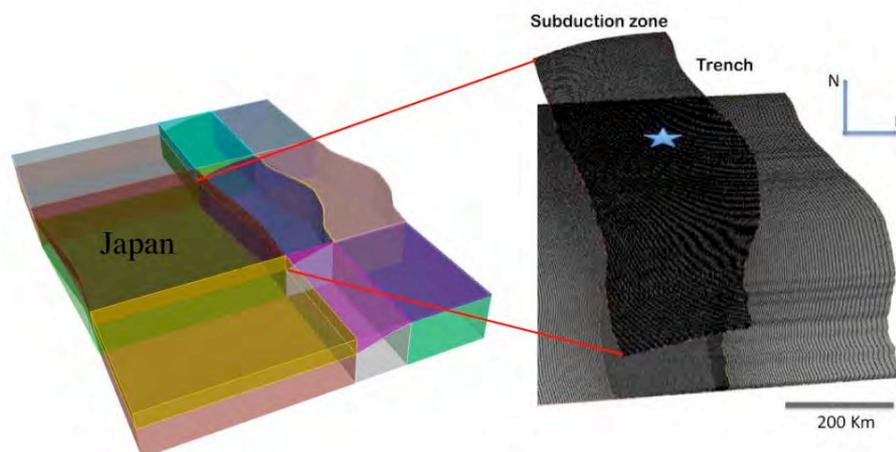


Figure. Mesh of a realistic non-planar fault geometry of the megathrust interface of the Mw9.0 2011 Tohoku earthquake in Japan. Start represents the hypocenter location.

Publications:

Galvez, P., J.-P. Ampuero, L. Dalguer, and T. Nissen-Meyer (2011), Dynamic rupture modeling of the 2011M9 Tohoku earthquake with unstructured 3D spectral element method, Eos Trans. AGU, 1(1), Fall Meet. Suppl., Abstract U51B.

Title: Investigating the reliability of kinematic source inversion with dynamic rupture models

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

Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: In this project we develop dynamic rupture simulation of a vertical strike slip fault. Our source model is composed by well-defined asperities (patches of large stress drop) and we assume that fault rupture is governed by the linear slip weakening friction model. The resulting near-source ground motion dominated by low frequency (up to 1Hz) is used for testing our inversion method. We performed various inversion tests and compared estimated solutions with true solutions obtained by the forward dynamic rupture modeling. Assuming the kinematic model generated displacements as recorded data to inverse source slip distribution. Our preliminary results show that estimated model spaces could be significantly perturbed, depending on data and modeling schemes used in the inversion, not only in terms of spatial distribution of model parameters, but also in terms of their auto- and cross-correlation structure. In addition, the recent emergence of high-rate Global Navigation Satellite Systems (GNSS) data can considerably improve the observation capabilities for dynamic surface movements (sampling up to 100 Hz) during large earthquakes. GNSS receivers are used to accurately measure both dynamic and static ground displacements without saturation or sensitivity to tilt and with a sampling interval below 1 second and sub-centimeter accuracy across the frequency spectrum. We expect that we can resolve an issue of relative weighting we often face in multiple data inversion, i.e., joint inversion of both geodetic and seismic data, by inverting ground displacement data recorded by the GNSS receivers

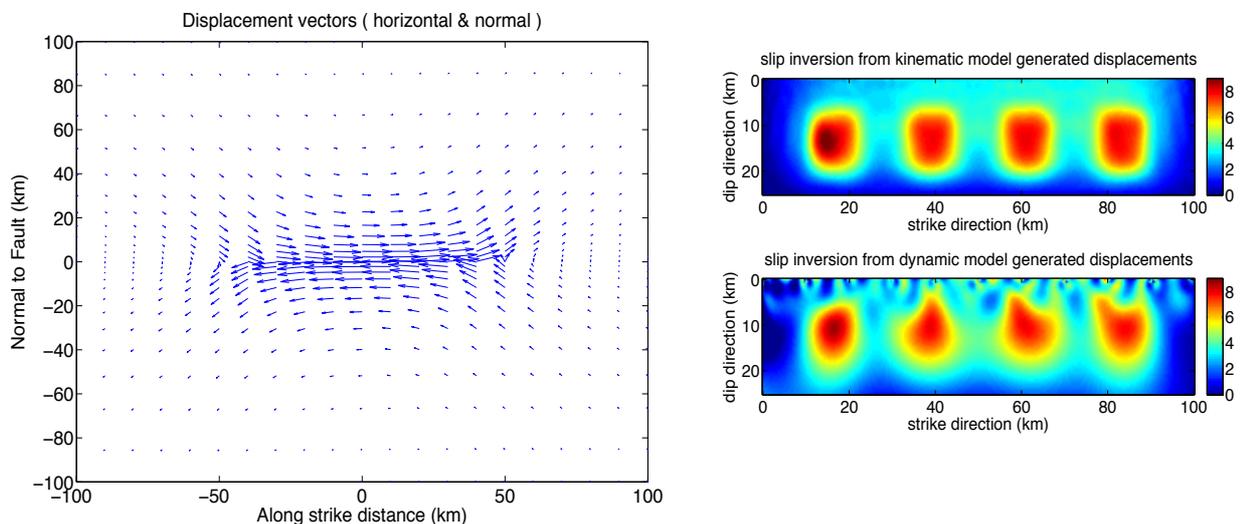


Figure: (left) Displacement field generated by dynamic rupture model. (right) Slip inversion from displacement field generated by a kinematic (top) and a dynamic (bottom) rupture model.

Publications:

Zhang J.; S. Song; L. A. Dalguer, and J. Clinton (2011), Investigating the reliability of kinematic source inversion with dynamic rupture models, Eos Trans. AGU 2011, Fall Meet. Suppl., Abstract S43C.

Title: Pseudo Dynamic Source Characterization Incorporating Effects of Super-shear Rupture and Stress Heterogeneity for Strong Ground Motion Prediction

Researchers: Dr. Banu Mena (ETHZ), Dr. Luis Dalguer, (ETHZ), Prof. Martin P. Mai (King Abdullah University of Science and Technology)

Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: Reliable prediction of ground motions for future earthquakes strongly depends on the ability to simulate realistic earthquake source models. Though full dynamic rupture calculations can be used for this purpose, they are still computationally challenging. An alternative is to invoke the framework of kinematic pseudo-dynamic procedures. This approach uses simple relationships between kinematic and dynamic source parameters to build physically consistent kinematic models. Based in the pseudo-dynamic approach proposed by Guatteri et al. (2004), here we propose new relationships to build pseudo-dynamic models that capture effects of super-shear rupture speed and local changes due to stress heterogeneities for moderate to large earthquake size. We carried out dynamic rupture simulations using stochastic initial stress distributions to generate a dataset that covers a wider range of magnitude (M_w 6-8). This set of models show first, local super shear rupture speed prevails at all earthquake sizes and second, local rise time distributions are not controlled by the global fault geometry, but by the local changes on the faults associated with the stress heterogeneous (asperities). Based on these findings, a new set of pseudo-dynamic relations is derived for the proposed pseudo-dynamic source characterization, which takes into account earthquake size, buried and surface rupturing ruptures, local rise time variations, and local super shear rupture speed. We performed further validation tests using the proposed pseudo-dynamic source characterization and obtained significant improvements in the synthetic ground motions when comparing with the model of Guatteri et al. (2004). The results are promising for the implementation of the proposed pseudo-dynamic methodology into the ground motion simulation tools and its application for ground motion prediction of future earthquakes.

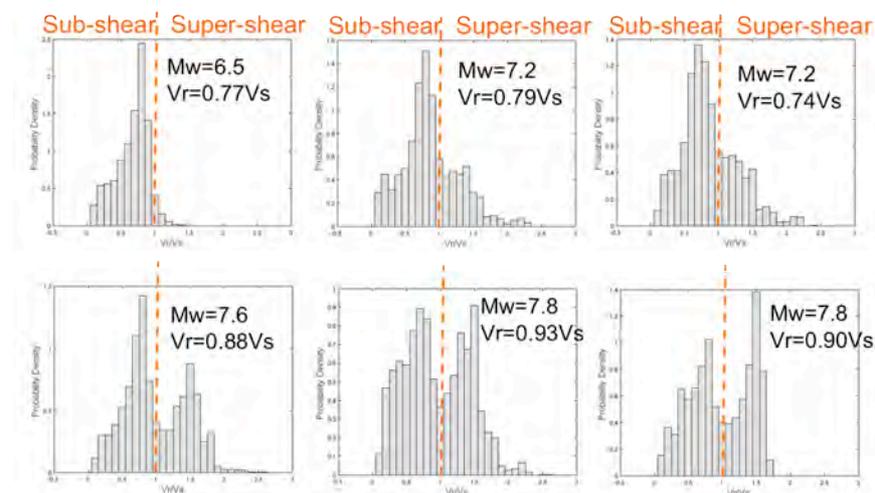


Figure. Histograms of local rupture speed distribution in strike-slip faults with earthquake size

Publications:

Mena, B.; L.A. Dalguer and P.M. Mai (2011), Pseudo Dynamic Source Characterization Incorporating Effects of Super-shear Rupture and Stress Heterogeneity for Strong Ground Motion Prediction. *Bull. Seismol. Soc. Am.*, in review.

Title: Understanding earthquake source processes with spatial random field models
Researchers: Dr. Seok Goo Song, (ETHZ)
Institute/Group: Swiss Seismological Service, Computational Seismology Group

Description: A finite-fault earthquake rupture model generator (SongRMG, Ver 1.0) has been developed, based on 1-point and 2-point statistics of kinematic source parameters such as slip, rupture velocity, slip velocity and duration. 1-point statistics define a marginal probability density function for a certain source parameter at a given point on a fault. 2-point statistics, i.e. auto- and cross-coherence between source parameters, control the heterogeneity of each source parameter and their coupling, respectively. Given the rupture model generator, we can generate physics-based rupture scenarios for simulation-based seismic hazard assessment as shown in Figures 1 and 2. This study was and will be presented at the following two meetings given below.

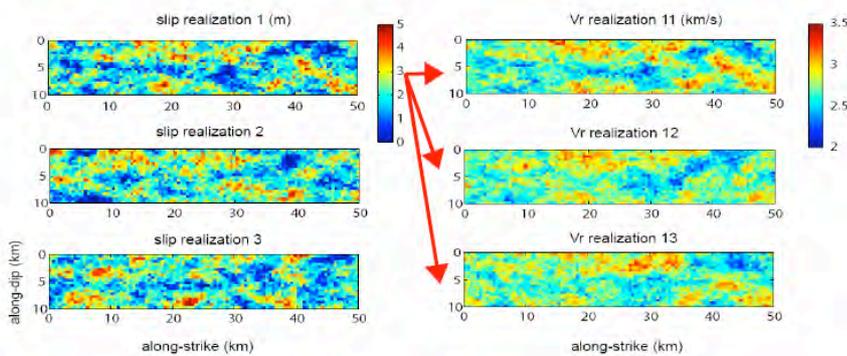


Figure 1. Slip and rupture velocity realizations for Mw 7.0 events obtained by sequential Gaussian simulation. Three slip realizations were obtained based on the target auto-coherence structure and marginal PDF given in Figure 2 (a) and (b). Three

rupture velocity distributions are obtained conditioning on the slip realization 1 with cross- and auto-coherence and marginal PDF for the rupture velocity given in Figure 2 (a) and (b). Note that high rupture velocity patches are coupled with high slip patches because of the positive cross-coherence introduced in the random sampling procedure.

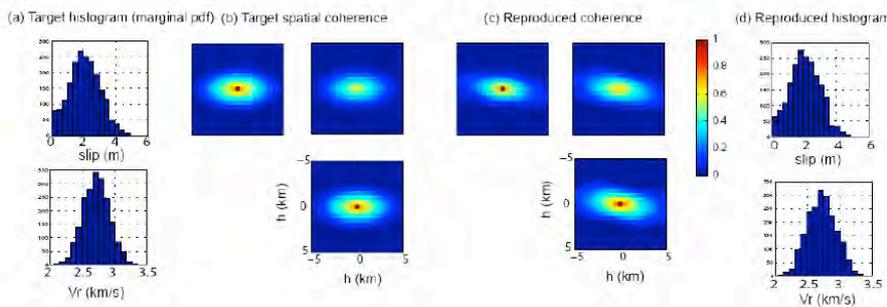


Figure 2. Target and reproduced coherence structure with target and reproduced histograms, respectively. Horizontally elongated auto- and cross-coherence structures

are assumed with Gaussian marginal probability density function for both slip and rupture velocity. Slip is truncated at zero in the modeling. Note that the target coherence structures as well as target histograms are successfully reproduced in the stochastic modeling.

Publications

Song, S., Understanding earthquake source processes with spatial random field models, Fall meeting of American Geophysical Union (AGU), San Francisco, California, 2011.

Song, S., Developing a physics-based rupture model generator based on 1-point and 2-point statistics of kinematic source parameters, annual meeting of Southern California Earthquake Center (SCEC), Palm Springs, California, 2011.

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, Computational Seismology Group

Description: This is a production project at Swiss National Supercomputing Center (CSCS). This project is oriented specifically to request computational resources at CSCS to use the Cray XT5 Rosa Super computer. We have been awarded an allocation of 3 millions of CPU hrs per year during 3 years (from August 2010 to August 2013). 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. This project is part of an ensemble of ongoing projects carried out by our Computational Seismology group. These projects are well integrated with each other in their goals and target, and include:

· *“Site-specific numerical simulations of earthquake rupture dynamics and strong ground motion: An application to Swiss NPP’s”*. This is part of the High-Impact User project, currently with an allocation of 1.0 MCPHU hrs (from October 1st to December 30th). In this project we are developing a suite of earthquake models for an existing nuclear-power-plant (NPP) site in Switzerland to investigate near-source ground motion variability where source processes and/or geological effects are dominant.

· *“Earthquake rupture dynamic in large aspect-ratio faults ($L \gg W$)”*. This is a project in collaboration with Dr. Jean Paul Ampuero (Caltech, USA). The main goal of this project is the study of the effect of large strike slip fault models with $L \gg W$ on the rupture propagation and ground motion (where L and W are the length and width of the fault, respectively).

· *“Development of earthquake source physics models for the seismological assessment of future earthquakes and ground motion prediction in the Alpine regions”* This is a project in collaboration with Cyrill Baumann (PhD student). This project is integrated in the Coupled Seismogenic GeoHazards in Alpine Regions (COGEAR) project. COGEAR is an interdisciplinary project to investigate the hazard chain induced by earthquakes in Valais, particularly in parts of the Rhone, Visper and Matter valleys.

· *“Coherence of near-fault ground motion spatial distribution and ground strain”*. This is a sub-module (JRA3) of the NERA projects: Network of European Research Infrastructures for Earthquake Risk Assessment and Mitigation. Here we will develop intensive earthquake numerical simulations to adequately assess the level and variability of near-source ground and to supplement the lack of data near the fault.

Publications:

Dalguer L.A. and P. M. Mai (2011), Near- Source Ground Motion Variability from M~6.5 Dynamic Rupture Simulations. *4th IASPEI / IAEE International Symposium: Effects of Surface Geology on Seismic Motion*, In CD. August 23–26, 2011, University of California Santa Barbara, CA, USA.

- Mai P. M. and **L.A. Dalguer** (2011), Broadband Ground-Motion from Rupture Dynamic. *4th IASPEI / IAEE International Symposium: Effects of Surface Geology on Seismic Motion*, In CD. August 23–26, 2011, University of California Santa Barbara, CA, USA.

Title: Example-Based Elastic Materials

Researchers: Sebastian Martin¹
Bernhard Thomaszewski^{1,2}
Eitan Grinspun³
Markus Gross^{1,2}

Institutes:

¹ Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich

² Disney Research Zurich

³ Columbia Computer Graphics Group, Columbia University

Description:

Different materials deform in different ways. Therefore, physically-based animations offer control of material properties as a way of controlling the final deformation. But in creative applications such as computer animation, material properties are just middlemen in a process that really focuses on obtaining some desired deformation.

Indeed, we can flip the causality between materials and deformation: when we witness the deformation of an object, we implicitly draw conclusions about its underlying, constitutive material. By controlling the deformation of an animated object, we can imply complex material behaviors. Therefore, if we can expand the repertoire of possible deformations of an object, we can broaden the expressive palette available for physics-based computer animation.

The computational mechanics literature already describes many mathematical models for myriad materials, alas these models are intended for problems where material coefficients are easily quantified. In artistic endeavors, we typically envision a desired deformation. Yet quantifying material coefficients that lead to a desired deformation behavior is difficult if not impossible.



Inspired by example-based graphical methods, we present an intuitive and direct method for artistic design and simulation of complex material behavior. Our method accepts a set of poses that provide examples of characteristic desirable deformations, created either by hand, with a modeling tool, or by taking 3D "snapshots" of previously run simulations. With these examples in hand, we provide a novel forcing term for dynamical integration that causes materials to obey the "physical laws" implied by the provided examples.

References: S. Martin, B. Thomaszewski, E. Grinspun, M. Gross, Example-based Elastic Materials. ACM Transaction on Graphics (Proc. SIGGRAPH), vol. 30, no. 4, 2011, pp. 72:1-72:8.

Title: Two-Scale Particle Simulation

Researchers: Barbara Solenthaler¹
Markus Gross^{1,2}

Institutes:

¹ Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich

² Disney Research Zurich

Description:

The physical and visual quality of particle-based solvers like SPH are defined by the number of particles that are used to discretize the fluid. Generally, the more particles that are used, the smaller the damping artifacts and the more small-scale details like splashes, spray, and surface waves can be reproduced. However, doubling the resolution of a simulation increases the particle number by a factor of 8. This increases the computational cost notably since it depends linearly on the number of particles. To cope with the increasing demand for more detailed flow structures, we present a new level-of-detail technique that follows the idea to allocate computing resources to regions where complex flow behavior emerges. Instead of recursively subdividing particles we use a hierarchy of several resolution levels. While the number of resolution levels is not fundamentally limited with our method, we focus on two scales only. We use two distinct but coupled simulations; one simulation that computes the whole fluid with a coarse resolution, and a high-resolution level that simulates a subset of the fluid with small particles.

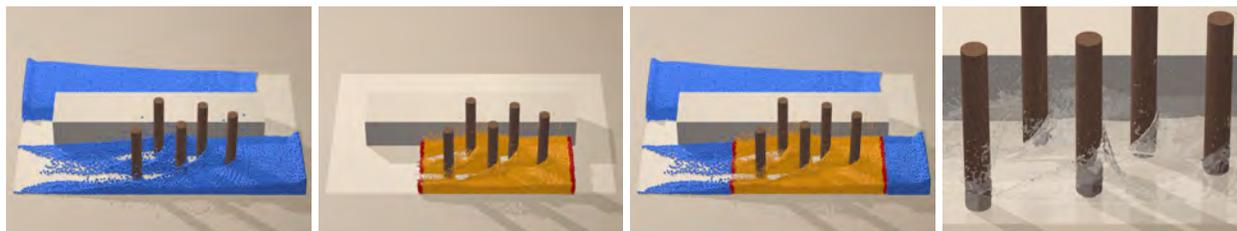


Figure 1: From left to right: Low-resolution level, high-resolution level, merged particles, rendered surface.

Our method reduces the particle number and hence the total computational cost by almost a factor of 7 compared to the single-scale reference simulation while producing corresponding flow details.

References: B. Solenthaler and M. Gross, Two-Scale Particle Simulation. ACM Transaction on Graphics (Proc. SIGGRAPH), vol. 30, no. 4, 2011, pp. 81:1-81:8.

Title: Development and application of numerical methods for computational electromagnetics

Researchers: Christian Hafner
Christian Engström
Jürg Fröhlich
Aytac Alparslan
Christoph Böcklin
Alexander Dorodnyy
Nikolay Komarvesky
Patrick Leidenberger
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.

The applications include 1) metamaterials for 50 Hz magnetic field shielding, for radar absorption, microwave sealing, thermal protection, and highly 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, etc.

Currently we develop and combine various field solvers based on boundary discretization methods - the Multiple Multipole Program (MMP), the Method of Auxiliary Sources (MAS), Method of Moments (MoM), as well as domain discretization methods in frequency and time domain, namely Finite Elements Methods (FEM), Discontinuous Galerkin (DG), Finite Difference Time Domain (FDTD), Finite Volume Time Domain (FVTD), and mesh-free techniques. 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, FEM and FDTD are favorable at least as long as moderate accuracy of the results is sufficient.

Our MMP and FDTD codes are contained in the OpenMaX platform, which is an OpenSource project (see <http://openmax.ethz.ch/>).

References:

From fall 2010 till fall 2011, eight papers on various topics of computational electromagnetics were published in reviewed journals.

Title: The FuturICT Knowledge Accelerator:
Creating Socially Interactive Information Technologies for a Sustainable
Future

Researchers: Dirk Helbing

Institute/ Chair of Sociology;
Group: in particular of Modeling and Simulation

Description:

Humanity faces enormous challenges ranging from financial and economic instability over conflict to environmental destruction and climate change, all linked directly to the difficulties in understanding and managing the consequences of our collective activities. Now, a diverse group of leading scientists has unveiled an extraordinary plan to meet these challenges through a project inspired by large-scale enterprises such as the Apollo Project.

The ultimate goal of the FuturICT flagship project is to understand and manage complex, global, socially interactive systems, with a focus on sustainability and resilience. Revealing the hidden laws and processes underlying societies constitutes the most pressing grand challenge of our century and is equally important for the development of novel robust, trustworthy and adaptive information and communication technologies (ICT), based on socially inspired concepts. Integrating ICT, Complexity Science and the Social Sciences will create a paradigm shift, facilitating a symbiotic co-evolution of ICT and society. Data from the complex globe spanning ICT system will be used to develop models of techno-socio-economic systems. In turn, insights from these models will inform the development of a new generation of socially adaptive, self-organized ICT systems.

The FuturICT Flagship will develop the Innovation Accelerator and include:

- The Living Earth Simulator, an open participatory platform to simulate global-scale systems involving the interactions of up to 10 billion agents. It will enable the identification of challenges and opportunities on a global scale. The systemic risk analysis will become possible through the integration of a number of crisis observatories.
- Crisis Observatories, specialized competence centres running massive data mining and large scale computer simulations. They will detect possible crises, such as bubbles or crashes in financial markets, reveal advance warning signs of critical shortages, identify risks of wars or social unrests, emerging epidemics, or environmental instabilities, and explore policy options, including their possible side effects..

Title: Fractality of eroded coastlines of correlated landscapes

Researchers: Pablo A. Morais
Erneson A. Oliveira
Dr. Nuno A. M. Araújo
Prof. Hans J. Herrmann
Prof. José S. Andrade Jr.

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Using numerical simulations of a simple sea-coast mechanical erosion model, we investigate the effect of spatial long-range correlations in the lithology of coastal landscapes on the fractal behavior of the corresponding coastlines. In the model, the resistance of a coast section to erosion depends on the local lithology configuration as well as on the number of neighboring sea sides. For weak sea forces, the sea is trapped by the coastline and the eroding process stops after some time. For strong sea forces erosion is perpetual. The transition between these two regimes takes place at a critical sea force, characterized by a fractal coastline front. For uncorrelated landscapes, we obtain, at the critical value, a fractal dimension $D = 1.33$, which is consistent with the dimension of the accessible external perimeter of the spanning cluster in two-dimensional percolation. For sea forces above the critical value, our results indicate that the coastline is self-affine and belongs to the Kardar-Parisi-Zhang universality class. In the case of landscapes generated with power-law spatial long-range correlations, the coastline fractal dimension changes continuously with the Hurst exponent H , decreasing from $D = 1.34$ to 1.04 , for $H = 0$ and 1 , respectively. This nonuniversal behavior is compatible with the multitude of fractal dimensions found for real coastlines.

References:

- [1] P.A. Morais, E.A. Oliveira, N.A.M. Araújo, H.J. Herrmann, and J.S. Andrade Jr., *Fractality of eroded coastlines of correlated landscapes*, Phys. Rev. E **84**, 016102 (2011).

Title: Simulation of particle mixing in turbulent channel flow due to intrinsic fluid velocity fluctuation

Researchers: Thomas Burgener
Dr. Dirk Kadau
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Particle transport in turbulent flows plays an important role in a variety of different applications. The influence of the intrinsic velocity fluctuations in fully developed turbulence on the mixing properties of a granular medium is currently not well understood.

We combine a DEM simulation with a stochastic process to model the movement of spherical particles in a turbulent channel flow. With this model we investigate the mixing properties of two species of particles flowing through the channel in two and three spatial dimensions. We find a linear increase of the mixing zone with the length of the pipe. Flows at different Reynolds number and different particle densities are studied. Below a critical Reynolds number at the Taylor microscale of around $R_c \approx 300$ the mixing rate is strongly dependent on the Reynolds number. Above R_c the mixing rate stays nearly constant.

References:

- [1] T. Burgener and D. Kadau and H.J. Herrmann, *Simulation of particle mixing in turbulent channel flow due to intrinsic fluid velocity fluctuation*, Phys. Rev. E **83**, 066301 (2011)

Title: Jump at the onset of saltation

Researchers: M.V. Carneiro
H.J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We simulate aeolian sand transport using the Discrete Elements Method. Our model simulates the behavior of a disordered particle bed under the influence of a logarithmic wind profile. The momentum transfer between particles and wind is considered and therefore, the wind is decelerated with the particle drag. We reveal that the transition in the saturated flux for aeolian saltation is generically discontinuous by simulating explicitly 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. We analyze the metastable behavior in the presence of perturbations and lift forces. The dimensionless saturated flux \tilde{q} was fitted according to $\tilde{q}_s = \tilde{q}_0 + A(\theta - \theta_c)\theta^{1/2}$ with $\theta = \frac{u_*^2}{(s-1)gD_{mean}}$.

References:

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

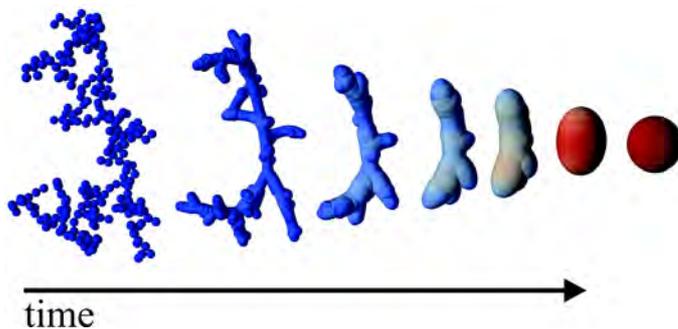
Title: Multi-Particle Sintering Dynamics: from Fractal-like Aggregates to Compact Structures

Researchers: Max L. Eggersdorfer
Dr. Dirk Kadau
Prof. Hans J. Herrmann
Prof. Sotiris E. Pratsinis

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Multi-particle sintering is encountered in almost all high temperature processes for material synthesis (titania, silica, nickel) and energy generation (e.g. fly ash formation) resulting in aggregates of primary particles (hard- or sinter-bonded agglomerates). This mechanism of particle growth is investigated quantitatively by mass and energy balances during viscous sintering of amorphous aerosol materials (e.g. SiO₂, polymers) that typically have a distribution of sizes and complex morphology. This model is validated at limited cases of sintering between two (equally or unequally sized) particles, and chains of particles. The evolution of morphology, surface area and radii of gyration of multi-particle aggregates are elucidated for various sizes and initial fractal dimension. For each of these structures that had been generated by diffusion limited (DLA), cluster-cluster (DLCA) and ballistic particle-cluster agglomeration (BPCA) the surface area evolution is monitored and found to scale differently than that of the radius of gyration (moment of inertia).



Snapshots of an aggregate undergoing viscous sintering and consisting of initially 256 monodisperse primary particles generated by diffusion limited cluster-cluster (DLCA, $D_f = 1.79$) agglomeration.

References:

- [1] Max L. Eggersdorfer, D. Kadau, H.J. Herrmann, Sotiris E. Pratsinis, Multi-particle sintering dynamics: from fractal-like aggregates to compact structures, *Langmuir* 27(10), 63586367 (2011).

Title: Scaling Relations for Watersheds

Researchers: Eric Fehr
Julian K. Schrenk
Dr. Dirk Kadau
Dr. Nuno A. M. Araújo
Prof. José S. Andrade
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Watersheds are the lines separating adjacent drainage basins (catchments). They play a fundamental role in water management, landslides, and flood prevention. Natural watersheds are fractal. Geographers and geomorphologists have found the evolution of watersheds to be driven by local events classified as stream captures or drainage rearrangements. These events can affect the biogeography, and may occur due to various mechanisms like erosion, natural damming, tectonic motion, as well as volcanic activity.

We study the morphology of watersheds in two and three dimensional systems subjected to different degrees of spatial correlations. The response of these objects to small, local perturbations is also investigated with extensive numerical simulations. We find the fractal dimension of the watersheds to generally decrease with the Hurst exponent, which quantifies the degree of spatial correlations. Moreover, in two dimensions, our results match the range of fractal dimensions $1.10 \leq d_f \leq 1.15$ observed for natural landscapes. We report that the watershed is strongly affected by local perturbations. For perturbed two and three dimensional systems, we observe a power-law scaling behavior for the distribution of areas (volumes) enclosed by the original and the displaced watershed, and for the distribution of distances between outlets. Finite-size effects are analyzed and the resulting scaling exponents are shown to depend significantly on the Hurst exponent. The intrinsic relation between watershed and invasion percolation, as well as relations between exponents conjectured in previous studies with two dimensional systems, are now confirmed by our results in three dimensions.

References:

- [1] E. Fehr, D. Kadau, J.S. Andrade, Jr., and H.J. Herrmann, *Impact of Perturbations on Watersheds*, Phys. Rev. Lett. 106, 048501 (2011).
- [2] E. Fehr, D. Kadau, N.A.M. Araújo, J.S. Andrade, Jr., and H.J. Herrmann, *Scaling Relations for Watersheds*, accepted for Phys. Rev. E.
- [3] E. Fehr, K.J. Schrenk, D. Kadau, N.A.M. Araújo, P. Grassberger, J.S. Andrade, Jr., and H.J. Herrmann, *Corrections-to-Scaling for Watersheds, Optimal Path Cracks, and Bridge Lines*, in preparation.

Title: Modeling the Growth and Impact of Wood Decay Fungi

Researchers: Matthias Fuhr
Prof. Dr. H.J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The selective degradation of pit membranes in refractory wood species e.g. Norway spruce (*Picea abies* [L.] Kast.) by the basidiomycete *Physisporinus vitreus* increases the permeability of the wood. This process which has been termed biocising can be used to improve the uptake of wood preservatives and environmentally-benign wood modification substances. The biocised wood can be used for a range different industrial purpose. The objective of this Project is to develop a mathematical model of hyphal growth and expansion of *P. vitreus* by means of stochastic processes both in space and time (Fig. 1). Irreversible growth has been investigated for a long time in the context of cancer growth, dendritic growth and gelation and penetration in porous media. In addition, the Project allows to examine degradation patterns of the fungus and its enzyme activity. By focusing on these fundamental processes, we hope to improve our knowledge on how the complex system (fungus - wood) interacts under defined conditions. This information is crucial for the scaling up of the biocising process. This work is a joint project of the two research groups Wood Protection and Biotechnology, EMPA St. Gallen (Prof. Dr. F.W.M.R. Schwarze) and Computational Physics for Engineering Materials (Prof. Dr. H.J. Herrmann).

References:

- [1] M.J. Fuhr, M. Schubert, F.W.M.R. Schwarze, H.J. Herrmann, *Modeling the hyphal growth of the wood decay fungus Physisporinus vitreus*, Fungal Biol. (2011), doi:10.1016/j.funbio.2011.06.017, in press
- [2] M.J. Fuhr, C. Stührk, B. Münch, F.W.M.R. Schwarze, M. Schubert, *Automated Quantification of the Impact of the Wood-decay fungus Physisporinus vitreus on the Cell Wall Structure of Norway spruce by Tomographic Microscopy*, Wood Sci. Technol. (2011), doi:10.1007/s00226-011-0442-y, in press

Title: Micro-Mechanical Modeling of Swelling in Wood

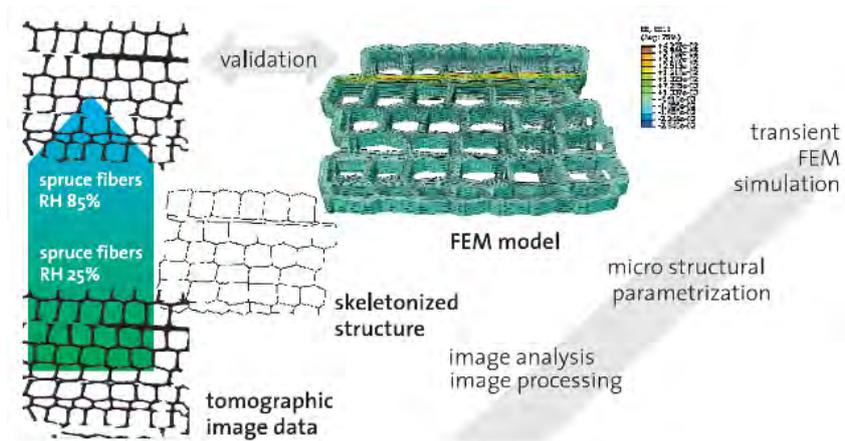
Researchers: François Gaignat
Dr. Falk K. Wittel
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Wood is a complex material that is at a microscopic level neither isotropic nor homogeneous. Its properties are mainly determined by the cell walls, that are composed of several layers which are themselves composed of different materials. Computational models are needed to forecast the relation between the applied loads (mechanical and/or moisture) and the respective hygrothermal and mechanical response.

In this work a multiscale model is used for describing the mechano-sorptive behavior of wood. Some properties of the nanoscopic constituents (mainly cellulose, hemicellulose, and lignin) are already known from research in paper industry. We use a micromechanical model for describing the properties of individual cell wall layers, a model for layered materials and finally a Finite Element Model to describe a cellular microstructure of a spruce wood sample. The predictions of this model are compared to values that come from the analysis of micro-tomographic insitu experiments under varying environmental conditions.



The comparison of the FEM-result and the synchrotron tomography data allows to understand the physical role of different model parameters on the cellular scale. A good microscopic model is the foundation for a valid macroscopic model of the wood.

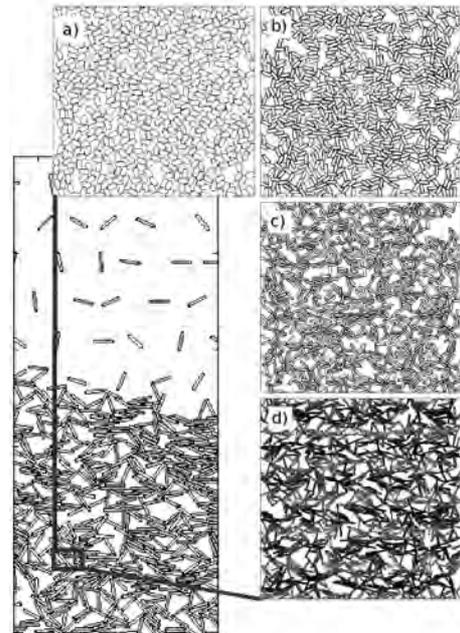
Title: Granular packings of cohesive elongated particles

Researchers: Dr. Raul C. Hidalgo
Dr. Dirk Kadau
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We investigate numerically the effect of attractive forces on the packing properties of two-dimensional elongated grains. In deposits of non-cohesive rods in 2D, the topology of the packing is mainly dominated by the formation of ordered structures of aligned rods. Elongated particles tend to align horizontally and the stress is mainly transmitted from top to bottom, revealing an asymmetric distribution of local stress. However, for deposits of cohesive particles, the preferred horizontal orientation disappears. Very elongated particles with strong attractive forces form extremely loose structures, characterized by an orientation distribution, which tends to a uniform behavior when increasing the Bond number. As a result of these changes, the pressure distribution in the deposits changes qualitatively. The isotropic part of the local stress is notably enhanced with respect to the deviatoric part, which is related to the gravity direction. Consequently, the lateral stress transmission is dominated by the enhanced disorder and leads to a faster pressure saturation with depth.



Simulated packings of elongated cohesive particles settled by gravity. Final configurations are shown for the same granular bond number $Bo_g = 10^4$ and increasing elongation: (a) $d = 2$, (b) $d = 3$, (c) $d = 5$ and (d) $d = 10$.

References:

[1] R.C. Hidalgo, D. Kadau, T. Kanzaki, H.J. Herrmann, Granular packings of cohesive elongated particles, *Granular Matter*, submitted.

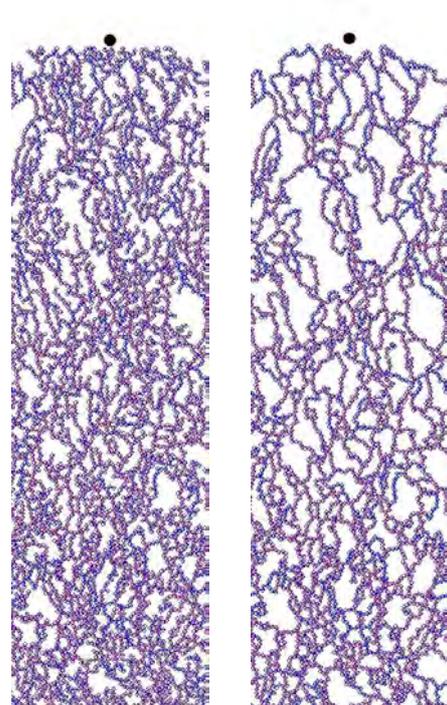
Title: A micromechanical model of collapsing quicksand

Researchers: Dr. Dirk Kadau
Prof. José S. Andrade
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The discrete element method constitutes a general class of modeling techniques to simulate the microscopic behavior (i.e. at the particle scale) of granular/soil materials. We present a contact dynamics method, accounting for the cohesive nature of fine powders and soils. A modification of the model adjusted to capture the essential physical processes underlying the dynamics of generation and collapse of loose systems is able to simulate “quicksand” behavior of a collapsing soil material, in particular of a specific type, which we call “living quicksand”. We investigate the penetration behavior of an object for varying density of the material. We also investigate the dynamics of the penetration process, by measuring the relation between the driving force and the resulting velocity of the intruder, leading to a “power law” behavior with exponent $1/2$, i.e. a quadratic velocity dependence of the drag force on the intruder.



Maximal density of a configuration after settling without change (left) and minimal density after removing all possible loose ends (right).

References:

[1] D. Kadau, H.J. Herrmann and J.S. Andrade Jr., A micromechanical model of collapsing quicksand, *Granular Matter* 13(3), 219-223 (2011), Special Issue in memory of I. Vardoulakis.

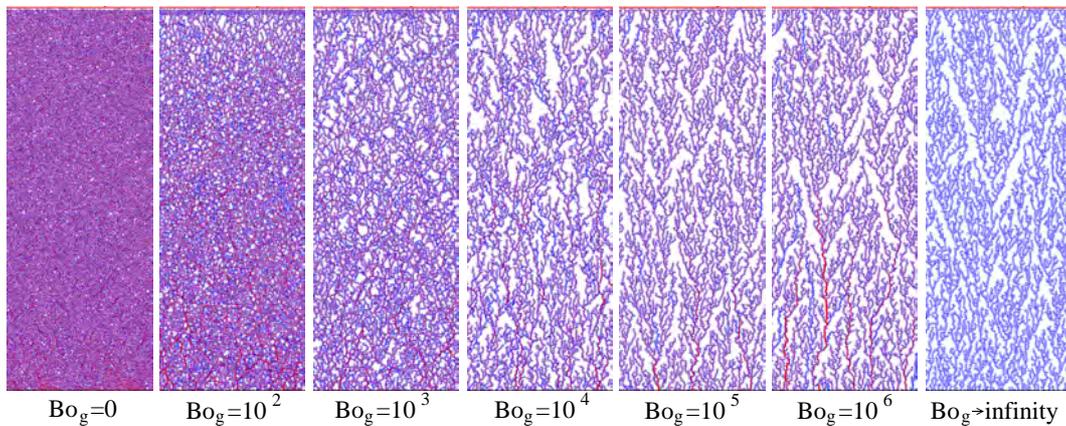
Title: Density profiles of loose and collapsed cohesive granular structures

Researchers: Dr. Dirk Kadau
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Loose granular structures stabilized against gravity by an effective cohesive force are investigated on a microscopic basis using contact dynamics. We study the influence of the granular Bond number on the density profiles and the generation process of packings, generated by ballistic deposition under gravity. The internal compaction occurs discontinuously in small avalanches and we study their size distribution. We also develop a model explaining the final density profiles based on insight about the collapse of a packing under changes of the Bond number.



Final structures achieved by the deposition and collapse process for different granular Bond numbers Bo_g . In addition to the particles, compressive forces are illustrated by red (dark-gray) lines connecting the center of masses between the particles. In the case of $Bo_g \rightarrow \infty$ no forces are present, as is realized in the simulations by switching off gravity.

References:

- [1] D. Kadau, H.J. Herrmann, Density profiles of loose and collapsed cohesive granular structures generated by ballistic deposition, *Physical Review E* 83, 031301 (2011).

Title: Investigation of the Liquid-Liquid Critical Point in ST2 Water Using Finite Size Scaling

Researchers: Tobias Kesselring
Prof. Dr. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We perform molecular dynamics simulations using the ST2 atomic water potential, mainly in the NPT ensemble, for different pressures, temperatures, and system sizes. Using finite size scaling of the Binder cumulant, we find a first-order phase transition between HDL and LDL for high pressures at 210MPa. The HDL and LDL structures compare in excellent way with experimental data for D_2O in similar conditions. This first order phase transition does not occur at lower pressures such as 190MPa. In between, at 208MPa and 246K, we find strong evidence for a critical point falling into the same universality class as the three-dimensional Ising model. Runs near to phase transition line or near to the Widom line are observed to sample both phases, LDL and HDL. The LDL equilibrates much slower than HDL, but with a relaxation time (10ns) 2 orders of magnitude smaller than our simulation time (1000ns). Hence, we equilibrate the LDL phase.

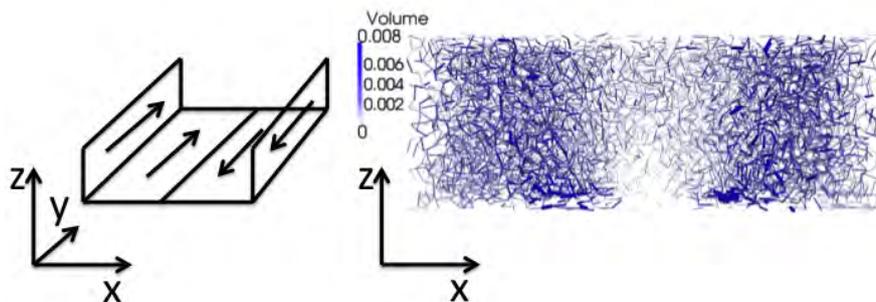
Title: Numerical modeling of liquid transport in wet granular matter

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Where does liquid migrate in shear bands formed in granular matter? It is known that in fully saturated granular media the liquid content increases in dilating shear bands. However, it is not clear what happens at low liquid contents. 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. We use contact dynamics to model spherical particles interacting via coulombian friction as well as via cohesive capillary forces [1,2]. 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. It predicts that liquid is driven out of shear bands despite the increased porosity due to dilatancy. A stable and stationary



shear band is achieved e.g. in the linear split bottom cell. A sketch of it is shown in the figure on the left. The shear zone is lens shaped and increases with increasing height. On the right we see the capillary bridge network after shearing. The liquid content has clearly decreased in the shear zone and acquires a lens shape similar to the velocity profile.

References:

- [1] R. Mani, D. Kadau and H. J. Herrmann, *Fluid transport in sheared wet granular matter*, Preprint (2011)

Title: Three-dimensional lattice Boltzmann model for electro-dynamics

Researchers: Miller Mendoza
Prof. Jose Daniel Muñoz

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

In this paper we introduce a three-dimensional Lattice-Boltzmann model that recovers in the continuous limit the Maxwell equations in materials. In order to build conservation equations with antisymmetric tensors, like the Faraday law, the model assigns four auxiliary vectors to each velocity vector. These auxiliary vectors, when combined with the distribution functions, give the electromagnetic fields. The evolution is driven by the usual Bhatnager-Gross-Krook (BGK) collision rule, but with a different form for the equilibrium distribution functions. This lattice Bhatnager-Gross-Krook (LBGK) model allows us to consider for both dielectrics and conductors with realistic parameters, and therefore it is adequate to simulate the most diverse electromagnetic problems, like the propagation of electromagnetic waves (both in dielectric media and in waveguides), the skin effect, the radiation pattern of a small dipole antenna and the natural frequencies of a resonant cavity, all with 2% accuracy. Actually, it shows to be one order of magnitude faster than the original Finite-difference time-domain (FDTD) formulation by Yee to reach the same accuracy. It is, therefore, a valuable alternative to simulate electromagnetic fields and opens lattice Boltzmann for a broad spectrum of new applications in electrodynamics.

References:

- [1] M. Mendoza and J.D. Muñoz, *Three-dimensional lattice Boltzmann model for electrodynamics*, Phys. Rev. E 82, 056708 (2010)
- [2] M. Mendoza and J.D. Muñoz, *A Reliable Lattice-Boltzmann Solver for Electrodynamics: New Applications in Non-linear Media*, PIERS Proceedings, 1632 - 1636, March 20-23, Marrakesh, MOROCCO 2011

Title: Fast Lattice Boltzmann Methods for Relativistic Hydrodynamics

Researchers: Miller Mendoza
Dr. Paul Romatschke
Prof. Bruce Boghosian
Prof. Hans J. Herrmann
Prof. Sauro Succi

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

A lattice Boltzmann formulation for relativistic fluids is presented and numerically validated through quantitative comparison with recent hydrodynamic simulations of relativistic fluids. In order to illustrate its capability to handle complex geometries, the scheme is also applied to the case of a three-dimensional relativistic shock wave, generated by a supernova explosion, impacting on a massive interstellar cloud. This formulation opens up the possibility of exporting the proven advantages of lattice Boltzmann methods, namely, computational efficiency and easy handling of complex geometries, to the context of (mildly) relativistic fluid dynamics at large, from quark-gluon plasmas up to supernovae with relativistic outflows.

References:

- [1] M. Mendoza, B. M. Boghosian, H. J. Herrmann, and S. Succi, *Fast Lattice Boltzmann Solver for Relativistic Hydrodynamics*, Phys. Rev. Lett. 105, 014502 (2010)
- [2] M. Mendoza, B. M. Boghosian, H. J. Herrmann, and S. Succi, *Derivation of the lattice Boltzmann model for relativistic hydrodynamics*, Phys. Rev. D 82, 105008 (2010)
- [2] P. Romatschke, M. Mendoza, and S. Succi, *Fully relativistic lattice Boltzmann algorithm*, Phys. Rev. C 84, 034903 (2011)

Title: Simulation of flow of mixtures through anisotropic porous media using a lattice Boltzmann model

Researchers: Miller Mendoza
Dr. Falk K. Wittel
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We propose a description for transient penetration simulations of miscible and immiscible fluid mixtures into anisotropic porous media, using the lattice Boltzmann (LB) method. Our model incorporates hydrodynamic flow, advection-diffusion, surface tension, and the possibility for global and local viscosity variations to consider various types of hardening fluids. The miscible mixture consists of two fluids, one governed by the hydrodynamic equations and one by advection-diffusion equations. We validate our model on standard problems like Poiseuille flow, the collision of a drop with an impermeable, solid interface and the deformation of the fluid due to surface tension forces. To demonstrate the applicability to complex geometries, we simulate the invasion process of mixtures into wood spruce samples.

References:

- [1] M. Mendoza, F.K. Wittel and H.J. Herrmann, *Simulation of flow of mixtures through anisotropic porous media using a lattice Boltzmann model*, Eur. Phys. J. E 32, 339-348 (2010)

Title: Optimal-path cracks in correlated and uncorrelated lattices

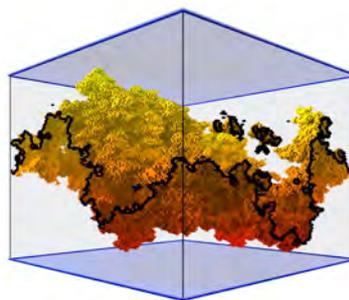
Researchers: K.J. Schrenk
Dr. N.A.M. Araújo
Prof. H.J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

In this project, the optimal path crack (OPC) model on uncorrelated surfaces, recently introduced by Andrade *et al.* [Phys. Rev. Lett. **103** (2009) 225503], is studied by extensive Monte Carlo simulations and its main percolation exponents computed. The analysis is extended to surfaces with spatial long-range power-law correlations, where non-universal fractal dimensions are obtained when the degree of correlation is varied. Finding the optimal path between two points in a disordered system is a relevant challenge for science and technology. If intensively used, this path is prone to fail, and a new path needs to be found. Studying how the successive paths evolve until the final configuration, where connectivity is no longer possible, is a challenge in itself which we address in this project. Exploring the large parameter space of the OPC model is a challenging computational task. Therefore, efficient algorithms for optimum path search and calculation of percolation cluster properties were implemented.

The figure shows a snapshot of a representative configuration of the OPC model in 3D in a strongly disordered energy landscape. The rugged surface of failed sites disconnects the top and bottom layers of the system.



References:

- [1] E. A. Oliveira, K. J. Schrenk, N. A. M. Araújo, H. J. Herrmann, and J. S. Andrade Jr., *Optimal-path cracks in correlated and uncorrelated lattices*, Phys. Rev. E **83** (2011) 046113

Title: Failures in Complex Networks

Researchers: Nuri Yazdani
Dr. Nuno A.M. Araújo

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The importance of considering the network structure in studying the behavior of many modern infrastructures and naturally occurring complex systems, has become increasingly clear. The topology of many real world networks makes them vulnerable with respect to targeted attacks or random failures of their components. There has been a recent surge of interest in determining how one can optimize the structure of these networks to minimize this vulnerability. Given a measure of robustness as objective function and an edge-swap procedure as operator, one can design an iterative algorithm to this purpose. Similar work exists with trajectory-based meta-heuristics and has shown that this method can largely improve the robustness of a given network. For the optimization process, one can introduce an evolutionary algorithm, and one can achieve significantly improved results with modest additional investment of computational resources. Another system which has been studied extensively over the past couple of years is that of two dependent networks, where a failure of a node in one network may cause the failure of a node in the other network. The nature of the collapse of the system was studied in detail by analysing the critical exponents of the model. While the problem was treated analytically, the resulting set of equations needed to be solved numerically to high precision, requiring modern numerical techniques.

Title: Preconditioning of a Robust Maxwell Formulation

Researchers: Florian Krämer
Prof. Dr. Ralf Hiptmair (ETH), Dr. Jörg Ostrowski (ABB), Prof. Dr. Mario Bebendorf (Univ. Bonn)

Institute: Seminar for Applied Mathematics, ETH Zürich

Partner: ABB Corporate Research, Baden-Dättwil

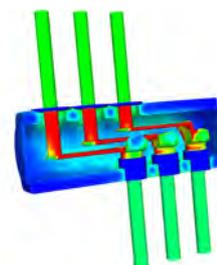
Description:

In this project we investigated the usage of hierarchical matrices (\mathcal{H} -matrices) as a fast and robust preconditioners for a recent formulation of Maxwell's equations. This formulation was introduced in [1] and remains stable in the stationary limit for non-conductive domains. The preconditioner is the inverse of (1), a matrix which has a construction based on a decoupling of magnetic and electric potential. This preconditioner is real, symmetric and positive definite.

We have used a approximative $UDU_{\mathcal{H}}^T$ factorization to overcome the problem that the approximation with \mathcal{H} -matrices could destroy the positive definiteness of the discretization of the first operator in (1) and therefore the stabilization parameter α could be chosen as 1. In (1) σ, μ, ϵ are material parameters and ω denotes the angular frequency.

$$\begin{pmatrix} \mathbf{curl}_{\mu}^1 \mathbf{curl} + \sigma\omega + \alpha & 0 & 0 \\ 0 & -\text{div}(\epsilon \mathbf{grad}) & 0 \\ 0 & 0 & -\text{div}(\epsilon \mathbf{grad})|_{\Omega_C} \end{pmatrix} \quad (1)$$

We have not used to \mathcal{H} -Matrices for all blocks, but just to approximate the inverse of the first block, since this is by far the largest block (\approx five times larger then the other blocks) and the other blocks are still small enough to use a direct decomposition. The solution was computed with a BiCGStab iterative solver, since the preconditioner was applied on the complex valued matrix that results from the finite element discretization of the operator in [1]. A proof that (1) can be approximated with \mathcal{H} -Matrices was given in [2]. Furthermore, we have also been able to approximate the inverse the real-life geometry in the shown figure.



Publications:

- [1] R. Hiptmair, F. Krämer and J. Ostrowski, A Robust Maxwell Formulation For All Frequencies, IEEE Transactions on Magnetics Volume 44, Issue 6, 2008.
- [2] M. Bebendorf and J. Ostrowski. Parallel hierarchical matrix preconditioners for the curl-curl operator. J. of Comp. Math., issue on Adapt. and Multilevel Methods for EM, 27(5):624-641, 2009.

Title: Implementation of a Boundary Element Template Library

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

Institute: Seminar for Applied Mathematics
ETH Zürich

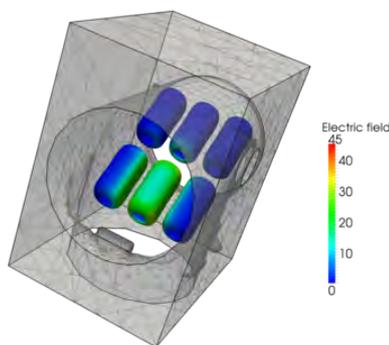
Description:

In the past decade there has been an explosion of available Open Source libraries dealing with Finite Element Methods. But unfortunately, there exist only very few approaches being devoted to the development of Open Source libraries which are well-suited to tackle the discretisation of Boundary Integral operators.

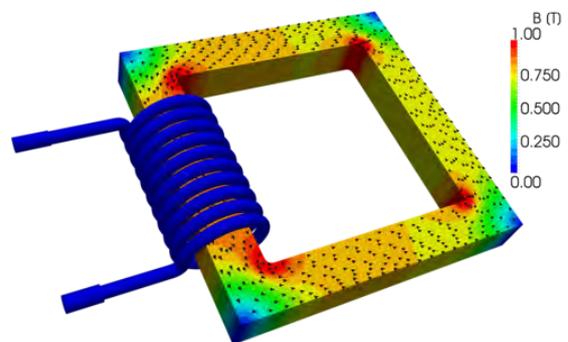
It is inherent to the method itself, that the development of Boundary Element codes is more challenging than it might be for Finite Element codes. Contrary, there are many applications where the usage of Boundary Element Methods is almost mandatory. Important fields of applications are exterior domain problems as well as acoustic and electromagnetic wave propagation phenomena. A Boundary Element library would lead to considerable shorter development times of new Boundary Element codes.

This project is about an unified approach on the implementation of discrete Boundary Integral operators. The implementation is done with C++ and it is done by making exhaustive use of the language's template mechanism. This guarantees not only a fast and robust runtime behavior of the final applications but also establishes a loose binding between the data structures by what the library can be easily enhanced and adopted to special requirements.

Up to now the library has been applied to electrostatic, to magnetostatic as well as to eddy-current problems. While further development on the library will continue it is additionally planned to publish it as an Open Source Project for non-commercial use.



Electrostatic simulation



FEM-BEM Magnetostatics

Title: Process Integrated Virtual Control (PIVC) for the Zero Failure Manufacturing of Deep Drawn Car Body Parts

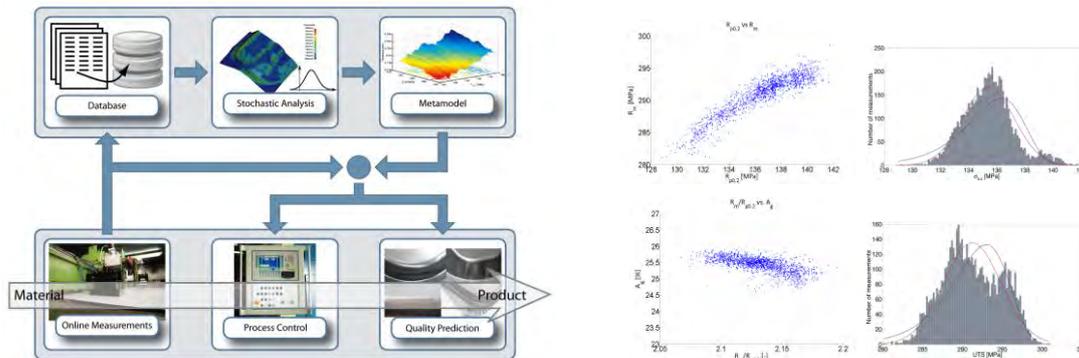
Researchers: N. Manopulo
P. Hora

Institute/ Group: Institute of Virtual Manufacturing

Description:

The use of numerical simulation techniques in the design of manufacturing processes has experienced a rapidly growing acceptance in industry during the past decades. The application of computational techniques remains however still very limited in the production phase. This is mainly because the production conditions are often very dynamic, where the effect of short term (temperature, lubrication etc.) and long term (e.g. tool wear) time dependent effects as well as stochastic influences (e.g. scattering material properties) can no longer be neglected. The mentioned effects can only be captured by substantial computational effort which is clearly unfeasible at production rates of 15-20 parts per minute.

The present work aims to implement an online control system, which can detect potential failures in the process and adapt the manufacturing conditions in a way to avoid their occurrence. The response of the system to the aforementioned scattering process conditions is predicted numerically through stochastic FE simulations and stored into a database. In order to make this information instantly available for an inline control during production, the predicted system response is approximated with a metamodel. In the scope of the project advanced numerical models able to match the real manufacturing conditions, as well as software tools for the setup and validation of metamodels have been developed.



References:

[1] Hora P., Heingärtner J., Manopulo N., Tong L.: Zero Failure Production Methods Based on a Process Integrated Virtual Control. In: *Proceedings of the 8th International Conference and Workshop on Numerical Simulation of 3D Sheet Metal Forming Processes (NUMISHEET 2011)*, Seoul, Korea, 2011.

[2] Manopulo, N., Heingärtner, J., Hora, P.: Numerical Methods and Hardware components for an adaptive robustness control during the production of stamped parts. In: *Proceedings of the 7th International Conference and Workshop on Numerical Simulation of 3D Sheet Metal Forming Processes (NUMISHEET 2008)*, Interlaken, Switzerland, pp. 871-876, 2008.

Title: Numerical simulation of microformed industrial components.

Researchers: F. Dallinger
P. Hora

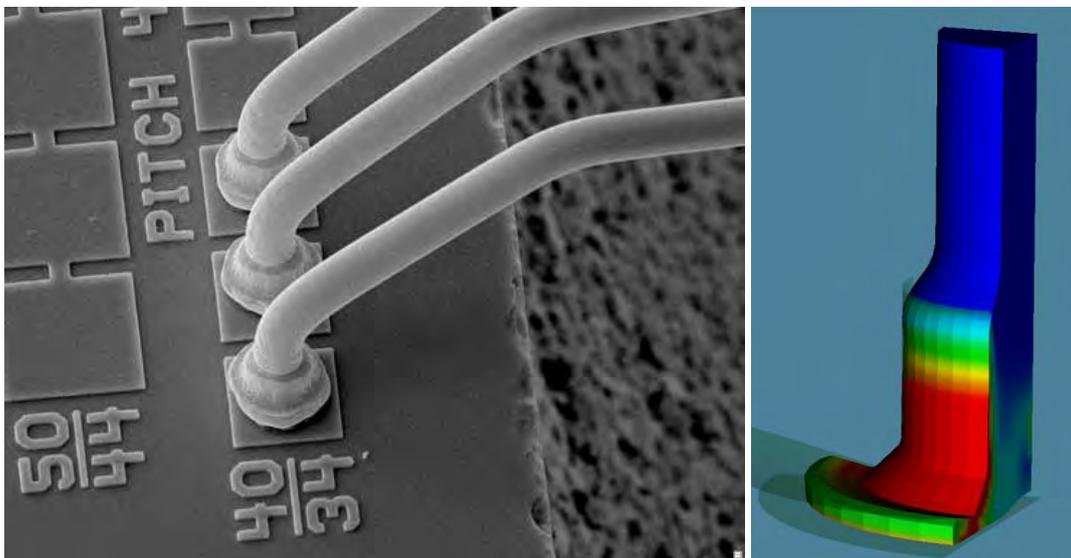
**Institute/
Group:** Institute of Virtual Manufacturing

Description:

Precision industrial products, such as electronic equipment, watches and medical appliances require the feasible series manufacturing of very small components. An increasingly greater share of the latter is being produced by forming operations. Although the numerical computation of conventional forming processes have reached wide industrial acceptance, the virtual control of micro-formed products still represents a major challenge. This is mainly caused by the fact that the continuum mechanics assumptions lying at the base of most state of the art simulation tools are no longer valid at the micro-scale.

The present work aims to develop a multi-scale approach in order to model all the phenomena that influence the forming and failure behavior of micro-formed components. This ranges from nano-level crystal-plasticity considerations such as the orientation and displacement of dislocations, to meso-level issues such as the behavior of the different material phases and the presence of micro-cracks, together with classical macroscopic techniques.

These different approaches are combined into a simulation software by using the Representative Volume Element (RVE) approach, where the different levels of detail are crossed in a hierarchical manner depending on the required accuracy.



Title: Theoretical investigation of solvent effects on glycosylation reactions: Stereoselectivity controlled by preferential conformations of the intermediate oxacarbenium-counterion complex.

Researchers: H. Satoh**
H.S. Hansen*
S. Manabe***
W.F. van Gunsteren*
P.H. Hünenberger*

**Institute/
Group:** * Laboratory of Physical Chemistry
** National Institute of Informatics
Tokyo, Japan
*** RIKEN Advanced Science Institute
Saitama, Japan

Description :

The mechanism of solvent effects on the stereoselectivity of glycosylation reactions is investigated using quantum-mechanical (QM) calculations and molecular dynamics (MD) simulations, considering a methyl-protected glucopyranoside triflate as a glycosyl donor equivalent and the solvents acetonitrile, ether, dioxane, or toluene, as well as gas-phase conditions (vacuum). The QM calculations on oxacarbenium-solvent complexes do not provide support to the usual solvent-coordination hypothesis, suggesting that an experimentally observed β -selectivity (α -selectivity) is caused by the preferential coordination of a solvent molecule to the reactive cation on the α -side (β -side) of the anomeric carbon. Instead, explicit-solvent MD simulations of the oxacarbenium-counterion (triflate ion) complex (along with corresponding QM calculations) are compatible with an alternative mechanism, termed here the conformer and counterion distribution hypothesis. This new hypothesis suggests that the stereoselectivity is dictated by two interrelated conformational properties of the reactive complex, namely, (1) the conformational preferences of the oxacarbenium pyranose ring, modulating the steric crowding and exposure of the anomeric carbon toward the α or β face, and (2) the preferential coordination of the counterion to the oxacarbenium cation on one side of the anomeric carbon, hindering a nucleophilic attack from this side. For example, in acetonitrile, the calculations suggest a dominant B_{2,5} conformation of the cation with preferential coordination of the counterion on the α side, both factors leading to the experimentally observed β selectivity. Conversely, in dioxane, they suggest a dominant ⁴H₃ ring conformation with preferential counterion coordination on the β side, both factors leading to the experimentally observed α selectivity.

References: H. Satoh, H.S. Hansen, S. Manabe, W.F. van Gunsteren and P.H. Hünenberger
J. Chem. Theory Comput. **6** (2010) 1783-1797.

Title: Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers: A comparative molecular dynamics study.

Researchers: B.A.C. Horta*
L. Perić-Hassler*
and P.H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group:

Description :

The disaccharide α,α -trehalose (TRH) is known for its bioprotective action in organisms subject to stressful environmental conditions. However, the mechanisms whereby TRH stabilizes biomolecules remains matter of debate, the five main hypotheses being the water replacement (WRH), headgroup bridging (HBH), vitrification (VIH), water entrapment (WEH) and hydration forces (HFH) hypotheses. Four hypotheses (all except HFH) are in principle compatible with a preferential affinity of the sugar molecules (compared to water) for the biomolecular surface. According to the recently proposed sugar-like mechanism (Pereira & Hünenberger, *Mol. Simul.* **4**, 403, 2008), preferential affinity would result from the entropy gain of releasing many water molecules from the surface region to the bulk, at the cost of immobilizing and rigidifying fewer sugar molecules. Thus, a more flexible disaccharide such as gentiobiose (GNT) should evidence a weaker preferential affinity, limiting its bioprotective ability. In this work, molecular dynamics (MD) simulations of a dipalmitoyl-phosphatidylcholine (DPPC) bilayer patch in the presence of either pure water or aqueous solutions of GNT or TRH are performed in order to assess the validity of this suggestion. At 475 K and 1.6 m (molal), TRH indeed preserves the bilayer structure to a larger extent compared to GNT. However, the present investigation does not unambiguously indicate which of the above mechanism takes place, since the simulations reveal characteristic features of all of them. This suggests either that multiple mechanisms may be simultaneously active or that their definitions are not precise enough.

References: B.A.C. Horta, L. Perić-Hassler and P.H. Hünenberger
J. Mol. Graph. Model. **29** (2010) 331-346.

Title: New interaction parameters for oxygen compounds in the GROMOS force field: Improved pure-liquid and solvation properties for alcohols, ethers, aldehydes, ketones, carboxylic acids and esters.

Researchers: B.A.C. Horta*
P.F.J. Fuchs**
W.F. van Gunsteren*
P.H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group: ** INSERM UMR-S66, Université Paris-Diderot
UFR Sciences du Vivant & Institut National
de Transfusion Sanguine, Paris, France

Description :

A new parameter set (53A6_{OXY}) is developed for the GROMOS force field, that combines reoptimized parameters for the oxygen containing chemical functions (alcohols, ethers, aldehydes, ketones, carboxylic acids and esters) with the current biomolecular force field version (53A6) for all other functions. In the context of oxygen containing functions, the 53A6_{OXY} parameter set is obtained by optimization of simulated pure-liquid properties, namely the density ρ_{liq} and enthalpy of vaporization ΔH_{vap} , as well as solvation properties, namely the free energies of solvation in water ΔG_{wat} and in cyclohexane ΔG_{che} , against experimental data for 10 selected organic compounds, and further tested for 25 other compounds. The simultaneous refinement of atomic charges and Lennard-Jones interaction parameters against the four mentioned types of properties provides a single parameter set for the simulation of both liquid and biomolecular systems. Small changes in the covalent parameters controlling the geometry of the oxygen containing chemical functions are also undertaken. The new 53A6_{OXY} force-field parameters reproduce the mentioned experimental data within root-mean-square deviations of 22.4 kg m⁻³ (ρ_{liq}), 3.1 kJ mol⁻¹ (ΔH_{vap}), 3.0 kJ mol⁻¹ (ΔG_{wat}) and 1.7 kJ mol⁻¹ (ΔG_{che}) for the 35 compounds considered.

References: B.A.C. Horta, P.F.J. Fuchs, W.F. van Gunsteren and P.H. Hünenberger
J. Chem. Theory Comput. **7** (2011) 1016-1031.

Title: Enantiometric segregation in the gel phase of lipid bilayers.

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

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

Description :

Enantiospecific interactions within a monoglyceride lipid bilayer are investigated using molecular dynamics simulations. Preferential homochiral interactions are observed in the gel phase, whereas no detectable enantiospecificity is seen in the liquid-crystal phase. On the basis of these results and available experimental data, a mechanism is proposed for the formation of the coagel phase of monoglycerides. Enantiomeric segregation in the gel phase is also discussed in terms of its possible implications for prebiological evolution and membrane raft function.

References: B.A.C. Horta and P.H. Hünenberger
J. Am. Chem. Soc. **133** (2011) 8464-8465.

Title: Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: Enthalpic and entropic driving forces.

Researchers: A. Choutko*
W.F. van Gunsteren*
P.H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group:

Description :

The modulation of the properties of lipid membranes by polyhydroxylated cosolutes such as sugars is a phenomenon of considerable biological, technological and medicinal relevance. A few years ago, we proposed the so-called sugar-like mechanism - binding driven by release of water molecules - as an attempt to rationalize the preferential affinity of carbohydrate molecules compared to water for the surface of lipid bilayers, presumably related to the bioprotective action of these compounds. The goal of the present work is to gain a better understanding of the driving force underlying this mechanism, in terms of specific interactions or effects, as well as in terms of energy-entropy partitioning. This is done in the simplest possible context of an apolar rigid-wall model representing the membrane, and mixtures of closely related and possibly artificial species in solution, namely monomers or dimers of Lennard-Jones particles, water with physical or reduced charges, and hydroxymethyl groups. The results indicate that although the sugar-like mechanism seems phenomenologically reasonable, the main driving force underlying this mechanism is not the entropy gain upon releasing water molecules into the bulk, as originally suggested, but rather the hydrophobic effect. Note that the latter effect is a generic concept and may in principle involve both a solvent release and an interaction component, depending on the solute considered.

References: A. Choutko, W.F. van Gunsteren and P.H. Hünenberger
Chem. Phys. Chem., submitted (2011)

Title: Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: Influence on the folding properties of two β -peptides.

Researchers: B.A.C. Horta*
Z. Lin*
W.F. van Gunsteren*
P.H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group:

Description :

Considering N-methylacetamide (NMA) as a model compound, new interaction parameters are developed for the amide function in the GROMOS force field, that are compatible with the recently derived 53A6_{OXY} parameter set for oxygen-containing chemical functions. The resulting set is referred to here as 53A6_{OXY+A}. This new set represents a significant improvement over the earlier GROMOS force-field versions in the context of the pure-liquid properties of NMA, including the density, heat of vaporization, self-diffusion constant, and viscosity. The agreement with experiment in terms of the hydration free energy of NMA is also improved. Since NMA represents the simplest possible peptide-backbone model compound, 53A6_{OXY+A} is expected to provide an improved description of polypeptide chains. As an initial test for the performance of 53A6_{OXY+A} in this context, simulations are also reported for two β -peptides characterized by very different folding properties in methanol. For these systems, earlier force-field versions provided good agreement with experimental NMR data, and the test shows that the improved description achieved in the context of NMA is not accompanied with any deterioration in the representation of the conformational properties of these peptides. Work is currently in progress following the same strategy to define improved interaction parameters for all nitrogen-containing, sulfur-containing and aromatic compounds necessary for spanning the entire range of amino-acid side chains occurring in natural polypeptides.

References: B.A.C. Horta, Z. Lin, W.F. van Gunsteren and P.H. Hünenberger
J. Chem. Theory Comput., submitted (2011).

Title: Single-ion solvation. Experimental and theoretical approaches to elusive thermodynamic quantities.

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

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

Description :

This book provides an up-to-date and consistent account of a research field that has over hundred years of history and remains nowadays largely unsettled: single-ion solvation thermodynamics. Ions are ubiquitous in chemical, technological, ecological and biological processes. Characterizing their role in these processes requires in the first place the evaluation of the thermodynamic parameters associated with the solvation of a given ion. Yet, due to the constraint of electroneutrality, the involvement of surface effects and the ambiguous connection between microscopic and macroscopic descriptions, the determination of single-ion solvation properties *via* both experimental and theoretical approaches has turned out to be a very difficult and highly controversial problem. By reviewing the various approaches employed to date, establishing the relevant connections between single-ion thermodynamics and electrochemistry, resolving conceptual ambiguities, and reporting an exhaustive data compilation (in the context of alkali and halide hydration, along with relevant values for the proton), this book provides a consistent synthesis of a large and sometimes very confusing research field. It represents an essential text for in-depth understanding and further research.

References: P. Hünenberger and M. Reif
RSC Theoretical and Computational Chemistry Series, ISBN: 978-1-84755-187-0 (2011).
See http://www.csms.ethz.ch/single_ion_solvation

Title: Turbulent reactive flow

Researchers: Michael Wild
Mathias Hack (now Sulzer Innotec)
Michael Hegetschweiler (now MAN)
Benjamin Zoller
Daniel Meyer
Patrick Jenny

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

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:

P. Jenny and D. W. Meyer. Transported probability and mass density function (PDF/MDF) methods for uncertainty assessment and multi-scale problems. In Numerical Analysis of Multiscale Problems. Springer, 2011.

- D. W. Meyer. A new particle interaction mixing model for turbulent dispersion and turbulent reactive flows. *Physics of Fluids*, 22, 2010.
- M. L. Hack. Joint PDF Closure for Turbulent Premixed Flames. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.
- M. L. Hack and P. Jenny. Joint PDF closure of turbulent premixed flames. In *Proceedings of Mediterranean Combustion Symposium*, 2011.
- M. Hegetschweiler, B. Zoller, and P. Jenny. Reactive parametrized scalar profile (R-PSP) mixing model for partially premixed combustion. *Combustion and Flame*, 2011.
- B. T. Zoller, J. Allegrini, U. Maas, and P. Jenny. PDF model for NO calculations with radiation and consistent NO-NO₂ chemistry in non-premixed turbulent flames. *Combustion and Flame*, 2011.
- B. T. Zoller and P. Jenny. Combustion model to predict local and global extinction of partially premixed flames. In *Proceedings of Mediterranean Combustion Symposium*, 2011.
- G. Anand. PDF Modeling of Turbulent Evaporating Sprays. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.
- M. Hegetschweiler. Hybrid PDF Algorithm and PDF Modeling of Partially Premixed Turbulent Combustion. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.
- M. Hegetschweiler, C. Handwerk, and P. Jenny. Partially premixed turbulent combustion model based on joint statistics of progress variable, mixture fraction, and scalar dissipation rate. *Combust. Sci. and Tech.*, 182:480–490, 2010.

Title: Flow and transport in porous and fractured media

Researchers: Dimitrios Karvounis
Florian Müller
Karim Khayrat
Manav Tyagi (now PSI)
Hadi Hajibeygi (now Stanford)
Giuseppe Bonfigli (now Andritz Hydro)
Daniel Meyer
Patrick Jenny

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

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, CO₂ 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 choice of the coarse cell boundaries.

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 is currently being 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 will be resolved. The cloud of small fractures will be homogenized and treated by effective permeabilities.

Recent developments include consistent corrections of transmissibility values and currently convergence studies and comparisons with established methods are performed.

Uncertainty assessment of scalar 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 sub-

stances 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. Alternatively, polynomial chaos and Karhunen-Loève expansion techniques are applied to investigate and simulate the transfer of uncertainty from the soil parameters to the flow- and transport-dependent quantities.

Currently a Lagrangian approach for multi-phase flow in combination with a multi-level Monte-Carlo method is developed.

Stochastic particle method for non-equilibrium multi-phase flow: This is a collaboration with Prof. Hamdi Tchelepi (Stanford University). A related topic with high relevance is motivated by CO₂ sequestration. Currently, storing CO₂ in geological sub-surface formations seems to be one of the most promising feasible technologies to stabilize the CO₂ concentration in the Earth's atmosphere. Our research in this area is conducted in collaboration with the Department of Energy Resources Engineering at Stanford University. The prime objective 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 developed a PDF modeling framework. A stochastic particle method (SPM), in which individual (infinitesimal) fluid volumes are modeled, is employed to solve the PDF transport equation. These fluid volumes are represented by computational particles, whose evolution depends on their phase, composition and other properties including memory. Such a Lagrangian approach offers an alternative viewpoint and allows to describe various complex non-equilibrium processes in a more general and natural way than in a classical Eulerian framework. Non-equilibrium dissolution and trapping model was incorporated and it was demonstrated that it is possible to treat complex processes in a very natural and intuitive way, which would lead to additional assumptions at the moment closure level.

The current effort deals with a quantitative validation of the approach. Using reference data from pore-network simulations it shall be demonstrated that the stochastic model can be closed by extracting minimal empirical information and then allows to make predictions.

References:

D. W. Meyer, P. Jenny, and H. A. Tchelepi. A joint velocity-concentration PDF method for tracer flow in heterogeneous porous media. *Water Resources Research*, 46, 2010.

D. W. Meyer and H. A. Tchelepi. Particle-based transport model with Markovian velocity processes for tracer dispersion in highly heterogeneous porous media. *Water Resources Research*, 46, 2010.

- F. Müller, D. W. Meyer, and P. Jenny. Probabilistic collocation and Lagrangian sampling for advective tracer transport in randomly heterogeneous porous media. *Advances in Water Resources*, 2011 (accepted).
- H. Hajibeygi. Iterative Multiscale Finite Volume Method for Multiphase Flow in Porous Media with Complex Physics. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.
- H. Hajibeygi, R. Deb, and P. Jenny. Multiscale finite volume method for non-conformal coarse grids arising from faulted porous media. In *Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 142205-PP)*, 2011.
- H. Hajibeygi and P. Jenny. Adaptive iterative multiscale finite volume method. *Journal of Computational Physics*, 230(3), 2011.
- H. Hajibeygi, D. Karvounis, and P. Jenny. A hierarchical fracture model for the iterative multiscale finite volume method. *Journal of Computational Physics*, 2011 (submitted).
- H. Hajibeygi, D. Karvounis, and P. Jenny. A loosely coupled hierarchical fracture model for the iterative multiscale finite volume method. In *Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141991-PP)*, 2011.
- H. Hajibeygi, I. Lunati, and S. H. Lee. Accurate and efficient simulation of multiphase flow in a heterogeneous reservoir by using error estimate and control in the multiscale finite-volume framework. In *Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141954-PP)*, 2011.
- H. Hajibeygi, I. Lunati, and S. H. Lee. Error estimate and control in the MSFV method for multiphase flow in porous media. In *Proceedings of CMWR XIII*, 2010.
- M. Tyagi and P. Jenny. Probability density function framework for modeling multi-phase ganglia flow in porous media. *Journal of Fluid Mechanics*, pages 1–39, 2011.
- M. Tyagi and P. Jenny. Probability density function modeling of multi-phase flow in porous media with density-driven gravity currents. *Transp. Porous Media*, 87(2), 2011.
- M. Tyagi. Probability Density Function (PDF) Approach for Modeling Multi-Phase Flow in Porous Media. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.
- M. Tyagi and P. Jenny. PDF-approach for modeling dissolution-driven gravity currents. In *Proceedings of CMWR XIII*, 2010.

D. Karvounis and P. Jenny. Modeling of flow and transport in Enhanced Geothermal Systems. In Proceedings, Thirty-Sixth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, January 31 - February 2, 2011.

G. Bonfigli. High-order finite-difference implementation of the immersed-boundary technique for incompressible flows. Computers and Fluids, 2010.

Title: Fluid dynamics in biological systems and biomedical optics

Researchers: Johannes Reichold
Milos Sormaz (now EMPA)
Prof. Patrick Jenny

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

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), Prof. Alfred Buck (University Hospital Zürich) and Prof. Marco Stampanoni (University of Zürich and Paul Scherrer Institut). 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.

References:

J. Reichold. Cerebral Blood Flow Modeling in Realistic Cortical Microvascular Networks. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

K. Erbertseder, J. Reichold, R. Helmig, P. Jenny, and B. Flemisch. A coupled discrete / continuum model for describing cancer therapeutic transport in the lung. PLoS ONE, 2011 (submitted).

B. Misselwitz, N. Barrett, S. Kreibich, P. Vonasch, S. Rout, K. Weidner, M. Sormaz, P. Songhet, P. Horvath, M. Chabria, V. Vogel, D. Spori, N. Spencer, P. Jenny, and W.-D. Hardt. Sliding of salmonella typhimurium on epithelial surfaces explains target cell selection and cooperative invasion, 2011 (submitted).

M. Sormaz and P. Jenny. Monte Carlo study of subsurface imaging in the time-domain with co-axial laser-detector setup and a novel scheme for the target reconstruction. Journal of Optical Society of America, 2011 (submitted).

S. Hirsch, J. Reichold, G., Székely, and B. Weber. Topology of the Cortical Cerebrovascular System. Invited Review for Journal of Cerebral Blood Flow & Metabolism, 2011 (invited).

D. Obrist, B. Weber, A. Buck, and P. Jenny. Red blood cell distribution in simplified capillary networks. Philosophical Transactions of the Royal Society, 368(1921):2897–2918, 2010.

M. Sormaz. On the Stochastic Modeling of Light Scattering Applied in Remote Sensing and Ballistic- Photon Imaging. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

M. Sormaz and P. Jenny. Contrast improvement by selecting ballistic-photons using polarization gating. Optical Society of America, 18(23), 2010.

M. Sormaz, T. Stamm, and P. Jenny. Influence of linear birefringence in the computation of scattering phase functions. Journal of Biomedical Optics, 15(5), 2010.

M. Sormaz, T. Stamm, and P. Jenny. Stochastic modeling of polarized light scattering using a Monte Carlo based stencil method. Optical Society of America, pages 1–29, 2010.

Title: PDF modeling of non-equilibrium gas flow

Researchers: Hossein Gorji
Patrick Jenny

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

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 are a generalization for diatomic gas and a wall model, which can account for redistribution of internal energy modes.

References:

H. Gorji and P. Jenny. Continuous stochastic equations for diatomic rarefied gas flows. In Proceedings of the 3rd GASMEMS Workshop - Bertinoro, June 9-11, 2011.

H. Gorji, M. Torrilhon, and P. Jenny. Fokker–Planck model for computational studies of monatomic rarefied gas flows. *J. Fluid Mech.*, 680:574–601, 2011.

H. Gorji and P. Jenny. A generalized stochastic solution algorithm for simulations of rarefied gas flows. In Proceedings of the 2nd European Conference on Microfluidics, Toulouse, France, 2010.

P. Jenny, M. Torrilhon, and S. Heinz. A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion. *Journal of Computational Physics*, 229:1077–1098, 2010.

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:

H. Xiao, M. Wild, and P. Jenny. Preliminary evaluation and applications of a consistent hybrid LES/RANS method. In HRLM-4, 2011 (submitted).

H. Xiao and P. Jenny. A consistent dual-mesh framework for hybrid LES/RANS modeling. *Journal of Computational Physics*, 2011 (submitted).

Title: Morphing wing aerodynamics

Researchers: Vitali 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:

G. Molinari, M. Quack, V. Dmitriev, M. Morari, P. Jenny, and P. Ermanni. Aero-structural optimisation of morphing aerofoils for adaptive wings. *Journal of Intelligent Material Systems and Structures*, Vol 22, 2011.

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-collexes. 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 nontrivial 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) 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:

Ruben S. Andrist, Helmut G. Katzgraber, H. Bombin, and M.-A. Martin-Delgado, *New. J. Phys.*, 13, 083006 (2011)

Helmut G. Katzgraber, H. Bombin, Ruben S. Andrist and M.-A. Martin-Delgado, *Phys. Rev. A* 81, 012319 (2010)

Helmut G. Katzgraber, H. Bombin, and M.-A. Martin-Delgado, *Phys. Rev. Lett.* 103, 090501 (2009)

Title: Three-spin spin-glass models as toy models to understand structural glasses

Researchers: D. Larson*
Helmut Katzgraber**
M. A. Moore***
A. Peter Young*

Institute/Group: * Department of Physics, University of California Santa Cruz, USA
** Theoretische Physik, ETH Zürich
***Department of Physics, University of Manchester, UK

Description:

We study a p-spin spin-glass model to understand if the finite-temperature glass transition found in the mean-field regime of p-spin models, and used to model the behavior of structural glasses, persists in the nonmean-field regime. By using a three-spin spin-glass model with long-range power-law diluted interactions we are able to continuously tune the (effective) space dimension via the exponent of the interactions. Monte Carlo simulations of the spin-glass susceptibility and the two-point finite-size correlation length show that deep in the nonmean-field regime, the finite-temperature transition is lost whereas this is not the case in the mean-field regime, in agreement with the prediction of Moore and Drossel [Phys. Rev. Lett. 89, 217202 (2002)] that three-spin models are in the same universality class as an Ising spin glass in a magnetic field. However, slightly in the nonmean-field region, we find an apparent transition in the three-spin model, in contrast to results for the Ising spin glass in a field. This may indicate that even larger sizes are needed to probe the asymptotic behavior in this region.

References:

Derek Larson, H. G. Katzgraber, M. A. Moore and A. P. Young, Phys. Rev. B 81, 064415 (2010)

Title: Evidence of a thermodynamic glass transition in the 10-state non-mean-field Potts glass

Researchers: Ruben S. Andrist*
D. Larson**
H. G. Katzgraber*

Institute/Group: *Theoretische Physik, ETH Zürich
**National University of Taiwan

Description:

Potts glasses are prototype models that have been used to understand the structural glass transition. However, in finite space dimensions a glass transition remains to be detected in the 10-state Potts glass. Using a one-dimensional model with long-range power-law interactions we present evidence that a glass transition below the upper critical dimension can exist for short-range systems at low enough temperatures. Gaining insights into the structural glass transition for short-range systems using spin models is thus potentially possible, yet difficult.

References:

Ruben S. Andrist, D. Larson, H. G. Katzgraber, Phys. Rev. E **83**, 030106(R) (2011)

Title: Universality in phase boundary slopes for spin glasses on self dual lattices

Researchers: Masayuki Ohzeki*
Creighton K. Thomas**
Helmut G. Katzgraber***
Hector Bombin****
Miguel Angel Martin-Delgado*****

Institute/Group: * Department of Physics, Kyoto University
** Texas A&M University
***Theoretische Physik, ETH Zurich
****Perimeter Institute, Canada
*****Universidad Complutense de Madrid, Spain

Description:

We study the effects of disorder on the slope of the disorder--temperature phase boundary near the Onsager point ($T_c = 2.269\dots$) in spin-glass models. So far, studies have focused on marginal or irrelevant cases of disorder. Using duality arguments, as well as exact Pfaffian techniques we reproduce these analytical estimates. In addition, we obtain different estimates for spin-glass models on hierarchical lattices where the effects of disorder are relevant. We show that the phase-boundary slope near the Onsager point can be used to probe for the relevance of disorder effects.

References:

Masayuki Ohzeki, Creighton K. Thomas, H. G. Katzgraber, H. Bombin, M. A. Martin-Delgado, J. Stat. Mech. P02004 (2011)

Title: Density of States and Critical Behavior of the Coulomb Glass

Researchers: B. Surer*
H. G. Katzgraber*
G. Blatter*
A. Glatz**
G. T. Zimanyi***
B. A. Allgood****

Institute/Group: * Theoretische Physik, ETH Zürich
** Argonne National Lab, USA
*** University of California Davis, USA
**** Numerate Inc., USA

Description:

We present zero-temperature simulations for the single-particle density of states of the Coulomb glass. Our results in three dimensions are consistent with the Efros and Shklovskii prediction for the density of states. Finite-temperature Monte Carlo simulations show no sign of a thermodynamic glass transition down to low temperatures, in disagreement with mean-field theory. Furthermore, the random-displacement formulation of the model undergoes a transition into a distorted Wigner crystal for a surprisingly broad range of the disorder strength.

References:

Brigitte Surer, H. G. Katzgraber, G. T. Zimanyi, B. A. Allgood, and Gianni Blatter, Phys. Rev. Lett. 102, 067205 (2009)

Brigitte Surer, A. Glatz, H. G. Katzgraber, G. T. Zimanyi, B. A. Allgood, and Gianni Blatter, Phys. Rev. Lett. 105, 039702 (2010)

Title: Optimizing glassy p-spin models

Researchers: Creighton K. Thomas*
H. G. Katzgraber**

Institute/Group: *Texas A&M University
**Theoretische Physik, ETH Zürich

Description:

Computing the ground state of Ising spin-glass models with p-spin interactions is, in general, an NP-hard problem. In this work we show that unlike in the case of the standard Ising spin glass with two-spin interactions, computing ground states with $p=3$ is an NP-hard problem even in two space dimensions. Furthermore, we present generic exact and heuristic algorithms for finding ground states of p-spin models with high confidence for systems of up to several thousand spins. Finally, we demonstrate that our heuristic optimization algorithm that combines a local search with triadic crossover genetic updates is capable of sampling uniformly among ground-state configurations in spin-glass-like Hamiltonians with p-spin interactions in d space dimensions that have highly degenerate ground states. Using this algorithm we probe the zero-temperature ferromagnet--spin-glass transition of two example models, the disordered version of the two-dimensional three-spin Baxter-Wu model [$q_c = 0.1072(1)$] and the three-dimensional Edwards-Anderson model [$q_c=0.2253(7)$], by computing the Binder ratio of the ground-state magnetization.

References:

Creighton K. Thomas and H. G. Katzgraber, Phys. Rev. E 83, 046709 (2011)

Creighton K. Thomas and H. G. Katzgraber, (arXiv:cond-mat/1108.1953).

Title: Critical behavior and universality in Levy spin glasses

Researchers: Juan Carlos Andresen*
Katharina Janzen**
Helmut G. Katzgraber*

Institute/Group: *Theoretische Physik, ETH Zürich
**Carl von Ossietzky Universitaet Oldenburg

Description:

Using large-scale Monte Carlo simulations that combine parallel tempering with specialized cluster updates, we show that Ising spin glasses with Levy-distributed interactions share the same universality class as Ising spin glasses with Gaussian or bimodal-distributed interactions. Corrections to scaling are large for Levy spin glasses. In order to overcome these and show that the critical exponents agree with the Gaussian case, we perform an extended scaling of the two-point finite size correlation length and the spin glass susceptibility. Furthermore, we compute the critical temperature and compare its dependence on the disorder distribution width to recent analytical predictions [J. Stat. Mech. (2008) P04006].

References:

Juan Carlos Andresen, Katharina Janzen and H. G. Katzgraber, Phys. Rev. B 83, 174427 (2011)

Title: Reentrance in Physical Systems

Researchers: Creighton K. Thomas*
H. G. Katzgraber**

Institute/Group: *Texas A&M University
**Theoretische Physik, ETH Zürich

Description:

We numerically investigate the necessary ingredients for reentrant behavior in the phase diagram of physical systems. Studies on the possibly simplest model that exhibits reentrance, the two-dimensional random bond Ising model, show that reentrant behavior is generic whenever frustration is present. For both discrete and continuous disorder distributions, the phase diagram in the disorder-temperature plane is found to be reentrant, where for some disorder strengths a paramagnetic phase exists at both high and low temperatures, but an ordered ferromagnetic phase exists for intermediate temperatures.

References:

Creighton K. Thomas and H. G. Katzgraber, Phys. Rev. B., in press, (arXiv:cond-mat/1104.2582).

Title: Fluid Mechanics of the Inner Ear

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

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

Description:

The inner ear hosts the balance sense (semicircular canals and otolith organs) as well as the sensory hearing organ (cochlea).

We study the (patho-)physiology of the semicircular canals and the cochlea with numerical simulations. While the cochlea requires a careful simulation of a highly unsteady flow with tight fluid-structure interaction (FSI), the simulation of the semicircular canals involves the simulation of particle sedimentation. Settling particles in the semicircular canals (SCC) of the inner ear are suspected to be the most common cause for vertigo. This pathological condition is known as benign paroxysmal positional vertigo (BPPV) and affects almost 10% of all elderly people. However, only little is known about the mechanisms of BPPV.

Another pathologic mechanism for vertigo is known as Tullio's phenomenon. For affected patients, energy transfer is possible between the organs of hearing and balance. Therefore the sensation of sound results in a misleading flow inside the SCCs which triggers abnormal eye movement and thus vertigo. Numerical investigations are performed with the open source software OpenFOAM and include pulse propagation and FSI on a finite-volume grid of the SCCs.

In order to study BPPV, we chose the method of fundamental solutions (MFS) to develop a numerical model of the flow in two- and three-dimensional semicircular canals. MFS is a meshless method but, unlike the traditional boundary element methods, the source points of the fundamental solutions are located outside the computational domain. An optimal location of the collocation points on the boundary and of the source points outside the domain yields spectral convergence. Unfortunately, this optimal configuration is not known a priori and sub-optimal configurations may lead to numerical instability. Based on several numerical experiments, we proposed a stable and efficient multilayer version of MFS for the solution of Stokes problems.

The proposed MFS solver is easily extended for the simulation of BPPV and first numerical experiments with particles have been performed. Moreover, a morphological model of the anatomy of the inner ear labyrinth has been reconstructed from bio-images and is available for numerical simulations.

References: See separate list.

Title: Large-Eddy Simulation of Transitional and Turbulent Wall-Bounded Flows

Researchers: Lars Gräf and Leonhard Kleiser

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

Description:

Most engineering and geophysical flows occur at high Reynolds numbers and are turbulent. A direct simulation of turbulent flows which resolves all relevant length and time scales (direct numerical simulation, DNS) is practicable only for very low Reynolds numbers. For larger Reynolds numbers the computational cost is prohibitive. Therefore, computationally less expensive but still accurate simulation methods have to be developed. This can be achieved by decreasing the spatial resolution while the effects of the non-resolved scales are modeled. Such simulations are known as large-eddy simulations (LES). In recent years, a number of different LES models have been developed, one of which is the approximate-deconvolution model (ADM) developed at our Institute. Large-eddy simulations with ADM were found to give excellent results for a wide range of flows, all at a fraction (on the order of one percent) of the cost needed for a DNS.

We implemented ADM in the semi-industrial finite-volume code NSMB with full support of domain decomposition and parallel computing. We used NSMB with ADM to investigate film cooling of turbine blades, a state-of-the-art cooling technique. First, the dominant vortex structures (counter-rotating vortex pair, horseshoe vortex, hairpin vortices) of the flow were visualized. Furthermore, the flow inside and beneath the cooling holes, which is generally inaccessible to experimental measurements, has been analyzed. Second, the cooling efficiency is strongly influenced by the turbulence properties of the oncoming boundary layer. Using a recent technique for turbulent inflow generation which uses randomly distributed synthetic eddies of deterministic size, we have been able to demonstrate the effect of turbulent versus laminar boundary layer flow on this specific scenario. Third, we investigated the flow field and cooling performance of an arrangement with two rows of cooling holes that are yawed. The beneficial effect of this arrangement on the cooling performance, that has been demonstrated experimentally in the literature, were simulated for realistic blowing ratios. Furthermore, the impact of the yaw angle on the cooling distribution was studied by parameter variation.

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, Leonhard Kleiser

Institute/ Institute of Fluid Dynamics
Group: 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.

In the work of Keiderling (Diss. ETH No. 17955, 2008) large-eddy simulations (LES) were performed using ADM as a subgrid-scale model. Based on this and other numerical and experimental work it became obvious that the jet nozzle itself plays an important role in the jet noise simulations in order to bring results in closer agreement with experiments. The present work deals with the integration of the nozzle into the existing simulation setup. The computational expense for the simulation at relevant Reynolds numbers is immense and will be further increased as the viscous sublayer of the flow within the nozzle now needs to be resolved in order to obtain reliable results with the LES approach. A massively parallel version of the existing code was developed using the Message Passing Interface (MPI) to achieve acceptable turn-around times of the jet simulations. The perceived noise at remote observer locations can be determined most efficiently with an acoustic far-field solver which extrapolates the information of the underlying LES to the acoustic far-field.

Furthermore, we investigate the stability and transitional behaviour of swirling jets at medium to high swirl numbers. At sufficiently high azimuthal velocity the jets breaks down and an elongated recirculation zone around the centerline develops. This flow state is governed by strong helical modes dominating the conical shear layers. A single helix instability is believed to undergo a change from a convectively to a globally unstable state overwhelming the entire flow. The global mode then acts as a ‘wave-maker’ for the flow field imposing a dominant frequency on the conical shear layer.

We study the influence of the nozzle on the breakdown behaviour of this swirling jet. The nozzle lip is believed to have an important impact on the mode selection in the flow region behind the nozzle. Our investigation also includes the influence of the azimuthal shear layers within and outside the nozzle on the mode selection mechanism. Our aim is to get a better more insight on the swirl numbers necessary for a vortex breakdown (for our specific setup) and to understand the hysteresis behaviour of the swirling jet at high swirl number.

References: See separate list.

Title: Simulation of Particle-Laden Flows (2 Projects)

Researchers: R. Henniger, Y. Reinhardt, O. Häuselmann, and L. Kleiser

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

Description:

The first project deals with direct and large-eddy simulations of miscible fluid flows. 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 4th or 6th 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 3D 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 on the Eulerian grid. Further, a Lagrangian particle approach has been implemented where additional momentum equations are solved for each particle. In return, the transported concentrations and particles give 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 model estuaries and turbidity currents. In model estuaries, the focus is on the mixing of freshwater with saltwater as well as the transport of suspended sediment particles or pollutants in the fluid. In turbidity currents, the Lagrangian particle description is used to gather more information on particle-settling mechanisms due to turbulence.

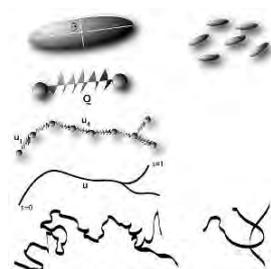
The second project deals with abrasive water jet cutting. In recent years the use of abrasive water jet technology has become increasingly popular for material cutting applications. The aim of this project is to model the abrasive water jet, more precisely the mixing process between particles and the jet in the cutting head.

For the computations, the open source code OpenFOAM is used. High Reynolds numbers and particle loadings require the use of the Reynolds-averaged Navier-Stokes equations and turbulence models. Preliminary numerical studies were carried out on jets where good agreement with analytical solutions for single-phase configurations and reasonable and perspicuous results for two-phase flows were achieved. With OpenFOAM, wall bounded flow simulations of single- and two-phase configurations were carried out at low Reynolds numbers and different particle loadings. The current work focuses on accurately modeling the turbulence of the different phases.

References: See separate list.

Title: Computational Polymer Physics

Researchers: Prof. Martin Kröger¹
Prof. Avraham Halperin²
Prof. Manuel Laso³
Prof. Juan J. de Pablo⁴
Prof. Ekaterina B. Zhulina,⁵
Prof. Igal Szleifer,⁶



Institutes: ¹ Computational Polymer Physics, D-MATL, ETH Zürich
² CEA Grenoble, France
³ ETSII Madrid, Spain
⁴ University of Wisconsin, Madison, WI, USA
⁵ Russian Academy of Sciences, St. Petersburg, Russia
⁶ Northwestern University, Chicago, CA, USA

Description:

During the beginning of 2011 we focused on studying the influence of nanorod inclusions on structure and primitive path network of polymer nanocomposites at equilibrium and under deformation [1], we developed a method for the smooth full field reconstruction of velocity and its gradients from noisy scattered velocimetry data [2], proposed a method for the morphology control of hairy nanopores [3], obtained the ideal contribution to the macroscopic, quasiequilibrium entropy of anisotropic fluids [4], developed a numerical method to molecularly derive a constitutive equation for low-molecular polymer melts from thermodynamically guided simulation [5], studied the effect of solvent quality on colloid-brush interactions [6], of relevance for dendronized polymers, large synthetic structures with molecular precision [7]. We currently attempt to extend the simulation methods towards the modeling of CNT buckypaper, systems containing copolymers and nanoinclusions, and crosslinked polymer brushes. Details available at <http://www.complexfluids.ethz.ch>

- [1] G.N. Toepferwein, N.C. Karayiannis, R.A. Riggleman, M. Kröger, J.J. de Pablo, *Macromolecules* **44** (2011) 1034-1045.
- [2] M. Sadati, C. Luap, M. Kröger, A.A. Gusev, H.C. Öttinger, *J. Rheol.* **55** (2011) 353-377.
- [3] O. Peleg, M. Tagliazucchi, M. Kröger, Y. Rabin, I. Szleifer, *ACS Nano* **5** (2011) 4737-4747.
- [4] P. Ilg, M. Hütter, M. Kröger, *Phys. Rev. E* **83** (2011) 061713.
- [5] P. Ilg, M. Kröger, *J. Rheol.* **55** (2011) 69-93.
- [6] A. Halperin, M. Kröger, E.B. Zhulina, *Macromolecules* **44** (2011) 3622-3638.
- [7] B. Zhang, R. Wepf, K. Fischer, M. Schmidt, S. Besse, P. Lindner, B.T. King, R. Sigel, P. Schurtenberger, Y. Talmon, Y. Ding, M. Kröger, A. Halperin, A.D. Schlüter, *Angew. Chem. Int. Ed.* **50** (2011) 737-740.

Title: Computational Solid State Electronics

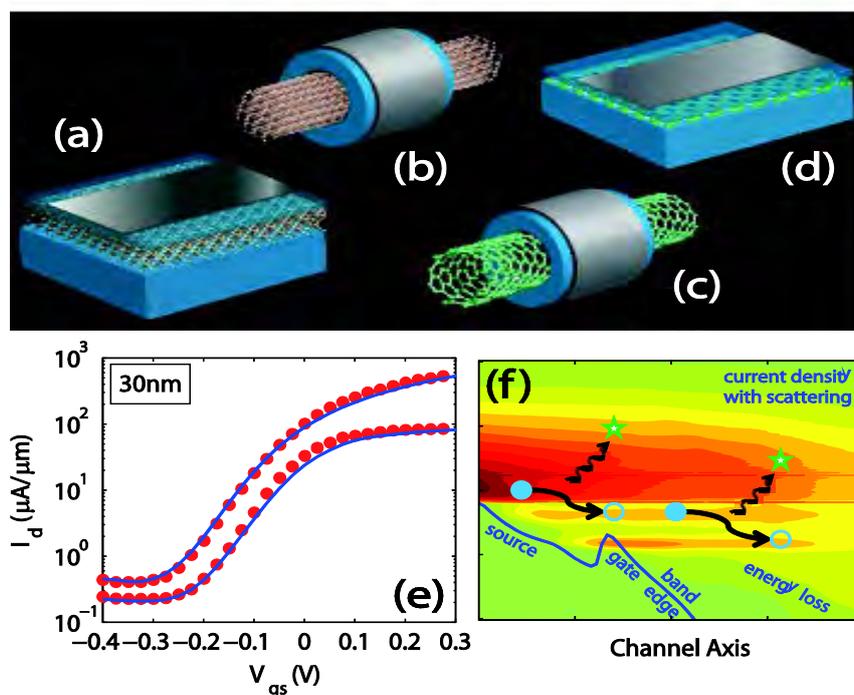
Researchers: Mathieu Luisier
Andreas Schenk
Mauro Ciappa

Institute/ Integrated Systems Laboratory/
Group: Nano-TCAD and Physical Characterization Groups

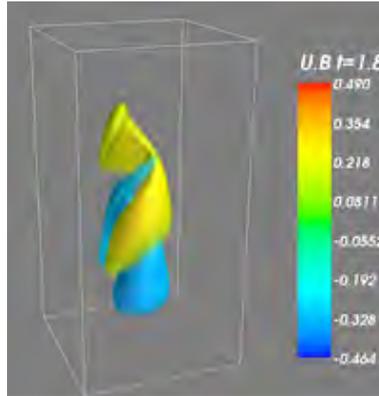
Description:

Advanced numerical simulation tools can greatly accelerate the development and facilitate the design of novel nanoelectronic devices, provided that they contain enough physics and rapidly deliver reliable results. After 40 years of aggressive scaling according to Moore's law, the dimensions of transistors, the active components of integrated circuits, have reached the nanometer scale and do not exceed a few atomic layers. Investigating the performance of such devices demands for state-of-the-art computational models with an atomistic resolution of the simulation domain and a proper inclusion of the required quantum mechanical effects.

We are developing and applying different parallel numerical tools in order to determine how transistors will look like in 10 years from now, how they can become more efficient, and how their power consumption can be reduced. To help experimentalists visualize the ultra-scaled structures they fabricate, we are also working on new numerical models to improve the resolution of images from scanning electron microscopy (SEM). One of the codes that we have developed, *OMEN*, a massively parallel and multi-dimensional quantum transport simulator recently reached a sustained performance of more than 1 petaflop/s on 222,000 cores of the CRAY-XT5 Jaguar at Oak Ridge National Laboratory (ORNL) Most of the simulations are carried either on Jaguar or Kraken at ORNL or on Rosa at CSCS in Manno. The following pictures illustrate some of our research activities:



Example of nanoscale devices: (a) Ultra-thin-body field-effect transistor (FET), (b) Nanowire FET, (c) Carbon nanotube FET, (d) Graphene Nanoribbon FET, (e) comparison between experimental (solid blue lines) and simulation results (red points) for a III-V high electron mobility transistor (HEMT) fabricated at MIT (f) spectral current through a nanowire FET illustrating the electron-phonon scattering mechanism



Title: Simulation of waves in the outer solar atmosphere.

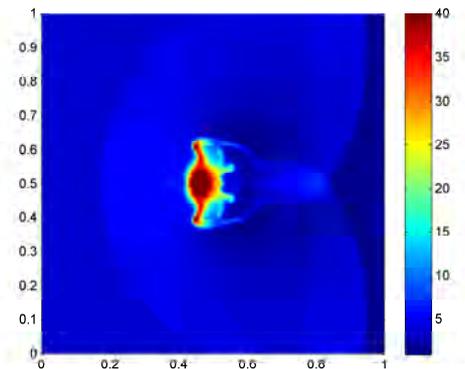
Researchers: S. Mishra, F. Fuchs, A. D. McMurry (U. Oslo), K. Waagan (U. Washington).

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

Description: We have developed a high-resolution massively parallel robust finite volume code termed SURYA to simulate the outer solar atmosphere (photosphere, chromosphere and corona). The code is based on high-order finite volume schemes for the Godunov-Powell form of the MHD equations and a well-balanced discretization to preserve magneto-hydrostatic equilibria. Highlights include the simulation of Alfvén waves and the ability of the code to handle real data sets. Ongoing work focuses on the inclusion of radiation by designing an efficient scheme for radiation MHD. Further validation with observed data sets from SOHO and HINODE is ongoing.

Publications:

1. Well balanced high-order finite volumes schemes for the simulation of wave propagation in three-dimensional non-isothermal stratified magneto-atmospheres, F. Fuchs, A. McMurry, S. Mishra, N.H. Risebro and K. Waagan, SAM report, 2010-27.
2. Simulating waves in the upper solar atmosphere with SURYA: A well-balanced high-order finite volume code, F. Fuchs, A. McMurry, S. Mishra and K. Waagan, Astrophysical Journal, To appear, SAM report 2010-47.



Title: Arbitrarily high-order entropy stable finite volume schemes for systems of conservation laws.

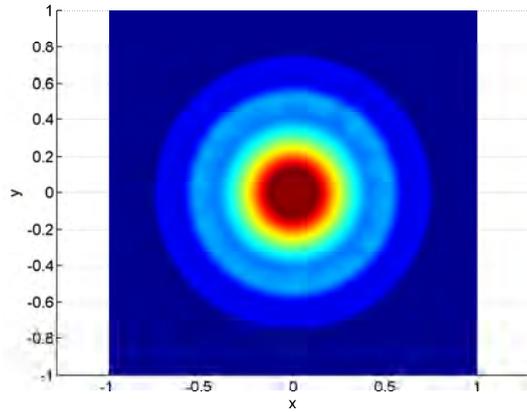
Researchers: S. Mishra, U.S. Fjordholm, E. Tadmor (U. Maryland).

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 arbitrarily high-order entropy stable schemes for a general system of conservation laws by combining entropy conservative fluxes with high-order numerical diffusion operators based on the ENO (essentially non-oscillatory) reconstruction. The schemes are applied to the shallow water equations and the Euler equations of gas dynamics. Ongoing work focuses on extension these high-order entropy stable schemes to unstructured grids and to the MHD equations.

Publications:

1. U.S. Fjordholm, S. Mishra and E. Tadmor, Energy preserving and energy stable schemes for shallow water equations with bottom topography, *Jl. Comput. Phys*, 230, 2011, 5587-5609.
2. U.S. Fjordholm, S. Mishra and E. Tadmor, ENO reconstruction and ENO interpolation are stable, *Research Report 2011-38*, SAM, ETH Zürich.
3. U.S. Fjordholm, S. Mishra and E. Tadmor, Arbitrarily high order accurate entropy stable essentially non-oscillatory schemes for systems of conservation laws, *Research Report 2011-39*, SAM, ETH Zürich.



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

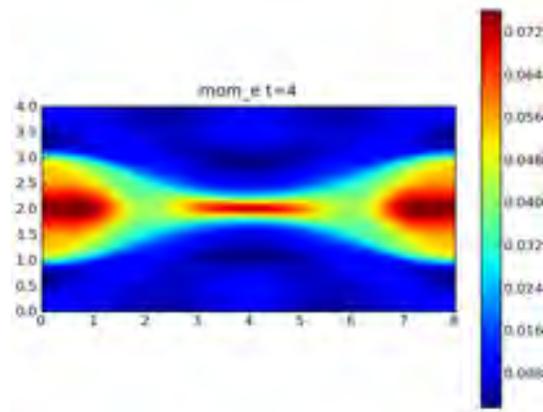
Researchers: S. Mishra, A. Hildebrand

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 needed for stability. Various theoretical estimates have been obtained and implementation issues addressed. 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 multi-dimensional systems of conservation laws, A. Hildebrand and S. Mishra, In preparation, 2011.



Title: High-order schemes for the two-fluid MHD equations.

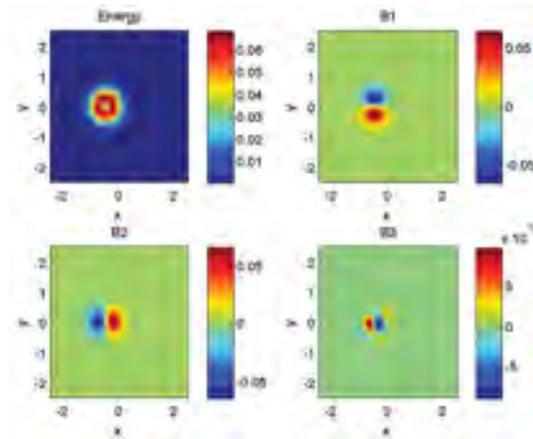
Researchers: S. Mishra, H. Kumar (U. Bordeaux).

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

Description: The two-fluid MHD equations consist of the Euler equations for the ion and electron plasmas coupled to the Maxwell equations of electromagnetism through the Lorentz force. The two-fluid MHD equations model finite Larmor radius effects like fast magnetic reconnection. The current project aims at the development of a robust numerical framework to discretize the two-fluid MHD equations for realistic parameters. We have designed high-resolution entropy stable schemes for the two-fluid MHD equations and novel IMEX time stepping algorithms to handle stiff source terms. Ongoing research aims at the development of a fully unstructured Discontinuous Galerkin (DG) scheme to simulate the two-fluid MHD equations for realistic charge to mass ratios.

Publications:

1. Entropy stable numerical schemes for two-fluid MHD equations, H. Kumar and S. Mishra, SAM report 2011-22.
2. Implicit-Explicit Runge-Kutta methods for two-fluid MHD equations, H. Kumar, SAM report 2011-26.



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

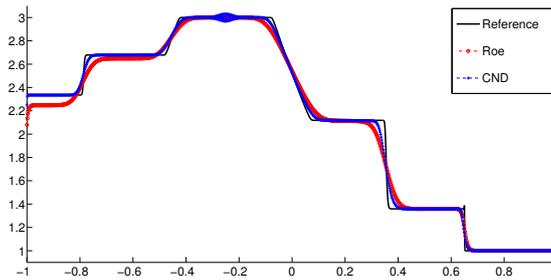
Researchers: S. Mishra, P. Corti.

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 finite difference schemes for the magnetic induction equation with Hall effect, P. Corti and S. Mishra, SAM report 2011-23.



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

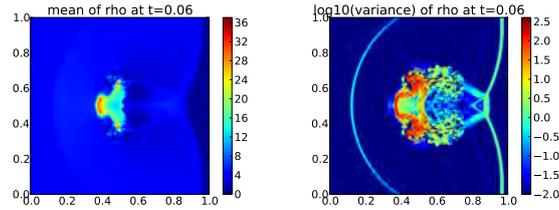
Researchers: S. Mishra, U. S. Fjordholm, M. Castro and C. Parés (U. Malaga), L. V. Spinolo (U. Zurich)

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. For non-conservative hyperbolic systems, such as the multi-layer shallow water equations, we design a new class of entropy conservative (ECPC) and entropy stable (ESPC) path conservative schemes with the numerical viscosity being based on the underlying physical viscosity. Similarly for boundary value problems, we design schemes whose equivalent equation matches the underlying PDE, to leading order. In both cases, the schemes approximate the physically relevant solution.

Publications:

1. U. S. Fjordholm and S. Mishra, Accurate numerical discretizations of non-conservative hyperbolic systems, *M2AN Math. Model. Num. Anal* to appear. Research Report N. 2010–25, Seminar für Angewandte Mathematik ETH Zürich, 2010.
2. M. J. Castro, U. S. Fjordholm, S. Mishra and C. Parés, Entropy conservative and entropy stable schemes for non-conservative hyperbolic systems, Research report NN. 2011-49, SAM ETH Zurich.
3. S. Mishra and L. V. Spinolo. Accurate numerical schemes for approximating initial-boundary value problems for systems of conservation laws, Research report NN. 2011-58, SAM ETH Zurich.



Title: Multi-level Monte-Carlo (MLMC) methods for quantifying uncertainty in hyperbolic PDEs

Researchers: S. Mishra, C. Schwab and J. Sukys.

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 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. Furthermore, they are superior to deterministic methods such as stochastic Galerkin and Collocation as they are robust with respect to the presence of very large number of sources of uncertainty as well as when the solutions can be discontinuous wrt to the stochastic variables (as in nonlinear hyperbolic equations). We have design a novel load balancing strategy to efficiently parallelize the method such that it scales on massively parallel hardware platforms.

Publications:

1. S. Mishra and C. Schwab, Sparse tensor multi-level Monte Carlo finite volume methods for hyperbolic conservation laws with random initial data. *Math. Comput.*, to appear, 2011.
2. S. Mishra, Ch. Schwab and J. Sukys, Multi-level Monte carlo finite volume methods for non-linear systems of conservation laws in multi-dimensions, *Research Report 2011-2*, SAM, ETH Zürich.
3. J. Sukys, S. Mishra and Ch. Schwab Static load balancing for multi-level Monte Carlo nite volume solvers , *Research Report 2011-32*, SAM, ETH Zürich.

Title: Multiple routes and milestones in the folding HIV-1 protease monomer

Researchers: M. Bonomi
A. Barducci
F.L. Gervasio*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900
*Computational Biophysics Group, Structural Biology and Biocomputing Programme, Spanish National Research Centre, Madrid, Spain

Description:

Proteins fold on a time scale incompatible with a mechanism of random search in conformational space thus indicating that somehow they are guided to the native state through a funneled energetic landscape. At the same time the heterogeneous kinetics suggests the existence of several different folding routes. Here we propose a scenario for the folding mechanism of the monomer of HIV-1 protease in which multiple pathways and milestone events coexist. A variety of computational approaches supports this picture. These include very long all-atom molecular dynamics simulations in explicit solvent, an analysis of the network of clusters found in multiple high-temperature unfolding simulations and a complete characterization of free-energy surfaces carried out using a structure-based potential at atomistic resolution and a combination of metadynamics and parallel tempering. Our results confirm that the monomer in solution is stable toward unfolding and show that at least two unfolding pathways exist. In our scenario, the formation of a hydrophobic core is a milestone in the folding process which must occur along all the routes that lead this protein towards its native state. Furthermore, the ensemble of folding pathways proposed here substantiates a rational drug design strategy based on inhibiting the folding of HIV-1 protease.

References: *PLoS ONE*, 5 (10), 13208, 2010, DOI: 10.1371/journal.pone.0013208

Title: Efficient stochastic thermostating of path integral molecular dynamics

Researchers: M. Ceriotti
M. Parrinello
T.E. Markland*
D.E. Manolopoulos

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom

Description:

The path integral molecular dynamics (PIMD) method provides a convenient way to compute the quantum mechanical structural and thermodynamic properties of condensed phase systems at the expense of introducing an additional set of high frequency normal modes on top of the physical vibrations of the system. Efficiently sampling such a wide range of frequencies provides a considerable thermostating challenge. Here we introduce a simple stochastic path integral Langevin equation (PILE) thermostat which exploits an analytic knowledge of the free path integral normal mode frequencies. We also apply a recently developed colored noise thermostat based on a generalized Langevin equation (GLE), which automatically achieves a similar, frequency-optimized sampling. The sampling efficiencies of these thermostats are compared with that of the more conventional Nosé–Hoover chain (NHC) thermostat for a number of physically relevant properties of the liquid water and hydrogen-in-palladium systems. In nearly every case, the new PILE thermostat is found to perform just as well as the NHC thermostat while allowing for a computationally more efficient implementation. The GLE thermostat also proves to be very robust delivering a near-optimum sampling efficiency in all of the cases considered. We suspect that these simple stochastic thermostats will therefore find useful application in many future PIMD simulations.

References: *J. Chem. Phys.* 133, 124104, 2010, DOI: 10.1063/1.3489925

Title: The delta-thermostat: selective normal-modes excitation by colored-noise Langevin dynamics

Researchers: M. Ceriotti
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Description:

The authors introduced a comprehensive framework to use a custom-tailored Langevin equation with correlated-noise in the context of molecular-dynamics simulations. Here it is established how such a framework can be used to selectively excite normal modes whose frequency falls within a prescribed, narrow range. Possible application of this technique to the diagonalization of large matrices is also discussed.

References: T. Schneider and E. Stoll, Molecular-dynamics study of a three-dimensional one-component model for distortive phase transitions, *Phys. Rev. B* **17** (3) (1978), pp. 1302–1322
Procedia Computer Science, 1, 1607-1614, 2010

Title: A self-learning algorithm for biased molecular dynamics

Researchers: G.A. Tribello
M. Ceriotti
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Description:

A new self-learning algorithm for accelerated dynamics, reconnaissance metadynamics, is proposed that is able to work with a very large number of collective coordinates. Acceleration of the dynamics is achieved by constructing a bias potential in terms of a patchwork of one-dimensional, locally valid collective coordinates. These collective coordinates are obtained from trajectory analyses so that they adapt to any new features encountered during the simulation. We show how this methodology can be used to enhance sampling in real chemical systems citing examples both from the physics of clusters and from the biological sciences.

References: *PNAS*, 107 (41), 17509-17514, 2010,
DOI:10.1073/pnas.1011511107/-/DCSupplemental

Title: First principle study of the $\text{LiNH}_2/\text{Li}_2\text{NH}$ transformation

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

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, 20125 Milano, Italy

Description:

Based on ab-initio simulations, we propose a scenario for the decomposition pathway of Li amide into Li imide and ammonia ($2 \text{LiNH}_2 \rightarrow \text{Li}_2\text{NH} + \text{NH}_3$) which represents the first step of the dehydrogenation reaction of the $\text{LiNH}_2 / \text{LiH}$ mixture. Activation energies for formation of NH_3 in LiNH_2 , for diffusion of charged species (H^+ , Li^+) in LiNH_2 and Li_2NH , for H^+/Li^+ transfer across the $\text{LiNH}_2 / \text{Li}_2\text{NH}$ interface and for NH_3 desorption at the surface of LiNH_2 and Li_2NH have been computed from first principles. The results actually suggest that the transformation path depends on the surface-to-volume ratio of the LiNH_2 crystallites.

References: *J. Phys. Chem. C*, 114 (35), 15174-15183, 2010,
DOI: 10.1021/jp100723p

Title: Nuclear quantum effects in *ab initio* dynamics: theory and experiments for lithium imide

Researchers: M. Ceriotti
G. Miceli*
A. Pietropaolo**
D. Colognesi***
A. Nale*
M. Catti*
M. Bernasconi*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Dipartimento di Scienza dei Materiali and CNISM, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125 Milano, Italy
**CNISM UdR Roma Tor Vergata and Centro NAST, Università degli Studi di Roma Tor Vergata, via della Ricerca Scientifica 1, I-0133 Roma, Italy
***Istituto dei Sistemi Complessi, CNR, via Madonna del Piano 10, 50019 Firenze, Italy

Description:

Owing to their small mass, hydrogen atoms exhibit strong quantum behavior even at room temperature. Including these effects in first-principles calculations is challenging because of the huge computational effort required by conventional techniques. Here we present the first *ab initio* application of a recently developed stochastic scheme, which allows to approximate nuclear quantum effects inexpensively. The proton momentum distribution of lithium imide, a material of interest for hydrogen storage, was experimentally measured by inelastic neutron-scattering experiments and compared with the outcome of quantum thermostatted *ab initio* dynamics. We obtain favorable agreement between theory and experiments for this purely quantum-mechanical property, thereby demonstrating that it is possible to improve the modeling of complex hydrogen-containing materials without additional computational effort.

References: *Phys. Rev. B*, 82, 174306, 2010, DOI: 10.1103/PhysRevB.82.174306

Title: Static disorder and structural correlations in the low-temperature phase of lithium imide

Researchers: M. Ceriotti
G. Miceli*
M. Bernasconi*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Dipartimento di Scienza dei Materiali and CNISM, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125 Milano, Italy

Description:

Based on *ab initio* molecular dynamics simulations, we investigate the low-temperature crystal structure of Li_2NH which in spite of its great interest as H-storage material is still a matter of debate. The dynamical simulations reveal a precise correlation in the fractional occupation of Li sites which leads average atomic positions in excellent agreement with diffraction data and solves the inconsistencies of previous proposals.

References: *Phys. Rev. B*, 83, 054119, 2011, DOI: 10.1103/PhysRevB.83.054119

Title: Structural diversity and energetic in anhydrous lithium tartrates: experimental and computational studies of novel chiral polymorphs and their racemic and meso analogues

Researchers: H.H.-M. Yeung
M. Kosa*
M. Parrinello*
P.M. Forster**
A.K. Cheetham

Institute/Group: Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge, U.K., CB2 3QZ
*ETH Zürich, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via G. Buffi 13, 6900 Lugano, Switzerland
** Department of Chemistry, University of Nevada, Las Vegas, 4505 South Maryland Parkway, Box 454003, Las Vegas, Nevada 89154-4003, United States

Description:

Five novel anhydrous inorganic–organic frameworks based on crystalline modifications of lithium tartrate ($\text{tart}^{2-} = \text{C}_4\text{H}_4\text{O}_6^{2-}$) have been synthesized by solvothermal means and investigated by single crystal X-ray and computational methods. Reactions between lithium acetate dihydrate and l-tartaric acid yielded three chiral compounds, $\text{LiH}(\text{l-tart})$ in space group $P2_1$ (**1**), $\text{Li}_2(\text{l-tart})$, $P2_12_12_1$ (**2**), and $\text{Li}_2(\text{l-tart})$, $C222_1$ (**3**), a polymorph of **2**. Two achiral compounds, $\text{Li}_2(\text{meso-tart})$, $P2_1/c$ (**4**) and $\text{Li}_2(\text{d,l-tart})$, $C2/c$ (**5**), were obtained from the reaction of lithium acetate dihydrate with meso-tartaric acid and d,l-tartaric acid, respectively. The singly deprotonated tartrate **1** contains isolated LiO_4 tetrahedra, while the tetrahedra in the doubly deprotonated tartrates **2–5** share corners to form parallel chains. The tartaric acid ligands employ a variety of binding modes to connect the inorganic moieties, resulting in nonporous three-dimensional frameworks in all cases. The relative formation energies of structures **2–5** were calculated using density functional theory (DFT) methods and are found to be within the narrow range of ca. 5 kJ mol^{-1} when electronic energies only are considered. However, when the contributions of zero point vibrational energy (ZPVE) and thermal vibrational energy are considered, the relative energy range increases to ca. 15 kJ mol^{-1} . Analysis of the vibrational modes shows that the non-negligible difference in ZPVE arises from degrees of freedom associated with the heavy backbone atoms rather than, for example, O–H modes.

References: *Crystal Growth & Design*, 11, 221 – 230, 201, DOI: 10.1021/cg101170k

Title: Accelerating the convergence of path integral dynamics with a generalized Langevin equation

Researchers: M. Ceriotti
D.E. Manolopoulos*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom

Description:

The quantum nature of nuclei plays an important role in the accurate modelling of light atoms such as hydrogen, but it is often neglected in simulations due to the high computational overhead involved. It has recently been shown that zero-point energy effects can be included comparatively cheaply in simulations of harmonic and quasiharmonic systems by augmenting classical molecular dynamics with a generalized Langevin equation (GLE). Here we describe how a similar approach can be used to accelerate the convergence of path integral (PI) molecular dynamics to the exact quantum mechanical result in more strongly anharmonic systems exhibiting both zero point energy and tunnelling effects. The resulting PI-GLE method is illustrated with applications to a double-well tunnelling problem and to liquid water.

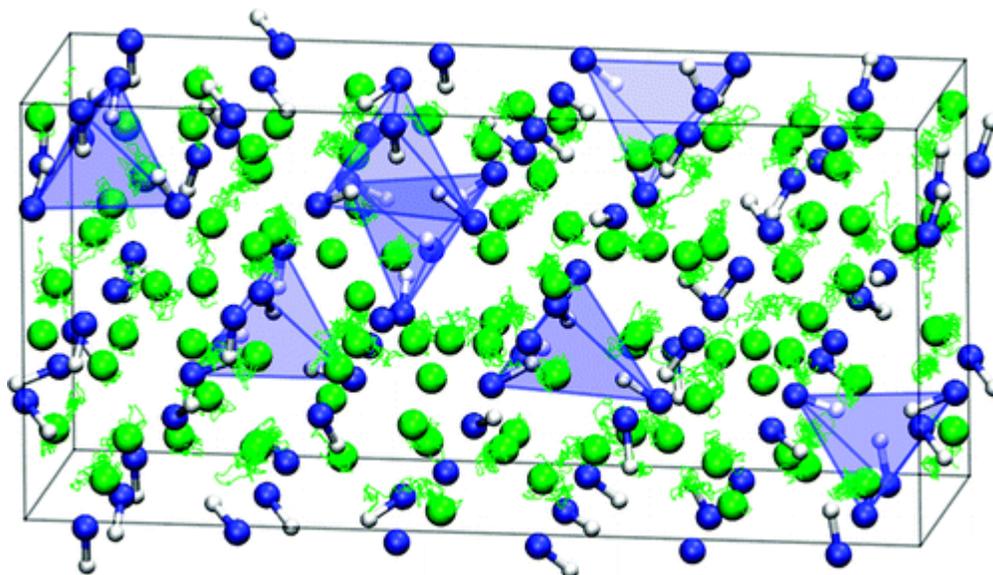
References: *J. Chem. Phys.*, 134, 084104, 2011, DOI: 10.1063/1.3556661

Title: First-principles study of the high-temperature phase of Li_2NH

Researchers: G. Miceli*
M. Ceriotti
S. Angioletti-Uberti*
M. Bernasconi*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125, Milano, Italy

Description:



On the basis of ab initio molecular dynamics simulations, we propose that the $Fm\bar{3}m$ symmetry of the high-temperature (above 356 K) phase of Li_2NH results from dynamical disorder due to fast diffusion of Li interstitials and a slower diffusion of Li vacancies. Still, most of the NH groups point tetrahedrally toward the nearest Li vacancy in a geometry reminiscent of the low-temperature $Fd\bar{3}m$ phase. Li diffusion appears at high temperature due to breaking of the tetrahedral clusters of Li interstitials present in our model of the low-temperature $Fd\bar{3}m$ phase.

References: *J. Phys. Chem. C*, 115, 7076-7080, 201, DOI: 10.1088/0952-8984/23/26/265801

Title: Momentum distribution, vibrational dynamics, and the potential of mean force in ice

Researchers: L. Lin
J.A. Morrone*
R. Car**
M. Parrinello***

Institute/Group: Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544, USA
*Department of Chemistry, Princeton University, Princeton, NJ 08544, USA
**Department of Physics, Princeton University, Princeton, NJ 08544, USA
***ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 12, CH-6900 Lugano, Switzerland

Description:

By analyzing the momentum distribution obtained from path integral and phonon calculations we find that the protons in hexagonal ice experience an anisotropic quasiharmonic effective potential with three distinct principal frequencies that reflect molecular orientation. Due to the importance of anisotropy, anharmonic features of the environment cannot be extracted from existing experimental distributions that involve the spherical average. The full directional distribution is required, and we give a theoretical prediction for this quantity that could be verified in future experiments. Within the quasiharmonic context, anharmonicity in the ground-state dynamics of the proton is substantial and has quantal origin, a finding that impacts the interpretation of several spectroscopies.

References: *Phys. Rev. B*, 83, 220302, 2011, DOI: 10.1103/PhysRevB.83.220302

Title: First-principles study of nitrogen doping in cubic and amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$

Researchers: S. Caravati
D. Colleoni
R. Mazzarello**
T.D. Kühne***
M. Krack****
M. Bernasconi*
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R Cozzi 53, I-20125 Milano, Italy
**Institute for Theoretical Solid State Physics and JARA—Fundamentals of Future Information Technology, RWTH Aachen, D-52056 Aachen, Germany
***Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany
**** Paul Scherrer Institut, CH-5232 Villigen, Switzerland

Description:

We investigated the structural, electronic and vibrational properties of amorphous and cubic $\text{Ge}_2\text{Sb}_2\text{Te}_5$ doped with N at 4.2 at.% by means of large scale *ab initio* simulations. Nitrogen can be incorporated in molecular form in both the crystalline and amorphous phases at a moderate energy cost. In contrast, insertion of N in the atomic form is very energetically costly in the crystalline phase, though it is still possible in the amorphous phase. These results support the suggestion that N segregates at the grain boundaries during the crystallization of the amorphous phase, resulting in a reduction in size of the crystalline grains and an increased crystallization temperature.

References: *J. Phys. Condens. Matter*, 23, 265801, 2011, DOI: 10.1021/jp200076p

Title: Replica Temperatures for Uniform Exchange and Efficient Roundtrip Times in Explicit Solvent Parallel Tempering Simulations

Researchers: M. K. Prakash
A. Barducci
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Description:

The efficiency of parallel tempering simulations is greatly influenced by the distribution of replica temperatures. In explicit solvent biomolecular simulations, where the total energy is dominated by the solvent, specific heat is usually assumed to be constant. From this, it follows that a geometric distribution of temperatures is optimal. We observe that for commonly used water models (TIP3P, SPC/E) under constant volume conditions and in the range of temperatures normally used, the specific heat is not a constant, consistent with experimental observations. Using this fact, we derive an improved temperature distribution which substantially reduces the round-trip times, especially when working with a small number of replicas.

References: *J. Chem. Theory Comput.*, 7 (7), 2025–2027, 2011,
DOI: 10.1021/ct200208h

Title: A quantitative measure of chirality inside nucleic acid databank

Researchers: A. Pietropaolo
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Description:

We show the capability of a chirality index (Pietropaolo et al., *Proteins* 2008;70:667–677) to investigate nucleic acid structures because of its high sensitivity to helical conformations. By analyzing selected structures of DNA and RNA, we have found that sequences rich in cytosine and guanine have a tendency to left-handed chirality, in contrast to regions rich in adenine or thymine which show strong negative, right-handed, chirality values. We also analyze RNA structures, where specific loops and hairpin motifs are characterized by a well-defined chirality value. We find that in nucleosome the chirality is exalted, whereas in ribosome it is reduced. Our results illustrate the sensitivity of this descriptor for nucleic acid conformations.

References: *Chirality*, 23 (7), 534–542, 2011, DOI: 10.1002/chir.20961

Title: Simplifying the representation of complex free-energy landscapes using sketch-map

Researchers: M. Ceriotti
G.A. Tribello*
M. Parrinello*

Institute/Group: Physical and Theoretical Chemistry Laboratory, University of Oxford,
South Parks Road, Oxford OX1 3QZ, United Kingdom
*ETH Zürich, Computational Science, Department of Chemistry and
Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe
Buffi 13, CH-6900 Lugano, Switzerland

Description:

A new scheme, sketch-map, for obtaining a low-dimensional representation of the region of phase space explored during an enhanced dynamics simulation is proposed. We show evidence, from an examination of the distribution of pairwise distances between frames, that some features of the free-energy surface are inherently high-dimensional. This makes dimensionality reduction problematic because the data does not satisfy the assumptions made in conventional manifold learning algorithms. We therefore propose that when dimensionality reduction is performed on trajectory data one should think of the resultant embedding as a quickly sketched set of directions rather than a road map. In other words, the embedding tells one about the connectivity between states but does not provide the vectors that correspond to the slow degrees of freedom. This realization informs the development of sketch-map, which endeavors to reproduce the proximity information from the high-dimensionality description in a space of lower dimensionality even when a faithful embedding is not possible.

References: *PNAS*, 108 (3)13023-1302, 2011,
DOI: 10.1073/pnas.1108486108/-/DCSupplemental

Title: Nucleation mechanism for the direct graphite-to-diamond phase transition

Researchers: R.Z. Khaliullin
H. Eshet
T.D. Kühne*
J. Behler**
M. Parrinello

Institute/Group: ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
*Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, 55128 Mainz, Germany
**Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Description:

Graphite and diamond have comparable free energies, yet forming diamond from graphite in the absence of a catalyst requires pressures that are significantly higher than those at equilibrium coexistence. At lower temperatures, the formation of the metastable hexagonal polymorph of diamond is favoured instead of the more stable cubic diamond. These phenomena cannot be explained by the concerted mechanism suggested in previous theoretical studies. Using an *ab initio* quality neural-network potential, we carried out a large-scale study of the graphite-to-diamond transition assuming that it occurs through nucleation. The nucleation mechanism accounts for the observed phenomenology and reveals its microscopic origins. We demonstrate that the large lattice distortions that accompany the formation of diamond nuclei inhibit the phase transition at low pressure, and direct it towards the hexagonal diamond phase at higher pressure. The proposed nucleation mechanism should improve our understanding of structural transformations in a wide range of carbon-based materials.

References: *Nature Materials* 10, 693–697, 2011, DOI: 10.1038/NMAT3078

Title: A Chirality-Based Metrics for Free-Energy Calculations in Biomolecular Systems

Researchers: A. Pietropaolo
D. Branduardi*
M. Bonomi**
M. Parrinello**

Institute/Group: Università Catania, Dipartimento Scienze Chimiche, I-95125 Catania, Italy and
Magna Graecia Università Catanzaro, Dipartimento Scienze Farmacobiologico, Catanzaro, Italy
*Ist Italiano Tecnol IIT, Drug Discovery & Dev Dept, I-16163 Genoa, Italy
**ETH Zürich, Computational Science, Department of Chemistry and Applied Biosciences and Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Description:

In this work, we exploit the chirality index introduced in (Pietropaolo et al., *Proteins* 2008, 70, 667) as an effective descriptor of the secondary structure of proteins to explore their complex free-energy landscape. We use the chirality index as an alternative metrics in the path collective variables (PCVs) framework and we show in the prototypical case of the C-terminal domain of immunoglobulin binding protein GB1 that relevant configurations can be efficiently sampled in combination with well-tempered metadynamics. While the projections of the configurations found onto a variety of different descriptors are fully consistent with previously reported calculations, this approach provides a unifying perspective of the folding mechanism which was not possible using metadynamics with the previous formulation of PC Vs.

References: *J. of Computational Chemistry*, 32 (12), 2627, 2011,
DOI: 10.1002/jcc.21842

Title: Nodes on Ropes: A comprehensive Data and Control Flow for Steering Ensemble Simulations

Researchers: J. Waser, H. Ribičić, R. Fuchs, C. Hirsch, B. Schindler, G. Blöschl, E. Gröller

Institute/ Chair of Computational Science /
Group: Scientific Visualization Group

Description:

Flood disasters are the most common natural risk and tremendous efforts are spent to improve their simulation and management. However, simulation-based investigation of actions that can be taken in case of flood emergencies is rarely done. This is in part due to the lack of a comprehensive framework which integrates and facilitates these efforts. In this paper, we tackle several problems which are related to steering a flood simulation. One issue is related to uncertainty. We need to account for uncertain knowledge about the environment, such as levee-breach locations. Furthermore, the steering process has to reveal how these uncertainties in the boundary conditions affect the confidence in the simulation outcome. Another important problem is that the simulation setup is often hidden in a black-box. We expose system internals and show that simulation steering can be comprehensible at the same time. This is important because the domain expert needs to be able to modify the simulation setup in order to include local knowledge and experience. In the proposed solution, users steer parameter studies through the World Lines interface to account for input uncertainties. The transport of steering information to the underlying data-flow components is handled by a novel meta-flow. The meta-flow is an extension to a standard data-flow network, comprising additional nodes and ropes to abstract parameter control. The meta-flow has a visual representation to inform the user about which control operations happen. Finally, we present the idea to use the data-flow diagram itself for visualizing steering information and simulation results. We discuss a case-study in collaboration with a domain expert who proposes different actions to protect a virtual city from imminent flooding. The key to choosing the best response strategy is the ability to compare different regions of the parameter space while retaining an understanding of what is happening inside the data-flow system.

References:

IEEE Transactions on Visualization and Computer Graphics, (to appear), 2011.

Title: Time-Varying Data Visualization Using Functional Representations

Researchers: Y. Jang, D. Ebert, K. Gaither

Institute/ Chair of Computational Science /
Group: Scientific Visualization Group

Description:

In many scientific simulations, the temporal variation and analysis of features are important. Visualization and visual analysis of time series data is still a significant challenge because of the large volume of data. Irregular and scattered time series datasets are even more problematic to visualize interactively. Previous work proposed functional representation using basis functions as one solution for interactively visualizing scattered data by harnessing the power of modern PC graphics boards. In this paper, we use the functional representation approach for time-varying datasets and develop an efficient encoding technique utilizing temporal similarity between time steps. Our system utilizes a graduated approach of three methods with increasing time complexity based on the lack of similarity of the evolving datasets. Using this system, we are able to enhance the encoding performance for the time-varying datasets, reduce the data storage by saving only changed or additional basis functions over time, and interactively visualize the time-varying encoding results. Moreover, we present efficient rendering of the functional representations using binary space partitioning tree textures to increase the rendering performance.

References:

IEEE Transactions on Visualization and Computer Graphics, (to appear), 2011.

Title: Handbook of High-Resolution Spectroscopy

Researchers: M. Quack
F. Merkt

Institute/Group: Physical Chemistry, ETH Zürich

Description:

This three volume handbook [1] describes the state of the art of current theory and experiment for high-resolution spectroscopy in numerous articles by experts in the field. It is the first comprehensive survey of the field since the famous 3 volume textbook series by G. Herzberg, of which the last volume appeared in 1966.

References:

1. M. Quack, F. Merkt (Eds.), *Handbook of High Resolution Spectroscopy*. Wiley, Chichester, New York, **2011**, (Foreword pages xv-xvi).

Title: Molecular Quantum Mechanics and Molecular Spectra, Molecular Symmetry, and Interaction of Matter with Radiation

Researchers: F. Merkt
M. Quack

Institute/Group: Physical Chemistry, ETH Zürich

Description:

The basic experimental and theoretical concepts underlying molecular spectroscopy are presented. The equations and relations needed in practical applications of high-resolution spectroscopy are provided. Group theoretical tools and their use in high-resolution spectroscopy are introduced and illustrated by simple examples. Time-dependent processes and quantum dynamics are presented and discussed in relation to spectroscopic observations. Coherent and incoherent radiative excitation and radiationless transitions are treated in relation to applications in molecular spectroscopy. The importance in relation to theory computation is discussed.

References:

F. Merkt, M. Quack, in *Handbook of High-Resolution Spectroscopy, Vol. 1*, Chapt. 1, pp. 1-55 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: Fundamentals of Rotation-Vibration Spectra

Researchers: S. Albert
K. Keppler Albert
H. Hollenstein
C. Manca Tanner
M. Quack
G. Seyfang

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

Description:

We provide a survey of fundamental aspects of vibration–rotation spectra. A basic understanding of the concepts is obtained from a detailed discussion of vibration–rotation spectra of diatomic molecules with only one vibrational degree of freedom. This includes approximate and exact separation of rotation and vibration, effective spectroscopic constants, the effects of nuclear spin and statistics, and transition probabilities derived from the form of the electric dipole moment function. The underlying assumptions and accuracy of the determination of molecular structure from spectra are discussed. Polyatomic molecules show many interacting vibrational degrees of freedom. Energy levels and spectra are discussed on the basis of normal coordinates and effective Hamiltonians of interacting levels in Fermi resonance, and in more complex resonance polyads arising from anharmonic potential functions. The resulting time-dependent dynamics of intramolecular energy flow is introduced as well. Effective Hamiltonians for interacting rotation–vibration levels are derived and applied to the practical treatment of complex spectra. Currently available computer programs aiding assignment and analysis are outlined.

References:

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*, Chapt. 3, pp. 117-173 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular Spectroscopy

Researchers: J. Stohner*
M. Quack**

Institute/Group: * Zürich University of Applied Sciences (ZHAW), ICBC Institute of Chemistry & Biological Chemistry, 8820 Wädenswil
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

A summary of conventions, symbols, quantities, units, and constants which are important for high-resolution molecular spectroscopy is provided. In particular, great care is taken to provide definitions which are consistent with the recommendations of the IUPAC “Green Book”, from which large parts of this article are drawn. While the recommendations in general refer to the SI (Système International), the relation to other systems and recommendations, which are frequently used in spectroscopy, for instance atomic units, is also provided. A brief discussion of quantity calculus is provided as well as an up-to-date set of fundamental constants and conversion factors together with a discussion of conventions used in reporting uncertainty of experimentally derived quantities. The article thus should provide an ideal compendium of many quantities of practical importance in high-resolution spectroscopy. The importance of the use of accurate definitions in computation and theory as in experiment is made clear.

References:

J. Stohner, M. Quack, *Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular Spectroscopy*, in *Handbook of High-Resolution Spectroscopy, Vol. 1*, Chapt. 5, pp. 263-324 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: Global Analytical Potential Energy Surfaces for High Resolution Molecular Spectroscopy and Reaction Dynamics

Researchers: R. Marquardt*
M. Quack**

Institute/Group: * Laboratoire de Chimie Quantique, Institut de Chimie, Université de Strasbourg, 4, F-67081 Strasbourg
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Analytical representations of potential energy hypersurfaces for the nuclear motion in polyatomic molecules from ab initio theory and experiment are discussed in a general way. The qualification of potential hypersurface representations from ab initio theory regarding the description of experimental data from rovibrational high-resolution spectroscopy and chemical reaction kinetics is analyzed in more detail for a restricted group of molecules including methane, CH₄, ammonia, NH₃, H₂O₂, and (HF)₂. Current methods for the derivation of analytical representations of potential energy surfaces as well as some applications are reviewed.

References:

R. Marquardt, M. Quack, *Global Analytical Potential Energy Surfaces for High Resolution Molecular Spectroscopy and Reaction Dynamics*, in *Handbook of High-Resolution Spectroscopy, Vol. 1*, Chapt. 12, pp. 511-549 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy

Researchers: M. Quack

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

Description:

Parity (P), together with time reversal symmetry (T) and charge conjugation (C) constitute a fundamental set of discrete symmetries in physics. We review the current status of molecular parity violation in the framework of the fundamental symmetries of physics in general and in relation to intramolecular quantum dynamics. Work of the last decade in electroweak quantum chemistry, including the weak force of the standard model of particle physics in quantum calculations on chiral molecules, has resulted in an increase of the predicted parity violating energies by one to two orders of magnitude. This results in a new outlook on possible experiments which are discussed. We discuss furthermore the conceptual foundations of molecular symmetry breaking (spontaneous, de facto, de lege) in relation to molecular chirality, the evolution of biomolecular homochirality and irreversibility and the origin of the second law of thermodynamics. It is shown that there arise closely parallel situations in the lack of our current understanding of the true physical origins of all three phenomena. For molecular chirality some of the fundamental questions have been answered quantitatively by recent theory. The new theoretical approaches are summarized briefly, as well as some current results. Recent results on a new molecular isotope effect arising from parity violation are reviewed as well.

References:

M. Quack, *Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy*, in *Handbook of High Resolution Spectroscopy, Vol. 1*, Chapt. 18, pp. 659-722 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: High Resolution Fourier Transform Infrared Spectroscopy

Researchers: S. Albert
K. Keppler Albert
M. Quack

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

Description:

Recent developments and applications of high-resolution Fourier transform spectroscopy are reviewed. A short historical summary of the development of high-resolution interferometric Fourier transform infrared (FTIR) spectrometers is given and the possibilities of the currently most highly resolving FTIR spectrometers, including a current prototype built for the Zürich group at the Swiss Light Source SLS as a synchrotron light source, are discussed. A short description of the principles of FTIR spectroscopy is given and the resolution of current spectrometers is illustrated by FTIR spectra of CO, CO₂, OCS, N₂O, CS₂, and CH₄ and its isotopomers. The computational tools necessary to analyze FTIR spectra are described briefly. As examples of rovibrational analysis of more complex spectra, selected molecules CHCl₂F, CDBrClF, pyridine (C₆H₅N) and pyrimidine (C₄H₄N₂), and naphthalene (C₁₀H₈) are discussed. The spectrum of CHCl₂F, a fluorochlorocarbon, is of interest for a better understanding of the chemistry of the Earth's atmosphere. It also possesses an isotopically chiral isotopomer CH₃₅Cl₃₇ClF analyzed in natural abundance. CDBrClF is a chiral molecule and therefore the analysis of its rovibrational spectra provides the basis for carrying out further experiments toward the detection of molecular parity violation. The analyses of the pyridine, pyrimidine, and naphthalene FTIR spectra illustrate the potential of the new generation of FTIR spectrometers in the study of spectra and rovibrational dynamics of aromatic systems and molecules of potential biological interest. In particular, naphthalene is a prototype molecule useful in gaining an understanding of the unidentified infrared bands (UIBs) detected in several interstellar objects. Computations support the analysis of spectra.

References:

S. Albert, K. Keppler Albert, M. Quack, *High Resolution Fourier Transform Infrared Spectroscopy*, in *Handbook of High Resolution Spectroscopy*, Vol. 2, Chapt. 26, pp. 965-1019 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: High Resolution FTIR and Diode Laser Spectroscopy of Supersonic Jets

Researchers: M. Snels*
V. Horká-Zelenková**
H. Hollenstein**
M. Quack**

Institute/Group: * Istituto di Scienze dell' Atmosfera e del Clima (ISAC), Sezione di Roma, Consiglio Nazionale delle Ricerche (CNR), I-00133 Roma
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Fourier transform infrared (FTIR) spectrometers and tunable diode lasers in combination with a supersonic molecular beam expansion are a perfect tool for the investigation of molecules, ions, and radicals at low temperatures. The internal degrees of freedom of the molecules are adiabatically cooled to very low temperatures and thus only low-lying energy levels are populated. The reduction of the number of populated levels at low temperatures makes the assignment of the spectra much easier as compared to the congested room-temperature spectra. Under certain conditions, the Doppler linewidths are greatly reduced, corresponding to very low effective translational temperatures. Supersonic expansion also provides a suitable method for producing and investigating van der Waals clusters and hydrogen-bonded complexes. Unstable species such as radicals and ions can be efficiently produced and studied in a molecular beam. The low rotational temperature allows for the study of nuclear spin symmetry conservation or conversion between nuclear spin isomers. A molecular beam expansion can be obtained by expanding gas through a slit or a circular nozzle. Both expansion geometries can be used in combination with a multipass optical setup and with cavity ring down spectroscopy, which enhances the effective absorption path length. Cooling of the molecules can be promoted by seeding in noble gases. This article summarizes the general aspects of the experimental technique as well as current developments. To demonstrate how powerful the combination of a molecular beam expansion with tunable diode laser and FTIR spectroscopy can be, we report results on some important current examples. Computations aid the analysis of spectra.

References:

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, Chapt. 27, pp. 1021-1067 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: Mass and Isotope Selective Infrared Spectroscopy

Researchers: M. Hippler*
E. Miloglyadov**
M. Quack**
G. Seyfang**

Institute/Group: * Dept of Chemistry, University of Sheffield, Sheffield S3 7HF, United Kingdom
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Recent advances in laser spectroscopic techniques make it possible to obtain mass- and isotope-selective infrared spectra of gas-phase species at high resolution and reduced hot-band spectral congestion. In these techniques, infrared excitation is coupled with ultraviolet multiphoton ionization and detection of the resulting ions in a mass spectrometer, which allows the separation of contributions of different isotopomers and, more generally, species of different mass in a mixture. In combination with jet cooling techniques, spectra are obtained for very cold molecules. These spectra can then be analyzed to extract information on dynamical processes such as intramolecular vibrational redistribution or tunneling and rearrangement processes, and on how intramolecular dynamics is influenced by vibrational excitation and isotope effects. In this review, we introduce isotope-selective infrared spectroscopic techniques and present some selected applications on isotope effects and intramolecular dynamics of vibrationally excited chloroform, aniline, and benzene obtained by isotope-selective infrared spectroscopy. Computations aid the analyses of spectra.

References:

M. Hippler, E. Miloglyadov, M. Quack, G. Seyfang, *Mass and Isotope Selective Infrared Spectroscopy*, in *Handbook of High Resolution Spectroscopy, Vol. 2*, Chapt. 28, pp. 1069-1118 (Eds.: M. Quack, F. Merkt), Wiley, Chichester; New York, **2011**.

Title: Synchrotron-based highest resolution Fourier transform infrared spectroscopy of naphthalene (C₁₀H₈) and indole (C₈H₇N) and application to astrophysical problems

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

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

Description:

We report a rotationally resolved analysis of the high resolution FTIR spectrum of naphthalene which can be considered as a prototypical molecule for polycyclic aromatic hydrocarbons (PAHs), and a similar analysis for the prototypical heterocyclic aromatic molecule indole. The spectra have been measured using a resolution of 0.0008 cm⁻¹ (21 MHz) with the new high resolution FTIR prototype spectrometer of the Molecular Kinetics and Spectroscopy Group at ETH Zürich. The spectrometer is connected to the infrared port available at the Swiss Light Source (SLS) at the Paul-Scherrer-Institute (PSI). Due to the high brightness of the synchrotron radiation in the spectral region of interest, effectively up to 20 times brighter than thermal sources, and the high resolution of the new interferometer, it was possible to record the rotationally resolved infrared spectra of naphthalene and indole at room temperature, and to analyse the ν_{46} *c*-type band ($\tilde{\nu}_0 = 782.330949$ cm⁻¹) of naphthalene as well as the ν_{35} *c*-type band ($\tilde{\nu}_0 = 738.483592$ cm⁻¹) of indole and an *a*-type band at $\tilde{\nu}_0 = 790.864370$ cm⁻¹ tentatively assigned as the overtone $2\nu_{40}$ of indole. The results of the naphthalene band analysis are discussed in relation to the Unidentified Infrared Band (UIB) found in interstellar spectra at 12.8 mm. The analysis of the spectra needs extensive computations.

References:

S. Albert, K. Keppler Albert, P. Lerch, M. Quack, *Faraday Discuss.*, **2011**, *150*, 71-99, 146-151.

Title: Frontiers in Spectroscopy

Researchers: M. Quack

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

Description:

We review the frontiers of spectroscopy from a historical perspective, starting with the development of atomic spectroscopy about 150 years ago, followed by some comments on selected previous Faraday Discussions. As the spectrum of frontiers at the Faraday Discussion 150 is very broad, we give only a brief survey providing a map of the various frontiers approached today. This is followed by an exemplary discussion of one particular frontier towards the spectroscopic detection of symmetry violations in fundamental physics. In particular the understanding of parity violation in chiral molecules has recently made great progress. We briefly describe the advances made in recent decades as well as the current status of theory and experiments in this exciting field of research. We conclude with an outlook on open questions and frontiers of the future in spectroscopy. The importance of relating theory and experiment by computations is made clear.

References:

M. Quack, *Frontiers in Spectroscopy*, in *Faraday Discussions*, Vol. 150, pp. 533-565, 2011.

Title: On parity violating frequency shifts

Researchers: J. Stohner*/**
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical
Chemistry, ETH Zürich
** Zurich University of Applied Sciences (ZHAW)

Description:

A brief description of the current status of computing parity violating frequency shifts is presented.

References:

J. Stohner, M. Quack, *Faraday Discuss.*, **2011**, *150*, 113-114 and 117-118.

Title: On nuclear spin symmetry relaxation in supersonic jets of H₂O

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

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

Description:

We report a brief analysis of the title topic.

References:

C. Manca Tanner, M. Quack, D. Schmidiger, *Faraday Discuss.*, **2011**, *150*, 118-122.

Title: On experiments to detect parity violation in chiral molecules

Researchers: M. Quack

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

Description:

Computations predict parity violating effects in chiral molecules. Here we describe possible experiments.

References:

M. Quack, *Faraday Discuss.*, **2011**, *150*, 123-127.

Title: On nuclear spin symmetry conservation in methane

Researchers: H. M. Niederer*
S. Albert*
S. Bauerecker**
V. Boudon***
G. Seyfang*
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig
*** Sciences et Techniques, Université de Bourgogne

Description:

The title subject is treated [1], see also [2, 3, 4]

References:

- [1] H. M. Niederer, S. Albert, S. Bauerecker, V. Boudon, G. Seyfang, M. Quack, *Faraday Discuss.*, **2011**, *150*, 128-130.
- [2] A. Amrein, M. Quack, U. Schmitt, *J. Phys. Chem.*, **1988**, *92*, 5455-5466.
- [3] M. Quack, *Mol. Phys.*, **1977**, *34*, 477-504.
- [4] M. Quack, *Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy*, in *Handbook of High Resolution Spectroscopy, Vol. 1*, Chapt. 18, pp. 659-722 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: On tunneling and parity violation in ClOOC1

Researchers: R. Prentner*
M. Quack*
J. Stohner*/**

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical
Chemistry, ETH Zürich
** Zurich University of Applied Sciences (ZHAW)

Description:

We report computations of the title subject.

References:

R. Prentner, M. Quack, J. Stohner, M. Willeke, *Faraday Discuss.*, **2011**, *150*, 130-132.

Title: On coupled cluster calculations of parity violating potentials in chiral molecules

Researchers: L. Horný
M. Quack

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

Description:

We report theory and computations of the title subject [1] (see also [2, 3]).

References:

- [1] L. Horný, M. Quack, *Faraday Discuss.*, **2011**, *150*, 152-154.
- [2] M. Quack, J. Stohner, M. Willeke, *Annu. Rev. Phys. Chem.*, **2008**, *59*, 741-769.
- [3] M. Quack, *Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy*, in *Handbook of High Resolution Spectroscopy, Vol. 1*, Chapt. 18, pp. 659-722 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: On isotope selective infrared spectroscopy and tunneling in substituted aniline derivatives

Researchers: E. Miloglyadov
M. Quack
G. Seyfang

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

Description:

We report results on the title subject.

References:

E. Miloglyadov, M. Quack, G. Seyfang, *Faraday Discuss.*, **2011**, *150*, 277 – 278.

Title: On the high resolution FTIR spectroscopy of phenol and torsional tunneling

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

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

Description:

We report results on the title subject [1] (see also [2]).

References:

- [1] S. Albert, K. Keppler Albert, P. Lerch, M. Quack, *On the high resolution FTIR spectroscopy of phenol and torsional tunneling*, in *Faraday Discussions*, Vol. 150, pp. 517-519, **2011**.
- [2] 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, Chapt. 3, pp. 117-173 (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**.

Title: On femtosecond pump probe experiments in bichromophoric acetylenic compounds

Researchers: A. Kushnarenko
E. Miloglyadov
M. Quack
G. Seyfang

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

Description:

We report results on the title subject.

References:

A. Kushnarenko, E. Miloglyadov, M. Quack, G. Seyfang, *Faraday Discuss.*, **2011**, *150*, 520-521.

Title: Die Asymmetrie des Lebens und die Symmetrieverletzungen der Physik:
Molekulare Paritätsverletzung und Chiralität

Researchers: M. Quack

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

Description:

We review the title subject in the light of current computations of parity violation in molecules.

References:

M. Quack, *Die Asymmetrie des Lebens und die Symmetrieverletzungen der Physik: Molekulare Paritätsverletzung und Chiralität*, in *Reise zum Ursprung des Lebens*, Chapt. 12, pp. 277 – 310 (Eds.: K. Al-Shamery, U. Neubauer), Wiley VCH, Weinheim, **2011**.

Title: Accurate Frozen-density Embedding Potentials as a First Step Towards a Subsystem Description of Covalent Bonds

Researchers: Samuel Fux¹
Christoph R. Jacob¹
Johannes Neugebauer²
Lucas Visscher³
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Gorlaeus Laboratories, Leiden Institute of Chemistry, Universiteit Leiden, 2300 RA Leiden, The Netherlands
³Amsterdam Center for Multiscale Modeling, VU University Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

Description:

The frozen-density embedding (FDE) scheme [Wesolowski and Warshel, *J. Phys. Chem.* 97, 8050 (1993)] relies on the use of approximations for the kinetic-energy component $v_T[\rho_1, \rho_2]$ of the embedding potential. While with approximations derived from generalized-gradient approximation kinetic-energy density functional weak interactions between subsystems such as hydrogen bonds can be described rather accurately, these approximations break down for bonds with a covalent character. Thus, to be able to directly apply the FDE scheme to subsystems connected by covalent bonds, improved approximations to v_T are needed. As a first step toward this goal, we have implemented a method for the numerical calculation of accurate references for v_T . We presented accurate embedding potentials for a selected set of model systems, in which the subsystems are connected by hydrogen bonds of various strength (water dimer and F–H–F⁻), a coordination bond (ammonia borane), and a prototypical covalent bond (ethane). These accurate potentials are analyzed and compared to those obtained from popular kinetic-energy density functionals.

References: S. Fux, Ch. R. Jacob, J. Neugebauer, L. Visscher, M. Reiher, *J. Chem. Phys.*, **2010**, 132, 164101.

Title: Basis Set Representation of the Electron Density at an Atomic Nucleus

Researchers: Remigius Mastalerz¹
Per-Olof Widmark²
Björn Olof Roos²
Roland Lindh³
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

²Department of Theoretical Chemistry, Chemical Center, Lund University, P.O. Box 124, 221 00 Lund, Sweden

³Department of Physical and Analytical Chemistry, Quantum Chemistry, Uppsala University, P.O. Box 518, SE-751 20 Uppsala, Sweden

Description:

In this paper a detailed investigation of the basis set convergence for the calculation of relativistic electron densities at the position of finite-sized atomic nuclei is presented. The development of Gauss-type basis sets for such electron densities is reported and the effect of different contraction schemes is studied. Results are then presented for picture-change corrected calculations based on the Douglas-Kroll-Hess Hamiltonian. Moreover, the role of electron correlation, the effect of the numerical integration accuracy in density functional calculations, and the convergence with respect to the order of the Douglas-Kroll-Hess Hamiltonian and the picture-change-transformed property operator are studied.

References: R. Mastalerz, P.-O. Widmark, B.O. Roos, R. Lindh, M. Reiher, *J. Chem. Phys.*, **2010**, *133*, 144111.

Title: Spin Interactions in Cluster Chemistry

Researchers: Maren Podewitz
Markus Reiher

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

Description:

The accurate description of spin-spin interactions in transition-metal cluster chemistry is a mandatory step to understanding and modelling the properties and reactivities of such systems. It cannot be achieved without a profound knowledge of the basic theory. Therefore, we provided a survey from the most fundamental relativistic quantum chemical concepts and subsequent approximations towards conceptual problems such as the definition of local spin which does not emerge naturally from quantum theory. The concept of local spins plays a central role because it allows for a rigorous interpretation of the wave function in terms of magnetic coupling behavior of the interacting (metal) centers. We discussed the relevance and consequences of these concepts for transition-metal chemistry and point to problems and pitfalls that may arise from state-of-the-art DFT calculations on transition-metal clusters.

References: R. Podewitz, M. Reiher, *Adv. Inorg. Chem.*, **2010**, *62*, 177.

Title: Catalytic Synthesis of Vinylphosphanes via Calcium-Mediated Intermolecular Hydrophosphanylation of Alkynes and Butadiynes

Researchers: ¹Tareq M. A. Al-Shboul
²Villő K. Palfi
²Lian Yu
¹Robert Kretschmer
¹Katja Wimmer
¹Reinald Fischer
¹Helmar Görls
²Markus Reiher
¹Matthias Westerhausen

Institute/Group: ¹Institut für Anorganische und Analytische Chemie, Friedrich-Schiller-Universität, D-07743 Jena, Germany
²Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

Description:

The calcium complex [(thf)₄Ca(PPh₂)₂] is a very effective catalyst for the hydrophosphanylation of substituted alkynes; yielding (E)-1,2-diphenyl-1-diphenylphosphanylene and (Z)-1-phenyl-2-diphenylphosphanyl-1-propene. The calcium-mediated hydrophosphanylation of butadiynes proceeds less selectively and diverse products are obtained such as 1,4-substituted 1,4-bis(diphenylphosphanyl)-1,3-butadienes, 1,4-diphenyl-1,2-bis(diphenylphosphanyl)-1,3-butadiene, and 1,4-di(tert-butyl)-1,4-bis(diphenylphosphanyl)buta-1,2-diene. Besides these regioisomers also several configuration isomers with respect to the C=C double bonds [(E)/(Z) isomerism] are obtained. A catalytic cycle can be formulated with the first addition of a Ca-P bond of the catalyst to a C-C triple bond always leading to the formation of an intermediate with the newly formed C-P bond in 1-position whereas the remaining phosphanido calcium fragment binds to the carbon in 2-position. The addition of a second diphenylphosphane is much faster and therefore, only two-fold hydrophosphanylated butadiynes are observed. Neither addition products with only one HPPH₂ group nor those with more than two PPh₂ substituents are obtained.

References: T. M. A. Al-Shboul, V. K. Palfi, L. Yu, R. Kretschmer, K. Wimmer, R. Fischer, H. Görls, M. Reiher, M. Westerhausen, *Organomet. Chem.*, **2010**, 696, 216.

Title: Construction of CASCI-type Wave Functions for very large active spaces

Researchers: Katharina Boguslawski
Konrad H. Marti
Markus Reiher

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

Description:

We present a procedure to construct a configuration-interaction expansion containing arbitrary excitations from an underlying full-configuration-interaction-type wave function defined for a very large active space. Our procedure is based on the density-matrix renormalization group (DMRG) algorithm that provides the necessary information in terms of the eigenstates of the reduced density matrices to calculate the coefficient of any basis state in the many-particle Hilbert space. Since the dimension of the Hilbert space scales binomially with the size of the active orbital space, a sophisticated Monte Carlo sampling routine is employed to collect the most important configurations. This sampling algorithm can also construct configuration-interaction-type wave functions from any other type of tensor network states. The configuration-interaction information obtained serves several purposes. It yields a qualitatively correct description of the molecule's electronic structure, it allows us to analyze DMRG wave functions converged for the same molecular system but with different parameter sets (e.g., different numbers of active-system (block) states), and it can be considered a balanced reference for the application of a subsequent standard multi-reference configuration-interaction method.

References: K. Boguslawski, K. H. Marti, M. Reiher, *J. Chem. Phys.*, **2011**, *134*, 224101.

Title: Can DFT Accurately Predict Spin Densities? Analysis of Discrepancies in Iron Nitrosyl Complexes

Researchers: Katharina Boguslawski¹
Christoph R. Jacob²
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Karlsruhe Institute of Technology (KIT), Center for Functional Nanostructures, Wolfgang-Gaede-Straße 1a, 76131 Karlsruhe, Germany

Description:

Iron nitrosyl complexes are a notably challenging case for density functional theory. In particular for the low-spin states, different exchange–correlation functionals yield disparate spin density distributions [Conradie and Ghosh, *J. Phys. Chem. B*, 2007, **111**, 12621-12624]. We investigate the origin of these differences in detail by analyzing the Kohn–Sham molecular orbitals. Furthermore, to decide which exchange–correlation functionals yield the most accurate spin densities, we compare to complete-active-space self-consistent-field calculations. To ensure that the spin density distribution is converged with respect to the dimension of the active orbital space, this comparison is performed for the $[\text{Fe}(\text{NO})]^{2+}$ molecule as a model system. We find that none of the investigated exchange–correlation functionals is able to reproduce the CASSCF spin densities accurately.

References: K. Boguslawski, Ch. R. Jacob, M. Reiher, *J. Chem. Theory Comp.*, **2011**, *7*, 2740.

Title: Oxygen Coordination to the Active Site of Hmd
in Relation to [FeFe] Hydrogenase

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

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

Description:

The application of [FeFe] hydrogenases for renewable energy production is limited by the generally high O₂-sensitivity of this class of enzymes. The process of O₂ induced inhibition is still not well understood.

In this work we studied energetical differences in oxygen coordination at the active sites of [FeFe] and monoiron (Hmd) hydrogenase as obtained from DFT calculations. Whereas O₂ addition is clearly exothermic in the case of [FeFe] hydrogenase it is endothermic for monoiron hydrogenase. By applying a recently proposed concept [*Inorg. Chem.* **2010**, *49*, 5818] that allows us to structurally and electronically relate both active sites we showed that we obtain an inversion in oxygen affinity when we mutually exchange the first ligand sphere of the central iron atoms of both catalytic centers. Modified Hmd active sites can bind O₂ exothermically whereas O₂ addition to the altered H-cluster variants is less exothermic than in the wild-type configuration. Our results show that oxygen affinity is not very strong when measured in terms of the coordination energy. Hence, changes in the first ligand shell of the reactive iron atoms under retaining similar ligand spheres, i.e., same type of ligands in the same positions of the coordination octahedron, can render oxygen coordination endo- or exothermic. This observation could explain the difference in oxygen sensitivity of Hmd and [FeFe] hydrogenases.

References: M. T. Stiebritz, A. R. Finkelmann, M. Reiher, *Eur. J. Inorg. Chem.*, **2011**, *7*, 1163.

Title: Electron Density in Quantum Theory

Researchers: Samuel Fux
Markus Reiher

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

Description:

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

References: S. Fux, M. Reiher, *Struct. Bonding*, **2011**
DOI: 10.1007/430_2010_37.

Title: Mössbauer Spectroscopy for Heavy Elements: a Relativistic Benchmark Study of Mercury

Researchers: Stefan Knecht¹
Samuel Fux²
Robert van Meer³
Lucas Visscher³
Markus Reiher²
Trond Saue⁴

Institute/Group: ¹Institute de Chimie de Strasbourg, CNRS et Université de Strasbourg, 67070 Strasbourg
²Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
³Amsterdam Center for Multiscale Modeling, VU University Amsterdam, 1081 HV Amsterdam
⁴Laboratoire de Chimie et Physique Quantique, Université Paul Sabatier, 31062 Toulouse Cedex

Description:

The electrostatic contribution to the Mössbauer isomer shift of mercury for the series HgF_n ($n = 1, 2, 4$) has been investigated in the framework of four- and two-component relativistic theory. Replacing the integration of the electron density over the nuclear volume by the contact density leads to a 10 % overestimation of the isomer shift. The systematic nature of this error suggests that it can be incorporated into a correction factor, thus justifying the use of the contact density for the calculation of the Mössbauer isomer shift. The performance of several density functionals for the calculation of contact densities has been assessed by comparing with finite-field four-component relativistic CCSD(T) calculations. For the absolute contact density of the mercury atom, the Density Functional Theory (DFT) calculations are in error by about 0.5 %, a result that must be judged against the observation that the change in contact density along the series HgF_n ($n = 1, 2, 4$), relevant for the isomer shift, is on the order of 50 ppm with respect to absolute densities. Projection analysis shows the expected reduction of the $6s_{1/2}$ population at the mercury center with an increasing number of ligands, but also brings into light an opposing effect, namely the increasing polarization of the $6s_{1/2}$ orbital due to increasing effective charge of the mercury atom, which explains the nonmonotonous behavior of the contact density along the series. The same analysis shows increasing covalent contributions to bonding along the series with the effective charge of the mercury atom reaching a maximum of around +2 for HgF_4 at the DFT level, far from the formal charge +4 suggested by the oxidation state of this recently observed species.

References: S. Knecht, S. Fux, R. van Meer, L. Visscher, M. Reiher, T. Saue, *Theor. Chem. Acc.*, **2011**, *129*, 631-650.

Title: Generation of Potential Energy Surfaces in High Dimensions and their Haptic Exploration

Researchers: Moritz P. Haag
Konrad H. Marti
Markus Reiher

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

Description:

A method was proposed for the automated generation of potential energy surfaces in high dimensions. It combines the existing algorithm for the definition of new energy data points based on the interpolating moving least squares algorithm with a simulated annealing procedure. This method was then studied in a haptic quantum chemistry environment that requires a fast evaluation of gradients on a potential energy surface with automatic improvement of its accuracy. As an example we investigated the nitrogen binding pathway in the Schrock dinitrogen fixation complex with this set-up.

References: M. P. Haag, K. H. Marti, M. Reiher, *ChemPhysChem*, **2011**, DOI: [10.1002/cphc.201100539](https://doi.org/10.1002/cphc.201100539).

Title: Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides

Researchers: Noah S. Bieler¹
Moritz P. Haag¹
Christoph R. Jacob²
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Karlsruhe Institute of Technology (KIT), Center for Functional Nanostructures, Wolfgang-Gaede-Str. 1a, 76131 Karlsruhe, Germany

Description:

The Cartesian Tensor Transfer Method (CTTM) was proposed by Bour, Keiderling and co-workers as an efficient way to calculate infrared, Raman, and Raman Optical Activity (ROA) spectra for large molecules from the Hessian matrix and property tensor derivatives calculated for smaller molecular fragments. Although this approach has been widely used, its reliability has not been analyzed in depth yet. Especially for ROA spectra, such an analysis became only recently possible because of methodological advances that allow for the calculation of full ROA spectra of fairly large molecules with large basis sets. In this work, we investigated an α -helical polypeptide of 20 alanine amino acids, for which we reported the full ROA spectra earlier, in order to study the CTTM for protein subunits. By comparing the full first-principles calculation of the vibrational spectra with spectra reconstructed with the CTTM from different fragment sizes, we found that infrared and Raman spectra are mostly well reproduced. However, this is not the case for the ROA spectrum. This might have implications for peptide and protein CTTM ROA spectra that have already been published in the literature.

References: N. S. Bieler, M. P. Haag, Ch. R. Jacob, M. Reiher, *J. Chem. Theory Comput.*, **2011**, *7*, 1867.

Title: New Electron Correlation Theories for Transition Metal Chemistry

Researchers: Konrad Marti
Markus Reiher

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

Description:

Electronic structure theory faces many computational challenges in transition metal chemistry. Usually, density functional theory is the method of choice for theoretical studies on transition metal complexes and clusters mostly because it is the only feasible one, although its results are not systematically improvable. By contrast, multireference ab initio methods could provide a correct description of the electronic structure, but are limited to small molecules because of the tremendous computational resources required. In recent years, conceptually new ab initio methods emerged that turned out to be promising for theoretical coordination chemistry. We discussed two efficient parametrization schemes for the electronic wave function, the matrix product states and the complete-graph tensor network states. Their advantages are demonstrated at the example of transition metal complexes. Especially, tensor network states might provide the key to accurately describe strongly correlated and magnetic molecular systems in transition metal chemistry.

References: K. Marti, M. Reiher, *Phys. Chem. Chem. Phys.*, **2011**, *13*, 6750.

Title: Quantum-information Analysis of Electronic States of Different Molecular Structures

Researchers: G. Barcza¹
Ö. Legeza¹
K. Marti²
M. Reiher²

Institute/Group: ¹Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany Research Institute for Solid State Physics and Optics
²Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

Description:

We have studied transition metal clusters from a quantum information theory perspective using the density-matrix renormalization group (DMRG) method. We demonstrated the competition between entanglement and interaction localization and discuss the application of the configuration interaction-based dynamically extended active space procedure, which significantly reduces the effective system size and accelerates the speed of convergence for complicated molecular electronic structures. Our results indicate the importance of taking entanglement among molecular orbitals into account in order to devise an optimal DMRG orbital ordering and carry out efficient calculations on transition metal clusters. Apart from these algorithmic observations, which lead to a recipe for black-box DMRG calculations, our work provides physical understanding of electron correlation in molecular and cluster structures in terms of entropy measures of relevance also to recent work on tensor-network representations of electronic states. We also identify those molecular orbitals which are highly entangled and discuss the consequences for chemical bonding and for the structural transition from an dioxygen binding copper cluster to an bis-oxygen-bridged system with broken O-O bond.

References: G. Barcza, Ö. Legeza, K. Marti, M. Reiher, *Phys. Rev. A*, **2011**, *83*, 012508.

Title: On the Emergence of Molecular Structure

Researchers: Edit Mátyus
Jürg Hutter
Ulrich Müller-Herold
Markus Reiher

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

Description:

The structure of $\{a^\pm, a^\pm, b^\mp\}$ -type Coulombic systems is characterized by the effective ground-state density of the a -type particles, computed via non-relativistic quantum mechanics without the introduction of the Born–Oppenheimer approximation. A structural transition is observed when varying the relative mass of the a - and b -type particles, *e.g.*, between atomic H^- and molecular H_2^+ . The particle-density profile indicates a molecular-type behavior for the positronium ion, Ps^- .

References: E. Mátyus, J. Hutter, U. Müller-Herold, and M. Reiher, *Phys. Rev. A*, **2011**, *83*, 052512.

Title: An Enquiry into Theoretical Bioinorganic Chemistry: How Heuristic is the Character of Present-day Quantum Chemical Methods?

Researchers: Maren Podewitz
Martin Tillmann Stiebritz
Markus Reiher

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

Description:

We elaborated on the state of the art in computational bioinorganic chemistry and aim at identifying and defining the most difficult obstacles in the process of obtaining unambiguous and predictive results from quantum chemical calculations. We proposed and analysed well-known as well as new concepts for overcoming some of these obstacles.

References: M. Podewitz, M.T. Stiebritz, M. Reiher, *Faraday Discuss.*, **2011**, *148*, 119.

Title: Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster

Researchers: Maren Podewitz
Thomas Weymuth
Markus Reiher

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

Description:

The past decades have witnessed considerable progress in the development of theoretical methods and tools to calculate a large variety of properties of chemical interest—including structural parameters, reaction energies, or spectroscopic parameters—from the first principles of quantum mechanics. Among these methods, density functional theory (DFT) is today the technique of choice for many applications in a wide range of areas, and especially for the description of transition metal complexes. Unfortunately, present-day DFT still suffers from major deficiencies which are mostly due to the approximate nature of the exchange-correlation functionals. Recent developments in the analysis of the shortcomings of standard density functionals have been reviewed, and the difficulties encountered in a study of a water-splitting dinuclear ruthenium catalyst have been studied.

References: M. Podewitz, T. Weymuth, M. Reiher, *in Modeling of Molecular Properties* (Ed. P. Comba), p. 139, **2011**, Wiley-VCH.

Title: Identifying Protein β -Turns with Vibrational Raman Optical Activity

Researchers: Thomas Weymuth¹
Christoph R. Jacob²
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76131 Karlsruhe

Description:

β -turns belong to the most important secondary structure elements in proteins. On the basis of density functional calculations, vibrational Raman optical activity signatures of different types of β -turns are established and compared as well as related to other signatures proposed in the literature earlier. Our findings indicate that there are much more characteristic ROA signals of β -turns than have been hitherto suggested. These suggested signatures are, however, found to be valid for the most important type of β -turns. Moreover, we compare the influence of different amino acid side chains on these signatures and investigate the discrimination of β -turns from other secondary structure elements, namely α - and 3_{10} -helices.

References: T. Weymuth, Ch. R. Jacob, M. Reiher, *ChemPhysChem*, **2011**, *12*, 1165.

Title: Targeting Intermediates of [FeFe]-hydrogenase by CO and CN Vibrational Signatures

Researchers: ¹L. Yu
²C. Greco
²M. Bruschi
³U. Ryde
²L. De Gioia
¹M. Reiher

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Department of Biotechnology and Biosciences, and Department of Environmental Science, University of Milano-Bicocca, 20126 Milan, Italy
³Department of Theoretical Chemistry, Lund University, Chemical Center, POB 124, Lund 22100, Sweden

Description:

We employed density functional theory to assign vibrational signatures of [FeFe]-hydrogenase intermediates to molecular structures. For this purpose, we performed an exhaustive analysis of structures and harmonic vibrations of a series of CN and CO containing model clusters of the [FeFe]-hydrogenase enzyme active site considering also different charges, counterions, and solvents. The pure density functional BP86 in combination with a triple- ζ polarized basis set produce reliable molecular structures as well as harmonic vibrations. Calculated CN and CO stretching vibrations are analyzed separately. Scaled vibrational frequencies are then applied to assign intermediates in [FeFe]-hydrogenase's reaction cycle. The results nicely complement the previous studies of Darensbourg and Hall, and Zilberman et al. The infrared spectrum of the H_{ox} form is in very good agreement with the calculated spectrum of the Fe(I)Fe(II) model complex featuring a free coordination site at the distal Fe atom, as well as, with the calculated spectra of the complexes in which H_2 or H_2O are coordinated at this site. The spectrum of H_{red} measured from *Desulfovibrio desulfuricans* is compatible with a mixture of a Fe(I)Fe(I) species with all terminal COs, and a Fe(I)Fe(I) species with protonated dtma ligand, while the spectrum of H_{red} recently measured from *Chlamydomonas reinhardtii* is compatible with a mixture of a Fe(I)Fe(I) species with a bridged CO, and a Fe(II)Fe(II) species with a terminal hydride bound to the Fe atom.

References: L. Yu, C. Greco, M. Bruschi, U. Ryde, L. De Gioia, M. Reiher, *Inorg. Chem.*, **2011**, *50*, 3888.

Title: Self-organizing adaptive-resolution particle methods for continuum problems

Researchers: Birte Schrader¹⁾
Sylvain Reboux¹⁾
Rajesh Ramaswamy¹⁾
Nicolas Fiétier¹⁾
Ivo F. Sbalzarini¹⁾

**Institute/
Group:** ¹⁾MOSAIC Group

Description:

We envision an adaptive hybrid particle-mesh method that can be efficiently implemented on large distributed-memory parallel computers. In this method, the particles and meshes self-organize according to adjustable interaction potentials akin to those used in molecular dynamics simulations. This provides flexibility to redistribute the available resolution, even during a simulation. In deterministic simulations, this is achieved by consistently computing the particle kernels (basis functions for function and operator approximation) on the fly, at no additional cost. In stochastic simulations, we use van-Kampen (volume) expansions to factorize the Master equation, yielding algorithms of high computational efficiency, even for high-dimensional problems.

References:

- R. Ramaswamy and I. F. Sbalzarini. A partial-propensity formulation of the stochastic simulation algorithm for chemical reaction networks with delays. *J. Chem. Phys.*, 134(1):014106, 2011.
Also published in: *Virtual Journal of Biological Physics Research* 21(2), 2011.
- J. A. Helmuth, S. Reboux, and I. F. Sbalzarini. Exact stochastic simulations of intra-cellular transport by mechanically coupled molecular motors. *J. Computational Science*, in print, 2011.
- O. Awile, F. Büyükkeçeci, S. Reboux, and I. F. Sbalzarini. Fast neighbor lists for adaptive-resolution particle simulations. *Comput. Phys. Commun.*, in revision, 2011.
- S. Reboux, B. Schrader, and I. F. Sbalzarini. Adaptive-resolution particle method using self-organizing Lagrangian particles. *J. Comput. Phys.*, in revision, 2011.
- R. Ramaswamy and I. F. Sbalzarini. Exact on-lattice stochastic reaction-diffusion simulations using partial-propensity methods. *J. Chem. Phys.*, submitted, 2011.
- B. Schrader, S. Reboux, and I. F. Sbalzarini. Choosing the best kernel: performance models for diffusion operators in particle methods. *SIAM J. Sci. Comput.*, submitted, 2011.
- O. Demirel, B. Schrader, and I. F. Sbalzarini. A parallel particle method for solving the EEG source localization forward problem. In *Proc. 6th Intl. Symp. Health Informatics and Bioinformatics (HIBIT)*, pages 154–158, Izmir, Turkey, May 2011.
- Oral presentation at the 6th international symposium on health informatics and bioinformatics (HiBIT), Izmir, Turkey.

Title: Middleware and code generation for parallel high-performance computing

Researchers: Omar Awile¹⁾
Ömer Demirel¹⁾
Nicolas Fiétier¹⁾
Ivo F. Sbalzarini¹⁾
Jens H. Walther²⁾
Petros Koumoutsakos³⁾

Institute/ ¹⁾MOSAIC Group
Group: ²⁾Technical University of Denmark, Copenhagen, Denmark
³⁾Computational Science and Engineering Laboratory, ETH Zurich

Description:

While the need for supercomputing is spreading from traditional applications to all areas of science and engineering, programming and using multi-core distributed-memory computers has not become any easier. We conceive of an abstract language in which the semantics of parallel simulations can be specified at a high level, and then automatically translated to source code containing the appropriate sequence of calls to a middleware. The paradigm is based on a sufficient set of abstract distributed data types and operations. These abstractions provide a semantic view that separates computation from communication and hence enables predicting the parallel efficiency of a simulation from its abstract high-level description. We plan to implement such abstractions in a parallel middleware akin to the PPM Library we co-developed earlier. Further, a code generator will be developed that automatically translates high-level descriptions of particle-mesh simulations to the corresponding source code containing the appropriate calls to the middleware.

References:

I. F. Sbalzarini. Abstractions and middleware for petascale computing and beyond. *Intl. J. Distr. Systems & Technol.*, 1(2):40–56, 2010.

O. Awile, O. Demirel, and I. F. Sbalzarini. Toward an object-oriented core of the PPM library. In *Proc. ICNAAM, Numerical Analysis and Applied Mathematics, International Conference*, pages 1313–1316, Rhodes, Greece, September 2010. AIP.

I. F. Sbalzarini, J. H. Walther, M. Bergdorf, S. E. Hieber, E. M. Kotsalis, and P. Koumoutsakos. PPM – A Highly Efficient Parallel Particle-Mesh Library for the Simulation of Continuum Systems, *J. Comput. Phys.*, 215(2):566-588, 2006.

Oral presentation at the International Conference on Numerical Analysis and Applied Mathematics (ICNAAM), Rhodes, Greece, 2010.

Title: Particle methods for image processing and model-based bio-image analysis

Researchers: Grégory Paul¹⁾
Janick Cardinale¹⁾
Arun Shivanandan¹⁾
Aurélien Rizk¹⁾
Yuanhao Gong¹⁾
Ivo F. Sbalzarini¹⁾

Institute/ ¹⁾MOSAIC Group
Group: Industry partner: BitPlane AG, Zürich

Description:

Many biological experiments are based on light microscopy to observe dynamic processes in living cells. Manual analysis and intuitive interpretation of image data are hereby more and more replaced by automated analysis. The use of large data sets and high degrees of automation results in improved significance and results that are less biased by prior expectations, i.e., that have better reproducibility. We develop computational methods to automatically analyze, quantify, and annotate biological image data from fluorescence and phase-contrast microscopy. The development focuses on robust and proven (validated, with known and guaranteed error bounds and on-line confidence estimates) methods for image quantification, segmentation, and tracking as they pertain to biological systems. The methods are rooted in the algorithmic and computational framework of particle methods.

References:

- M. E. Ambühl, C. Brepsant, J.-J. Meister, A. B. Verkhovsky, and I. F. Sbalzarini. High-resolution cell outline segmentation and tracking from phase-contrast microscopy images. *J. Microscopy*, in print, doi: 10.1111/j.1365-2818.2011.03558.x, 2011.
- C. Bottier, C. Gabella, B. Vianay, L. Buscemi, I. F. Sbalzarini, J.-J. Meister, and A. B. Verkhovsky. Dynamic measurement of the height and volume of migrating cells by a novel fluorescence microscopy technique. *Lab on Chip*, in print, doi: 10.1039/C1LC20807A, 2011.
- J. Cardinale, G. Paul, and I. F. Sbalzarini. Fast region competition with topological control for multi-region segmentation using a black-box optimizer. *IEEE Trans. Image Proc.*, in revision, 2011.

Oral presentations at the International Conference on Systems Biology (ICSB), Mannheim, Germany (invited talk); SystemsX.ch retreat, Murten, Switzerland; NCCBI annual meeting, Zurich, Switzerland; Bio-Image Informatics Conference, Washington D.C., USA (invited talk).

Title: Randomized algorithms for black-box optimization

Researchers: Christian L. Müller¹⁾
Grégory Paul¹⁾
Sebastian Stich¹⁾
Ivo F. Sbalzarini¹⁾

**Institute/
Group:** ¹⁾MOSAIC Group

Description:

Evolutionary computing is a promising concept for the off-line optimization of complex black-box systems and for adaptive Monte Carlo sampling in high-dimensional and non-linear probability spaces. The lack of theoretical understanding and of higher-order information (e.g., about uncertainties) has, however, limited its practical application. We plan to exploit recently discovered connections between optimization and sampling theory to develop robust algorithms for optimization and uncertainty quantification in complex (multi-funnel) objective functions. Further, we plan to derive an unbiased sensitivity measure on arbitrary sampling-point distributions.

References:

- C. L. Müller and I. F. Sbalzarini. Energy landscapes of atomic clusters as black-box optimization benchmarks. *Evolutionary Computation*, in revision, 2011.
- C. L. Müller and I. F. Sbalzarini. A conjecture about an upper bound of the RMSD between linear chains. In *Proc. EuroCG, 27th European Workshop on Computational Geometry*, pages 31–34, Morschach, Switzerland, March 2011.
- C. L. Müller and I. F. Sbalzarini. Global characterization of the CEC 2005 fitness landscapes using fitness-distance analysis. In *Proc. EvoStar*, volume 6624 of *Lecture Notes in Computer Science*, pages 294–303, Torino, Italy, April 2011.
- C. L. Müller. Continuous black-box optimization in linearly constrained domains using efficient Gibbs sampling. In *Proc. EVOLVE, Workshop on Probability, Set Oriented Numerics and Evolutionary Computation*, Luxembourg, May 2011.
- G. Paul, C. L. Müller, and I. F. Sbalzarini. Sensitivity analysis from evolutionary algorithm search paths. In *Proc. EVOLVE, Workshop on Probability, Set Oriented Numerics and Evolutionary Computation*, Luxembourg, May 2011.
- C. L. Müller and I. F. Sbalzarini. Gaussian Adaptation for robust design centering. In *Evolutionary and deterministic methods for design, optimization and control, Proc. EuroGen*, pages 736–742, Capua, Italy, September 14–16 2011.
- Oral presentations at the International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control (EuroGen), Capua, Italy; 5th workshop on Theory of Randomized Search Heuristics (ThRaSh), Copenhagen, Denmark; Workshop on Computational Geometric Learning, Paris, France; EVOLVE Workshop on Probability, Set-Oriented Numerics, and Evolutionary Computation, Luxembourg; EvoStar Joint European Conference on Evolutionary Computation, Torino, Italy; 27th European Workshop on Computational Geometry (EuroCG), Morschach, Switzerland; International Conference on Operations Research (OR), Zurich, Switzerland.

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

Researchers: Nikolina Ban, Omar Bellprat, Adeline Bichet, Thomas Bosshard, Marc Chiacchio, Lukas Egloff, Erich Fischer, Doris Folini, Hanieh Hassanzadeh, Sven Kotlarski, Wolfgang Langhans, Daniel Lüthi, Pardeep Pall, Christoph Schär, Linda Schlemmer, Jürg Schmidli, 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 summer climate. Comprehensive European-scale climate-change scenario simulations will be conducted in the framework of IPCC-AR5 at a horizontal resolution of 12 km covering the period 1950-2100. Current work is addressing potential changes in heat-wave and heavy precipitation events, snow cover, the height dependence of the change signals and 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. 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 Dr. Daniel Lüthi.

The global scale simulations are carried out with the climate model ECHAM5-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.

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

Title: Computational Finance: Advanced Methods for Option pricing beyond Black-Scholes Market Models

Researchers: Prof. D. Marazzina (Politecnico di Milano), O. Reichmann, Prof. Ch. Schwab,

Institute: Seminar for Applied Mathematics
ETH Zürich

Description: We consider the numerical solution of high-dimensional partial(-integro) differential equations arising in option pricing problems in computational finance along the following two axes.

Drift dominated markets We deal with the discretization of non-local degenerate parabolic type equations. This class of equation arises in option pricing problems when dealing with Lévy driven stochastic volatility models. Well-posedness of the arising equations is addressed. We develop and analyse stable discretization schemes.

Time-inhomogeneous markets We analyze parabolic PDEs with certain type of weakly singular or degenerate time-dependent coefficients and prove existence and uniqueness of weak solutions in an appropriate sense. A localization of the PDEs to a bounded spatial domain is justified. For the numerical solution a space-time wavelet discretization is employed. An optimality result for the iterative solution of the arising systems can be obtained. Finally, applications to fractional Brownian motion models in option pricing are presented.

References

- [1] D. MARAZZINA, O. REICHMANN, AND C. SCHWAB, *hp-dgfem for kolmogorov equations of multivariate lévy processes*, Tech. Rep. 17, SAM, ETH Zurich, 2011. <http://www.sam.math.ethz.ch/reports/2011/03> (accepted for M3AS).
- [2] O. REICHMANN, *Optimal space-time adaptive wavelet methods for degenerate parabolic PDEs*, Tech. Rep. 03, SAM, ETH, 2011. <http://www.sam.math.ethz.ch/reports/2011/03> (accepted for Numer. Math.).

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 (SPDEs) driven by square integrable martingales. SPDEs 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 multi-level 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 multiplicative noncontinuous martingale noises*. SAM report 2011-36, May 2011.
- [4] ———, *Simulation of stochastic partial differential equations using Finite Element methods*, Stochastics, (2011), pp. 1–15.
- [5] A. BARTH, A. LANG, AND C. SCHWAB, *Multi-level Monte Carlo Finite Element method for parabolic stochastic partial differential equations*. SAM report 2011-30, May 2011.
- [6] A. LANG, *Almost sure convergence of a Galerkin approximation for SPDEs of Zakai type driven by square integrable martingales*. SAM report 2011-35, June 2010.
- [7] ———, *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] 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.

Title: Generalized FEM for High Frequency Wave Propagation
in Locally Periodic Media

Researchers: Prof. C. Schwab
Prof. D. Kressner
Holger Brandsmeier
Dr. Kersten Schmidt

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 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*.

References

- [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: 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] C. SCHWAB AND S. TOKAREVA, *High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data*, SAM Research report No. 2011-53, (2011). <http://www.sam.math.ethz.ch/reports/2011/53>.

Title: Sparse techniques for stochastic PDEs

Researchers: Roman Andreev, Claude Gittelsohn
Markus Hansen, Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description: The project encompasses the analysis and implementation of algorithms for the deterministic numerical solution of elliptic and parabolic boundary value problems and associated eigenvalue problems with stochastic coefficients. A separation of deterministic and stochastic parts reduces the original stochastic problem to a high-dimensional parametric deterministic problem. In order to overcome this high complexity we use sparse techniques to approximate the random behavior of the solution, a priori and a posteriori adaptivity to represent it by as few terms as possible, and computer parallelism to efficiently overcome potential bottlenecks.

We apply sparse approximation techniques and adaptivity in the context of *stochastic Galerkin FEM*, *stochastic collocation FEM* and *multi level Monte Carlo* methods, see references below. All methods allow for parallelization. Numerical analysis as well as implementation, parallelization and testing of the proposed algorithms form the major part of this project.

- [1] R. ANDREEV AND C. SCHWAB, *Sparse Tensor Approximation of Parametric Eigenvalue Problems*, in press, ETH Zürich, 2010. Available at <http://www.sam.math.ethz.ch/reports/2010/40>.
- [2] A. COHEN, R. DEVORE, AND C. SCHWAB, *Analytic regularity and polynomial approximation of parametric stochastic elliptic PDEs*, Tech. Rep. 2010-3, Seminar for Applied Mathematics, ETH Zürich, 2010. In review.
- [3] C. J. GITTELSON, *Adaptive Galerkin Methods for Parametric and Stochastic Operator Equations*, PhD thesis, ETH Zürich, 2011. ETH Dissertation No. 19533.
- [4] ———, *An adaptive stochastic Galerkin method*, Tech. Rep. 2011-11, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [5] ———, *Adaptive stochastic Galerkin methods: Beyond the elliptic case*, Tech. Rep. 2011-12, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [6] ———, *Adaptive wavelet methods for elliptic partial differential equations with random operators*, Tech. Rep. 2011-37, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [7] ———, *Representation of gaussian fields in series with independent coefficients*, IMA Journal of Numerical Analysis, (2011).
- [8] ———, *Stochastic Galerkin approximation of operator equations with infinite dimensional noise*, Tech. Rep. 2011-10, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [9] ———, *Uniformly convergent adaptive methods for parametric operator equations*, Tech. Rep. 2011-19, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [10] C. J. GITTELSON, J. KÖNNÖ, C. SCHWAB, AND R. STENBERG, *The multi-level monte carlo finite element method for a stochastic brinkman problem*, Tech. Rep. 2011-31, Seminar for Applied Mathematics, ETH Zürich, 2011.

- [11] M. HANSEN AND C. SCHWAB, *Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic PDEs*, Tech. Rep. 2011-29, Seminar for Applied Mathematics, ETH Zürich. Available at <http://www.sam.math.ethz.ch/reports/2011/29>.
- [12] C. SCHWAB AND C. J. GITTELSON, *Sparse tensor discretization of high-dimensional parametric and stochastic PDEs*, in Acta Numerica, vol. 20 of Acta Numer., Cambridge Univ. Press, Cambridge, 2011, pp. 291–467.

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

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

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.

One direction of work are new function systems designed to efficiently capture anisotropic features in two dimensions. *Shearlets* represent such a system forming a multiresolution *frame*. The assumed advantage of using shearlets is their suitability for capturing spatial directional irregularities, yielding an efficient adaptive method. The disadvantages are that shearlets lack a good refinement relation, which complicates the computational work, and that they are not well suited to use on bounded domains. The shearlet types investigated appear not to form a frame.

In a different direction, we succeeded in developing a discretization of the radiative transfer equation which for the first time can be shown to converge at an optimal rate in terms of arithmetic operations [4].

Furthermore we develop sparse tensor versions of popular solution approaches such as the discrete ordinates method and the spherical harmonics method to overcome the curse of dimensionality. These sparse tensor methods achieve convergence rates equal to those of 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. Depending on the problem size, this reduction can correspond to an order of magnitude fewer degrees of freedom.

Numerical experiments in two physical and one angular dimension show evidence for the theoretical estimates to hold in practice.

- [1] E. FONN, *Shearlet galerkin for transport equations: implementation and stability*, tech. rep., SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2011/50>.
- [2] K. GRELLA AND C. SCHWAB, *Sparse discrete ordinates method in radiative transfer*, tech. rep., SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2010/46>.
- [3] ———, *Sparse tensor spherical harmonics approximation in radiative transfer*, J. of Comput. Phys., (2011).
- [4] P. GROHS AND C. SCHWAB, *Sparse twisted tensor frame discretizations of parametric transport equations*, tech. rep., SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2010/41>.

Title: Free Surface Influence on Plate Tectonics and Mantle Convection

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

Institute/ Institute of Geophysics
Group: 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.

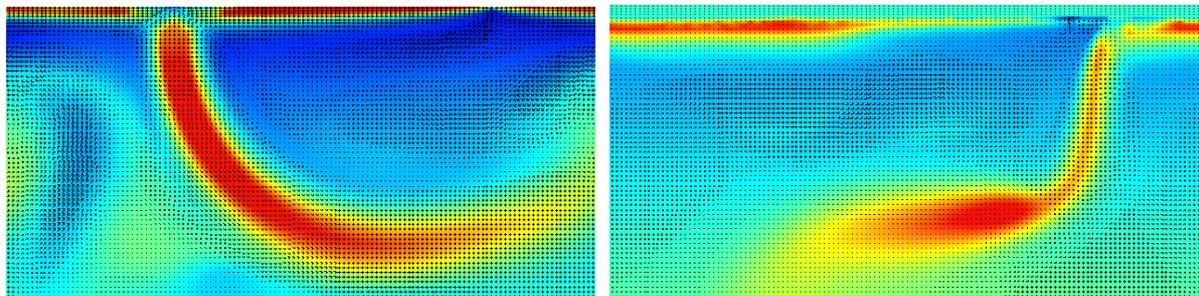


Figure. Convection with strongly temperature-dependent and yield stress-dependent viscosity. Shown is $\log(\text{viscosity})$. The left case has a free-slip surface and develops a symmetric downwelling, whereas the right case has a free surface and develops single-sided downwelling resembling subducting oceanic plates (slabs) on Earth.

References: A manuscript is submitted to *Geophysical Research Letters*

Title: Reservoirs of Dense Material in the Deep Earth's Mantle as the Source of Ocean Island Basalts

Researchers: F. Deschamps, P.J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Description:

A major result established by seismological observations is the existence of large scale compositional heterogeneities in the Earth's deep mantle. The exact nature of these heterogeneities is still debated. A likely hypothesis, which is supported by rare gases signatures of Ocean Island Basalt, is that they consist in reservoirs of primitive material that differentiated early in the Earth's history. This hypothesis is supported by. In this project, we demonstrate that appropriate models of thermo-chemical convection quantitatively agree with Ocean Island Basalt data. For this, we performed numerical experiments varying the chemical density contrast between the primitive and regular materials in the range 60-110 kg/m³, and the slope of the coexistence curve (Clapeyron) of the 660-km phase transition between -3.0 and 0 MPa/K. Reservoirs of primitive material are forming at the bottom of the system with shape and stability that depend on the chemical density contrast (Figure 1). For each model, we determined the entrainment of primitive material by plumes generated at the top of the primitive reservoirs. In the most likely models, *i.e.* fitting tomography, the entrainment never exceeds 9%. Our results clearly indicate that the presence of primitive reservoirs in the deep mantle is dynamically feasible and satisfies both seismological and geochemical constraints.

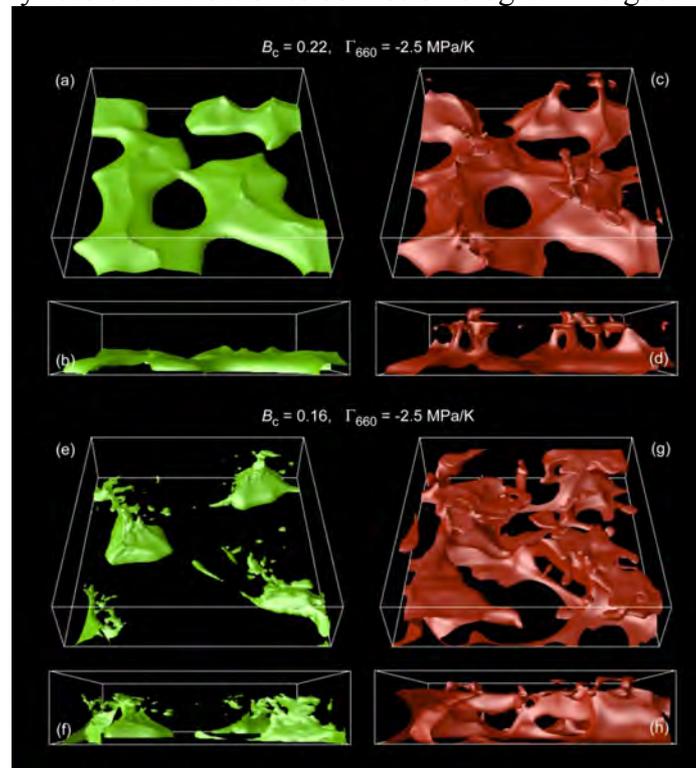


Figure. Isosurfaces of composition (left column) and residual temperature (right column) for two numerical experiments. (a-d) Buoyancy ratio $B_c = 0.22$, $\Gamma_{660} = -2.5$ MPa/K. (e-h) $B_c = 0.16$, and $\Gamma_{660} = -2.5$ MPa/K. Snapshots are taken at time $t = 6.3$ Gyr.

Reference: Nature Geoscience (2011), in press

Title: Discretization Errors and Free Surface Stabilization in the Finite Difference and Marker-in-cell Method

Researchers: Thibault Duretz, Dave May, Taras Gerya, Paul Tackley

Institute/ Institute of Geophysics
Group: Geophysical Fluid Dynamics

Description:

The finite difference-marker-in-cell (FD-MIC) method is a popular method in thermomechanical modeling in geodynamics. Although no systematic study has investigated the numerical properties of the method, numerous applications have shown its robustness and flexibility for the study of large viscous deformations. The model setups used in geodynamics often involve large smooth variations of viscosity (e.g., temperature-dependent viscosity) as well large discontinuous variations in material properties (e.g., material interfaces). In this study, we numerically investigate the discretization errors and order of accuracy of the velocity and pressure solution obtained from the FD-MIC scheme using two-dimensional analytic solutions (Fig.3). We also introduce a stabilization algorithm that damps the potential oscillations that may arise from quasi free surface calculations in numerical codes that employ the strong form of the Stokes equations. This correction term is of particular interest for topographic modeling, since the surface of the Earth is generally represented by a free surface. Including the stabilization enables physically meaningful solutions to be obtained from our simulations, even in cases where the time step value exceeds the isostatic relaxation time.

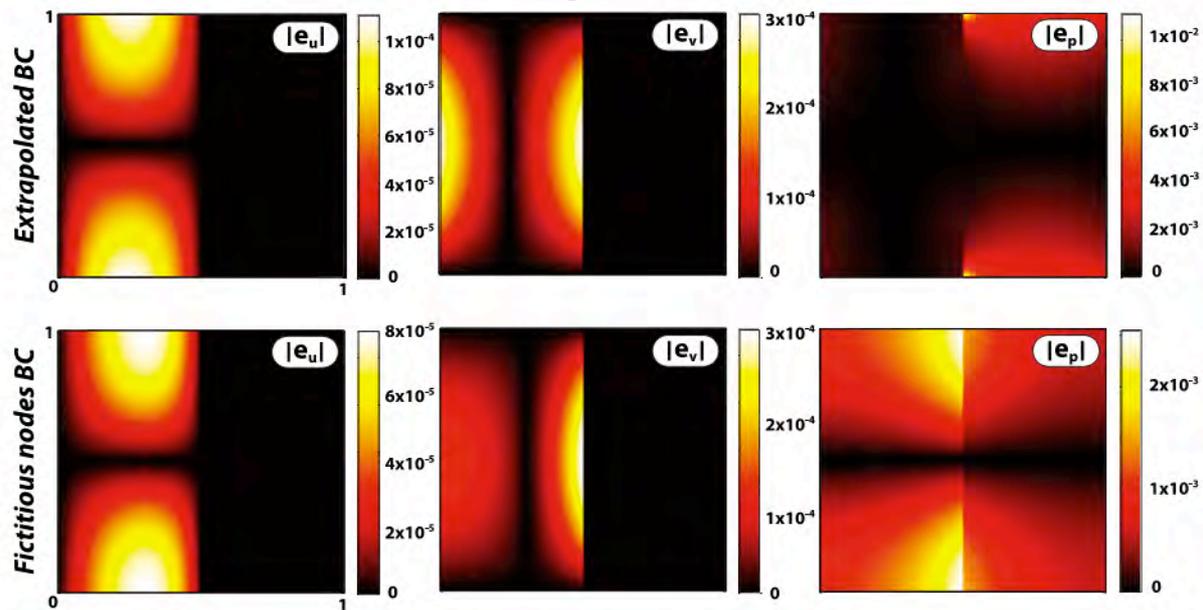


Figure. Absolute value of the discretization error for the primitive variables u , v , and p . Results are produced with the analytical solution SolCx with a viscosity jump of 10^6 and a grid resolution of 101×101 nodes. Extrapolated and fictitious node boundary condition implementations produce a similar velocity error pattern. The pressure error is dominant at the location of the viscosity jump. (Duretz et al., 2011).

References:

Duretz T., May D.A., Gerya T.V., Tackley, P.J. (2011) Discretization errors and free surface stabilization in the finite difference and marker-in-cell method for applied geodynamics: A numerical study. *Geochemistry, Geophysics, Geosystems*, 12 Article Number: Q07004.

Title: Numerical Modelling of Sedimentary Basins and Mid-ocean Ridges

Researchers: Taras Gerya, Filippo Schenker, Jie Liao

Institute/ Institute of Geophysics
Group: Geophysical Fluid Dynamics

Description:

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

- Development of transform faults at mid-ocean ridges (Gerya, 2011)
- Lithospheric extension (Fig.2)

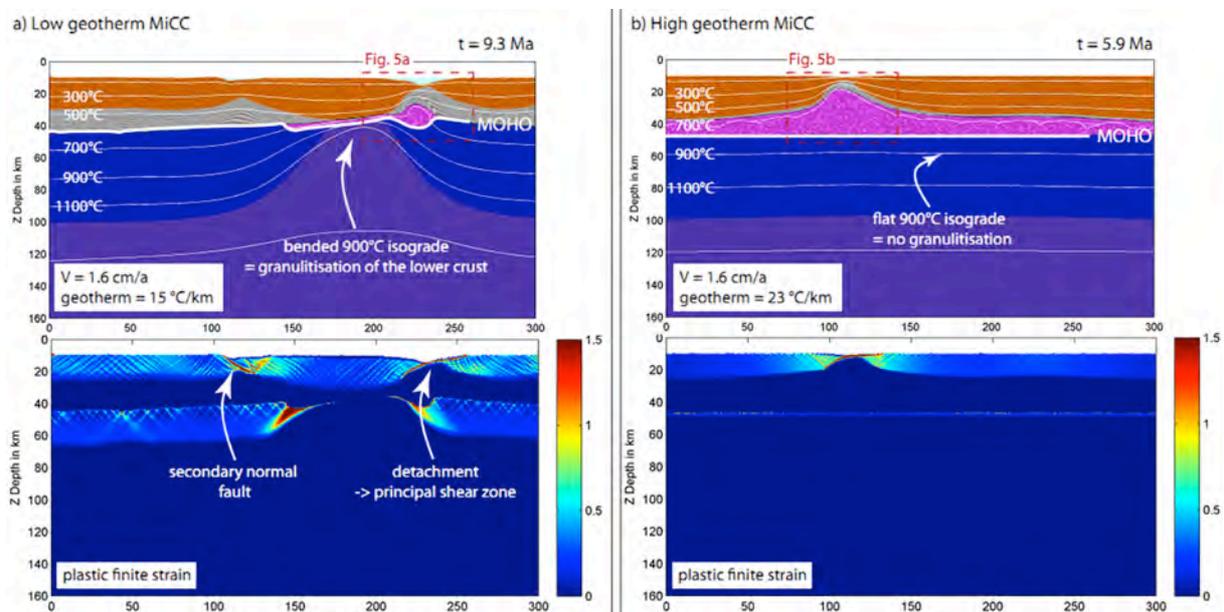


Figure. Different types of extensional doming (Schenker et al., in preparation)

References:

Gerya, T. (2011) Origin and models of oceanic transform faults. *Tectonophysics*, doi: 10.1016/j.tecto.2011.07.006

Title: Numerical Modeling of Planetary Differentiation Processes
Researchers: Gregor Golabek, Tobias Keller, Ja-Ren Lin, Taras Gerya, Paul Tackley

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

Description:

Various aspects of planetary formation processes are modelled in 2D and 3D with the use of the original codes I2ELVIS, I3ELVIS and STAG_YY 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 the martian dichotomy and Tharsis (Fig. 4, Golabek et al., 2011)
- Protocore destabilization in planetary embryos (Lin et al., 2011). The study highlighted in NATURE GEOSCIENCE, VOL 4, APRIL 2011.

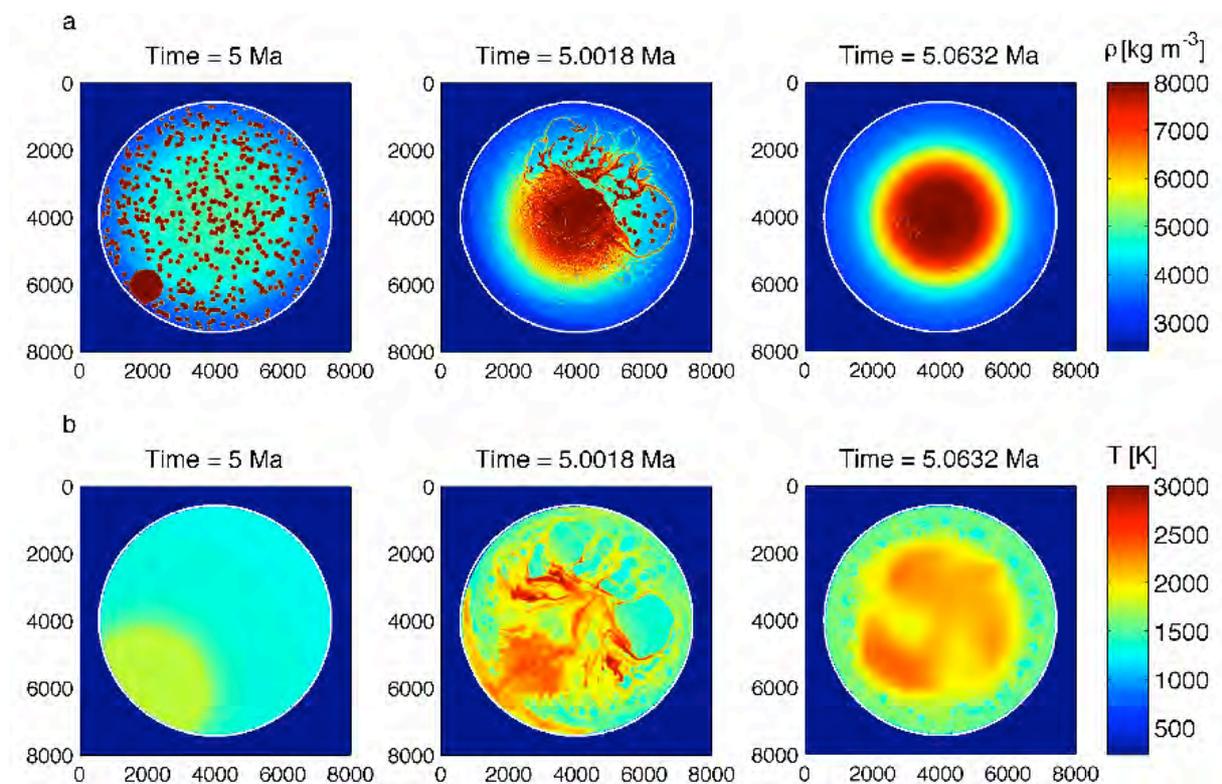


Figure. Formation of a thermal anomaly due to the sinking of the giant impactor core during runaway differentiation. Evolution of (a) density and (b) temperature in a Mars-sized body at the time of core formation (Golabek et al., 2011).

References

- Golabek, G.J., Keller, T., Gerya, T.V., Zhu, G., Tackley, P.J., Connolly, J.A.D. (2011) Origin of the martian dichotomy and Tharsis from a giant impact causing massive magmatism. *Icarus*, 215, 346–357.
- Lin, J.-R., Gerya, T.V., Tackley, P.J., Yuen, D.A., Golabek, G.J. (2011) Protocore destabilization in planetary embryos formed by cold accretion: Feedbacks from non-Newtonian rheology and energy dissipation. *Icarus*, 213, 24-42 .

Title: Influence of Curvature on Thermo-chemical Convection in Spherical Geometry

Researchers: Y. Li, F. Deschamps, P.J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Description:

In this project, we performed a series of experiments of thermo-chemical convection in a spherical shell (located in between a core and the surface) to study the effect of the core's size on the stability of reservoirs of dense material located at the bottom of the spherical shell (Figure 1). For this, we varied the core's size, which is controlled by the ratio of the core radius to the total radius $f = rc/R$. The dense material is initially distributed in a layer located at the bottom of the shell representing 10% of the total volume of the shell. We found that the core's size does not have any influence on the stability of reservoirs that form at the bottom of the shell. However, the detailed shape of these reservoirs is strongly affected by the core's size. The number of reservoirs increases with the core's radius, but the size of these reservoirs decreases. In a second series of experiments, we studied the influence of the buoyancy ratio B , which measures the density contrast between the dense and regular material. We found that the buoyancy ratio has a major influence on the stability of the dense layer. For small (< 0.18) values of the buoyancy ratio, the dense layer is progressively swept out and the dense and regular materials are well mixed. Large (> 0.30) values of the buoyancy ratio induce stable layering, i.e., the initial layer remains stable during the entire experiment, and only has some moderate topography at its surface. For intermediate values of the buoyancy ratio, we observe the formation of reservoirs of dense material, which remains stable until the end of the experiments.

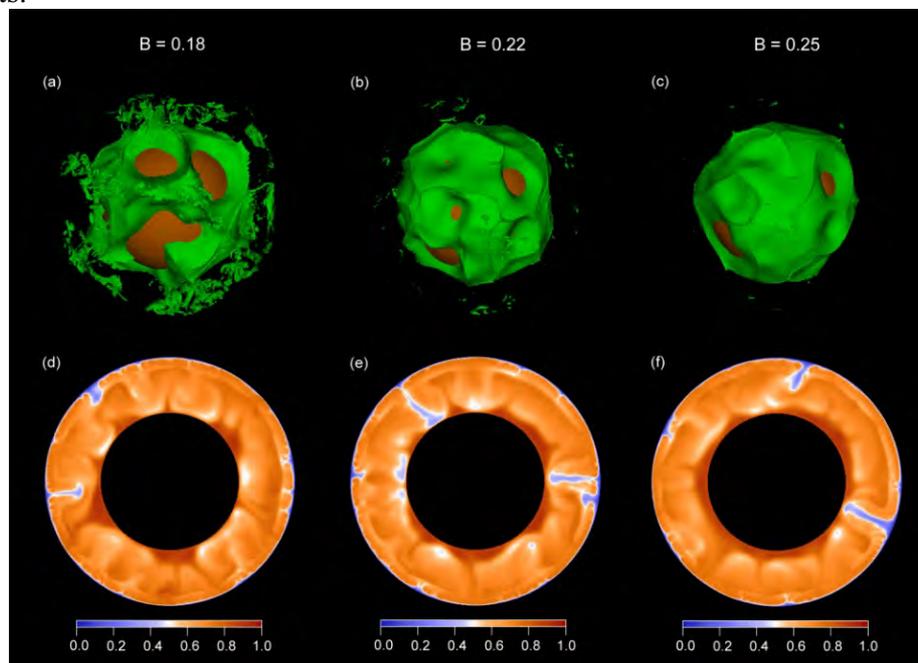


Figure 1. Experiments of thermo-chemical convection for three values of the buoyancy ratio (B), from left to right $B = 0.18$, $B = 0.22$, and $B = 0.25$. For each case, the top row shows an isosurface (with $C = 0.5$) of the composition, and the bottom row shows a slice of the temperature (see color scale). Snapshots are taken at non-dimensional time $t = 0.0170$ (corresponding to 7.2 Gyr). The ratio of the core's radius to the total radius is $f = 0.55$.

Title: Decoupled and Coupled Multilevel Preconditioners for Problems in Elasticity and Variable Viscosity Stokes Flow

Researchers: Dave A. May
Jed Brown

Institute/Group: Institute of Geophysics
Geophysical Fluid Dynamics

Description:

In this work, we focus on the development and comparison of several multilevel preconditioners for solving problems in elasticity and Stokes flow applied to geodynamic applications. The main barrier to developing robust, scalable multilevel preconditioners for these applications is that the coefficients in the differential operator (e.g Youngs modulus, viscosity) typically exhibit large variations in space. For the applications we consider, we requiree that our methods can solve problems which exhibit coefficient variations which are either continuous or discontinuous.

When considering coupled partial differential equations, we have several options in how to construct the multilevel preconditioner. For example we can (i) choose to split the PDE into individual scalar components and apply a multilevel precondition to each scalar sub-problem and couple the entire system with a stationary block iterative method like Jacobi, or SOR(SSOR), (ii) generate the multilevel hierarchy of the coupled problem and on each level, define the smoother using a node based decoupling of the individual fields or (iii) consider some hybrid method where we generate the multilevel hierarchy of the coupled problem and define the smoother by splitting the discrete coarse grid PDE into individual scalar components (as in (i)).

The performance of the three styles of multilevel preconditioners are compared for a range of different coefficient structures associated with elasticity and Stokes flow for prototypical geodynamic problems. The problems consist of setups with rigid inclusions employing a range of different geometries (dimensionality) and length scales. We also examine some cases in the Stokes regime involving a von-Mises yield surface. The trade-offs between the different strategies are compared.

Title: Optimal, Scalable Forward Models for Computing Gravity Anomalies

Researchers: Dave A. May
Matthew G. Knepley

Institute/Group: Institute of Geophysics
Geophysical Fluid Dynamics

Description:

We describe three approaches for computing a gravity signal from a density anomaly. The first approach consists of the classical ‘summation’ technique, while the remaining two methods solve the Poisson problem for the gravitational potential using either a finite-element (FE) discretization employing a multilevel pre-conditioner, or a Green’s function evaluated with the fast multipole method (FMM). The methods using the Poisson formulation described here differ from previously published approaches used in gravity modelling in that they are optimal, implying that both the memory and computational time required scale linearly with respect to the number of unknowns in the potential field. Additionally, all of the implementations presented here are developed such that the computations can be performed in a massively parallel, distributed memory-computing environment. Through numerical experiments, we compare the methods on the basis of their discretization error, CPU time and parallel scalability. We demonstrate the parallel scalability of all these techniques by running forward models with up to 108 voxels on 1000s of cores.

Reference:

D. A. May, M. G. Knepley
Optimal, scalable forward models for computing gravity anomalies
Geophysical Journal International 187(1) (2011) 161-177

Title: High Resolution, 3-D Finite Element Modelling of Continental Collision

Researchers: Dave A. May
Sarah M. Lechmann
Stefan M. Schmalholz

Institute/Group: Institute of Geophysics
Geophysical Fluid Dynamics

Description:

Various models have been proposed to explain tectonic deformations during continent collision. A frequently applied model is the thin viscous sheet model which is however not fully 3-D and assumes *a priori* diffuse thickening as the dominant deformation style.

We compare a fully 3-D multilayer numerical model with a corresponding thin viscous sheet numerical model for the scenario of continent indentation. In our comparison we focus on the three basic viscous deformation styles thickening, buckling (folding) and lateral crustal flow.

3-D multilayer models provide a more complete picture of continental collision than thin-sheet models as they enable studying the timing, locality and relative importance of different processes simultaneously which is especially important for the hundreds of kilometre scale around the collision zone and indenter corners. 3-D models are, however, still computationally challenging and we, therefore, also present results of a computational performance test of several solution algorithms.

Work is under way to greatly increase the resolution used in the preliminary study of Lechmann et al., (2011). This is achieved by using a lower order finite element (Q1-Q1 stabilised) and exploiting a matrix-free, geometric multigrid preconditioner. A careful study has been performed to verify that the stabilized low order finite element is adequate to study continental collision processes. The use of optimized, matrix-free kernels within both the Krylov method and preconditioner allow us to perform simulations with approximately 128 x 128 x 128 elements per subdomain. The strong and weak scalability of the proposed continental collision models is being investigated.

Reference:

S. M. Lechmann, D. A. May, B. J. P. Kaus, S. M. Schmalholz
Comparing thin-sheet models with 3-D multilayer models for continental collision
Geophysical Journal International 187(1) (2011) 10-33

Title: Effects of Low-Viscosity Post-Perovskite on Thermo-Chemical Mantle Convection in a 3-D Spherical Shell

Researchers: T. Nakagawa, P. J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Description:

Numerical simulations of thermo-chemical, multi-phase mantle convection in a 3-D spherical shell are performed to determine how a low viscosity of post-perovskite affects dynamics and structures in the deep mantle. Low-viscosity post-perovskite weakens the deepest part of slabs, allowing them to more effectively spread over the core-mantle boundary (CMB), and it also results in a greater volume of basalt segregating, both of which increase the size of dense chemical piles, the horizontal lengthscale of regions of pooled slab material, and the steepness of piles' edges (in composition and phase), consistent with the existence of steep, sharp-sided edges found in seismic analyses. CMB heat flux is strongly enhanced in regions of low-viscosity post-perovskite (consistent with a theoretical prediction) and both CMB and surface heat flux are increased on average by a low-viscosity of post-perovskite, which could have important implications for the evolution of Earth's core and mantle.

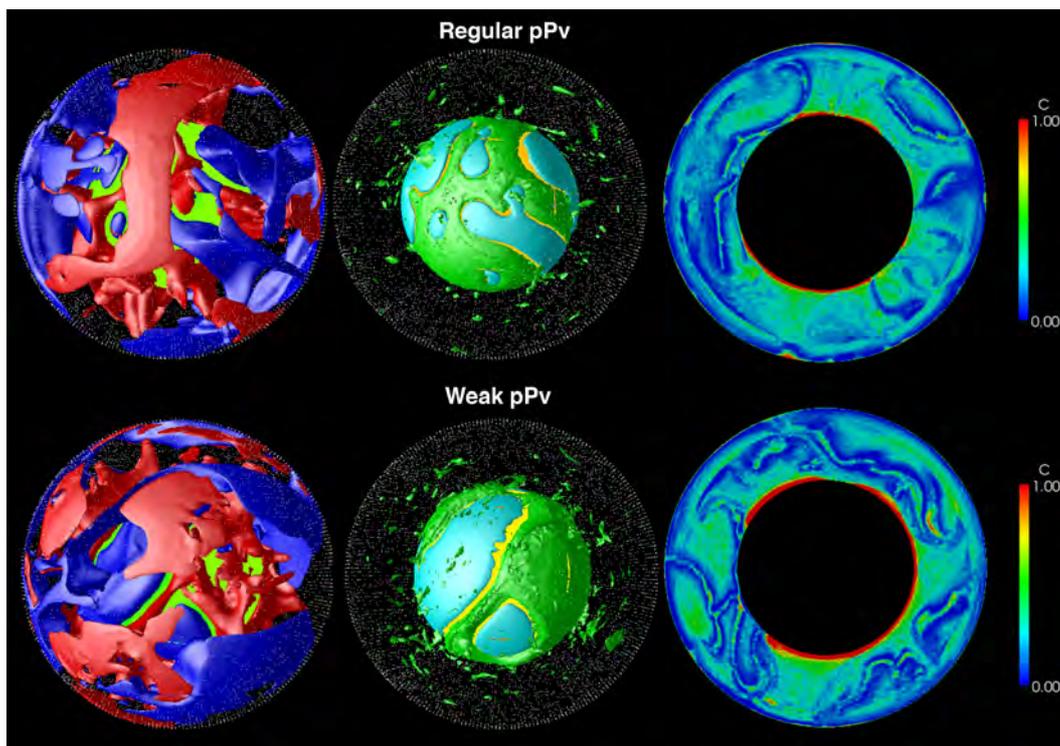


Figure. Comparison of mantle convection simulation with regular (top row) and weak (bottom row) post-perovskite. Shown are isosurfaces of T (red and blue), C (green) and post-perovskite (light blue); and cross-sections of composition (right).

References: Nakagawa, T. and P. J. Tackley, Effects of low-viscosity post-perovskite on thermo-chemical mantle convection in a 3-D spherical shell (2011) *Geophys. Res. Lett.*, 38, L04309, doi:10.1029/2010GL046494, 2011.

Title: Numerical Modelling of Subduction and Collision Zones

Researchers: Ksenia Nikolaeva, Guizhi Zhu, Katharina Vogt, Taras Gerya, Boris Kaus, Diana Dymkova, Thibault Duretz, Bettina Baitsch-Ghirardello

Institute/ Institute of Geophysics
Group: Geophysical Fluid Dynamics

Description:

Various aspects of subduction zone dynamics 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:

- Subduction initiation risks along American Atlantic margins (Fig. 1) (Nikolaeva et al., 2011) http://www.ethlife.ethz.ch/archive_articles/110524_Subduktion_Atlantik_su/index_EN
- 3-D plume patterns and melt productivity above retreating slabs (Zhu et al., 2011)
- Subduction of young oceanic plates (Blanco-Quintero et al., 2011)
- Defining future directions in subduction modeling (Gerya, 2011)

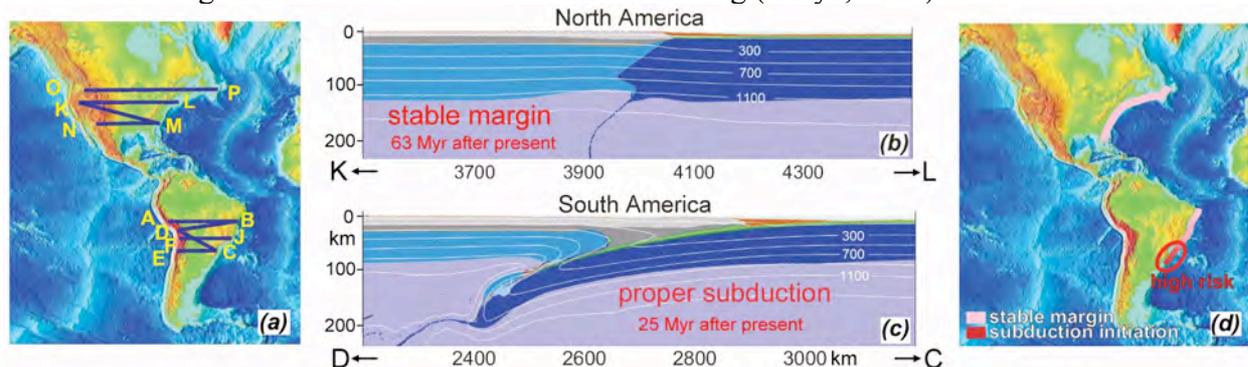


Figure. Dynamics of subduction initiation at a passive margin (Nikolaeva et al., 2010).

References:

- Blanco-Quintero, I.F., Gerya, T.V., García-Casco, A., Castro, A. (2011) Subduction of young oceanic plates: A numerical study with application to aborted thermal-chemical plumes
- Gerya, T.V. (2011) Intra-oceanic subduction zones. In: D. Brown and P.D. Ryan (Eds.) Arc-Continent Collision, *Frontiers in Earth Sciences*. Springer-Verlag, Berlin Heidelberg, pp.23-51.
- Gerya, T. (2011) Future directions in subduction modeling. *Journal of Geodynamics*, 52, 344-378.
- Nikolaeva, K., Gerya, T.V., Marques, F.O. (2011) Numerical analysis of subduction initiation risk along the Atlantic American passive margins. *Geology*, 39, 463-466.
- Zhu, G., Gerya, T.V., Honda, S., Tackley, P.J., Yuen., D.A. (2011) Influences of the buoyancy of partially molten rock on 3-D plume patterns and melt productivity above retreating slabs. *Phys. Earth Planet. Interiors*, 185, 112-121.
- Zhu, G., Gerya, T.V., Yuen., D.A. (2011) Melt evolution above a spontaneously retreating subducting slab in a three-dimensional model. *Journal of Earth Science*, 22, 137-142.

Title: Modelling the Influence of Continents on Plate Tectonics

Researchers: T. Rolf
P. J. Tackley

Institute/ Institute of Geophysics
Group: 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.

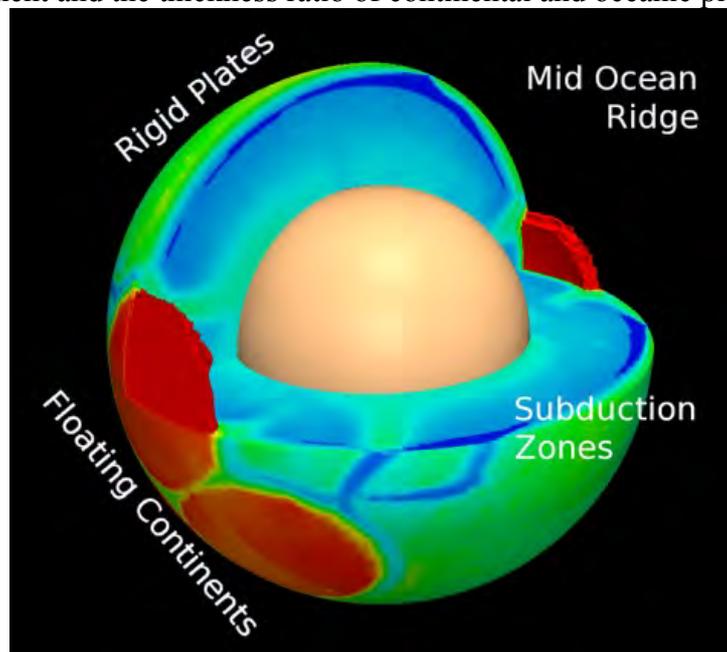


Figure. Numerical simulation of plate tectonics with buoyant continents in 3-D spherical geometry. Plotted is effective viscosity (red=high to blue=low).

References: Rolf, T., and P. J. Tackley (2011) Focussing of stress by continents in 3D spherical mantle convection with self-consistent plate tectonics, *Geophys. Res. Lett.*, 38, L18301, doi:10.1029/2011GL048677.

Title: Modelling The Dynamics of Slabs in the Core-Mantle Boundary Region

Researchers: P. J. Tackley

Institute/ Institute of Geophysics

Group: Geophysical Fluid Dynamics, D-ERDW

Description:

Subducted oceanic plates, known as slabs, sink to the core-mantle boundary (CMB), where the crustal layer, made of basalt, might peel off and segregate into a layer above the CMB, which could have a strong influence on the evolution of Earth's mantle and core. Here, three-dimensional (3-D) and two-dimensional (2-D) simulations of a compositionally-stratified slab reaching the CMB are performed. Slab-CMB interaction is characterised by heating up of the slab followed by separation of the basalt and harzburgite layers, with harzburgite rising in vigorous plumes. Plumes form at the edges and sides of slabs at the CMB as well as in their interiors with plume heads dominated by depleted harzburgitic material, while plume tails entrain basaltic material. Segregation of basalt depends strongly on the presence or absence of a preexisting dense layer at the CMB and by dimensionality. A preexisting dense layer greatly increases the fraction of basalt that segregates from the slab. A range of "interesting" structures are observed in the model CMB region, which may be useful in interpreting seismic observations. Structures include plumes next to vertical slab segments, inverted slab sections perched above the CMB and harzburgite curtains. 2-D simulations give a good first-order guide to the dynamics obtained in fully 3-D geometry, but inherently 3-D structures are missed (plumes versus sheets, fingering) and there is a quantitative difference in the fraction of basalt segregated.

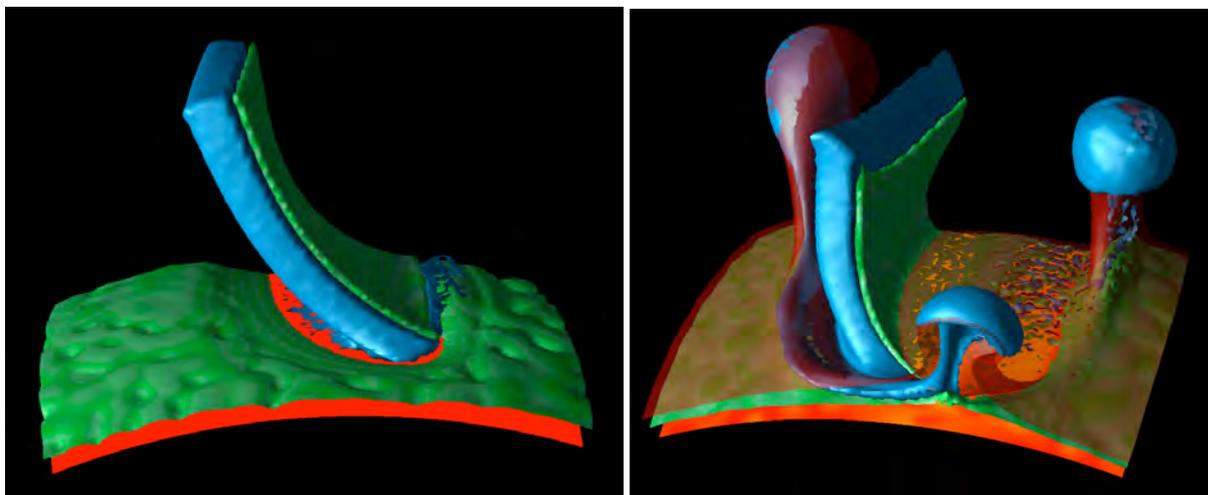


Figure. Numerical simulation of a subducted oceanic plate (slab) reaching the hot CMB. The slab contains basaltic (green) and harzburgitic (blue) layers. Red isosurfaces show hot temperature.

References: Living dead slabs in 3-D: The dynamics of compositionally-stratified slabs entering a 'slab graveyard' above the core-mantle boundary, *Phys. Earth Planet. Inter.*, in press, doi:10.1016/j.pepi.2011.04.013.

Title: Stagnant Lid Convection in Spherical Geometry and the Thermal Evolution of Large Icy Moons of Giant Planets

Researchers: C. Yao
F. Deschamps
P.J. Tackley

Institute/Group: Institute of Geophysics/Geophysical Fluid Dynamics

Description:

The thermal evolution of large icy moons orbiting around giant planets (*e.g.*, Ganymede and Callisto around Jupiter, and Titan around Saturn) is controlled by the heat transfer through the outer ice I layer of these moons. The viscosity of ice I strongly depends on the temperature, suggesting that convection in the ice I layer of icy moons undergoes the so-called stagnant lid regime. This regime has been studied in 2D and 3D-Cartesian geometry, but so far few numerical experiments have been carried out in spherical geometry. We started a systematic study of thermal convection with strongly temperature dependent viscosity in spherical geometry. Figure 1 shows two models with a ratio of the core to total radius equal to 0.80. We then use our calculations to parameterize the heat flux and the average temperature as a function of the Rayleigh number (Ra) and the thermal viscosity contrast ($\Delta\mu$). Preliminary results indicate some substantial differences compared to the Cartesian cases. In particular, for given values of the Ra and $\Delta\mu$, the stagnant lid regime is less developed in spherical geometry than in Cartesian geometry.

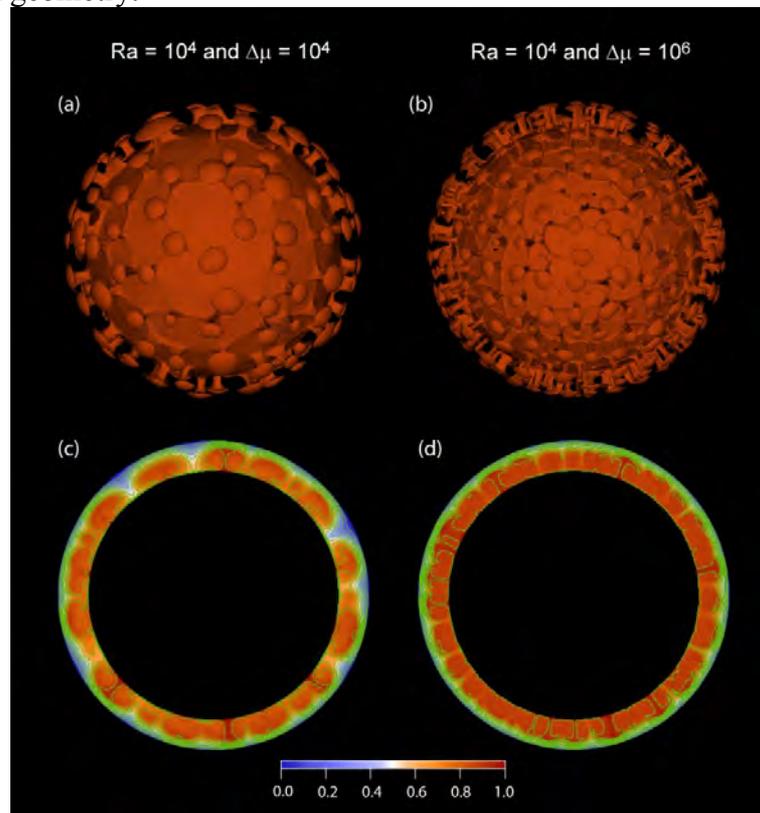


Figure. Experiments of thermal convection for a top to bottom thermal viscosity ratio of 10^4 (left column) and 10^6 (left column). For each case, the top row shows an isosurface of the non-dimensional temperature, and the bottom row shows a slice of the temperature. The ratio of the core's radius to the total radius is $f = 0.80$.

Title: The effect of using a polarizable solvent model upon the folding equilibrium of different β -peptides

Researchers: Z. Lin^{a,b}
N. Schmid^a
W. F. van Gunsteren^{a*}

Institute/ ^aLaboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
^bSchool of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

Folding and unfolding of β -peptides has been studied extensively by molecular dynamics (MD) simulation in the past decade. In these simulations, a non-polarizable model for the solvent (mostly methanol) was used. This work has investigated the effect of using a polarizable methanol solvent model upon the folding equilibrium of β -peptides. Thirteen MD simulations covering a total simulation length of 1.25 μ s for three differently folding β -peptides were analyzed. The agreement with experimental data was slightly improved by applying the polarizable solvent. In the polarizable solvent, helical structures, which have a large dipole moment, are stabilized, while no obvious effect was detected in the simulations of peptides that have a hairpin structure as the dominant fold. The introduction of electronic polarizability into the solvent model appears of importance to a proper description of folding equilibria if these are determined by competing solute conformations that have different dipole moments.

References: *Mol. Phys.* **109** (2011) 493-506

Title: A simple, efficient polarisable coarse-grained water model for molecular dynamics simulations

Researchers: S. Riniker
W. F. van Gunsteren^a

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

The development of coarse-grained (CG) models that correctly represent the important features of compounds is essential to overcome the limitations in time scale and system size currently encountered in atomistic molecular dynamics simulations. Most approaches reported in the literature model one or several molecules into a single uncharged CG bead. For water, this implicit treatment of the electrostatic interactions, however, fails to mimic important properties, e.g., the dielectric screening. Therefore, a coarse-grained model for water is proposed which treats the electrostatic interactions between clusters of water molecules explicitly. Five water molecules are embedded in a spherical CG bead consisting of two oppositely charged particles which represent a dipole. The bond connecting the two particles in a bead is unconstrained, which makes the model polarizable. Experimental and all-atom simulated data of liquid water at room temperature are used for parametrization of the model. The experimental density and the relative static dielectric permittivity were chosen as primary target properties. The model properties are compared with those obtained from experiment, from clusters of simple-point-charge water molecules of appropriate size in the liquid phase, and for other CG water models if available. The comparison shows that not all atomistic properties can be reproduced by a CG model, so properties of key importance have to be selected when coarse graining is applied. Yet, the CG model reproduces the key characteristics of liquid water while being computationally 1-2 orders of magnitude more efficient than standard fine-grained atomistic water models.

References: *J. Chem. Phys.* **134** (2011) 084110

Title: Influence of variation of a side chain on the folding equilibrium of a β -peptide

Researchers: Z. Lin^{a,b}
H. Hodel^a
W. F. van Gunsteren^{*a}

Institute/ ^aLaboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
^bSchool of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

The ability to design well-folding β -peptides with a specific biological activity requires detailed insight into the relationship between the β -amino acid sequence and the three-dimensional structure of the peptide. Here, we present a molecular-dynamics (MD) study of the influence of a variation of a side chain on the folding equilibrium of a β -heptapeptide that folds into a 3_{14} -helical structure. The side chain of the 5th residue, a valine, was changed into five differently branched side chains of different lengths and polarity, Ala, Leu, Ile, Ser, and Thr. Two computational techniques, long-time MD simulations and the one-step perturbation method, were used to obtain free enthalpies of folding. The simulations show that all six peptides exhibit similar folding behavior, and that their dominant fold is the same, i.e., a 3_{14} -helix. Despite the similarities of their structural properties, a small stabilization effect of ca. 2 kJ mol⁻¹ on the folding equilibrium of the 3_{14} -helical structure due to a branching C $_{\gamma}$ -atom in the β^3 -side chain is observed. These results confirm those of previous circular dichroism (CD) studies. The length of side chain and its polarity seem to have no apparent (de)stabilization effect. Application of the cost-effective one-step perturbation method to predict free-enthalpy differences appeared to yield an overall accuracy of about $k_B T$, which is not sufficient to detect the small stabilization effect.

References: *Helv. Chim. Acta.* **94** (2011) 597-610

Title: A refined, efficient mean solvation force model that includes the interior volume contribution

Researchers: J. R. Allison[†]
K. Boguslawski[†]
F. Fraternali[‡]
W. F. van Gunsteren^{*,†}

Institute/ [†]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[‡]Randall Division of Cell and Molecular Biophysics, King's College London SE1 1UL, United Kingdom

Group: Computer-aided chemistry

Description:

A refined implicit aqueous solvation model is proposed for the simulation of biomolecules without the explicit inclusion of the solvent degrees of freedom. The mean force due to solvation is approximated by the derivative of a simple analytic function of the solvent accessible surface area combined with two atomic solvation parameters, as described previously, with the addition of a novel term to account for the interaction of the interior atoms of the solute with the solvent. The extended model is parametrized by comparing the structural properties and energies computed from simulations of six test proteins of varying sizes and shapes using the new solvation energy term with the corresponding values obtained from simulations in vacuum, using the original implicit solvent model and in explicit water, and from the X-ray or NMR model structures. The mean solvation model proposed here improves the structural properties relative to vacuum simulations and relative to the simpler model that neglects the volume contribution, while remaining significantly more efficient than simulations in explicit water.

References: *J. Phys. Chem. B* **115** (2011) 4547-4557

Title: Enhancing the configurational sampling of ions in aqueous solution using adiabatic decoupling with translational temperature scaling

Researchers: A. P. E. Kunz
W. F. van Gunsteren*

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

Three methods to enhance the configurational sampling of ions in aqueous solution, temperature and Hamiltonian replica exchange and adiabatic decoupling with translational temperature scaling, were compared for a system of CaSO_4 in water. It took 11 replicas in the case of temperature replica exchange to make use of a diffusion coefficient that is a factor of 1.5 larger at 350 K compared to that at 300 K. Thirty replicas were required in the Hamiltonian replica exchange with charge reduction to reach uncharged ions that have a diffusion coefficient that is 2-7 times larger than the fully charged ones. The adiabatic decoupling technique with translational temperature scaling yielded a diffusion coefficient that was 15 times larger while keeping the distribution of the water molecules around the ions unaltered with respect to the standard temperature simulation. This result illustrates the efficiency of the adiabatic decoupling technique to enhance configurational sampling

References: *J. Phys. Chem. B* **115** (2011) 2931-2936

Title: On the calculation of the dielectric permittivity and relaxation time of molecular models in the liquid phase

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

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

Methodology to compute the relative static dielectric permittivity and dielectric relaxation time of molecular liquids is reviewed and explicit formulas are given for the external field method in the case of simulations using a spherical cutoff, in which the background dielectric permittivity (ϵ_{cs}) can be larger than one, in combination with a Poisson-Boltzmann reaction-field approximation for long-range electrostatic interactions. The external field method is simple to implement and computationally efficient. It is particularly suitable for polarizable molecular models with zero permanent dipole moment and for coarse-grained molecular models with $\epsilon_{cs} > 1$. The dielectric permittivities and relaxation times of water (H₂O), dimethylsulfoxide (DMSO), methanol (MeOH), and chloroform (CHCl₃), which range from 2 to 80 and from 5 ps to 50 ps, respectively, were calculated as an illustration.

References: *J. Chem. Theory Comput.* **7** (2011) 1469-1475

Title: Validation of the GROMOS 54A7 force field with respect to β -peptide folding

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

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology,
ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

The recently developed GROMOS 54A7 force field, a modification of the 53A6 force field, is validated by simulating the folding equilibrium of two β -peptides which show different dominant folds, i.e., a 3_{14} -helix and a hairpin, using three different force fields, i.e., GROMOS 45A3, 53A6, and 54A7. The 54A7 force field stabilizes both folds, and the agreement of the simulated NOE atom-atom distances with the experimental NMR data is slightly improved when using the 54A7 force field, while the agreement of the 3J couplings with experimental results remains essentially unchanged when varying the force field. The 54A7 force field developed to improve the stability of α -helical structures in proteins can thus be safely used in simulations of β -peptides.

References: *J. Chem. Theory Comput.* **7** (2011) 1237-1243

Title: Conformational state-specific free energy differences by one-step perturbation: protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields

Researchers: Z. Lin^{1,2}
W. F. van Gunsteren²
H. Liu¹

Institute/ ¹School of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China
²Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

The one-step free energy perturbation approach can be applied to obtain conformational state-specific free energy differences (FEDs) associated with changes in force field parameters, and thus offers the possibility to consider conformational equilibria during force field parameterization. In this work, using the alanine decapeptide in explicit water solution as a model, the α -helical and β -hairpin state-specific FEDs associated with force field changes between two widely used parameter sets of the GROMOS force field, namely, 43A1 and 53A6, were determined using one-step perturbation. The results mostly deviated by only 1 kJ mol⁻¹ in absolute or a few percent in relative values from thermodynamic integration results, suggesting that the convergence ranges of one-step perturbation were large enough to cover the substantial changes in nonbonded parameters between the two parameter sets. It was also found that one-step perturbation may give larger errors when the changes from the reference state include a large decrease in van der Waals radius, as indicated by the result for the β -hairpin state-specific free energy change going from 53A6 to 43A1. According to the free energy results, the α -helical state of the alanine decapeptide is destabilized by 15 kJ mol⁻¹, i.e., 1.5 kJ mol⁻¹ per residue, relative to the β -hairpin state when going from 43A1 to 53A6, in agreement with previous direct simulations in which native α -helices were often found to be unstable in simulations using 53A6, despite that the 53A6 parameters better reproduce a range of thermodynamic properties of small molecular systems. By applying one-step perturbation to analyze the effects of perturbing individual parameters, the differential stabilization of the two secondary structure states can be traced to the changes in van der Waals parameters, especially a van der Waals parameter involved in third-neighbor interactions. This study provides an example of the efficiency of one-step perturbation in force field development, reducing the computational cost by orders of magnitude

References: *J. Comput. Chem.* **32** (2011) 2290-2297

Title: Definition and testing of the GROMOS force-field versions: 54A7 and 54B7

Researchers: N. Schmid¹
A. P. Eichenberger¹
A. Choutko¹
S. Riniker¹
M. Winger²
A. E. Mark²
W. F. van Gunsteren¹

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
²School of Chemistry and Molecular Biosciences, University of Queensland, St. Lucia, QLD 4072, Brisbane, Australia

Group: Computer-aided chemistry

Description:

New parameter sets of the GROMOS biomolecular force field, 54A7 and 54B7, are introduced. These parameter sets summarise some previously published force field modifications: The 53A6 helical propensities are corrected through new φ/ψ torsional angle terms and a modification of the N-H, C=O repulsion, a new atom type for a charged -CH₃ in the choline moiety is added, the Na⁺ and Cl⁻ ions are modified to reproduce the free energy of hydration, and additional improper torsional angle types for free energy calculations involving a chirality change are introduced. The new helical propensity modification is tested using the benchmark proteins hen egg-white lysozyme, fox1 RNA binding domain, chorismate mutase and the GCN4-p1 peptide. The stability of the proteins is improved in comparison with the 53A6 force field, and good agreement with a range primary experimental data is obtained.

References: *Eur. Biophys. J.* **40** (2011) 843-856

Title: Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors

Researchers: S. Riniker¹
C. D. Christ^{2,b}
N. Hansen¹
A. E. Mark³
P. C. Nair³
W. F. van Gunsteren^{1,a}

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
²Lead Identification and Optimization Support, Boehringer Ingelheim Pharma GmbH & Co. KG, 88397 Biberack, Germany
³School of Chemistry and Molecular Biosciences, University of Queensland, St. Lucia, QLO 4072, Brisbane, Australia

Group: Computer-aided chemistry

Description:

The relative binding free energy between two ligands to a specific protein can be obtained using various computational methods. The more accurate and also computationally more demanding techniques are the so-called free energy methods which use conformational sampling from molecular dynamics or Monte Carlo simulations to generate thermodynamic averages. Two such widely applied methods are the thermodynamic integration (TI) and the recently introduced enveloping distribution sampling (EDS) methods. In both cases relative binding free energies are obtained through the alchemical perturbations of one ligand into another in water and inside the binding pocket of the protein. TI requires many separate simulations and the specification of a pathway along which the system is perturbed from one ligand to another. Using the EDS approach, only a single automatically derived reference state enveloping both end states needs to be sampled. In addition, the choice of an optimal pathway in TI calculations is not trivial and a poor choice may lead to poor convergence along the pathway. Given this, EDS is expected to be a valuable and computationally efficient alternative to TI. In this study, the performances of these two methods are compared using the binding of ten tetrahydroisoquinoline derivatives to phenylethanolamine N-transferase as an example. The ligands involve a diverse set of functional groups leading to a wide range of free energy differences. In addition, two different schemes to determine automatically the EDS reference state parameters and two different topology approaches are compared.

References: *J. Chem. Phys.* **135** (2011) 024105

Title: Enhanced sampling of particular degrees of freedom in molecular systems based on adiabatic decoupling and temperature or force scaling

Researchers: A. P. E. Kunz¹
H. Liu²
W. F. van Gunsteren^{1,a}

Institute: ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
²School of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

A method to enhance sampling of a small subset of N^h particular degrees of freedom of a system of $N^h + N^l$ degrees of freedom is presented. It makes use of adiabatically decoupling these degrees of freedom by increasing their mass followed by either increasing their temperature or reducing their interaction or the force acting on them. The appropriate statistical-mechanical expressions for use of these methods in simulation studies are derived. As long as the subset of mass-increased degrees of freedom is small compared to the total number of degrees of freedom of the system, sampling of this subset of degrees of freedom can be much enhanced at the cost of a slight perturbation of the configurational distribution. This is illustrated for a test system of 1000 SPC, simple point charge, water molecules at 300 K and a density of 997 kg m⁻³. Various fractions $N^h/(N^h + N^l)$ of water molecules were adiabatically decoupled to different degrees. The size of the diffusion coefficient of these decoupled water molecules was used as a measure for how much the sampling was enhanced and the average potential energy per water molecule was used as a measure of how much the configurational distribution of the system gets distorted. A variety of parameter values was investigated and it was found that for $N^h/(N^h + N^l) \leq 0.1$ the diffusion of the N^h molecules could be enhanced by factors up to 35 depending on the method, the ratio $N^h/(N^h + N^l)$, the extent of adiabatic decoupling, and the temperature or force scaling factors, at the cost of a slight perturbation of the configurational distribution.

References: *J. Chem. Phys.* **135** (2011) 104106

Title: Free energy calculations offer insights into the influence of receptor flexibility on ligand-receptor binding affinities

Researchers: J. Dolenc^{1,2}
S. Riniker¹
R. Gaspari^{1,4}
X. Daura³
W. F. van Gunsteren¹

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
²Faculty of Chemistry and Chemical Technology, University of Ljubljana, 1000 Ljubljana, Slovenia
³Catalan Institution for Research and Advanced Studies (ICREA) and Institute of Biotechnology and Biomedicine (IBB), Universitat Autònoma de Barcelona, Bellaterra, 08193, Barcelona, Spain
⁴Empa, Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Group: Computer-aided chemistry

Description:

Docking algorithms for computer-aided drug discovery and design often ignore or restrain the flexibility of the receptor, which may lead to a loss of accuracy of the relative free enthalpies of binding. In order to evaluate the contribution of receptor flexibility to relative binding free enthalpies, two host-guest systems have been examined: inclusion complexes of α -cyclodextrin (α -CD) with 1-chlorobenzene (ClBn), 1-bromobenzene (BrBn) and toluene (MeBn), and complexes of DNA with the minor groove binding ligands netropsin (Net) and distamycin (Dist). Molecular dynamics simulations and free energy calculations reveal that restraining of the flexibility of the receptor can have a significant influence on the estimated relative ligand-receptor binding affinities as well as on the predicted structures of the biomolecular complexes. The influence is particularly pronounced in the case of flexible receptors such as DNA, where a 50% contribution of DNA flexibility towards the relative ligand-DNA binding affinities is observed. The differences in the free enthalpy of binding do not arise only from the changes in ligand-DNA interactions but also from changes in ligand-solvent interactions as well as from the loss of DNA configurational entropy upon restraining.

References: *J. Comp. - Aided Mol. Des.* **25** (2011) 709-716

Title: A method for conformational sampling of loops in protein based on adiabatic decoupling and temperature or force scaling.

Researchers: A. P. E. Kunz
W. F. van Gunsteren^{*(a)}

Institute: ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

A method for conformational Boltzmann sampling of loops in proteins in aqueous solution is presented that is based on adiabatic decoupling molecular dynamics (MD) simulation with temperature or force scaling. To illustrate the enhanced sampling, the loop from residues 33 to 43 in the bovine protein ribonuclease A is adiabatically decoupled from the rest of the protein and the solvent with a mass scaling factor $s_m = 1000$ and the sampling is enhanced with a scaling of the temperature using $s_T = 2$ or of the force using $s_F = 0.667$. Over 5 ns of simulation the secondary structure of the protein remains unaltered while a combined dihedral-angle conformational cluster analysis shows an increase of conformations outside the first most populated cluster of loop conformations for adiabatic decoupling MD with temperature scaling using $s_T = 2$ or force scaling using $s_F = 0.667$ compared to the standard MD simulation. The atom-positional root-mean-square fluctuations of the C_α atoms of the loop show an increase in the movement of the loop as well, indicating that adiabatic decoupling MD with upscaling of the temperature or downscaling of the force is a promising method for conformational Boltzmann sampling.

References: *ChemPhysChem* (2011) online

Title: Architecture, implementation and parallelization of the GROMOS software for biomolecular simulation

Researchers: N. Schmid¹
C. D. Christ²
M. Christen³
A. P. Eichenberger¹
W. F. van Gunsteren^{1*}

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
²Lead Identification and Optimization Support, Boehringer Ingelheim Pharma GmbH & Co. KG, 88397 Biberach, Germany
³Swiss Re, 8002 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

In this work the design of the latest version of the GROMOS software for biomolecular simulation, GROMOS11 is discussed. Detailed organisation and class descriptions of the MD++ simulation program and the GROMOS++ analysis package are given. It is shown how the code was documented, how it can be easily modified and extended, how debugging of it is carried out. Additional efficiency and parallelisation concepts are presented and benchmarked.

References: *Comp. Phys. Comm. (2011) submitted*

Title: Biomolecular structure refinement using the GROMOS simulation software

Researchers: N. Schmid¹
J. R. Allison¹
J. Dolenc¹
A. P. Eichenberger¹
A. P. E. Kunz¹
W. F. van Gunsteren^{1,*}

Institute/ †Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

For the understanding of cellular processes the molecular structure of biomolecules has to be accurately determined. Initial models can be significantly improved by structure refinement techniques. Here, we present the refinement methods and analysis techniques implemented in the GROMOS software for biomolecular simulation. The methodology and some implementation details of the computation of NMR NOE data, ³J-couplings and residual dipolar couplings, X-ray scattering intensities from crystals and solutions and neutron scattering intensities used in GROMOS is described and refinement strategies and concepts are discussed using example applications. The GROMOS software allows structure refinement combining different types of experimental data with different types of restraining functions, while using a variety of methods to enhance conformational searching and sampling and the thermodynamically calibrated GROMOS force field for biomolecular simulation.

References: *J. Biomolecular NMR. (2011) online*

Title: Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software

Researchers: S. Riniker[†]
C. D. Christ[†]
H. S. Hansen[†]
P. H. Hünenberger[†]
C. Oostenbrink[‡]
D. Steiner[†]
W. F. van Gunsteren^{*,†}

Institute/ [†]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[‡]Institute of Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria

Group: Computer-aided chemistry

Description:

The calculation of the relative free energies of ligand-protein binding, of solvation for different compounds, and of different conformational states of a polypeptide is of considerable interest in the design or selection of potential enzyme inhibitors. Since such processes in aqueous solution generally comprise energetic and entropic contributions from many molecular configurations, adequate sampling of the relevant parts of configurational space is required and can be achieved through molecular dynamics simulations. Various techniques to obtain converged ensemble averages and their implementation in the GROMOS software for biomolecular simulation are discussed, and examples of their application to biomolecules in aqueous solution are given.

References: *J. Phys. Chem. (2011) in press*

Title: New functionalities in the GROMOS biomolecular simulation software

Researchers: A. P. E. Kunz[†]
J. R. Allison[†]
D. P. Geerke^{†,‡}
B. A. C. Horta
P. H. Hünenberger[†]
S. Riniker[†]
N. Schmid[†]
W. F. van Gunsteren^{*,†}

Institute/ [†]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology
ETH, 8093 Zürich, Switzerland
[‡]Present address: Division of Molecular and Computational Toxicology, VU
University Amsterdam, 1081 HV Amsterdam, the Netherlands

Group: Computer-aided chemistry

Description:

Since the most recent description of the functionalities of the GROMOS software for biomolecular simulation in 2005 many new functions have been implemented. In the present paper the new functionalities that involve modified forces in a molecular dynamics simulation are described: the treatment of electronic polarisability, an implicit surface area and internal volume solvation term to calculate interatomic forces, functions for the GROMOS coarse-grained supra-molecular force field, a multiplicative switching function for non-bonded interactions, adiabatic decoupling of a number of degrees of freedom with temperature or force scaling to enhance sampling, and non-equilibrium molecular dynamics to calculate the dielectric permittivity or viscosity. Examples that illustrate the use of these functionalities are given.

References: *J. Comput. Chem.* (2011) in press

Title: The GROMOS++ software for the analysis of biomolecular simulation trajectories

Researchers: A. P. Eichenberger¹
J. R. Allison¹
J. Dolenc¹
D. P. Geerke²
B. A. C. Horta¹
K. Meier¹
C. Oostenbrink³
N. Schmid¹
D. Steiner¹
D. Wang¹
W. F. van Gunsteren^{1,*}

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology
ETH, 8093 Zürich, Switzerland
²Division of Molecular and Computational Toxicology, VU University
Amsterdam, Amsterdam, the Netherlands.
³Institute of Molecular Modeling and Simulation, University of Natural
Resources and Life Sciences, Vienna, Austria

Group: Computer-aided chemistry

Description:

GROMOS++ is a set of C++ programs for pre- and post-processing of molecular dynamics simulation trajectories and as such part of the GRONingen MOlecular Simulation software for (bio)molecular simulation. It contains more than 70 programs that can be used to prepare data for the production of molecular simulation trajectories and to analyse these. These programs are reviewed and the various structural, dynamic and thermodynamic quantities that can be analysed using time series, correlation functions and distributions are described together with technical aspects of their implementation in GROMOS. A few examples of the use of GROMOS++ for the analysis of MD trajectories are given. A full list of all GROMOS++ programs, together with an indication of their capabilities, is given in the appendix.

References: *J. Chem. Theory. Comp. (2011) in press*

Title: Exploring the effect of side-chain substitutions upon the secondary structure preferences of β -peptides

Researchers: Z. Lin
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 well-folding β -peptides with a specific biological activity requires detailed insight into the relationship between the β -amino acid sequence and the dominant three-dimensional structure of such a peptide. To this end, secondary structure preferences of two sets of 16 β -peptides were investigated by means of one-step perturbation using molecular dynamics (MD) simulations. For each set of peptides, two reference-state simulations and one perturbed-state simulation were carried out to predict the secondary structure preferences for the other fifteen peptides. The results show that the substitution of a methyl group in the 3rd or 4th residue stabilizes the left-handed 3_{14} -helix over the right-handed $2.7_{10/12}$ -helix for the set of hexa-peptides **A**; for the set of hepta-peptides **B**, having methyl substitutions at both β - and α -carbon positions of the 4th or 5th residue stabilizes the left-handed 3_{14} -helix over the right-handed 2.5_{12} -helix. Not only the side-chain substitution pattern, but also the side-chain composition affects the relative stability of different secondary structures. The approach described here may be of use in peptide design with an eye to obtaining peptides with particular folds and biological activities.

References: *J. Phys. Chem. (2011) in press*

Title: A method for sampling the internal degrees of freedom of a flexible solute molecule based on adiabatic decoupling and temperature or force scaling

Researchers: A.P.E. Kunz^a
Z. Lin^{a,†}
W.F. van Gunsteren^{a,*}

Institute/ ^aLaboratory of Physical Chemistry, Swiss Federal Institute of Technology ETH, 8093 Zürich, Switzerland
[†]School of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

Simulation of the folding equilibrium of a polypeptide in solution is a computational challenge. Standard molecular dynamics (MD) simulations of such systems cover hundreds of nanoseconds, which is barely sufficient to obtain converged ensemble averages for properties that depend both on folded and unfolded peptide conformations. If one is not interested in dynamical properties of the solute, techniques to enhance the conformational sampling can be used to obtain the equilibrium properties more efficiently. Here the effect on particular equilibrium properties at 298 K of adiabatically decoupling the motion of a β -heptapeptide from the motion of the solvent and subsequently up-scaling its temperature or down-scaling the forces acting on it is investigated. The ensemble averages and rate of convergence are compared to those for standard MD simulations at two different temperatures and a simulation in which the temperature of the solute is increased to 340 K while keeping the solvent at 298 K. Adiabatic decoupling with a solute mass scaling factor $s_m = 100$ and a temperature scaling factor of $s_T = 1.1$ seems to slightly increase the convergence of several properties such as enthalpy of folding, NMR NOE atom-atom distances and ³J-couplings compared to a standard MD simulation at 298 K. Convergence is still slower than that observed at 340 K. The system with a temperature of 340 K for the solute and 298 K for the solvent without scaling of the mass converges fastest. Using a force scaling factor $s_V = 0.909$ perturbs the system too much and leads to a destabilisation of the folded structure. The sampling efficiency and possible distortive effects on the configurational distribution of the solute degrees of freedom due to adiabatic decoupling and temperature or force scaling are also analysed for a simpler model, a dichloroethane molecule in water. It appears that an upscaling of the mass of the solute reduces the sampling more than the subsequent up-scaling of the temperature or down-scaling of the force enhances it. This means that adiabatic decoupling the solute degrees of freedom from the solvent ones followed by an up-scaling of temperature or down-scaling of the forces does not lead to significantly enhanced sampling of the folding equilibrium.

References: *Mol. Phys.* (2011) submitted

Title: Can computer modeling explain why two highly similar sequences fold into different structures?

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

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology
ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

The remarkable recent creation of two proteins that fold into two completely different and stable structures, exhibit different functions, and yet differ by only a few amino acids poses a conundrum to those hoping to understand how sequence encodes structure. Here, computer modeling uniquely allows the characterization of not only the native structure of each minimally-different sequence, but also systems in which each sequence was modeled onto the fold of the alternate sequence. The reasons for the different structural preferences of two pairs of highly similar sequences are explored by a combination of structure analyses, comparison of potential energies calculated from energy-minimized single structures and trajectories produced from molecular dynamics simulations, and application of a novel method for calculating free energy differences. The sensitivity of such analyses to the choice of force field is also explored. Many of the hypotheses proposed on the basis of the NMR model structures of the 95% sequence identity proteins are supported. However each level of analysis provides different predictions regarding which sequence/structure combination should be most favored, highlighting the fact that protein structure and stability result from a complex combination of interdependent factors.

References: *Biochemistry (2011) submitted*

Title: On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations

Researchers: K. Meier[†]
W. Thiel[‡]
W. F. van Gunsteren^{†*}

Institute/ ^{*}Laboratory of Physical Chemistry, Swiss Federal Institute of Technology
ETH, 8093 Zürich, Switzerland
[‡]Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr,
Germany

Group: Computer-aided chemistry

Description:

During the past years, the use of combined quantum-classical, QM/MM, methods for the study of complex biomolecular processes, such as enzymatic reactions and photocycles, has increased considerably. The quality of the results obtained from QM/MM calculations is largely dependent on five aspects to be considered when setting up a molecular model: the QM Hamiltonian, the MM Hamiltonian or force field, the boundary and coupling between the QM and MM regions, the size of the QM region and the boundary condition for the MM region. In this study, we systematically investigate the influence of a variation of the molecular mechanics force field and the size of the QM region in QM/MM MD simulations on properties of the photoactive part of the blue light photoreceptor protein AppA. For comparison, we additionally performed classical MD simulations and studied the effect of a variation of the type of spatial boundary condition. The classical boundary conditions and the force field used in a QM/MM MD simulation are shown to have non-negligible effects upon the structural and energetic properties of the protein.

References: *J. Comput. Chem. (2011) in press*

Title: Ester-linked hen egg white lysozyme shows a compact fold in a molecular dynamics simulation: possible causes and sensitivity of experimentally observable quantities to structural changes maintaining this compact fold

Researchers: A. P. Eichenberger¹
L. J. Smith²
W. F. van Gunsteren^{1*}

Institute/ ¹Laboratory of Physical Chemistry, Swiss Federal Institute of Technology
ETH, 8093 Zürich, Switzerland
²Department of Chemistry, University of Oxford, Inorganic Chemistry
Laboratory, South Parks Road, Oxford OX1 3QR, United Kingdom

Group: Computer-aided chemistry

Description:

Prediction and understanding of the folding and stability of the three-dimensional structure of proteins is still a challenge. The different atomic interactions, such as non-polar contacts and hydrogen bonding, are known but their exact relative weights and roles when contributing to protein folding and stability are not identified. Initiated by a previous molecular dynamics simulation of fully ester-linked hen egg white lysozyme (HEWL), which showed a more compact fold of the ester-linked molecule compared to the native one, three variants of this protein are analysed in this work. These are 129-residue native HEWL, partly ester-linked HEWL, in which only 35 peptide linkages that are not involved in the helical or β -strand parts of native HEWL were replaced by ester linkages, and fully (126 residues) ester-linked HEWL. Native and partly ester-linked HEWL showed comparable behaviour while fully ester-linked HEWL could not maintain the native secondary structure of HEWL in the simulation and adopted a more compact fold. The conformational changes were analysed by comparing simulation averaged values of quantities that can be measured by NMR, such as ¹H-¹⁵N backbone order parameters, proton-proton NOE distances and ³J-couplings with the corresponding values derived from experimental NMR data for native HEWL. The information content of the latter appeared insufficient to detect the local conformational rearrangements upon esterification of the loop regions of the protein. For fully ester-linked HEWL though a significantly reduced agreement was observed. Upon esterification the backbone-side chain and side chain- side chain hydrogen bonding pattern of HEWL changes such as to maintain its compactness and thus the structural stability of the ester-linked lysozymes.

References: *FEBS (2011) submitted*

Title: Helical content of a β^3 -octapeptide in methanol: Molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data

Researchers: D. A. Niggli[†]
M. O. Ebert•
Z. Lin^{†,‡}
D. Seebach
W. F. van Gunsteren

Institute/ [†]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[•]Laboratory of Organic Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[‡]School of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

Connecting experimental observables with the underlying conformational ensemble is a long-standing problem in structure determination of bio-molecules. The simulations described in this article attempt a resolution of a seeming discrepancy between conformational features derived from measured NOE intensities, ³J-coupling constants and CD spectra for two β -peptides differing in a linker between two side-chains. While both peptides are very similar in terms of r-6 averaged distances between atom-pairs involved in observed NOEs, the molecular dynamics trajectories suggest why CD spectra show a greater ₃₁₄-helical propensity for the linked, cyclic peptide than for the linear one, while for the latter slightly more NMR NOE peaks had been observed and assigned. The nine 100 ns unrestrained simulations show better agreement with the observed experimental data than single conformations derived from the published NMR structures by additional energy minimization with the GROMOS force field. They show why the seemingly contradictory quantities obtained by NMR and CD can arise from a single conformational ensemble.

References: *Chem. Eur. J. (2011) accepted*

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 on a protein from NMR experimental data is a non-trivial challenge to computational biochemistry. This is due to the low ratio of independent observables and molecular degrees of freedom, the approximations involved in the various relations between particular observable quantities and molecular conformation, and the averaged character of the experimental data. For example, 3J -coupling data on a protein is seldom used in structure refinement due to the multiple-valuedness and limited accuracy of the Karplus relation linking a 3J -coupling to a torsional angle. Moreover, sampling of the large conformational space is still problematic. Using the 99-residue protein plastocyanin as example it is investigated whether the 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 is producing a more realistic representation of the ensemble of protein conformations than standard single-structure refinement in non-explicit solvent using restraints that do not account for averaging and are partly based on non-observed data. Yielding better agreement with the observed experimental data the protein conformational ensemble is less restricted than when using standard single-structure refinement techniques, which thus are likely to yield a too rigid picture of a protein.

References: *J. Biomolecular NMR (2011) submitted*

Title: An effective force field for molecular dynamics simulations of dimethyl sulfone

Researchers: N. Hansen
P. Kraus
H. Sassmannshausen
T. Timmerscheidt
W. F. van Gunsteren*

Institute/ Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland

Group: Computer-aided chemistry

Description:

A rigid five-site united atom model for dimethyl sulfone (DMSO₂) compatible with the GROMOS force field is parametrized and tested. The parameters were optimized with respect to experimental quantities such as liquid density heat of vaporization, shear viscosity and excess free energy. Good agreement with pure component properties is achieved except for the static dielectric permittivity which is calculated too low. Together with the SPC model for water the new DMSO₂ model was used to study aqueous mixtures at low concentrations and compared to aqueous mixtures of DMSO. It is concluded that interaction parameters for sulfoxide oxygen are not transferable to sulfonyl oxygen unambiguously.

References: *Mol. Phys.* (2011) *in press*

Title: Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol

Researchers: J. R. Allison
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 time- and length-scale accessible to molecular dynamics simulations of biomolecular systems using atomic-level (AL) models is most limited by the calculation of the solvent-solvent interactions, which comprise the majority of the interactions and yet are seldom of specific interest. Coarse-graining (CG), in which multiple solvent molecules are subsumed into a single particle or bead, provides a means of overcoming this limitation without resorting to implicit solvation models, which misrepresent the hydrophobic effect. Most existing CG models, however, do not explicitly include electrostatic interactions, and thus fail to reproduce important properties of the solvent such as dielectric screening. Moreover, CG models for one type of solvent molecule are seldom compatible with those for other solvents. Here, we develop polarizable CG models for the solvents dimethyl sulfoxide, chloroform and methanol that are compatible with an existing CG model for water. The inclusion of polarizability greatly improves the reproduction of thermodynamic data measured experimentally and calculated from AL simulations for both the pure liquids and binary mixtures.

References: *J. Chem. Phys.* (2011) submitted

Title: On the use of enveloping distribution sampling (EDS) to compute free enthalpy differences between different conformational states of molecules: application to 3_{10} -, α -, and π helices

Researchers: Z. Lin^{†‡}
H. Liu[‡]
S. Riniker[†]
W. F. van Gunsteren

Institute/ [†]Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zürich, Switzerland
[‡]School of Life Sciences and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei, Anhui 230027, People's Republic of China

Group: Computer-aided chemistry

Description:

Enveloping distribution sampling (EDS) is a powerful method to compute relative free energies from simulation. So far, the EDS method has only been applied to alchemical free energy differences, *i.e.* between different Hamiltonians defining different systems, and not yet to obtain free energy differences between different conformations or conformational states of a system. In this article, we extend the EDS formalism such that it can be applied to compute free energy differences of different conformations, and apply it to compute the relative free enthalpy ΔG of 3_{10} -, α -, and π -helices of an alanine deca-peptide in explicit water solvent. The resulting ΔG values are compared to those obtained by standard thermodynamic integration (TI) and from so-called end-state simulations. A TI simulation requires the definition of a λ -dependent pathway which in the present case is based on hydrogen bonds of the different helical conformations. The values $\langle \delta V_{\pi} / \delta \lambda \rangle_{\lambda}$ show a sharp change for a particular range of λ -values which is indicative of an energy barrier along the pathway, which lowers the accuracy of the resulting ΔG value. In contrast, in a two-state EDS simulation, an unphysical reference-state Hamiltonian which connects the parts of conformational space that are relevant to the different end states is constructed automatically, that is, no pathway needs to be defined. In the simulation using this reference state, both helices were sampled, and many transitions between them occurred, thus ensuring the accuracy of the resulting free enthalpy difference. According to the EDS simulations, the free enthalpy difference of the π -helix and the 3_{10} -helix versus the α -helix are 5 kJ mol⁻¹ and 47 kJ mol⁻¹, respectively, for an alanine deca-peptide in explicit SPC water solvent using the GROMOS 53A6 force field. The EDS method is thus applicable to compute free energy differences between conformational states as well as between systems, and has definite advantages over the traditional TI and umbrella sampling methods to compute relative free energies.

References: *J. Chem. Theory. Comp.* (2011) submitted

Title: Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution

Researchers: N. Hansen
J. Dolenc
M. Knecht
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 performance of enveloping distribution sampling (EDS) simulations to estimate free enthalpy differences associated with seven alchemical transformations of A-T into G-C base pairs at the netropsin binding site in the minor groove of a 13 base pair DNA duplex in aqueous solution is evaluated. It is demonstrated that sufficient sampling can be achieved with a two-state EDS Hamiltonian even for large perturbations such as the simultaneous transformation of up to three A-T into three G-C base pairs. The two parameters required to define the EDS reference state Hamiltonian are obtained automatically using a modified version of a scheme presented in earlier work. The sensitivity of the configurational sampling to a variation of these parameters is investigated in detail. While for relatively small perturbations, i. e. one base pair, the free enthalpy estimate depends only weakly on the EDS parameters, the sensitivity is stronger for the largest perturbation. Yet, EDS offers various convenient measures to evaluate the degree of sampling and thus the reliability of the free enthalpy estimate and appears to be an efficient alternative to the conventional thermodynamic integration methodology to obtain free energy differences for molecular systems.

References: *J. Comput. Chem.* (2011) submitted

Title: Damping of Bloch Oscillations in the Hubbard Model

Researchers: M. Eckstein
P. Werner

Institute: Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

Using nonequilibrium dynamical mean-field theory, we study the isolated Hubbard model in a static electric field in the limit of weak interactions. Linear response behavior is established at long times, but only if the interaction exceeds a critical value, below which the system exhibits an ac-type response with Bloch oscillations. The transition from ac to dc response is defined in terms of the universal long-time behavior of the system, which does not depend on the initial condition.

References: Phys. Rev. Lett. 107, 186406 (2011)

Title: Superconductivity and Pairing Fluctuations in the Half-Filled Two-Dimensional Hubbard Model

Researchers: M. Sentef (1)
P. Werner (2)
E. Gull (3)
A. Kampf (1)

Institute: (1) Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg
(2) Theoretische Physik, ETH Zurich, 8093 Zurich
(3) Department of Physics, Columbia University, New York, New York 10027

Description:

The two-dimensional Hubbard model exhibits superconductivity with d-wave symmetry even at half-filling in the presence of next-nearest neighbor hopping. Using plaquette cluster dynamical mean-field theory with a continuous-time quantum Monte Carlo impurity solver, we reveal the non-Fermi liquid character of the metallic phase in proximity to the superconducting state. Specifically, the low-frequency scattering rate for momenta near $(\pi, 0)$ varies non-monotonously at low temperatures, and the dc conductivity is T-linear at elevated temperatures with an upturn upon cooling. Evidence is provided that pairing fluctuations dominate the normal-conducting state even considerably above the superconducting transition temperature.

References: Phys. Rev. Lett. 107, 126401 (2011)

Title: Low temperature properties of the infinite-dimensional attractive Hubbard model

Researchers: A. Koga (1)
P. Werner (2)

Institute: (1) Department of Physics, Tokyo Institute of Technology,
Tokyo 152-8551
(2) Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We investigate the attractive Hubbard model in infinite spatial dimensions by combining dynamical mean-field theory with a strong-coupling continuous-time quantum Monte Carlo method. By calculating the superfluid order parameter and the density of states, we discuss the stability of the superfluid state. In the intermediate coupling region above the critical temperature, the density of states exhibits a heavy fermion behavior with a quasi-particle peak in the dense system, while a dip structure appears in the dilute system. The formation of the superfluid gap is also addressed.

References: Phys. Rev. A 84, 023638 (2011)

Title: Thermalization of a pump-excited Mott insulator

Researchers: M. Eckstein
P. Werner

Institute: Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We use nonequilibrium dynamical mean-field theory in combination with a recently implemented strong-coupling impurity solver to investigate the relaxation of a Mott insulator after a laser excitation with frequency comparable to the Hubbard gap. The time evolution of the double occupancy exhibits a crossover from a strongly damped transient at short times toward an exponential thermalization at long times. In the limit of strong interactions, the thermalization time is consistent with the exponentially small decay rate for artificially created doublons, which was measured in ultracold atomic gases. When the interaction is comparable to the bandwidth, however, the double occupancy thermalizes within a few times the inverse bandwidth along a rapid thermalization path in which the exponential tail is absent. Similar behavior can be observed in time-resolved photoemission spectroscopy. Our results show that a simple quasi-equilibrium description of the electronic state breaks down for pump-excited Mott insulators characterized by strong interactions.

References: Phys. Rev. B 84, 035122 (2011)

Title: Dynamical mean-field theory for bosons

Researchers: P. Anders (1)
E. Gull (2)
L. Pollet (1)
M. Troyer (1)
P. Werner (1)

Institute: (1) Theoretische Physik, ETH Zurich, 8093 Zurich
(2) Department of Physics, Columbia University, New York, NY 10027

Description:

We discuss the recently developed bosonic dynamical mean-field theory (B-DMFT) framework, which maps a bosonic lattice model onto the selfconsistent solution of a bosonic impurity model with coupling to a reservoir of normal and condensed bosons. The effective impurity action is derived in several ways: (i) as an approximation to the kinetic energy functional of the lattice problem, (ii) using a cavity approach and (iii) using an effective medium approach based on adding a one-loop correction to the self-consistently defined condensate. To solve the impurity problem, we use a continuous-time Monte Carlo algorithm based on the sampling of a perturbation expansion in the hybridization functions and the condensate wave function. As applications of the formalism, we present finite-temperature B-DMFT phase diagrams for the bosonic Hubbard model on a three-dimensional (3D) cubic and a 2D square lattice, the condensate order parameter as a function of chemical potential, critical exponents for the condensate, the approach to the weakly interacting Bose gas regime for weak repulsions and the kinetic energy as a function of temperature.

References: New J. Phys. 13, 075013 (2011)

Title: Optimal ramp shapes for the fermionic Hubbard model in infinite dimensions

Researchers: N. Eurich
M. Eckstein
P. Werner

Institute: Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We use nonequilibrium dynamical mean field theory and a real-time diagrammatic impurity solver to study the heating associated with time-dependent changes of the interaction in a fermionic Hubbard model. Optimal ramp shapes $U(t)$ which minimize the excitation energy are determined for a noninteracting initial state and an infinitesimal change of the interaction strength. For ramp times of a few inverse hoppings, these optimal $U(t)$ are strongly oscillating with a frequency determined by the bandwidth. We show that the scaled versions of the optimized ramps yield substantially lower temperatures than linear ramps even for final interaction values comparable to the bandwidth. The relaxation of the system after the ramp and its dependence on the ramp shape are also addressed.

References: Phys. Rev. B 83, 155122 (2011)

Title: Dynamical band flipping in fermionic lattice systems: an ac-field driven change of the interaction from repulsive to attractive

Researchers: N. Tsuji (1)
T. Oka (1)
P. Werner (2)
H. Aoki (1)

Institute: (1) Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033
(2) Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We show theoretically that the sudden application of an appropriate ac field to correlated lattice fermions flips the band structure and effectively switches the interaction from repulsive to attractive. The nonadiabatically driven system is characterized by a negative temperature with a population inversion. We numerically demonstrate the converted interaction in an ac-driven Hubbard model with the nonequilibrium dynamical mean-field theory solved by the continuous-time quantum Monte Carlo method. Based on this, we propose an efficient ramp-up protocol for ac fields that can suppress heating, which leads to an effectively attractive Hubbard model with a temperature below the superconducting transition temperature of the equilibrium system.

References: Phys. Rev. Lett. 106, 236401 (2011)

Title: Superfluid state in the periodic Anderson model with attractive interactions

Researchers: A. Koga (1)
P. Werner (2)

Institute: (1) Department of Physics, Tokyo Institute of Technology,
Tokyo 152-8551
(2) Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We investigate the periodic Anderson model with attractive interactions by means of dynamical mean-field theory (DMFT). Using a continuous-time quantum Monte Carlo impurity solver, we study the competition between the superfluid state and the paramagnetic Kondo insulating state, and determine the phase diagram. At the chemical potential-induced phase transition from the Kondo insulating state to the superfluid state, a low-energy peak characteristic of the superfluid state appears inside the hybridization gap. We also address the effect of the confining potential in optical lattice systems by means of real-space DMFT calculations.

References: J. Phys. Soc. Jpn. 79, 114401 (2010)

Title: Dielectric breakdown of a Mott insulator in dynamical mean field theory

Researchers: M. Eckstein (1)
T. Oka (2)
P. Werner (1)

Institute: (1) Theoretische Physik, ETH Zurich, 8093 Zurich
(2) Department of Physics, University of Tokyo, Hongo,
Tokyo 113-0033

Description:

Using nonequilibrium dynamical mean-field theory, we compute the time evolution of the current in a Mott insulator after a strong electric field is turned on. We observe the formation of a quasistationary state in which the current is almost time independent although the system is constantly excited. At moderately strong fields this state is stable for quite long times. The stationary current exhibits a threshold behavior as a function of the field, in which the threshold increases with the Coulomb interaction and vanishes as the metal-insulator transition is approached.

References: Phys. Rev. Lett. 105, 146404 (2010)

Title: Nonequilibrium dynamical mean field calculations based on the non-crossing approximation and its generalizations

Researchers: M. Eckstein
P. Werner

Institute: Theoretische Physik, ETH Zurich, 8093 Zurich

Description:

We solve the impurity problem which arises within nonequilibrium dynamical mean-field theory for the Hubbard model by means of a self-consistent perturbation expansion around the atomic limit. While the lowest order, known as the noncrossing approximation (NCA), is reliable only when the interaction U is much larger than the bandwidth, low-order corrections to the NCA turn out to be sufficient to reproduce numerically exact Monte Carlo results in a wide parameter range that covers the insulating phase and the metal-insulator crossover regime at not too low temperatures. As an application of the perturbative strong-coupling impurity solver we investigate the response of the double occupancy in the Mott insulating phase of the Hubbard model to a dynamical change in the interaction or the hopping, a technique which has been used as a probe of the Mott insulating state in ultracold fermionic gases.

References: Phys. Rev. B 82, 115115 (2010)

Title: Continuous-time Monte Carlo methods for quantum impurity models

Researchers: E. Gull (1)
A. Lichtenstein (2)
A. Millis (1)
A. Rubtsov (3)
M. Troyer (4)
P. Werner (4)

Institute: (1) Department of Physics, Columbia University, New York, New York 10027, USA
(2) Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany
(3) Department of Physics, Moscow State University, 119992 Moscow, Russia
(4) Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

Quantum impurity models describe an atom or molecule embedded in a host material with which it can exchange electrons. They are basic to nanoscience as representations of quantum dots and molecular conductors and play an increasingly important role in the theory of correlated electron materials as auxiliary problems whose solution gives the dynamical mean-field approximation to the self-energy and local correlation functions. These applications require a method of solution which provides access to both high and low energy scales and is effective for wide classes of physically realistic models. The continuous-time quantum Monte Carlo algorithms reviewed in this article meet this challenge. Derivations and descriptions of the algorithms are presented in enough detail to allow other workers to write their own implementations, discuss the strengths and weaknesses of the methods, summarize the problems to which the new methods have been successfully applied, and outline prospects for future applications.

References: Rev. Mod. Phys. 83, 349 (2011)

Title: Continuous-time Quantum Monte Carlo impurity solvers

Researchers: E. Gull (1)
P. Werner (2)
S. Fuchs (3)
B. Surer (2)
T. Pruschke (3)
M. Troyer (1)

Institute: (1) Columbia University, New York, NY 10027, USA
(2) ETH Zurich, 8093 Zurich, Switzerland
(3) Georg-August-Universitt Gttingen, Gttingen, Germany

Description:

Continuous-time quantum Monte Carlo impurity solvers are algorithms that sample the partition function of an impurity model using diagrammatic Monte Carlo techniques. The present paper describes codes that implement the interaction expansion algorithm originally developed by Rubtsov, Savkin, and Lichtenstein, as well as the hybridization expansion method developed by Werner, Millis, Troyer, et al. These impurity solvers are part of the ALPS-DMFT application package and are accompanied by an implementation of dynamical mean-field self-consistency equations for (single orbital single site) dynamical mean-field problems with arbitrary densities of states.

References:

Computer Physics Communications 182, 1078 (2011)

High-performance Hardware

6.1 C4: The Year in Review

The Competence Center for Computational Chemistry (C4) is a network of computational chemists of the IBM Zürich Research Laboratory, the University of Zürich, and the ETH Zürich. The goal of C4 is to seek 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 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 2010 Fall- and 2011 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.

One C4 seminar was hosted by the IBM Research Laboratory, and two seminars were held jointly with the ETH Physical Chemistry Colloquium, and the Seminar for Theory, Spectroscopy and Dynamics, respectively.

C4 Workshop

On January 13, the 2011 C4 Workshop entitled “Advancing the Frontiers of Modeling and Simulation in Chemistry and Materials Science” was hosted by the IBM Research Laboratory in Rüschlikon. There were forty scientific presentations given (33 posters, 7 lectures), and there was also the opportunity to visit the Nanotech Center shortly before its inauguration in May 2011. This was the fourth time a C4 Workshop was held jointly with another institution, and the second time the event was held out-of-town.

Compute Resource

The C4 compute-cluster Obélix, a 32 node IBM Opteron cluster operated by the ETH Informatikdienste was decommissioned in May of 2011 after five years of nearly uninterrupted service. 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 are also 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 three resources respond to a specific demand, and the results and achievements reported in this 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 to Michele Ceriotti for his thesis entitled “A novel framework for enhanced molecular dynamics based on the generalized Langevin equation“.

The 2010 Award Ceremony, for the first time, took place at the ETH Tag with the Rector, Prof. Heidi Wunderli-Allenspach, handing out the award to the winner. Michele Ceriotti also presented his research at the occasion of a regular C4 Seminar held at the IBM Research Laboratory in Rüschlikon.

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 networks 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 27, 2011

6.2 Information Technology Services

The following resource is available:

The Information Technology Services operates a Linux Cluster co-owned with the departments Biology, Environmental Sciences, Earth Sciences, Physics, Mathematics, Material Sciences, Mechanical and Process Engineering, Civil, Environmental and Geomatic Engineering, Management, Technology and Economics and Computer Science.

This cluster consists of the following node types:

- 8 x eight processor dual-core AMD Opteron 8220 and 64-128 GB memory
- 324 x two processor AMD Opteron 250 systems with 8 GB memory
- 272 x two processor dual-core AMD Opteron 2220 systems with 16 GB memory and Ethernet network
- 4 x two processor six-core AMD Opteron 2435 CPUs and 32 GB memory
- 10 x four processor quad-core AMD Opteron 8380 CPUs and 128 GB memory
- 410 x four processor quad-core AMD Opteron 8380 systems with 32 GB memory
- 80 x four processor quad-core AMD Opteron 8384 systems with 32 GB memory
- 18 x two processor 12-core AMD Opteron 6174 systems with 32 GB memory and two NVIDIA Tesla M2050 (Fermi) GPUs with 2.6 GB memory
- 24 x two processor 12-core AMD Opteron 6174 systems with 32 GB memory

All nodes are connected to the cluster's internal Gigabit Ethernet backbone. Up to 272 nodes are connected to a high speed/low latency Quadrics QsNetII network. 512 nodes are connected to a high speed/low latency InfiniBand QDR network.

The peak performance of the cluster is more than 90 teraflops.

A Lustre parallel filesystem with a capacity of 250 TB is available as work storage for data and I/O intensive computations.

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 Quadrics QsNetII and 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 of the cluster is intended for single node throughput computing and not communication intensive parallel jobs. The eight processor dual core nodes as well as the four processor quad core nodes are suited well for up to 16-way symmetric multiprocessing jobs.

Starting 1st April 2011, this system and the team were transferred back to the Information Technology Services department after they were transferred to the Swiss National Supercomputing Center CSCS the year before, at 1st October 2010.

The Hewlett Packard Superdome Cluster has been decommissioned on 17. January 2011 after 10 years of successful operation.

7

Publications* in 2010/2011

*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 (2011), doi:10.1016/j.parco.2011.08.001.

C. Flaig, P. Arbenz: *A highly scalable matrix-free multigrid solver for μFE analysis based on a pointer-less octree*. Accepted for publication in the proceedings of LSSC 2011, Sozopol, Bulgaria, June 6-10, 2011.

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.

A. Adelman, 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. Adelman, P. Arbenz, Y. Ineichen: "Improvements of a fast parallel Poisson solver on irregular domains". Accepted for publication in the proceedings of PARA2010, Reykjavik, Iceland, June 6-9, 2010.

H. Guo, A. Adelman, P. Arbenz, A. Falone, C. Kraus, and 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. Adelman, 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*. 2011. Submitted for publication.

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. Hildebrand, D. Obrist: *A parallel space-time finite difference solver for periodic solutions of the shallow-water equation*. Accepted for publication in the proceedings of PPAM 2011, Torun, Poland, September 11-14, 2011.

Group of Sebastian Bonhoeffer

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-+

Kouyos, RD, zur Wiesch, PA, Bonhoeffer, S

On Being the Right Size: The Impact of Population Size and Stochastic Effects on the Evolution of Drug Resistance in Hospitals and the Community

PLOS PATHOGENS (2011) 7:-

Kouyos, RD, zur Wiesch, PA, Bonhoeffer, S

Informed Switching Strongly Decreases the Prevalence of Antibiotic Resistance in Hospital Wards

PLOS COMPUTATIONAL BIOLOGY (2011) 7:-

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

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) 6:-

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

Takizawa, H, Boddupalli, CS, Regoes, RR, Bonhoeffer, S, Manz, MG

Hematopoietic Stem Cell Cycling Dynamics In Steady State and Upon Hematopoietic

Challenge

BLOOD (2010) 116:253-253

Bonhoeffer, S, zur Wiesch, PA, Kouyos, RD

ROTATING ANTIBIOTICS DOES NOT MINIMIZE SELECTION FOR RESISTANCE

MATHEMATICAL BIOSCIENCES AND ENGINEERING (2010) 7:919-922

Alizon, S, von Wyl, V, Stadler, T, Kouyos, RD, Yerly, S, Hirschel, B, Boni, J, Shah, C, Klimkait, T, Furrer, H, Rauch, A, Vernazza, PL, Bernasconi, E, Battegay, M, Burgisser, P, Telenti, A, Gunthard, HF, Bonhoeffer, S

Phylogenetic Approach Reveals That Virus Genotype Largely Determines HIV Set-Point Viral Load

PLOS PATHOGENS (2010) 6:-

Mostowy, R, Salathe, M, Kouyos, RD, Bonhoeffer, S

ON THE EVOLUTION OF SEXUAL REPRODUCTION IN HOSTS COEVOLVING WITH MULTIPLE PARASITES

EVOLUTION (2010) 64:1644-1656

Kouyos, RD, von Wyl, V, Yerly, S, Boni, J, Taffe, P, Shah, C, Burgisser, P, Klimkait, T, Weber, R, Hirschel, B, Cavassini, M, Furrer, H, Battegay, M, Vernazza, PL, Bernasconi, E, Rickenbach, M, Ledergerber, B, Bonhoeffer, S, Gunthard, HF

Molecular Epidemiology Reveals Long-Term Changes in HIV Type 1 Subtype B Transmission in Switzerland

JOURNAL OF INFECTIOUS DISEASES (2010) 201:1488-1497

zur Wiesch, PS, Engelstadter, J, Bonhoeffer, S

Compensation of Fitness Costs and Reversibility of Antibiotic Resistance Mutations

ANTIMICROBIAL AGENTS AND CHEMOTHERAPY (2010) 54:2085-2095

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

Ambiguity in population-based sequencing of HIV-1 as a marker for the age of HIV infection

ANTIVIRAL THERAPY (2010) 15:A158-A158

Group of K. Boulouchos publications

1. G. Pizza, C.E. Frouzakis, J. Mantzaras, Chaotic dynamics in premixed hydrogen/air channel flow combustion, *Combust. Theory Modeling*, (in press).
2. 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.*, (submitted).
3. E. Chiavazzo and I. Karlin, Adaptive simplification of complex multiscale systems, *Phys. Rev. E* 83, 036706 (2011).
4. D. Lycett-Brown, I. Karlin and K. H. Luo, Droplet Collision Simulation by a Multi-Speed Lattice Boltzmann Method, *Commun. Comput. Phys.* 9, 1219-1234 (2011).
5. I.V. Karlin, P. Asinari and S. Succi, Matrix lattice Boltzmann reloaded, *Phil. Trans. R. Soc. A* 369, 2202-2210 (2011).

Group of Domenico Giardini

J. F. Schaefer, L. Boschi, E. Kissling

Adaptively parametrized surface wave tomography: methodology and a new model of the European upper mantle.

Geophysical Journal International (2011), 186: 1431–1453. doi: 10.1111/j.1365-246X.2011.05135.x.

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

Geophysical Journal International (2011), doi: 10.1111/j.1365-246X.2011.05044.x

P. M. Mai, W. Imperatori and K. B. Olsen

Hybrid Broadband Ground-Motion Simulations: Combining Long-Period Deterministic Synthetics with High-Frequency Multiple S-to-S Backscattering

Bulletin of the Seismological Society of America (2010), Vol. 100, No. 5A, pp. 2124–2142, doi: 10.1785/0120080194

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, and N. Abrahamson

Verifying a computational method for predicting extreme groundmotion at the proposed Yucca Mountain repository

Seismological Research Letters (2011); 82: 638-644.

Colombi, T. Nissen-Meyer, L. Boschi, D. Giardini

Seismic sensitivity to boundary topography

To be submitted to Geoph. J. Int. (2011)

J. F. Schaefer, L. Boschi, L., T. Becker, E. Kissling

Radial Anisotropy in the European Mantle: Tomographic Studies Explored in Terms of Mantle Flow

Submitted to Geophysical Research Letters (2011)

S. Della Mora, L. Boschi, T. W. Becker and D. Giardini

Can the Earth's harmonic spectrum be derived directly from the stochastic inversion of global travel-time data?

Submitted to Geophys. J. Int., (2011)

T. Nissen-Meyer, A. Fournier

Time-frequency sensitivity in global tomography

Submitted to Geoph. J. Int. (2011)

G. S. O'Brien, T. Nissen-Meyer, C. Bean

A lattice Boltzmann method for elastic wave propagation

subject to minor revision, Bull. Seis. Soc. America (2011)

A. Gabriel J. P. Ampuero, L. A. Dalguer, P. M. Mai
The Transition of Dynamic Rupture Styles in Elastic 1 Media Under Velocity-Weakening Friction
To be submitted to J. Geophys. Res. (2011)

D. Fäh, J. R. Moore, J. Burjanek, I. Iosifescu, L. Dalguer, et al
Coupled seismogenic geohazards in alpine regions
Bollettino di Geofisica Teorica e Applicada, in press (2011)

B. Mena, L.A. Dalguer, P.M. Mai
Pseudo Dynamic Source Characterization Incorporating Effects of Super-shear Rupture and Stress Heterogeneity for Strong Ground Motion Prediction
Bull. Seismol. Soc. Am, in review (2011)

Group of Markus Gross

B. Solenthaler and M. Gross

Two-Scale Particle Simulation

ACM Transaction on Graphics (Proceedings SIGGRAPH), vol. 30, no. 4, 2011, pp. 81:1–81:8.

S. Martin, B. Thomaszewski, E. Grinspun, M. Gross

Example-based Elastic Materials

ACM Transaction on Graphics (Proceedings SIGGRAPH), vol. 30, no. 4, 2011, pp. 72:1–72:8

Group of Ch. Hafner

Reviewed Journals

1. **T. Sannomiya, H. Dermutz, Ch. Hafner, J. Vörös, A. Dahlin**, Electrochemistry on localized surface plasmon sensor, *Langmuir*, Vol. 26, Issue 10, pp.Langmuir, October 2010.
2. **C. Engström, M. Wang**, Complex dispersion relation calculations with the symmetric interior penalty method, *Int. J. Numer. Methods Eng.*, Vol. 84, Issue 7, pp.849-863, November 2010.
3. **T. Kaufmann, C. Engström, C. Fumeaux, R. Vahldieck**, Eigenvalue Analysis and Longtime Stability of Resonant Structures for the Meshless Radial Point Interpolation Method in Time Domain, *IEEE Trans. Microwave Theory Tech.*, Vol. 58, Issue 12, pp.3399-3408, December 2010.
4. **V. Lotito, U. Sennhauser, Ch. Hafner**, Numerical analysis of novel asymmetric SNOM tips, *PIERS Online*, Vol. 7, Issue 4, pp.394-400, 2011.
5. **V. Lotito, U. Sennhauser, Ch. Hafner, G.-L. Bona**, Fully Metal-Coated Scanning Near-Field Optical Microscopy Probes with Spiral Corrugations for Superfocusing under Arbitrarily Oriented Linearly Polarised Excitation, *Plasmonics*, Vol. 6, pp.327-336, 2011.
6. **Ch. Hafner, J. Smajic**, Eigenvalue analysis of lossy dispersive waveguides, *J. of Modern Optics*, Vol. 58, Issue 5-6, pp.467-479, March 2011.
7. **A. Alparslan, Ch. Hafner**, Using Layered Geometry Green's Functions in the Multiple Multipole Program, *J. Comput. Theor. Nanosci.*, Issue 8, pp.1600-1608, Aug. 2011.
8. **M. Wang, Ch. Engström, K. Schmidt, Ch. Hafner**, On High-Order FEM Applied to Canonical Scattering Problems in Plasmonics, *J. Comput. Theor. Nanosci.*, Vol. 8, Issue 8, pp.1564-1572, August 2011.

Group of D. Helbing

C. P. Roca and D. Helbing

Emergence of social cohesion in a model society of greedy, mobile individuals.
Proceedings of the National Academy of Sciences USA (PNAS) **108**(28) (2011) 11370-11374.
DOI 10.1073/pnas.1101044108

J. Lorenz, H. Rauhut, F. Schweitzer, and D. Helbing

How social influence can undermine the wisdom of crowd effect.
Proceedings of the National Academy of Sciences USA (PNAS) **108**(28) (2011) 9020-9025. DOI
10.1073/pnas.1008636108

J. Wu, S. Lozano, and D. Helbing

Empirical study of the growth dynamics in real career h-index sequences.
Journal of Informetrics **5**(4) (2011) 489-497. DOI 10.1016/j.joi.2011.02.003

D. Helbing and S. Balietti

From social data mining to forecasting socio-economic crises
Eur. Phys. J. Special Topics **195** (2011) 3-68. DOI 10.1140/epjst/e2011-01401-8

D. Helbing and S. Balietti

From social simulation to integrative system design.
Eur. Phys. J. Special Topics **195** (2011) 69-100. DOI 10.1140/epjst/e2011-01402-7

D. Helbing and S. Balietti

How to create an innovation accelerator.
Eur. Phys. J. Special Topics **195** (2011) 101-136. DOI 10.1140/epjst/e2011-01403-6

D. Helbing, S. Balietti, S. Bishop, and P. Lukowicz

Understanding, creating, and managing complex techno-socio-economic systems: Challenges and perspectives.
Eur. Phys. J. Special Topics **195** (2011) 165-186. DOI 10.1140/epjst/e2011-01410-7

A. Mazloumian, Y-H. Eom, D. Helbing, S. Lozano, and S. Fortunato

How citation boosts promote scientific paradigm shifts and Nobel Prizes.
PLoS ONE **6**(5) (2011) e18975. DOI 10.1371/journal.pone.0018975

D. Helbing, W. Yu, and H. Rauhut

Self-organization and emergence in social systems: Modeling the coevolution of social environments and cooperative behavior.
Journal of Mathematical Sociology **35** (2011) 177-208. DOI 10.1080/0022250X.2010.532258

M. Moussaïd, D. Helbing, and G. Theraulaz

How simple rules determine pedestrian behavior and crowd disasters.
PNAS **108**(17) (2011) 6884-6888. DOI 10.1073/pnas.1016507108

- D. Roggen, M. Wirz, G. Tröster, and D. Helbing
 Recognition of crowd behavior from mobile sensors with pattern analysis and graph clustering methods.
Networks and Heterogeneous Media (NHM) **6**(3) (2011) 521-544. DOI 10.3934/nhm.2011.6.521
- K. Trantopoulos, M. Schlaepfer, and D. Helbing
 Toward Sustainability of Complex Urban Systems through Techno-Social Reality Mining.
Environ. Sci. Technol. **45**(15) (2011) 6231–6232. DOI 10.1021/es2020988
- T. Becker, M. E. Beber, K. Windt, M-T. Hütt, and D. Helbing
 Flow control by periodic devices: a unifying language for the description of traffic, production, and metabolic systems.
Journal of Statistical Mechanics: Theory and Experiment (2011) P05004. DOI 10.1088/1742-5468/2011/05/P05004
- D. Helbing and W. Yu
 The future of social experimenting.
Proceedings of the National Academy of Sciences USA (PNAS) **107**(12) (2010) 5265-5266. DOI 10.1073/pnas.1000140107
- D. Helbing
 Pluralistic modeling of complex systems.
Science and Culture **76**(9-10) (2010) 315-329.
- M. Mäs, A. Flache, and D. Helbing
 Individualization as driving force of clustering phenomena in humans.
PLoS Comput Biol **6**(10) (2010) e1000959. DOI 10.1371/journal.pcbi.1000959
- D. Helbing and A. Johansson
 Cooperation, norms, and revolutions: A unified game-theoretical approach.
PLoS ONE **5**(10) (2010) e12530. DOI 10.1371/journal.pone.0012530
- D. Helbing, A. Szolnoki, M. Perc, and G. Szabó
 Evolutionary establishment of moral and double moral standards through spatial interactions.
PLoS Computational Biology **6**(4) (2010) e1000758. DOI 10.1371/journal.pcbi.1000758
- W. Yu and D. Helbing
 Game theoretical interactions of moving agents.
Understanding Complex Systems **0/2010** (2010) 219-239. DOI 10.1007/978-3-642-12203-3_10
- D. Helbing
 Quantitative Sociodynamics.
Stochastic Methods and Models of Social Interaction Processes (2010) (Springer, Berlin).

- D. Helbing and W. Yu
The future of social experimenting.
Proceedings of the National Academy of Sciences USA (PNAS) **107**(12) (2010) 5265-5266. DOI 10.1073/pnas.1000140107
- D. Helbing and A. Johansson
Cooperation, norms, and revolutions: A unified game-theoretical approach.
PLoS ONE **5**(10) (2010) e12530. DOI 10.1371/journal.pone.0012530
- T. Chadeaux and D. Helbing
How wealth accumulation can promote cooperation.
PLoS ONE **5**(10) (2010) e13471. DOI 10.1371/journal.pone.0013471
- D. Helbing, A. Szolnoki, M. Perc, and G. Szabó
Punish, but not too hard: how costly punishment spreads in the spatial public goods game.
New J. Phys. **12** (2010) 083005. DOI 10.1088/1367-2630/12/8/083005
- D. Helbing, A. Szolnoki, M. Perc, and G. Szabó
Defector-accelerated cooperativeness and punishment in public goods games with mutations.
Physical Review E **81**(5) (2010) 057104. DOI 10.1103/PhysRevE.81.057104
- D. Helbing, A. Szolnoki, M. Perc, and G. Szabó
Evolutionary establishment of moral and double moral standards through spatial interactions.
PLoS Computational Biology **6**(4) (2010) e1000758. DOI doi:10.1371/journal.pcbi.1000758
- D. Helbing and S. Lozano
Phase transitions to cooperation in the prisoner's dilemma.
Physical Review E **81**(5) (2010) 057102. DOI 10.1103/PhysRevE.81.057102
- D. Helbing and A. Johansson
Evolutionary dynamics of populations with conflicting interactions: Classification and analytical treatment considering asymmetry and power.
Physical Review E **81** (2010) 016112. DOI 10.1103/PhysRevE.81.016112
- W. Yu and D. Helbing
Game theoretical interactions of moving agents.
Pages 219-239 in: A. G. Hoekstra, Jiří Kroc, and P. M.A. Slood (eds.) *Simulating Complex Systems by Cellular Automata* (2010) (Springer, Berlin).
- D. Helbing, A. Johansson
Pedestrian, Crowd and Evacuation Dynamics.
Encyclopedia of Complexity and Systems Science **16** (2010) 6476-6495.
- M. Moussaïd, N. Perozo, S. Garnier, D. Helbing, and G. Theraulaz

The walking behaviour of pedestrian social groups and its impact on crowd dynamics.
PLoS One **5**(4) (2010) e10047. DOI 10.1371/journal.pone.0010047

D. Helbing, L. Rarità, C. D'Apice, and B. Piccoli
Sensitivity analysis of permeability parameters for flows on Barcelona networks.
Journal of Differential Equations **249**(12) (2010) 3110-3131. DOI 10.1016/j.jde.2010.09.006

A. Kesting, M. Treiber, and D. Helbing
Enhanced intelligent driver model to access the impact of driving strategies on traffic capacity.
Phil. Trans. R. Soc. A **368**(1928) (2010) 4585-4605. DOI 10.1098/rsta.2010.0084

M. Treiber, A. Kesting, and D. Helbing
Three-phase traffic theory and two-phase models with a fundamental diagram in the light of
empirical stylized facts.
Transportation Research Part B **44**(8-9) (2010) 983-1000. DOI 10.1016/j.trb.2010.03.004

A. Kesting, M. Treiber, and D. Helbing
Connectivity statistics of store-and-forward intervehicle communication.
IEEE Transactions on Intelligent Transportation Systems **11**(1) (2010) 172-181. DOI
10.1109/TITS.2009.2037924

A. Mazlounian, N. Geroliminis and D. Helbing
The spatial variability of vehicle densities as determinant of urban network capacity.
Phil. Trans. R. Soc. A **368**(1928) (2010) 4627-4647. DOI 10.1098/rsta.2010.0099

R. Donner, K. Padberg, J. Höfener, and D. Helbing
Dynamics of supply chains under mixed production strategies.
Progress in Industrial Mathematics at ECMI 2008, Mathematics in Industry **15**(2) (2010) 527-
533. DOI 10.1007/978-3-642-12110-4_83

H. Rauhut and J. Lorenz
The wisdom of crowds in one mind: Methods and empirical examples of how decision-makers
can learn from societal effects. Accepted (with minor revisions) Journal of Mathematical
Psychology (2010).

Group of H.J. Herrmann

M.L. Eggersdorfer, D. Kadau, H.J. Herrmann, S.E. Pratsinis
Multi-particle sintering dynamics: from fractal-like aggregates to compact structures
Langmuir 27(10), 63586367 (2011).

E.A. Oliveira, K.J. Schrenk, N.A.M. Araújo, H.J. Herrmann, and J.S. Andrade Jr.
Optimal-path cracks in correlated and uncorrelated lattices
Phys.Rev.E **83** (2011) 046113.

N.A.M. Araújo and H.J. Herrmann
Explosive percolation via control of the largest cluster
Phys. Rev. Lett. **105** (2010) 035701.

N.A.M. Araújo, J.S. Andrade Jr., and H.J. Herrmann
Tactical voting in plurality elections
PLoS One **5** (2010) e12446.

N.A.M. Araújo, R.F.S. Andrade, and H.J. Herrmann
q-state Potts model on Apollonian network
Phys. Rev. E **82** (2010) 046109.

N.A.M. Araújo, J.S. Andrade Jr., R.M. Ziff, and H.J. Herrmann
Tricritical point in explosive percolation
Phys. Rev. Lett. **106** (2011) 095703.

H.J. Herrmann and N.A.M. Araújo
Watersheds and explosive percolation
Phys. Proc. **15** (2011) 37.

P.A. Morais, E.A. Oliveira, N.A.M. Araújo, H.J. Herrmann, and J.S. Andrade Jr.
Fractality of eroded coastlines of correlated landscapes
Phys. Rev. E **84** (2011) 016102.

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

E. Fehr, D. Kadau, J.S. Andrade, Jr., and H.J. Herrmann
Impact of Perturbations on Watersheds
Phys. Rev. Lett. 106, 048501 (2011).

E. Fehr, D. Kadau, N.A.M. Araújo, J.S. Andrade Jr., H.J. Herrmann
Scaling Relations for Watersheds
Physical Review E 84, 036116 (2011).

D. Kadau, H.J. Herrmann and J.S. Andrade Jr.
A micromechanical model of collapsing quicksand
Granular Matter 13(3), 219-223 (2011), Special Issue in memory of I. Vardoulakis.

- D. Kadau, H.J. Herrmann
Density profiles of loose and collapsed cohesive granular structures generated by ballistic deposition
Physical Review E 83, 031301 (2011).
- T. Burgener, D. Kadau, H.J. Herrmann
Simulation of particle mixing in turbulent channel flow due to intrinsic fluid velocity fluctuation
Physical Review E 83, 066301 (2011).
- M. Mendoza and J.D. Muñoz
Three-dimensional lattice Boltzmann model for electrodynamics
Phys. Rev. E 82, 056708 (2010)
- M. Mendoza and J.D. Muñoz
A Reliable Lattice-Boltzmann Solver for Electrodynamics: New Applications in Non-linear Media
PIERS Proceedings, 1632 - 1636, March 20-23, Marrakesh, MOROCCO 2011
- M. Mendoza, B.M. Boghosian, H.J. Herrmann, and S. Succi
Fast Lattice Boltzmann Solver for Relativistic Hydrodynamics
Phys. Rev. Lett. 105, 014502 (2010)
- M. Mendoza, B.M. Boghosian, H.J. Herrmann, and S. Succi
Derivation of the lattice Boltzmann model for relativistic hydrodynamics
Phys. Rev. D 82, 105008 (2010)
- M. Mendoza, F.K. Wittel and H.J. Herrmann
Simulation of flow of mixtures through anisotropic porous media using a lattice Boltzmann model
Eur. Phys. J. E 32, 339-348 (2010)
- P. Romatschke, M. Mendoza, and S. Succi
Fully relativistic lattice Boltzmann algorithm
Phys. Rev. C 84, 034903 (2011)
- M. Mendoza, H.J. Herrmann, and S. Succi
Preturbulent Regimes in Graphene Flow
Phys. Rev. Lett. 106, 156601 (2011)
- M.J. Fuhr, M. Schubert, F.W.M.R. Schwarze, H.J. Herrmann
Modeling the hyphal growth of the wood decay fungus *Physisporinus vitreus*
Fungal Biol. (2011), doi:10.1016/j.funbio.2011.06.017, in press.
- M.J. Fuhr, C. Stührk, B. Münch, F.W.M.R. Schwarze, M. Schubert
Automated Quantification of the Impact of the Wood-decay fungus *Physisporinus vitreus* on the Cell Wall Structure of Norway spruce by Tomographic Microscopy
Wood Sci. Technol. (2011), doi:10.1007/s00226-011-0442-y, in press.

S.J. Wettstein, F.K. Wittel, N.A.M. Araújo, B. Lanyon, and H.J. Herrmann
From invasion percolation to flow in rock networks
Accepted for publication in *Physica A*.

M. Mendoza, S. Succi, and H. J. Herrmann
Hydrodynamic Approach to the Conductivity in Graphene
Submitted to *Nature Physics*

R.C. Hidalgo, D. Kadau, T. Kanzaki, H.J. Herrmann
Granular packings of cohesive elongated particles
Granular Matter, submitted.

M.L. Eggersdorfer, D. Kadau, H.J. Herrmann, S.E. Pratsinis
Aggregate Coalescence or Sintering: Number & Diameter of Primary Particles
Journal of Aerosol Science, submitted.

E. Fehr, K. J. Schrenk, D. Kadau, N. A. M. Araújo, P. Grassberger, J. S. Andrade, Jr.,
and H. J. Herrmann
Corrections-to-Scaling for Watersheds, Optimal Path Cracks, and Bridge Lines
in preparation.

R. Mani, D. Kadau and H.J. Herrmann
Fluid transport in sheared wet granular matter
Preprint.

Group of P.H. Hünenberger

V. Kräutler, S. Hiller and P.H. Hünenberger

Residual structure in a peptide fragment of the outer membrane protein X under denaturing conditions: A molecular dynamics study.

Eur. Biophys. J. **39** (2010) 1421-1432.

H.S. Hansen and P.H. Hünenberger

Using the local elevation method to construct optimized umbrella sampling potentials: Calculation of the relative free energies and interconversion barriers of glucopyranose ring conformers in water.

J. Comput. Chem. **31** (2010) 1-23.

L. Perić-Hassler, H.S. Hansen, R. Baron and P.H. Hünenberger

Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling.

Carbohydr. Res. **345** (2010) 1781-1801.

L. Perić-Hassler and P.H. Hünenberger

Interaction of alginate single-chain polyguluronate segments with mono- and divalent metal cations: A comparative molecular dynamics study.

Mol. Simul. **36** (2010) 778-795.

D.P. Geerke, W.F. van Gunsteren and P.H. Hünenberger

Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: Preferential affinity/exclusion effects and their relevance for bioprotection.

Mol. Simul. **36** (2010) 708-728.

H. Satoh, H.S. Hansen, S. Manabe, W.F. van Gunsteren and P.H. Hünenberger

Theoretical investigation of solvent effects on glycosylation reactions: Stereoselectivity controlled by preferential conformations of the intermediate oxacarbenium-counterion complex.

J. Chem. Theory Comput. **6** (2010) 1783-1797.

B.A.C. Horta, A.H. de Vries and P.H. Hünenberger

Simulating the transition between gel and liquid-crystal phases of lipid bilayers: Dependence of the transition temperature on the hydration level.

J. Chem. Theory Comput. **6** (2010) 2488-2500.

H.S. Hansen, X. Daura and P.H. Hünenberger

Enhanced conformational sampling in molecular dynamics simulations of solvated peptides: Fragment-based local elevation umbrella sampling.

J. Chem. Theory Comput. **6** (2010) 2596-2621.

H.S. Hansen and P.H. Hünenberger

Ball-and-stick local elevation umbrella sampling : Molecular simulations involving enhanced sampling within conformational or alchemical subspaces of low internal dimensionalities, minimal irrelevant volumes and problem-adapted geometries.

J. Chem. Theory Comput. **6** (2010) 2622-2646.

B.A.C. Horta, L. Perić-Hassler and P.H. Hünenberger

Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers: A comparative molecular dynamics study.

J. Mol. Graph. Model. **29** (2010) 331-346.

M.M. Reif and P.H. Hünenberger

Computation of methodology-independent single-ion solvation properties from molecular simulations. III. Correction terms for the solvation free energies, enthalpies, entropies, heat capacities, volumes, compressibilities and expansivities of solvated ions.

J. Chem. Phys. **134** (2011) 144103/1-144103/30.

M.M. Reif and P.H. Hünenberger

Computation of methodology-independent single-ion solvation properties from molecular simulations. IV. Optimised Lennard-Jones interaction parameter sets for the alkali and halide ions in water.

J. Chem. Phys. **134** (2011) 144104/1-144104/25.

B. Keller, P.H. Hünenberger and W.F. van Gunsteren

An analysis of the validity of Markov state models for emulating the dynamics of classical molecular systems and ensembles.

J. Chem. Theory Comput. **7** (2011) 1032-1044.

H.S. Hansen and P.H. Hünenberger

A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers and glycosidic linkage conformers.

J. Comput. Chem. **32** (2011) 998-1032.

B.A.C. Horta, P.F.J. Fuchs, W.F. van Gunsteren and P.H. Hünenberger

New interaction parameters for oxygen compounds in the GROMOS force field: Improved pure-liquid and solvation properties for alcohols, ethers, aldehydes, ketones, carboxylic acids and esters.

J. Chem. Theory Comput. **7** (2011) 1016-1031.

B.A.C. Horta and P.H. Hünenberger

Enantiometric segregation in the gel phase of lipid bilayers.

J. Am. Chem. Soc. **133** (2011) 8464-8465.

P. Hünenberger and M. Reif

Single-Ion Solvation. Experimental and Theoretical Approaches to Elusive Thermodynamic Quantities.

Authored book, RSC Theoretical and Computational Chemistry Series (2011).

A. Choutko, W.F. van Gunsteren and P.H. Hünenberger

Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: Enthalpic and entropic driving forces.

Chem. Phys. Chem., submitted (2011)

A.-P.E. Kunz, N. Schmid, S. Riniker, J.R. Allison, B.A.C. Horta, D.J. Geerke, P.H. Hünenberger and W.F. van Gunsteren

New functionalities in the GROMOS biomolecular simulation software.

J. Comput. Chem., submitted (2011)

S. Riniker, C.D. Christ, H.S. Hansen, P.H. Hünenberger, C. Oostenbrink, D. Steiner and W.F. van Gunsteren

Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software.

J. Phys. Chem. B, submitted (2011)

B.A.C. Horta, Z. Lin, W.F. van Gunsteren and P.H. Hünenberger

Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: Influence on the folding properties of two beta-peptides.

J. Chem. Theory Comput., submitted (2011).

Group of P. Jenny

Dissertations since 2010:

G. Anand. PDF Modeling of Turbulent Evaporating Sprays. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

M. L. Hack. Joint PDF Closure for Turbulent Premixed Flames. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

H. Hajibeygi. Iterative Multiscale Finite Volume Method for Multiphase Flow in Porous Media with Complex Physics. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

M. Hegetschweiler. Hybrid PDF Algorithm and PDF Modeling of Partially Premixed Turbulent Combustion. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

J. Reichold. Cerebral Blood Flow Modeling. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2011.

E. Shahraeeni. Thermo-Evaporative Fluxes From Porous Media From Pore To Continuum Scale. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

M. Sormaz. On the Stochastic Modeling of Light Scattering Applied in Remote Sensing and Ballistic-Photon Imaging. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

M. Tyagi. Probability Density Function (PDF) Approach for Modeling Multi-Phase Flow in Porous Media. ETH Dissertation, ETH Zurich, Zurich, Switzerland, 2010.

Publications since 2010:

G. Bonfigli. High-order finite-difference implementation of the immersed-boundary technique for incompressible flows. *Computers and Fluids*, 2010.

H. Gorji and P. Jenny. A generalized stochastic solution algorithm for simulations of rarefied gas flows. In *Proceedings of the 2nd European Conference on Microfluidics*, Toulouse, France, 2010.

H. Gorji and P. Jenny. Continuous stochastic equations for diatomic rarefied gas flows. In *Proceedings of the 3rd GASMEMS Workshop - Bertinoro*, June 9-11, 2011.

H. Gorji, M. Torrilhon, and P. Jenny. Fokker-Planck model for computational studies of monatomic rarefied gas flows. *J. Fluid Mech.*, 680:574–601, 2011.

- M. L. Hack and P. Jenny. Joint PDF closure of turbulent premixed flames. In Proceedings of Mediterranean Combustion Symposium, 2011.
- H. Hajibeygi, R. Deb, and P. Jenny. Multiscale finite volume method for non-conformal coarse grids arising from faulted porous media. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 142205-PP), 2011.
- H. Hajibeygi and P. Jenny. Adaptive iterative multiscale finite volume method. Journal of Computational Physics, 230(3), 2011.
- H. Hajibeygi, D. Karvounis, and P. Jenny. A loosely coupled hierarchical fracture model for the iterative multiscale finite volume method. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141991-PP), 2011.
- H. Hajibeygi, I. Lunati, and S. H. Lee. Error estimate and control in the MSFV method for multiphase flow in porous media. In Proceedings of CMWR XIII, 2010.
- H. Hajibeygi, I. Lunati, and S. H. Lee. Accurate and efficient simulation of multiphase flow in a heterogeneous reservoir by using error estimate and control in the multiscale finite-volume framework. In Proceedings of Reservoir Simulation Symposium, Society of Petroleum Engineering (SPE 141954- PP), 2011.
- M. Hegetschweiler, C. Handwerk, and P. Jenny. Partially premixed turbulent combustion model based on joint statistics of progress variable, mixture fraction, and scalar dissipation rate. Combust. Sci. and Tech., 182:480–490, 2010.
- M. Hegetschweiler, B. Zoller, and P. Jenny. Reactive parametrized scalar profile (R-PSP) mixing model for partially premixed combustion. Combustion and Flame, 2011.
- P. Jenny and D. W. Meyer. Transported probability and mass density function (PDF/MDF) methods for uncertainty assessment and multi-scale problems. In Numerical Analysis of Multiscale Problems. Springer, 2011.
- P. Jenny, M. Torrilhon, and S. Heinz. A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion. Journal of Computational Physics, 229:1077–1098, 2010.
- D. Karvounis and P. Jenny. Modeling of flow and transport in enhanced geothermal systems. in proceedings. In In Proceedings of Thirty-Sixth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, January 2011.
- D. W. Meyer. A new particle interaction mixing model for turbulent dispersion and turbulent reactive flows. Physics of Fluids, 22, 2010.

- D. W. Meyer, P. Jenny, and H. A. Tchelepi. A joint velocity-concentration PDF method for tracer flow in heterogeneous porous media. *Water Resources Research*, 46, 2010.
- D. W. Meyer and H. A. Tchelepi. Particle-based transport model with Markovian velocity processes for tracer dispersion in highly heterogeneous porous media. *Water Resources Research*, 46, 2010.
- G. Molinari, M. Quack, V. Dmitriev, M. Morari, P. Jenny, and P. Ermanni. Aero-structural optimisation of morphing aerofoils for adaptive wings. *Journal of Intelligent Material Systems and Structures*, 22, 2011.
- F. Müller, D. W. Meyer, and P. Jenny. Probabilistic collocation and Lagrangian sampling for tracer transport in randomly heterogeneous porous media. *Advances in Water Resources* (accepted), 2011.
- D. Obrist, B. Weber, A. Buck, and P. Jenny. Red blood cell distribution in simplified capillary networks. *Philosophical Transactions of the Royal Society*, 368(1921):2897–2918, 2010.
- M. Sormaz and P. Jenny. Contrast improvement by selecting ballistic-photons using polarization gating. *Optical Society of America*, 18(23), 2010.
- M. Sormaz, T. Stamm, and P. Jenny. Influence of linear birefringence in the computation of scattering phase functions. *Journal of Biomedical Optics*, 15(5), 2010.
- M. Sormaz, T. Stamm, and P. Jenny. Stochastic modeling of polarized light scattering using a Monte Carlo based stencil method. *Optical Society of America*, pages 1–29, 2010.
- M. Tyagi and P. Jenny. PDF-approach for modeling dissolution-driven gravity currents. In *Proceedings of CMWR XIII*, 2010.
- M. Tyagi and P. Jenny. Probability density function framework for modeling multi-phase ganglia flow in porous media. *Journal of Fluid Mechanics*, pages 1–39, 2011.
- M. Tyagi and P. Jenny. Probability density function modeling of multi-phase flow in porous media with density-driven gravity currents. *Transp Porous Media*, 87(2), 2011.
- B. T. Zoller, J. Allegrini, U. Maas, and P. Jenny. PDF model for NO calculations with radiation and consistent NO-NO₂ chemistry in non-premixed turbulent flames. *Combustion and Flame*, 2011.
- B. T. Zoller and P. Jenny. Combustion model to predict local and global extinction of partially premixed flames. In *Proceedings of Mediterranean Combustion Symposium*, 2011.

Submitted Publications:

K. Erbertseder, J. Reichold, R. Helmig, P. Jenny, and B. Flemisch. A coupled discrete / continuum model for describing cancer therapeutic transport in the lung. PLoS ONE, 2011 (submitted).

H. Hajibeygi, D. Karvounis, and P. Jenny. A hierarchical fracture model for the iterative multiscale finite volume method. Journal of Computational Physics, 2011 (submitted).

B. Misselwitz, N. Barrett, S. Kreibich, P. Von Jasch, S. Rout, K. Weidner, M. Sormaz, P. Songhet, P. Horvath, M. Chabria, V. Vogel, D. Spori, N. Spencer, P. Jenny, and W.-D. Hardt. Sliding of Salmonella Typhimurium on epithelial surfaces explains target cell selection and cooperative invasion. 2011 (submitted).

M. Sormaz and P. Jenny. Monte Carlo study of subsurface imaging in the time-domain with co-axial laser-detector setup and a novel scheme for the target reconstruction. Journal of Optical Society of America, 2011 (submitted).

H. Xiao and P. Jenny. A consistent dual-mesh framework for hybrid LES/RANS modeling. Journal of Computational Physics, 2011 (submitted).

H. Xiao, M. Wild, and P. Jenny. Preliminary evaluation and applications of a consistent hybrid LES/RANS method. In HRLM-4, 2011 (submitted).

Group of Helmut G. Katzgraber

Creighton K. Thomas and H. G. Katzgraber

Fair sampling of the ground-state magnetization of d-dimensional p-body Ising models
Phys. Rev. B, in press, (arXiv:cond-mat/1108.1953)

Creighton K. Thomas and H. G. Katzgraber

The simplest model to study reentrance in physical systems
Phys. Rev. E, in press, (arXiv:cond-mat/1104.2582)

Juan Carlos Andresen, Katharina Janzen and H. G. Katzgraber

Critical behavior and universality in Levy spin glasses
Phys. Rev. B 83, 174427 (2011)

Creighton K. Thomas and H. G. Katzgraber

Optimizing glassy p-spin models
Phys. Rev. E 83, 046709 (2011)

Masayuki Ohzeki, Creighton K. Thomas, H. G. Katzgraber, H. Bombin, M. A. Martin-Delgado

Universality in phase boundary slopes for spin glasses on self dual lattices
J. Stat. Mech. P02004 (2011)

Ruben S. Andrist, D. Larson and Helmut G. Katzgraber

Evidence of a thermodynamic glass transition in the 10-state non-mean-field Potts glass
Phys. Rev. E 83, 030106(R) (2011)

Brigitte Surer, A. Glatz, H. G. Katzgraber, G. T. Zimanyi, B. A. Allgood, and Gianni Blatter

Reply to Comment on Density of States and Critical Behavior of the Coulomb Glass
Phys. Rev. Lett. 105, 039702 (2010)

Ruben S. Andrist, Helmut G. Katzgraber, H. Bombin, and M.-A. Martin-Delgado

Tricolored Lattice Gauge Theory with Randomness: Fault-Tolerance in Topological Color Codes
New J. Phys. 13, 083006 (2011)

Helmut G. Katzgraber, H. Bombin, Ruben S. Andrist and M.-A. Martin-Delgado

Topological color codes on Union Jack lattices: a stable implementation of the whole Clifford group
Phys. Rev. A 81, 012319 (2010)

H. G. Katzgraber

Random Numbers in Scientific Computing: An Introduction

lecture held at the second summer school "Modern Computation Science," Eds. A. K. Hartmann and R. Leidl, BIS-Verlag Oldenburg, Germany (2010)

Group of L. Kleiser

References

- F. Boselli, D. Obrist, and L. Kleiser. A new study on the fluid dynamics in the SCC and the utricle. *Journal of Vestibular Research*, 20(3):168–169, 01 2010a. doi: 10.3233/VES-2010-0373.
- F. Boselli, D. Obrist, and L. Kleiser. A meshless boundary method for computation of Stokes flow with particles in the semicircular canals of the inner ear. *Proc. Appl. Math. Mech.*, 10:459–460, 2010b. doi: 10.1002/pamm.201010222.
- S. Bühler, T. Luginsland, D. Obrist, and L. Kleiser. Parallel simulation of compressible jets including nozzle modelling. *Proc. Appl. Math. Mech.*, 10:443–444, 2010. doi: 10.1002/pamm.201010214.
- R. Erb, D. Obrist, P. W. Chen, J. Studer, and A. R. Studart. Predicting sizes of droplets made by microfluidic flow-induced dripping. *Soft Matter*, 7:8757–8761, 2011. doi: 10.1039/c1sm06231j.
- M. Gloor and J. Bellan. A new formulation of the large eddy simulation composition equations for two-phase fully-multicomponent turbulent flows. *Comp. Fluids*, 50(1):94–103, 2011. doi: 10.1016/j.compfluid.2011.06.017.
- L. Gräf and L. Kleiser. Large-Eddy Simulation of Double-Row Compound-Angle Film-Cooling: Setup and Validation. *Comp. Fluids*, 43:58–67, 2011. doi: 10.1016/j.compfluid.2010.09.032.
- O. Häuselmann, R. Henniger, and L. Kleiser. Numerical study on the influence of particle inertia in particle-driven gravity currents. *Proc. Appl. Math. Mech.*, 11:567–568, 2011.
- T. Luginsland, S. Bühler, D. Obrist, and L. Kleiser. A parallel code for large-eddy simulations of compressible swirling jet flows. *Proc. Appl. Math. Mech.*, 10:727–728, 2010. doi: 10.1002/pamm.201010348.
- D. Obrist. Acoustic emission from convected wave packets. *Phys. Fluids*, 23(2):026101–14, 2011. doi: 10.1063/1.3540693.
- D. Obrist and P. J. Schmid. Algebraically diverging modes upstream of a swept bluff body. *J. Fluid Mech.*, 683:346–356, 2011. doi: 10.1017/jfm.2011.269.
- D. Obrist, R. Henniger, P. Arbenz, and N. Kuroiwa. Parallelization of the time integration of time-periodic flow problems. *Proc. Appl. Math. Mech.*, 10:567–568, 2010. doi: 10.1002/pamm.201010276.
- F. Boselli, D. Obrist, and L. Kleiser. A multilayer method of fundamental solutions for Stokes flow problems. *J. Comput. Phys.*, 2011a. submitted.

- F. Boselli, D. Obrist, and L. Kleiser. Vortical flow in the utricle and the ampulla: A computational study on the fluid dynamics of the vestibular system. *Biomech. Model. Mechanobiol.*, 2011b. submitted.
- D. Obrist, R. Henniger, and L. Kleiser. Subcritical spatial transition of swept Hiemenz flow. *Int. J. Heat and Fluid Flow*, 2011. submitted.

P. Ilg, M. Hütter, M. Kröger, Ideal contribution to the macroscopic, quasiequilibrium entropy of anisotropic fluids,
Phys. Rev. E **83** (2011) 061713.

P. Ilg, M. Kröger, Molecularly derived constitutive equation for low-molecular polymer melts from thermodynamically guided simulation,
J. Rheol. **55** (2011) 69-93.

O. Peleg, M. Tagliacuzzi, M. Kröger, Y. Rabin, I. Szleifer, Morphology control of hairy nanopores,
ACS Nano **5** (2011) 4737-4747.

M. Sadati, C. Luap, M. Kröger, A.A. Gusev, H.C. Öttinger, Smooth full field reconstruction of velocity and its gradients from noisy scattered velocimetry data in a cross-slot flow,
J. Rheol. **55** (2011) 353-377.

G.N. Toepperwein, N.C. Karayiannis, R.A. Riggleman, M. Kröger, J.J. de Pablo, Influence of nanorod inclusions on structure and primitive path network of polymer nanocomposites at equilibrium and under deformation,
Macromolecules **44** (2011) 1034-1045.

B. Zhang, R. Wepf, K. Fischer, M. Schmidt, S. Besse, P. Lindner, B.T. King, R. Sigel, P. Schurtenberger, Y. Talmon, Y. Ding, M. Kröger, A. Halperin, A.D. Schlüter, The largest synthetic structure with molecular precision: Towards a molecular object,
Angew. Chem. Int. Ed. **50** (2011) 737-740.

A. Halperin, M. Kröger, E.B. Zhulina, Colloid-brush interactions: The effect of solvent quality,
Macromolecules **44** (2011) 3622-3638.

Y. Ding, M. Kröger, Rubik cylinder model for dendronized polymers,
J. Comput. Theor. Nanosci. **7** (2010) 661-674.

S. Fransson, O. Peleg, N. Loren, A.-M. Hermansson, M. Kröger, Modelling and confocal microscopy of biopolymer mixtures in confined geometries,
Soft Matter **6** (2010) 2713-2722.

P.S. Stephanou, C. Baig, G. Tsolou, V.G. Mavrantzas, M. Kröger, Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model,
J. Chem. Phys. **132** (2010) 124904.

M. Kröger, O. Peleg, A. Halperin, From dendrimers to dendronized polymers and forests: Scaling theory and its limitations,

Macromolecules **43** (2010) 6213-6224.

M. Kröger, M. Hütter, Automated symbolic calculations in nonequilibrium thermodynamics,
Comput. Phys. Commun. **181** (2010) 2149-2157.

C. Baig, V.G. Mavrantzas, M. Kröger, Flow effects on the melt structure and entanglement network of linear polymer melts: Results from a nonequilibrium molecular dynamics simulation study of a polyethylene melt in steady shear,
Macromolecules **43** (2010) 6886-6902.

C. Baig, P.S. Stephanou, G. Tsolou, V.G. Mavrantzas, M. Kröger, Understanding dynamics in binary mixtures of entangled cis-1,4-polybutadiene melts at the level of primitive path segments by mapping atomistic simulation data onto the tube model,
Macromolecules **43** (2010) 8239-8250.

Preprints

L. Isa, E. Amstad, K. Schwenke, E. del Gado, P. Ilg, M. Kröger, E. Reimhult, Adsorption of core-shell nanoparticles at liquid-liquid interfaces,
Soft Matter doi:DOI:10.1039/C1SM05407D in press

B. Zhang, R. Wepf, M. Kröger, A. Halperin, A.D. Schlüter, Height and width of adsorbed dendronized polymers: Electron and atomic force microscopy of homologous series,
Macromolecules doi:DOI:10.1021/ma2014707 in press

N.C. Karayiannis, R. Malshe, M. Kröger, J.J. de Pablo, M. Laso, Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings,
Soft Matter

Y. Li, M. Kröger, W.K. Liu, Primitive chain network study on uncrosslinked and crosslinked cis-polyisoprene polymers,
Polymers

M. Sadati, C. Luap, M. Kröger, H.C. ttinger, Hard vs. soft constraints in the full field reconstruction of incompressible flow kinematics from noisy scattered velocimetry data,
J. Rheol. in press

L.M.C. Sagis, M. Kröger, Two-dimensional phase-separation on a curved interface: effects of bulk mass transfer,
Phys. Rev. Lett.

A. Halperin, M. Kröger, Collapse of thermoresponsive brushes and the tuning of protein adsorption,
Macromolecules doi:DOI:10.1021/ma201006h in press

Group of M. Luisier

M. Luisier, "Investigation of thermal transport degradation in rough Si nanowires", *J. of Applied Physics* 110, 074510 (2011).

S. Cauley, M. Luisier, V. Balakrishnan, G. Klimeck, and C.-K. Koh, "Distributed NEGF Algorithms for the Simulation of Nanoelectronic Devices with Scattering", *J. of Applied Physics* 110, 043713 (2011).

N. Kharche, G. Klimeck, D. Kim, J. A. del Alamo, and M. Luisier, "Multiscale Metrology and Optimization of Ultra-Scaled InAs Quantum Well FETs", *IEEE Trans. on Elec Dev.* 58, 1963-1971 (2011).

Y. Liu, M. Luisier, and M. S. Lundstrom, "Temperature Dependence of the Transconductance in Ballistic III-V QWFETs", *IEEE Trans. on Elec. Dev.* 58, 1804-1808 (2011).

T. B. Boykin, M. Luisier, G. Klimeck, X. Jiang, N. Kharche, Y. Zhou, and S. K. Nayak, "Accurate six-band nearest-neighbor tight-binding model for the pi-bands of bulk graphene and graphene nanoribbons", *J. of Applied Physics* 109, 104304 (2011).

S. Kim, M. Luisier, A. Paul, T. B. Boykin, and G. Klimeck, "Full Three-Dimensional Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs", *IEEE Trans. on Elec Dev.* 58, 1271-1380 (2011).

P. M. Solomon, I. Lauer, A. Majumdar, J. T. Teherani, M. Luisier, J. Cai, and S.J. Koester, "Effect of Uniaxial Strain on the Drain Current of an Heterojunction Tunneling Field Effect Transistor" *IEEE Elec. Dev. Lett.* 34, 464-466 (2011).

M. Luisier, "Phonon-limited and effective low-field mobility in n- and p-type [100]-, [110]-, and [111]-oriented Si nanowire transistors", *App. Phys. Lett.* 98, 032111 (2011).

M. Frey, A. Esposito, and A. Schenk, "Computational comparison of conductivity and mobility models for silicon nanowire devices", *J. Appl. Phys.* 109, 083707 (2011).

D. Dolgos, H. Meier, A. Schenk, and B. Witzigmann, "Full-band Monte Carlo simulation of high-energy carrier transport in single photon avalanche diodes: Computation of breakdown probability, time to avalanche breakdown, and jitter", *J. Appl. Phys.* 110, 084507 (2011).

M. Ciappa, A. Koschik, M. Dapor, and W. Fichtner, "Modeling secondary electron images for linewidth measurement by critical dimension scanning electron microscopy", *Microelectronics Reliability* 50, 1407 (2011).

Group of S. Mishra

Published papers

1. U.Koley, S. Mishra, N.H.Risebro and M. Svärd, Higher order finite difference schemes for the magnetic induction equations, *BIT.*, 49 (2), 375-395, 2010.
2. F.Fuchs, A.McMurry, S. Mishra, N.H.Risebro and K.Waagan, Finite volume methods for wave propagation in stratified magneto-atmospheres, *Comm. Comput. Phys.*, 7 (3), 2010, 473-509.
3. F.Fuchs, A.McMurry, S. Mishra, N.H.Risebro and K.Waagan, High-order Well-balanced finite volume schemes for simulating waves in stratified magneto-atmospheres, *Jl. Comput. Phys.*, 229 (11), 2010, 4033-4058.
4. S. Mishra and M. Svärd, Implicit-Explicit schemes for flow equations with stiff source terms, *Jl. Comp. Appl. Math.*, 235 (6), 1564-1577, 2011.
5. S. Mishra and E. Tadmor, Constraint preserving schemes using potential based fluxes- I: Multi-dimensional transport equations, *Comm. Comput. Phys.*, 9, 2011, 688-710.
6. S. Mishra and E. Tadmor, Constraint preserving schemes using potential based fluxes- II: Genuinely multi-dimensional schemes for systems of conservation laws, *SIAM Jl. Num. Anal.*, 49 (3), 2011, 1023-1045.
7. U.S. Fjordholm, S. Mishra and E. Tadmor, Energy preserving and energy stable schemes for shallow water equations with bottom topography, *Jl. Comput. Phys.*, 230, 2011, 5587-5609.
8. F.Fuchs, A.McMurry, S. Mishra, N.H.Risebro and K.Waagan, Approximate Riemann solver based high-order finite volume schemes for the MHD equations in multi-dimensions, *Comm. Comput. Phys.*, 9, 2011, 324-362.
9. U.S. Fjordholm and S. Mishra, Vorticity preserving schemes for the shallow-water equations, *SIAM Jl. Sci. Comp.*, 33 (2), 588-611, 2011.

In Press

10. U.Koley, S. Mishra, N.H.Risebro and M. Svärd, Higher order SBP-SAT schemes for magnetic induction equations with resistivity, *IMA Jl. Num. Anal.*, to appear, 2011.
11. S. Mishra and E. Tadmor, Constraint preserving schemes using potential based fluxes- III: divergence preserving central schemes for MHD equations, *M2AN Math. Model. Num. Anal.*, to appear, 2011.
12. S. Mishra and C. Schwab, Sparse tensor multi-level Monte Carlo finite volume methods for hyperbolic conservation laws with random initial data. *Math. Comput.*, to appear, 2011.
13. U.S. Fjordholm and S. Mishra, Accurate Numerical discretizations of non-conservative hyperbolic systems, *M2AN Math. Model. Num. Anal.*, to appear, 2011.

14. F.Fuchs, A.McMurry, S. Mishra and K.Waagan, Simulating waves in the upper solar atmosphere with SURYA: A well-balanced high-order finite volume code, *Astrophysical Journal*, to appear, 2011.
15. G.M.Coclite, S. Mishra, K.H.Karlsen and N.H.Risebro, Existence of solutions to a model of two-phase flow in porous media, *Int. Jl. Num. Anal. Model.*, to appear, 2011.
16. U.S. Fjordholm, S. Mishra and E. Tadmor, Entropy stable ENO scheme, *Proc. of 13th Hyp. prob. conf.*, to appear, 2012.
17. J. Sukys, S. Mishra and Ch. Schwab Static load balancing for multi-level Monte Carlo finite volume solvers, *PPAM Par. Proc. Appl. Math.*, to appear 2012.

Preprints

18. U.S. Fjordholm, S. Mishra and E. Tadmor, ENO reconstruction and ENO interpolation are stable, *Research Report 2011-38*, SAM, ETH Zürich.
19. U.S. Fjordholm, S. Mishra and E. Tadmor, Arbitrarily high order accurate entropy stable essentially non-oscillatory schemes for systems of conservation laws, *Research Report 2011-39*, SAM, ETH Zürich.
20. Entropy stable numerical schemes for two-fluid MHD equations, H. Kumar and S. Mishra, SAM report 2011-22.
21. Implicit-Explicit Runge-Kutta methods for two-fluid MHD equations, H. Kumar, SAM report 2011-26.
22. Stable finite difference schemes for the magnetic induction equation with Hall effect, P. Corti and S. Mishra, SAM report 2011-23.
23. M. J. Castro, U. S. Fjordholm, S. Mishra and C. Parés, Entropy conservative and entropy stable schemes for non-conservative hyperbolic systems, Research report NN. 2011-49, SAM ETH Zurich.
24. S. Mishra and L. V. Spinolo. Accurate numerical schemes for approximating initial-boundary value problems for systems of conservation laws, Research report NN. 2011-58, SAM ETH Zurich.
25. S. Mishra, Ch. Schwab and J. Sukys, Multi-level Monte carlo finite volume methods for non-linear systems of conservation laws in multi-dimensions, *Research Report 2011-2*, SAM, ETH Zürich.

Group of M. Parrinello

- M. Bonomi, A. Barducci, F.L. Gervasio, M. Parrinello
Multiple routes and milestones in the folding of HIV-1 protease monomer”
PLoS ONE, **5** (10), 13208 (2010)
- M. Ceriotti, M. Parrinello, T.E. Markland, D.E. Manolopoulos
Efficient stochastic thermostating of path integral molecular dynamics
J. Chem. Phys., **133**, 124104 (2010)
- M. Ceriotti, M. Parrinello
The delta-thermostat: selective normal-modes excitation by colored-noise Langevin dynamics
Proceedings: International Conference on Computational Science, ICCS 2010
Procedia Computer Science, **1**, 1607-1614 (2010)
- G.A. Tribello, M. Ceriotti, M. Parrinello
A self-learning algorithm for biased molecular dynamics
PNAS, **107** (41), 17509-17514 (2010)
- G. Miceli, C.S. Cucinotta, M. Bernasconi, M. Parrinello
First principles study of the $\text{LiNh}_2/\text{Li}_2\text{NH}$ transformation
J. Phys. Chem. C, **114** (35), 15174-15183 (2010)
- M. Ceriotti, G. Miceli, A. Pietropaolo, D. Colognesi, A. Nale, M. Catti, M. Bernasconi, M. Parrinello
Nuclear quantum effects in *ab initio* dynamics: theory and experiments for lithium imide
Phys. Rev. B, **82**, 174306 (2010)
- G. Miceli, M. Ceriotti, M. Bernasconi, M. Parrinello
Static disorder and structural correlations in the low-temperature phase of lithium imide
Phys. Rev. B, **83**, 054119 (2011)
- H.H.-M. Yeung, M. Kosa, M. Parrinello, P.M. Forster, A.K. Cheetham
Structural diversity and energetic in anhydrous lithium tartrates: experimental and computational studies of novel chiral polymorphs and their racemic and meso analogues
Crystal Growth & Design, **11**, 221 – 230 (2011)
- M. Ceriotti, D.E. Manolopoulos, M. Parrinello
Accelerating the convergence of path integral dynamics with a generalized Langevin equation
J. Chem. Phys., **134**, 084104 (2011)
- G. Miceli, M. Ceriotti, S. Angioletti-Uberti, M. Bernasconi, M. Parrinello
First-principles study of the high-temperature phase of Li_2NH
J. Phys. Chem. C, **115**, 7076-7080 (2011)

- L. Lin, J.A. Morrone, R. Car, M. Parrinello
Momentum distribution, vibrational dynamics, and the potential of mean force in ice
Phys. Rev. B, **83**, 220302, 2011
- S. Caravati, D. Colleoni, R. Mazzarello, T.D. Kühne, M. Krack, M. Bernasconi, M. Parrinello
First-principles study of nitrogen doping in cubic and amorphous Ge₂Sb₂Te₅
J. Phys. Condens. Matter, **23**, 265801 (2011)
- M.K. Prakash, A. Barducci, M. Parrinello
Replica temperatures for uniform exchange and efficient roundtrip times in explicit solvent parallel tempering simulations
J. of Chemical Theory and Computation, **7** (7), 2025-2027 (2011)
- Pietro Paolo, M. Parrinello
A quantitative measure of chirality inside nucleic acid databank
Chirality, **23** (7), 534-542 (2011)
- M. Ceriotti, G.A. Tribello, M. Parrinello
Simplifying the representation of complex free-energy landscapes using sketch-map
PNAS, **108** (32), 13023-13028 (2011)
- R.Z. Khaliullin, H. Eshet, T.D. Kuehne, J. Behler, M. Parrinello
Nucleation mechanism for the direct graphite-to-diamond phase transition
Nature Materials, **10** (9), 693-697 (2011)
- A. Pietro Paolo, D. Branduardi, M. Bonomi, M. Parrinello
A Chirality-Based Metrics for Free-Energy Calculations in Biomolecular Systems
J. of Comput. Chem., **32** (12), 2627-2637, (2011)

Group of M. Quack

1. M. Quack, and F. Merkt, editors
Handbook of High-Resolution Spectroscopy,
Preface by the editors Frédéric Merkt and Martin Quack, Vol. 1, pages XV–XVI
Wiley, Chichester (2011), 3 volumes, ISBN-13: 978-0-470-06653-9
2. F. Merkt, and M. Quack
Molecular Quantum Mechanics and Molecular Spectra, Molecular Symmetry, and
Interaction of Matter with Radiation
in “Handbook of High-Resolution Spectroscopy”, Vol. 1, chapter 1, pages 1–55,
M. Quack, and F. Merkt, Eds. Wiley Chichester, 2011, ISBN-13: 978-0-470-06653-9.
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. J. Stohner, M. Quack
Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular
Spectroscopy
in “Handbook of High-Resolution Spectroscopy”, Vol. 1, chapter 5, pages 263–324,
M. Quack and F. Merkt, Eds., Wiley, Chichester, 2011, ISBN-13: 978-0-470-06653-9.
5. R. Marquardt, M. Quack
Global Analytical Potential Energy Surfaces for High Resolution Molecular
Spectroscopy and Reaction Dynamics
in “Handbook of High-Resolution Spectroscopy”, Vol. 1, chapter 12, pages 511–549,
M. Quack and F. Merkt, Eds., Wiley, Chichester, 2011, ISBN-13: 978-0-470-06653-9.
6. 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.
7. 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.
8. 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.

9. 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
10. S. Albert, K. Keppler Albert, P. Lerch, M. Quack,
Synchrotron-based highest resolution Fourier transform infrared spectroscopy of
naphthalene (C₁₀H₈) and indole (C₈H₇N) and application to astrophysical problems
Faraday Disc. **150**, 71 – 99 (2011), DOI:10.1039/C0FD00013B
11. M. Quack
Frontiers in Spectroscopy (Concluding Paper to Faraday Discussion 150, 2011)
Faraday Disc. **150**, 533–565, DOI:10.1039/C1FD00096A.
12. Discussion Contributions on the Frontiers in Spectroscopy
 - a) J. Stohner, and M. Quack
On parity violating frequency shifts
Faraday Disc. **150**, 113 – 114 and 117 – 118 (2011)
 - b) C. Manca Tanner, M. Quack, and D. Schmidiger
On nuclear spin symmetry relaxation in supersonic jets of H₂O
Faraday Disc. **150**, 118 – 122 (2011)
 - c) M. Quack
On experiments to detect parity violation in chiral molecules
Faraday Disc. **150**, 123 – 127 (2011)
 - d) H. M. Niederer, S. Albert, S. Bauerecker, V. Boudon, G. Seyfang, and M. Quack
On nuclear spin symmetry conservation in methane
Faraday Disc. **150**, 128 – 130 (2011)
 - e) R. Prentner, M. Quack, and J. Stohner
On tunneling and parity violation in ClOOCl
Faraday Disc. **150**, 130 – 132 (2011)
 - f) S. Albert, K. Keppler Albert, P. Lerch, and M. Quack
Discussion replies on synchrotron based high resolution Fourier Transform
Spectroscopy
Faraday Disc. **150**, 146 – 151 (2011)
 - g) L. Horný, and M. Quack
On coupled cluster calculations of parity violating potentials in chiral molecules
Faraday Disc. **150**, 152 – 154 (2011)

- h) E. Miloglyadov, M. Quack, and G. Seyfang
On isotope selective infrared spectroscopy and tunneling in substituted aniline derivatives
Faraday Disc. **150**, 277 – 278 (2011)
 - i) M. Quack
On observing line resolved spectra in molecules showing ultrafast intramolecular processes
Faraday Disc. **150**, 397 – 398 (2011)
 - j) M. Quack
On a general approach describing potentials for hydrogen bonded complexes (HF)_n and similar cases
Faraday Disc. **150**, 413 – 414 (2011)
 - k) S. Albert, K. K. Albert, P. Lerch, and M. Quack
On the high resolution FTIR spectroscopy of phenol and torsional tunneling
Faraday Disc. **150**, 517 – 519 (2011)
 - l) A. Kushnarenko, E. Miloglyadov, M. Quack, and G. Seyfang
On femtosecond pump probe experiments in bichromophoric acetylenic compounds
Faraday Disc. **150**, 520 – 521 (2011)
13. M. Quack
Die Asymmetrie des Lebens und die Symmetrieverletzungen der Physik:
Molekulare Paritätsverletzung und Chiralität
in „Moleküle aus dem All? Reise zum Ursprung des Lebens“, Kapitel 12, pages 277 – 310,
Katharina Al-Shamery Hrsg., Wiley VCH, Weinheim (2011).
(Nach einem Vortrag „Paritätsverletzung und Chiralität“ auf der Tagung „Chemische Evolution“, Manfred-Eigen-Nachwuchswissenschaftler-Gespräche Delmenhorst, 4.–6. Februar 2009)

Group of Prof. M. Reiher

S. Fux, Ch. R. Jacob, J. Neugebauer, L. Visscher, M. Reiher
Accurate Frozen-density Embedding Potentials as a First Step Towards a Subsystem Description of Covalent Bonds
J. Chem. Phys., **2010**, *132*, 164101.

R. Mastalerz, P.-O. Widmark, B. O. Roos, R. Lindh, M. Reiher
Basis Set Representation of the Electron Density at an Atomic Nucleus
J. Chem. Phys., **2010**, *133*, 144111.

M. Podewitz, M. Reiher
Spin Interactions in Cluster Chemistry
Adv. Inorg. Chem., **2010**, *62*, 177.

T. M. A. Al-Shboul, V. K. Palfi, L. Yu, R. Kretschmer, K. Wimmer, R. Fischer, H. Görls, M. Reiher, M. Westerhausen
Catalytic Synthesis of Vinylphosphanes via Calcium-Mediated Intermolecular Hydrophosphanylation of Alkynes and Butadiynes
Organomet. Chem., **2010**, *696*, 216.

K. Boguslawski, K. H. Marti, M. Reiher
Construction of CASCI-type wave functions for very large active spaces
J. Chem. Phys., **2011**, *134*, 224101.

K. Boguslawski, Ch. R. Jacob, M. Reiher
Can DFT accurately predict spin densities? Analysis of discrepancies in iron nitrosyl complexes
J. Chem. Theory Comp., **2011**, *7*, 2740.

Martin T. Stiebritz, Arndt R. Finkelmann, M. Reiher
Oxygen Coordination to the Active Site of Hmd in Relation to [FeFe] Hydrogenase
Eur. J. Inorg. Chem., **2011**, *7*, 1163.

S. Fux, M. Reiher
Electron Density in Quantum Theory
Struct. Bonding, **2011**, DOI: 10.1007/430-2010-37.

S. Knecht, S. Fux, R. van Meer, L. Visscher, M. Reiher, T. Saue
Mössbauer Spectroscopy for Heavy Elements: a Relativistic Benchmark Study of Mercury
Theor. Chem. Acc., **2011**, *129*, 631-650.

M. P. Haag, K. H. Marti, M. Reiher
Generation of Potential Energy Surfaces in High Dimensions
ChemPhysChem, **2011**, DOI: 10.1002/cphc.201100539.

- N. S. Bieler, M. P. Haag, Ch. R. Jacob, M. Reiher
Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides
J. Chem. Theory Comput., **2011**, *7*, 1867.
- K. Marti, M. Reiher
New Electron Correlation Theories for Transition Metal Chemistry
Phys. Chem. Chem. Phys., **2011**, *13*, 6750.
- G. Barcza, Ö. Legeza, K. Marti, M. Reiher
Quantum-information Analysis of Electronic States of Different Molecular Structures *Phys. Rev. A*, **2011**, *83*, 012508.
- E. Mátyus, J. Hutter, U. Müller-Herold, and M. Reiher
On the Emergence of Molecular Structure
Phys. Rev. A, **2011**, *83*, 052512.
- M. Podewitz, M.T. Stiebritz, M. Reiher
An Enquiry into Theoretical Bioinorganic Chemistry: How Heuristic is the Character of Present-day Quantum Chemical Methods?
Faraday Discuss., **2011**, *148*, 119.
- M. Podewitz, T. Weymuth, M. Reiher
Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster
in Modeling of Molecular Properties (Ed. P. Comba), p. 139, **2011**, Wiley-VCH.
- T. Weymuth, Ch. R. Jacob, M. Reiher
Identifying Protein β -Turns with Vibrational Raman Optical Activity
ChemPhysChem, **2011**, *12*, 1165.
- L. Yu, C. Greco, M. Bruschi, U. Ryde, L. De Gioia, M. Reiher
Targeting Intermediates of [FeFe]-hydrogenase by CO and CN Vibrational Signatures *Inorg. Chem.*, **2011**, *50*, 3888.

Group of I.F. Sbalzarini

A. A. Polyansky, R. Ramaswamy, P. E. Volynsky, I. F. Sbalzarini, S. J. Marrink, and R. G. Efremov. Antimicrobial peptides induce growth of phosphatidylglycerol domains in a model bacterial membrane. *J. Phys. Chem. Lett.*, 1:3108–3111, 2010.

R. Ramaswamy and I. F. Sbalzarini. A partial-propensity formulation of the stochastic simulation algorithm for chemical reaction networks with delays. *J. Chem. Phys.*, 134(1):014106, 2011.

Also published in: *Virtual Journal of Biological Physics Research* 21(2), 2011.

R. Ramaswamy, I. F. Sbalzarini, and N. González-Segredo. Noise-induced modulation of the relaxation kinetics around a non-equilibrium steady state of non-linear chemical reaction networks. *PLoS ONE*, 6(1):e16045, 2011.

Z. Smole, N. Nikolic, F. Supek, T. Smuc, I. F. Sbalzarini, and A. Krisko. Proteome sequence features carry signatures of the environmental niche of prokaryotes. *BMC Evolutionary Biology*, 11:26, 2011.

M. E. Ambühl, C. Brepsant, J.-J. Meister, A. B. Verkhovsky, and I. F. Sbalzarini. High-resolution cell outline segmentation and tracking from phase-contrast microscopy images. *J. Microscopy*, in print, doi: 10.1111/j.1365-2818.2011.03558.x, 2011.

C. Bottier, C. Gabella, B. Vianay, L. Buscemi, I. F. Sbalzarini, J.-J. Meister, and A. B. Verkhovsky. Dynamic measurement of the height and volume of migrating cells by a novel fluorescence microscopy technique. *Lab on Chip*, in print, doi: 10.1039/C1LC20807A, 2011.

J. A. Helmuth, S. Reboux, and I. F. Sbalzarini. Exact stochastic simulations of intra-cellular transport by mechanically coupled molecular motors. *J. Computational Science*, in print, 2011.

C. L. Müller, R. Ramaswamy, and I. F. Sbalzarini. Global parameter identification of stochastic reaction networks from single trajectories. *Adv. Sys. Biol.*, in print, 2011.

Y. Yamauchi, H. Boukari, I. Banerjee, I. F. Sbalzarini, P. Horvath, and A. Helenius. Influenza A virus entry, centrosome function, and endosome maturation are regulated by Class I Histone Deacetylases (HDACs 1 and 8). *PLoS Pathogens*, in print, 2011.

O. Awile, F. Büyükkeçeci, S. Reboux, and I. F. Sbalzarini. Fast neighbor lists for adaptive-resolution particle simulations. *Comput. Phys. Commun.*, in revision, 2011.

C. L. Müller and I. F. Sbalzarini. Energy landscapes of atomic clusters as black-box optimization benchmarks. *Evolutionary Computation*, in revision, 2011.

J. Cardinale, G. Paul, and I. F. Sbalzarini. Fast region competition with topological control for multi-region segmentation using a black-box optimizer. *IEEE Trans. Image Proc.*, in revision, 2011.

Group of Christoph Schär

Huber, M.B., R. Knutti, I. Mahlstein, and M. Wild, 2011: Constraints on climate sensitivity from radiation patterns in climate models. *Journal of Climate*, **24**, 1034-1052.

Kotlarski, S., T. Bosshard, D. Lüthi, P. Pall and C. Schär, 2011: Elevation Gradients of European climate change in the regional climate model COSMO-CLM. doi: 10.1007/s10584-011-0195-5

Liang, S., K. Wang, X. Zhang, and M. Wild, 2010: Review on Estimation of Land Surface Radiation and Energy Budgets From Ground Measurement. Remote Sensing and Model Simulations. *IEEE J. of Selected Topics in Applied Earth Observations and Remote Sensing*, **3**, 225-240.

Raible, C.C, B. Ziv, H. Saaroni, and M. Wild, 2010: Winter synoptic-scale variability over the Mediterranean Basin under future climate conditions as simulated by the ECHAM5, *Clim. Dyn.*, **35**, 473–488 DOI 10.1007/s00382-009-0678-5.

Shi, X., M. Wild, and D.P. Lettenmaier, 2010: Surface radiative fluxes over the pan-Arctic land region: variability and trends. *J. Geophys. Res.*, **115**, D22104, doi: 10.1029/2010JD014402.

Schlemmer, L., C. Hohenegger, J. Schmidli, C. Bretherton and C. Schär, 2011: An Idealized Cloud-Resolving Framework for the Study of Midlatitude Diurnal Convection over Land. *J. Atmos. Sci.*, **68** (5), 1041-1057

Schmidli, J., B. Billings, F.K. Chow, S.F.J De Wekker, J. Doyle, V. Grubisic, T. Holt, Q. Jiang, K.A. Lundquist, P. Sheridan, S. Vosper, C.D. Whiteman, A.A. Wyszogrodzki, and G. Zängl, 2011: Intercomparison of mesoscale model simulations of the daytime valley wind system. *Mon. Wea. Rev.*, **139**, 1389–1409.

Schmidli, J., and R. Rotunno, 2010: Mechanisms of along-valley winds and heat exchange over mountainous terrain. *J. Atmos. Sci.*, **67**, 3033–3047.

Zubler, E. M., D. Folini, U. Lohmann, D. Lüthi, A. Muhlbauer, S. Pousse-Nottelmann, C. Schär, and M. Wild, 2011: Implementation and evaluation of aerosol and cloud microphysics in a regional climate model. *J. Geophys. Res.*, **116**, D02211, doi:10.1029/2010JD014572, 2011.

Zubler, Elias M., Ulrike Lohmann, Daniel Lüthi, Christoph Schär, Andreas Muhlbauer, 2011: Statistical Analysis of Aerosol Effects on Simulated Mixed-Phase Clouds and Precipitation in the Alps. *J. Atmos. Sci.*, **68**, 1474–1492.

Zubler, E. M., U. Lohmann, D. Lüthi, and C. Schär, 2011: Intercomparison of aerosol climatologies for use in a regional climate model over Europe, *Geophys. Res. Lett.*, **38**, L15705, doi:10.1029/2011GL048081.

Zubler, E. M., D. Folini, U. Lohmann, D. Lüthi, C. Schär, and M. Wild (2011), Simulation of dimming and brightening in Europe from 1958 to 2001 using a regional climate model, *J. Geophys. Res.*, doi:10.1029/2010JD015396, in press.

In press, accepted, submitted:

Bichet, A., M. Wild, D. Folini, and C. Schär, 2011: Global precipitation response to changing external forcings since 1870, submitted to *ACP*

Doyle, J.D., S. Gabersek, L. Bernardet, J.M. Brown, A. Dörnbrack, E. Filaus, V. Grubisic, D.J. Kirshbaum, O. Knoth, S. Koch, J. Schmidli, I. Stiperski, S. Vosper, and S. Zhong, 2011: An intercomparison of T-REX mountain wave simulations and implications for mesoscale predictability. (in press).

- Folini, D., and M. Wild, 2011: Aerosol Emissions and Dimming / Brightening in Europe: sensitivity studies with ECHAM5-HAM, *J. Geophys. Res.*, submitted.
- Haywood, J., N. Bellouin, A. Jones, O. Boucher, K. Shine, and M. Wild, 2011: The roles of aerosol, water vapor and cloud in future global dimming/brightening, *J. Geophys. Res.*, in press.
- Langhans, W., J. Schmidli, and C. Schär, 2011: Mesoscale impacts of explicit numerical diffusion in a convection-permitting model. (accepted).
- Schlemmer, L., C. Hohenegger, J. Schmidli, C. Schär, 2011: Diurnal equilibrium convection and land surface-atmosphere interactions in an idealized cloud-resolving model. (submitted).
- Schmidli, J., and R. Rotunno, 2011: The influence of the valley surrounding on valley wind dynamics. (submitted)
- Schmidli, J., 2011: The diabatic pressure difference: A new diagnostic for the analysis of valley winds. (submitted)
- Wild, M. 2011: Enlightening global dimming and brightening, *Bull. Am. Meteorol. Soc.*, in press.
- Wild, M., and E. Schmucki, 2011: Assessment of global dimming and brightening in IPCC-AR4/CMIP3 models and ERA40 based on surface observations. *Clim. Dyn.*, in press.
- Zubler, E. M., D. Folini, U. Lohmann, D. Lüthi, A. Muehlbauer, S. Pousse-Nottelmann, C. Schär, and M. Wild, 2010: Implementation and evaluation of aerosol and cloud microphysics in a regional climate model. *J. Geophys. Res.*, in press.

Group of Ch. Schwab

References

- [1] Roman Andreev and Christoph Schwab. Sparse Tensor Approximation of Parametric Eigenvalue Problems. in press, ETH Zürich, 2010. Available at <http://www.sam.math.ethz.ch/reports/2010/40>.
- [2] Andrea Barth. A Finite Element method for martingale-driven stochastic partial differential equations. *Comm. Stoch. Anal.*, 4(3):355–375, September 2010.
- [3] Andrea Barth and Annika Lang. L^p and almost sure convergence of a Milstein scheme for stochastic partial differential equations. SAM report 2011-15, June 2009.
- [4] Andrea Barth and Annika Lang. Milstein approximation for advection-diffusion equations driven multiplicative noncontinuous martingale noises. SAM report 2011-36, May 2011.
- [5] Andrea Barth and Annika Lang. Simulation of stochastic partial differential equations using Finite Element methods. *Stochastics*, pages 1–15, 2011.
- [6] Andrea Barth, Annika Lang, and Christoph Schwab. Multi-level Monte Carlo Finite Element method for parabolic stochastic partial differential equations. SAM report 2011-30, May 2011.
- [7] H. Brandsmeier, K. Schmidt, and Ch. Schwab. A multiscale hp-FEM for 2d photonic crystal bands. *Journal of Computational Physics*, 230(2):349–374, 2011.
- [8] Albert Cohen, Ronald DeVore, and Christoph Schwab. Analytic regularity and polynomial approximation of parametric stochastic elliptic PDEs. Technical Report 2010-3, Seminar for Applied Mathematics, ETH Zürich, 2010. In review.
- [9] E. Fonn. Shearlet galerkin for transport equations: implementation and stability. Technical report, SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2011/50>.
- [10] Claude J. Gittelsohn. *Adaptive Galerkin Methods for Parametric and Stochastic Operator Equations*. PhD thesis, ETH Zürich, 2011. ETH Dissertation No. 19533.

- [11] Claude J. Gittelsohn. An adaptive stochastic Galerkin method. Technical Report 2011-11, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [12] Claude J. Gittelsohn. Adaptive stochastic Galerkin methods: Beyond the elliptic case. Technical Report 2011-12, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [13] Claude J. Gittelsohn. Adaptive wavelet methods for elliptic partial differential equations with random operators. Technical Report 2011-37, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [14] Claude J. Gittelsohn. Representation of gaussian fields in series with independent coefficients. *IMA Journal of Numerical Analysis*, 2011.
- [15] Claude J. Gittelsohn. Stochastic Galerkin approximation of operator equations with infinite dimensional noise. Technical Report 2011-10, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [16] Claude J. Gittelsohn. Uniformly convergent adaptive methods for parametric operator equations. Technical Report 2011-19, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [17] Claude J. Gittelsohn, Juho Könnö, Christoph Schwab, and Rolf Stenberg. The multi-level monte carlo finite element method for a stochastic brinkman problem. Technical Report 2011-31, Seminar for Applied Mathematics, ETH Zürich, 2011.
- [18] K. Grella and Ch. Schwab. Sparse discrete ordinates method in radiative transfer. Technical report, SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2010/46>.
- [19] K. Grella and Ch. Schwab. Sparse tensor spherical harmonics approximation in radiative transfer. *J. of Comput. Phys.*, 2011.
- [20] P. Grohs and Ch. Schwab. Sparse twisted tensor frame discretizations of parametric transport equations. Technical report, SAM, ETH Zürich, 2011. Available at <https://www.sam.math.ethz.ch/reports/2010/41>.
- [21] M. Hansen and C. Schwab. Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic PDEs. Technical Report 2011-29, Seminar for Applied Mathematics, ETH Zürich. Available at <http://www.sam.math.ethz.ch/reports/2011/29>.

- [22] Annika Lang. Almost sure convergence of a Galerkin approximation for SPDEs of Zakai type driven by square integrable martingales. SAM report 2011-35, June 2010.
- [23] Annika Lang. A Lax equivalence theorem for stochastic differential equations. *J. Comput. Appl. Math.*, 234(12):3387–3396, October 2010.
- [24] Annika Lang. Mean square convergence of a semidiscrete scheme for SPDEs of Zakai type driven by square integrable martingales. *Procedia Computer Science*, 1(1):1609–1617, 2010. ICCS 2010.
- [25] Annika Lang, Pao-Liu Chow, and Jürgen Potthoff. Almost sure convergence of a semidiscrete Milstein scheme for SPDEs of Zakai type. *Stochastics*, 82(3):315–326, June 2010.
- [26] D. Marazzina, O. Reichmann, and C. Schwab. *hp*-dgfem for kolmogorov equations of multivariate lévy processes. Technical Report 17, SAM, ETH Zurich, 2011. <http://www.sam.math.ethz.ch/reports/2011/03> (accepted for M3AS).
- [27] O. Reichmann. Optimal space-time adaptive wavelet methods for degenerate parabolic PDEs. Technical Report 03, SAM, ETH, 2011. <http://www.sam.math.ethz.ch/reports/2011/03> (accepted for Numer. Math.).
- [28] Ch. Schwab and S. Tokareva. High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data. *SAM Research report No. 2011-53*, 2011. <http://www.sam.math.ethz.ch/reports/2011/53>.
- [29] Christoph Schwab and Claude J. Gittelsohn. Sparse tensor discretization of high-dimensional parametric and stochastic PDEs. In *Acta Numerica*, volume 20 of *Acta Numer.*, pages 291–467. Cambridge Univ. Press, Cambridge, 2011.

Group of P. J. Tackley

M. D. Ballmer, G. Ito, J. van Hunen, P. J. Tackley
Small-scale sublithospheric convection reconciles geochemistry and geochronology of 'superplume' volcanism in the western and south Pacific
Earth Planet. Sci. Lett. **290** (2010) 224-232, doi:10.1016/j.epsl.2009.12.05

M. D. Ballmer, G. Ito, J. van Hunen, P. J. Tackley
Spatial and temporal variability in Hawaiian hotspot volcanism induced by small-scale convection
Nature Geoscience **4** (2011) 457-460, DOI: 10.1038/ngeo1187

C. Baumann, T. Gerya, J.A.D. Connolly
Numerical modelling of spontaneous slab breakoff dynamics during continental collision
In: Spalla, M.I., Marotta, A.M., Gosso, G. (eds), *Advances in Interpretation of Geological Processes*. Geological Society of London, Special Publications **332** (2010) 99-114.

I. F. Blanco-Quintero, T. V. Gerya, A. García-Casco, A. Castro
Subduction of young oceanic plates: A numerical study with application to aborted thermal-chemical plumes
Geochem. Geophys. Geosyst. (2011) online DOI: 10.1029/2011GC003717

S. Castelltort, S. Nagel, F. Mouthereau, A.T.-S. Lin, A. Wetzel, B.J.P. Kaus, S. Willett, S.-P. Chiang, W.-Y. Chiu
Sedimentology of Early Pliocene Sandstones in the south-western Taiwan foreland: implications for basin physiography in the early stages of collision.
Journal of Asian Earth Sciences **40** (2010) 52-71

A. Castro, T. Gerya, A.G. Casco, C. Fernandez, J. Diaz-Alvarado, I. Moreno-Ventas, I. Low
Melting relations of MORB-sediment melanges in underplated mantlewedge plumes; implications for the origin of cordilleran-type batholiths
Journal of Petrology **51** (2010) 1267-1295, DOI 10.1016/j.gr.2008.12.011

F. Crameri, B.J.P. Kaus
Parameters that control lithospheric-scale thermal localization on terrestrial planets.
Geophys. Res. Lett. **37** (2010) online DOI: 10.1029/2010GL042921

S. Della Morra, L. Boschi, P. J. Tackley, T. Nakagawa, D. Giardini
Low seismic resolution cannot explain S/P velocity decorrelation in the lower mantle
Geophys. Res. Lett. **38** (2011) online DOI: 10.1029/2011GL047559

F. Deschamps, P. J. Tackley, T. Nakagawa
Temperature and heat flux scalings for isoviscous thermal convection in spherical geometry
Geophys. J. Int. **182** (2010) 137-154, DOI 10.1111/j.1365-246X.2010.04637.x.

Y. Deubelbeiss, B.J.P. Kaus, J.A.D. Connolly
Direct numerical simulation of two-phase flow: Effective rheology and flow patterns of particle suspensions.
Earth and Planetary Science Letters. **290** (2010) 1-12, DOI 10.1016/j.epsl.2009.11.041

- Y. Deubelbeiss, B.J.P. Kaus, J.A.D. Connolly, L. Caricchi
 Potential causes for the non-Newtonian rheology of crystal-bearing magmas.
Geochemistry Geophysics Geosystems **12** (2010) online DOI:10.1029/2010GC003485
- T. Duretz, T.V. Gerya, D.A. May
 Numerical modelling of spontaneous slab breakoff and subsequent topographic response
Tectonophysics **502** (2011) 244-256, DOI 10.1016/j.tecto.2010.05.024
- T. Duretz, D. A. May, T. V. Gerya, P. J. Tackley
 Discretization errors and free surface stabilization in the finite difference and marker-in-cell
 method in geodynamic applications: A numerical study
Geochem. Geophys. Geosyst. **12** (2011) online DOI: 10.1029/2011GC003533
- T.M. Duretz, B.J.P. Kaus, K. Schulmann, D. Gapais
 Indentation as an extrusion mechanism of lower crustal rocks in the Eastern Bohemian
 Massif: Insight from analogue and numerical modelling
Lithos **124** (2011) 158-168
- R.J. Farrington, D.R. Stegman, L.N. Moresi, M. Sandiford, D.A. May
 Interactions of 3D mantle flow and continental lithosphere near
 passive margins
Tectonophysics **483** (2010) 20-28
- T. Gerya
 Dynamical instability produces transform faults at mid-ocean ridges
Science **329** (2010) 1047-1050, DOI 10.1126/science.1191349
- T. Gerya
 Origin and models of oceanic transform faults
Tectonophysics (2011) online DOI: 10.1016/j.tecto.2011.07.006
- T. Gerya
 Future directions in subduction modeling
Journal of Geodynamics **52** (2011) 344-378
- T.V. Gerya, F.I. Meilick
 Geodynamic regimes of subduction under an active margin: effects of rheological weakening
 by fluids and melts.
Journal of Metamorphic Geology (2010) online DOI: 10.1111/j.1525-1314.2010.00904.x
- G. J. Golabek, T. Keller, T. V. Gerya, G. Zhu, P. J. Tackley, J. A. D. Connolly
 Origin of the Martian dichotomy and Tharsis from a giant impact causing massive
 magmatism
Icarus **215** (2011) 346-357, doi:10.1016/j.icarus.2011.06.012
- S. Honda, T. Gerya, G. Zhu
 A simple three-dimensional model of thermo-chemical convection in the mantle wedge
Earth and Planetary Science Letters **290** (2010) 311-318, DOI 10.1016/j.epsl.2009.12.027
- B.J.P. Kaus

Factors that control the angle of shear bands in geodynamic numerical models of brittle deformation.

Tectonophysics **484** (2010) 36-47, DOI 10.1016/j.tecto.2009.08.042

B.J.P. Kaus, H. Mühlhaus, D.A. May

A stabilization algorithm for geodynamic numerical simulations with a free surface

Phys. Earth Planet. Inter. **181** (2010) 12-20, DOI 10.1016/j.pepi.2010.04.007

S.M. Lechmann, D.A. May, B.J.P. Kaus, S.M. Schmalholz

Comparing thin-sheet models with 3D multilayer models for continental collision

Geophys. J. Int. **87** (2011) 10-33

Z. Li, T.V. Gerya, J.P. Burg

Influence of tectonic overpressure on P-T paths of HP-UHP rocks in continental collision zones: Thermomechanical modelling

J. Metamorphic Geol. **28** (2010) 227-247, DOI 10.1111/j.1525-1314.2009.00864.x

Z. Li, Z.Q. Xu, T.V. Gerya

Flat versus steep subduction: contrasting modes for the formation and exhumation of high- to ultrahigh-pressure rocks in continental collision zones

Earth and Planetary Science Letters **301** (2010) 65-77

J.-R. Lin, T. V. Gerya, P. J. Tackley, D. A. Yuen, G. J. Golabek

Protocore destabilization during planetary accretion: Feedbacks from non-Newtonian rheology and energy dissipation

Icarus **213** (2011) 24-42

G. Lu, B.J.P. Kaus, L. Zhao

Thermal localization as a potential mechanism to rift cratons

Phys. Earth Planet. Inter. **186** (2010) 125-137.

D.A. May, M.G. Knepley

Optimal, scalable forward models for computing gravity anomalies

Geophysical Journal International **187** (2011) 161-77

C.A. Mériaux, J.A. Mansour, L.N. Moresi, R.C. Kerr, D.A. May

On the rise of strongly tilted mantle plume tails

Physics of the Earth and Planetary Interiors **184** (2011) 63-79

M. Morishige, S. Honda, P. J. Tackley

Construction of semi-dynamic model of subduction zone with given plate kinematics in 3D sphere

Earth Planets and Space **62** (2010) 665-673

G. Morra, D. A. Yuen, L. Boschi, P. Chatelain, P. Koumoutsakos, P. J. Tackley

The fate of slabs interacting with a viscosity hill in mid-mantle

Phys. Earth Planet. Inter. **180** (2010) 271-282, DOI 10.1016/j.pepi.2010.04.001

T. Nakagawa, P. J. Tackley, F. Deschamps, J. A. D. Connolly

The Influence of MORB and Harzburgite Composition on Thermo-Chemical Mantle

Convection in a 3-D Spherical Shell With Self-Consistently Calculated Mineral Physics
Earth Planet. Sci. Lett. **296** (2010) 403-412, DOI 10.1016/j.epsl.2010.05.026.

T. Nakagawa, P. J. Tackley

Influence of initial CMB temperature and other parameters on the thermal evolution of Earth's core resulting from thermo-chemical spherical mantle convection
Geochem. Geophys. Geosys. **11** (2010) online DOI 10.1029/2010GC003031

Nakagawa, T., P. J. Tackley

Effects of low-viscosity post-perovskite on thermo-chemical mantle convection in a 3-D spherical shell
Geophys. Res. Lett. **38** (2011) online doi:10.1029/2010GL046494.

K. Nikolaeva, T.V. Gerya, F.O. Marques

Subduction initiation at passive margins: numerical modeling
J. Geophys. Res. **115** (2010) online DOI 10.1029/2009JB006549

K. Nikolaeva, T. V. Gerya , F. O. Marques

Numerical analysis of subduction initiation risk along the Atlantic American passive margins
Geology **39** (2011) 463-466

K.D. Petersen, S.B. Nielsen, O.R. Clausen, R. Stephenson, T. Gerya

Small-scale mantle convection produces stratigraphic sequences in sedimentary basins.
Science **329** (2010) 827-830, DOI 10.1126/science.1190115

Rolf, T., P. J. Tackley

Focussing of stress by continents in 3D spherical mantle convection with self-consistent plate tectonics
Geophys. Res. Lett. **38** (2011) online DOI:10.1029/2011GL048677.

H. Samuel, P. J. Tackley, M. Evonuk

Heat Partitioning in Terrestrial Planets During Core Formation by Negative Diapirism
Earth Planet. Sci. Lett. **290** (2010) 13-19, DOI 10.1016/j.epsl.2009.11.050

E. Sizova, T. Gerya, M. Brown, L.L. Perchuk

Subduction styles in the Precambrian: Insight from numerical experiments
Lithos **116** (2010) 209-229, DOI 10.1016/j.lithos.2009.05.028

van Heck, H., P. J. Tackley

Plate tectonics on super-Earths: Equally or more likely than on Earth
Earth Planet. Sci. Lett. **310** (2011) 252-261.

P. Yamato, B.J.P. Kaus, F. Mouthereau, S. Castelltort

Dynamic constraints on crustal-scale rheology from the Zagros Mountains.
Geology **39** (2010) 815-818, DOI 10.1130/G32136.1

G. Zhu, T. V. Gerya, S. Honda, P. J. Tackley, D. A. Yuen Dynamical influences on plume patterns from thermo-chemical buoyancy in 3-D mantle wedge
Phys. Earth Planet. Inter. **185** (2011) 112-121.

G. Zhu, Y. Shi, P. Tackley

Subduction of the western Pacific plate underneath northeast China: Implications of numerical studies

Phys. Earth Planet. Inter. **178** (2010) 92-99, DOI 10.1016/j.pepi.2009.10.008

G. Zhu, T. V. Gerya, D. A. Yuen

Melt evolution above a spontaneously retreating subducting slab in a three-dimensional model

Journal of Earth Science **22** (2011) 137-142.

Submitted or in press

F. Crameri, H. Schmeling, G. J. Golabek, T. Duretz, R. Orendt, S. Buiter, D. A. May, B. J. P. Kaus, T. V. Gerya, P. J. Tackley

A benchmark comparison of numerical surface topography calculations in geodynamic modelling

Geophys. J. Int. (2011) submitted

F. Deschamps, E. Kaminski, P. J. Tackley

Thermo-chemical convection shows that the primitive flavor of Ocean Island Basalt has a deep origin

Nature Geoscience (2011) in press

M. Furuichi, D. A. May, P. J. Tackley

Development of a Stokes Flow Solver Robust to Large Viscosity Jumps Using a Schur Complement Approach with Mixed Precision Arithmetic

J. Comp. Phys. (2011) in press, corrected proof, doi:10.1016/j.jcp.2011.09.007

P. J. Tackley

Living dead slabs in 3-D: The dynamics of compositionally-stratified slabs entering a 'slab graveyard' above the core-mantle boundary

Phys. Earth Planet. Inter. (2011) in press, doi:10.1016/j.pepi.2011.04.013

P. Yamato, R. Tartèse, T. Duretz, D.A. May

Numerical modelling of magma transport in dykes

Tectonophysics (2011) in press

Group of M. Troyer

- R. N. C. Pfeifer, P. Corboz, O. Buerschaper, M. Aguado, M. Troyer, G. Vidal
Simulation of anyons using entanglement renormalisation
Phys. Rev. B **82**, 115126 (2010)
- D. Galanakis, Shuxiang Yang, F.F. Assaad, M. Jarrell, P. Werner, Matthias Troyer
Comment on "Exact bosonization for an interacting Fermi gas in arbitrary dimensions"
Phys. Rev. Lett. **105**, 159701 (2010)
- S. Trotzky, L. Pollet, F. Gerbier, U. Schnorrberger, I. Bloch, N.V. Prokof'ev, B. Svistunov, M. Troyer
Suppression of the critical temperature for superfluidity near the Mott transition: validating a quantum simulator
Nature Physics **6**, 998–1004 (2010)
- Konrad H Marti, Bela Bauer, Markus Reiher, Matthias Troyer, Frank Verstraete
Complete-Graph Tensor Network States: A New Fermionic Wave Function Ansatz for Molecules
New J. Phys. **12**, 103008 (2010).
- S. Fuchs, E. Gull, L. Pollet, E. Burovski, E. Kozik, T. Pruschke, M. Troyer
Thermodynamics of the 3D Hubbard model on approach to the Neel transition
Phys. Rev. Lett. **106**, 030401 (2011)
- Hao Wang, B. Bauer, M. Troyer, V. W. Scarola
Identifying Quantum Topological Phases Through Statistical Correlation
Phys. Rev. B **83**, 115119 (2011)
- Bela Bauer, P. Corboz, R. Orus, Matthias Troyer,
Implementing global abelian symmetries in projected entangled-pair state algorithms
Phys. Rev. B **83**, 125106 (2011)
- Andreas W.W. Ludwig, Didier Poilblanc, Simon Trebst, Matthias Troyer
Two-dimensional quantum liquids from interacting non-Abelian anyons
New J. Phys. **13**, 045014 (2011)
- Eddy Ardonne, Jan Gukelberger, Andreas W.W. Ludwig, Simon Trebst, Matthias Troyer
Microscopic models of interacting Yang-Lee anyons
New J. Phys. **13**, 045006 (2011)
- S.V. Isakov, P. Fendley, A.W.W. Ludwig, S. Trebst, M. Troyer
Dynamics at and near conformal quantum critical points
Phys. Rev. B **83**, 125114 (2011)
- [E. Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, P. Werner
Continuous-time Monte Carlo methods for quantum impurity models
Rev. Mod. Phys. **83**, 349 (2011)
- B. Bauer, L. D. Carr, A. Feiguin, J. Freire, S. Fuchs, L. Gamper, J. Gukelberger, E. Gull, S. Guertler, A. Hehn, R. Igarashi, S.V. Isakov, D. Koop, P.N. Ma, P. Mates, H. Matsuo, O. Parcollet, G. Pawłowski, J.D. Picon, L. Pollet, E. Santos, V.W. Scarola, U. Schollwöck, C. Silva, B. Surer, S. Todo, S. Trebst, M. Troyer, M.L. Wall, P. Werner, S.

Wessel

The ALPS project release 2.0: Open source software for strongly correlated systems

J. Stat. Mech., P05001 (2011)

- Didier Poilblanc, Andreas W.W. Ludwig, Simon Trebst, Matthias Troyer
Quantum spin ladders of non-Abelian anyons.
Phys. Rev. B **83**, 134439 (2011)
- M.H. Freedman, L. Gamper, C. Gils, S.V. Isakov, S. Trebst, M. Troyer
Topological Phases: An Expedition off Lattice
Annals of Physics **326**, 2108 (2011)
- Kai-Yu Yang, E. Kozik, Xin Wang, M. Troyer
Diagrammatic Quantum Monte Carlo solution of the two-dimensional Cooperon-Fermion model
Phys. Rev. B **83**, 214516 (2011)
- Sebastian Fuchs, Emanuel Gull, Matthias Troyer, Mark Jarrell, Thomas Pruschke
Spectral properties of the three-dimensional Hubbard model
Phys. Rev. B **83**, 235113 (2011)
- D. Koop, E. Santos, P. Mates, H.T. Vo, P. Bonnet, B. Bauer, B. Surer, M. Troyer, D.N. Williams, J.E. Tohline, Juliana Freire, C.T. Silva
A Provenance-Based Infrastructure for Creating Executable Papers
Procedia Computer Science, 2011. ICCS 2011
- Peter Anders, Emanuel Gull, Lode Pollet, Matthias Troyer, Philipp Werner
Dynamical mean field theory for bosons
New J. Phys **13**, 075013 (2011).
- P. Corboz, S. R. White, G. Vidal, M. Troyer
Stripes in the two-dimensional t - J model with infinite projected entangled-pair states
Phys. Rev. B **84**, 041108(R) (2011)
- Johannes Wilms, Matthias Troyer, Frank Verstraete
Mutual information in classical spin models
J. Stat Mech. P10011 (2011)
- Jia-Wei Huo, Fu-Chun Zhang, Weiqiang Chen, M. Troyer and U. Schollwöck
Trapped Ultracold Bosons in Periodic Lattice Modulations
Phys. Rev. A **84**, 043608 (2011)
- E. Gull, P. Werner, S. Fuchs, B. Surer, T. Pruschke and M. Troyer,
Continuous-time Quantum Monte Carlo impurity solvers
Computer Physics Communications 182, 1078 (2011)
- Philippe Corboz, Andreas M. Laeuchli, Karlo Penc, Matthias Troyer, Frederic Mila
Simultaneous dimerization and $SU(4)$ symmetry breaking of 4-color fermions on the square lattice
Phys. Rev. Lett. (in press)
- P.N. Ma, S. Pilati, X. Dai and M. Troyer
Density functional theory for atomic Fermi gases
Preprint, submitted to Nature Physics

- M.H. Freedman, J. Gukelberger, M.B. Hastings, S. Trebst, M. Troyer, Zhenghan Wang
Galois Conjugates of Topological Phases
Preprint, submitted to Phys. Rev. B
- S.V. Streltsov, E. Gull, A.O. Shorikov, M. Troyer, V.I. Anisimov, P. Werner
Magnetic susceptibility of Ce: an LDA+DMFT study
Preprint, submitted Phys. Rev. B
- B. Surer, M. Troyer, P. Werner, A.M. Läuchli, TO. Wehling, A. Wilhelm, A. I. Lichtenstein
Multi-orbital Kondo physics of Co in Cu hosts
Preprint, submitted Phys. Rev. B
- S. Pilati and M. Troyer
The bosonic superfluid-insulator transition in continuous space
Preprint, submitted Phys. Rev. Lett.

Group of W.F. van Gunsteren

K. Meier, W.F. van Gunsteren

A cyclic β -helical / β -hairpin D, L- α -peptide: study of its folding properties and structure refinement using molecular dynamics

J. Phys. Chem. A **114** (2010) 1852-1859, DOI: 10.1021/jp906218f

W.F. van Gunsteren, M. Winger

Reply to the comment on using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models

Phys. Chem. Chem. Phys. **12** (2010) 2257-2258, DOI: 10.1039/b922516c

B. Keller, Z. Gattin, W.F. van Gunsteren

What stabilizes the 3_{14} -helix in β^3 -peptides? A conformational analysis using molecular simulation

Proteins **78** (2010) 1677-1690, DOI: 10.1002/prot.22685

B. Keller, X. Daura, W.F. van Gunsteren

Comparing geometric and kinetic cluster algorithms for molecular simulation data

J. Chem. Phys. **132** (2010) 074110, DOI:10.1063/1.3301140

Z. Gattin, J. Zaugg, W.F. van Gunsteren

Structure Determination of a Flexible Cyclic Peptide Based on NMR and MD Simulation 3J -Coupling

Chem. Phys. Chem **11** (2010) 830-835, DOI: 10.1002/cphc.200900501

N. Schmid, M. Bötschi, W.F. van Gunsteren

A GPU solvent-solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software

J. Comput. Chem. **31** (2010) 1636-1643, DOI 10.1002/jcc

Z. Lin, H. Liu, W.F. van Gunsteren

Using one-step perturbation to predict the effect of changing force-field parameters on the simulated folding equilibrium of a β -peptide in solution

J. Comput. Chem. **31** (2010) 2419-2427, DOI: 10.1002/jcc.21534, incl. supp. mat.

Z. Lin, J. Kornfeld, M. Mächler, W.F. van Gunsteren

Prediction of folding equilibria of differently substituted peptides using one-step perturbation

J. Am. Chem. Soc. **132** (2010) 7276-7278, DOI: 10.1021/ja100879k, incl. supp. mat.

H. Satoh, H. Hansen, S. Manabe, P.H. Hünenberger, W.F. van Gunsteren
Theoretical Investigation of Solvent Effects on Glycosylation Reactions: Stereoselectivity
Controlled by Preferential Conformations of the Intermediate Oxocarbenium - Counterion
Complex

J. Chem. Theory Comput. **6** (2010) 1783-1797, DOI: 10.1021/ct1001347, incl. supp. mat.

D. Wang, M. Friedmann, Z. Gattin, B. Jaun, W.F. van Gunsteren
The propensity of aminoisobutyric acid (Aib) to induce helical secondary structure in an α -
heptapeptide: a computational study

Helv. Chim. Acta **93** (2010) 1513-1531, DOI: 10.1002/hlca.200900420

D. Wang, T. Merz, W.F. van Gunsteren

The thermal isomerization of the GFP chromophore: a computational study

Phys. Chem. Chem. Phys. **36** (2010) 11051-11061, DOI: 10.1039/C0CP00181C

A.P. Eichenberger, Z. Gattin, G. Yalak, W.F. van Gunsteren

Molecular dynamics simulation of ester-linked hen egg white lysozyme reveals the effect of
missing backbone hydrogen-bond donors on the protein structure

Helv. Chim. Acta **93** (2010) 1857-1869, DOI: 10.1002/hlca.201000077

J. Dolenc, J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren

Methods of NMR structure refinement: molecular dynamics simulations improve the
agreement with measured NMR data of a C-terminal peptide of GCN4-p1

J. Biomol. NMR **47** (2010) 221-235, DOI: 10.1007/s10858-010-9425-9

J.R. Allison, G.P. Moll, W.F. van Gunsteren

Investigation of stability and disulfide bond shuffling of lipid transfer proteins by molecular
dynamics simulation

Biochemistry **49** (2010) 6916-6927, DOI: 10.1021/bi100383m, incl. supp. mat

J. Dolenc, S. Gerster, W.F. van Gunsteren

Molecular dynamics simulations shed light on the enthalpic and entropic driving forces that
govern the sequence specific recognition between netropsin and DNA

J. Phys. Chem. B **114** (2010) 11164-11172, DOI: 10.1021/jp100483f, incl. supp. mat

Z. Lin, A.P.E. Kunz, W.F. van Gunsteren

A one-site polarizable model for liquid chloroform: COS/C

Mol. Phys. **108** (2010) 1749-1757, DOI: 10.1080/00268976.2010.489527

D.P. Geerke, W.F. van Gunsteren, P.H. Hünenberger
Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection
Mol. Simul. **36** (2010) 708-728, DOI: 10.1080/08927021003752804

S. Bachmann, B. Jaun, W.F. van Gunsteren, D. Wang
The effect of fluoro substitution upon the β -hairpin fold of a β -tetrapeptide in methanol
Helv. Chim. Acta **93** (2010) 1870-1881, DOI: 10.1002/hlca.201000179

A. Choutko, A. Glättli, C. Fernández, C. Hilty, K. Wüthrich, W.F. van Gunsteren
Membrane protein dynamics in different environments: simulation study of the outer membrane protein X in a lipid bilayer and in a micelle
Eur. Biophys. J. **40** (2011) 39-58, DOI: 10.1007/s00249-010-0626-7

Z. Lin, W.F. van Gunsteren
Using one step perturbation to predict the folding equilibrium of differently stereochemically substituted β -peptides
Phys. Chem. Chem. Phys. **12** (2010) 15442-15447, DOI: 10.1039/c0cp00833h

J.H. Missimer, J. Dolenc, M.O Steinmetz, W.F. van Gunsteren
Exploring the trigger sequence of the GCN4 coiled-coil: biased molecular dynamics resolves apparent inconsistencies in NMR measurements
Proteins **19** (2010) 2462-2474 DOI:10.1002/pro.528, incl. supp. mat.

S. Riniker, X. Daura, W.F. van Gunsteren
 α -Cyclodextrin host-guest binding: A computational study analyzing the different driving forces
Helv. Chim. Acta **93** (2010) 2318-2325 DOI: 10.1002/hlca.201000251, incl. supp. mat.

J. Allison, M. Müller, W.F. van Gunsteren
A comparison of the different helices adopted by α - and β - peptides suggests different reasons for their stability
Prot. Sci. **19** (2010) 2186-2195, DOI: 10.1002/pro.504

Z. Lin, N. Schmid, W.F. van Gunsteren
The effect of using a polarizable solvent model upon the folding equilibrium of different β -peptides
Mol. Phys. **109** (2011) 493-506, DOI: 10.1080/00268976.2010.532163

A.P.E. Kunz, A.P. Eichenberger, W.F. van Gunsteren
A simple, efficient polarisable molecular model for liquid carbon tetrachloride
Mol. Phys. **109** (2011) 365-372, DOI: 10.1080/00268976.2010.533208

S. Riniker, W.F. van Gunsteren
A simple, efficient polarisable coarse-grained water model for molecular dynamics simulations
J. Chem. Phys. **134** (2011) 084110, DOI: 10.1063/1.3553378

Z. Lin, F.H. Hodel, W.F. van Gunsteren
Influence of variation of a side chain on the folding equilibrium of a β -peptide
Helv. Chim. Acta. **94** (2011) 597-610, DOI: 10.1002/hlca.201100003, incl. supp. mat.

B. Keller, P.H. Hünenberger, W.F. van Gunsteren
An analysis of the validity of Markov state models for emulating the dynamics of classical molecular systems and ensembles
J. Chem. Theory Comput. **7** (2011) 1032-1044, DOI: 10.1021/ct200069c

J.R. Allison, K. Boguslawski, F. Fraternali, W.F. van Gunsteren
A refined, efficient mean solvation force model that includes the interior volume contribution
J. Phys.Chem. **B 115** (2011) 4547-4557, DOI: 10.1021/jp2017117, incl. supp. mat.

B.A.C. Horta, P.F.J. Fuchs, W.F. van Gunsteren, P.H. Hünenberger
New interaction parameters for oxygen compounds in the GROMOS force field: improved pure-liquid and solvation properties for alcohols, ethers, aldehydes, ketones, carboxylic acids and esters.
J. Chem. Theory Comput. **7** (2011) 1016-1031, DOI: 10.1021/ct200069c

- A.P.E. Kunz, W.F. van Gunsteren
Enhancing the configurational sampling of ions in aqueous solution using adiabatic decoupling with translational temperature scaling
J. Phys. Chem. B **115** (2011) 2931-2936, DOI: 10.1021/jp110778k
- D. Steiner, C. Oostenbrink, F. Diederich, M. Zürcher, W.F. van Gunsteren
Calculation of binding free energies of inhibitors to Plasmepsin II
J. Comput. Chem. **32** (2011) 1801-1812, DOI: 10.1002/jcc.21761, incl. supp. mat.
- S. Riniker, A.P. E. Kunz, W.F. van Gunsteren
On the calculation of the dielectric permittivity and relaxation time of molecular models in the liquid phase
J. Chem. Theory Comput. **7** (2011) 1469-1475, DOI: org/10.1021/ct100610v
- W. Huang, Z. Lin, W.F. van Gunsteren
Validation of the GROMOS 54A7 force field with respect to β -peptide folding
J. Chem. Theory Comput. **7** (2011) 1237-1243, DOI: org/10.1021/ct100747y
- Z. Lin, W.F. van Gunsteren, H. Liu
Conformational state-specific free energy differences by one-step perturbation: protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields
J. Comput. Chem. **32** (2011) 2290-2297, DOI: 10.1002/jcc.21818, incl. supp. mat.
- N. Schmid, A.P. Eichenberger, A. Choutko, S. Riniker, M. Winger, A.E. Mark, W.F. van Gunsteren
Definition and testing of the GROMOS force-field versions: 54A7 and 54B7
Eur. Biophys. J. **40** (2011) 843-856, DOI: 10.1007/s00249-011-0700-9, incl. supp. mat.
- S. Riniker, C.D. Christ, N. Hansen, A.E. Mark, P.C. Nair, W.F. van Gunsteren
Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors
J. Chem. Phys. **135** (2011) 024105, DOI: 10.1063/1.3604534, incl. supp. mat.
- A. Kuzmanic, D. Kruschel, W.F. van Gunsteren, B. Zagrovic
Dynamics may significantly influence the estimation of interatomic distances in biomolecular X-ray structures
J. Mol. Biol. **411** (2011) 286-297, DOI: 10.1016/j.jmb.2011.05.033, incl. supp. mat.

A.P.E. Kunz, H. Liu, W.F. van Gunsteren
Enhanced sampling of particular degrees of freedom in molecular systems based on adiabatic decoupling and temperature or force scaling
J. Chem. Phys. **135** (2011) 104106, DOI:10.1063/1.3629450, incl. supp. mat.

J. Dolenc, S. Riniker, R. Gaspari, X. Daura, W.F. van Gunsteren
Free energy calculations offer insights into the influence of receptor flexibility on ligand-receptor binding affinities
J. Comp. - Aided Mol. Des. **25** (2011) 709-716, DOI: 10.1007/s10822-011-9453-x

A.P.E. Kunz, W.F. van Gunsteren
A method for conformational sampling of loops in protein based on adiabatic decoupling and temperature or force scaling
ChemPhysChem (2011) online, DOI: 10.1002/cphc. 201100305

N. Schmid, C.D. Christ, M.Christen, A.P. Eichenberger, W.F. van Gunsteren
Architecture, implementation and parallelization of the GROMOS software for biomolecular simulation
Comp. Phys. Comm. (2011) submitted

N. Schmid, J.R. Allison, J. Dolenc, A.P. Eichenberger, A.P.E. Kunz, W.F. van Gunsteren
Biomolecular structure refinement using the GROMOS simulation software
J. Biomolecular NMR. (2011) online, DOI: 10.1007/s10858-011-9534-0

S. Riniker, C.D. Christ, H.S. Hansen, P.H. Hünenberger, C. Oostenbrink, D. Steiner, W.F. van Gunsteren
Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software
J. Phys. Chem. (2011) in press

A.P.E. Kunz, J.R. Allison, D.P. Geerke, B.A.C. Horta, P.H. Hünenberger, S. Riniker, N. Schmid,
W.F. van Gunsteren
New functionalities in the GROMOS biomolecular simulation software
J. Comput. Chem. (2011) in press

A.P. Eichenberger, J.R. Allison, J. Dolenc, D.P. Geerke, B.A.C. Horta, K. Meier, C. Oostenbrink,
N. Schmid, D. Steiner, D. Wang, W.F. van Gunsteren
The GROMOS++ software for the analysis of biomolecular simulation trajectories
J. Chem. Theory. Comp. (2011) in press

Z. Lin, W.F. van Gunsteren
Exploring the effect of side-chain substitutions upon the secondary structure preferences of β -peptides
J. Phys. Chem. (2011) in press

J. Kleinjung, W.R.P. Scott, J.R. Allison, W.F. van Gunsteren, F. Fraternali
Implicit solvation parameters derived from explicit water forces in large-scale molecular dynamics simulations
J. Chem. Theory. Comp. (2011) submitted, incl. supp. mat.

A.P.E. Kunz, Z. Lin, W.F. van Gunsteren
A method for sampling the internal degrees of freedom of a flexible solute molecule based on adiabatic decoupling and temperature or force scaling
Mol. Phys. (2011) submitted

J.R. Allison, M. Bergeler, N. Hansen, W.F. van Gunsteren
Can computer modeling explain why two highly similar sequences fold into different structures?
Biochemistry (2011) submitted, incl. supp. mat.

K. Meier, W. Thiel, W.F. van Gunsteren
On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations
J. Comput. Chem. (2011) in press

A.P. Eichenberger, L.J. Smith, W.F. van Gunsteren
Ester-linked hen egg white lysozyme shows a compact fold in a molecular dynamics simulation: possible causes and sensitivity of experimentally observable quantities to structural changes maintaining this compact fold
FEBS (2011) submitted, incl. supp. mat.

D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
Helical content of a β^3 -octapeptide in methanol:
Molecular dynamics simulations explain a seeming discrepancy between conclusions derived
from CD and NMR data
Chem. Eur. J. (2011) accepted, incl. supp. mat.

D. Steiner, W.F. van Gunsteren
An improved structural characterisation of reduced french bean plastocyanin
based on NMR data and local-elevation molecular dynamics simulation
J. Biomolecular NMR (2011) submitted, incl. supp. mat.

A. Choutko, W.F. van Gunsteren, P.H. Hünenberger
Preferential affinity of the components of liquid mixtures at a rigid non-polar surface:
Enthalpic and entropic driving forces
ChemPhysChem (2011) submitted

N. Hansen, P. Kraus, H. Sassmannshausen, T. Timmerscheidt, W.F. van Gunsteren
An effective force field for molecular dynamics simulations of dimethyl sulfone
Mol. Phys. (2011) in press

J.R. Allison, S. Riniker, W.F. van Gunsteren
Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
J. Chem. Phys. (2011) submitted, incl. supp. mat.

Z. Lin, H. Liu, S. Riniker, W.F. van Gunsteren
On the use of enveloping distribution sampling (EDS) to compute free enthalpy differences
between different conformational states of molecules: application to 3_{10} -, α -, and π helices
J. Chem. Theory. Comp. (2011) submitted, incl. supp. mat.

N. Hansen, J. Dolenc, M. Knecht, S. Riniker, W.F. van Gunsteren
Assessment of enveloping distribution sampling to calculate relative free enthalpies of
binding for eight netropsin-DNA duplex complexes in aqueous solution
J. Comput. Chem. (2011) submitted, incl. supp. mat.

Group of P. Werner

M. Eckstein and P. Werner

Damping of Bloch oscillations in the Hubbard model

Phys. Rev. Lett. **107**, 186406 (2011)

M. Sentef, P. Werner, E. Gull, and A. Kampf

Superconductivity and Pairing Fluctuations in the Half-Filled Two-Dimensional Hubbard Model,

Phys. Rev. Lett. **107**, 126401 (2011)

A. Koga and P. Werner

Low temperature properties of the infinite-dimensional attractive Hubbard model

Phys. Rev. A **84**, 023638 (2011)

M. Eckstein and P. Werner

Thermalization of a pump-excited Mott insulator

Phys. Rev. B **84**, 035122 (2011)

P. Anders, E. Gull, L. Pollet, M. Troyer, and P. Werner

Dynamical mean-field theory for bosons

New J. Phys. **13**, 075013 (2011)

N. Eurich, M. Eckstein, and P. Werner

Optimal ramp shapes for the fermionic Hubbard model in infinite dimensions

Phys. Rev. B **83**, 155122 (2011)

N. Tsuji, T. Oka, P. Werner, and H. Aoki

Dynamical band flipping in fermionic lattice systems: an ac-field driven change of the interaction from repulsive to attractive

Phys. Rev. Lett. **106**, 236401 (2011)

A. Koga and P. Werner

Superfluid state in the periodic Anderson model with attractive interactions

J. Phys. Soc. Jpn. **79**, 114401 (2010)

M. Eckstein, T. Oka and P. Werner

Dielectric breakdown of a Mott insulator in dynamical mean field theory

Phys. Rev. Lett. **105**, 146404 (2010)

M. Eckstein and P. Werner

Nonequilibrium dynamical mean-field calculations based on the non-crossing approximation and its generalizations

Phys. Rev. B **82**, 115115 (2010)

E. Gull, A. Lichtenstein, A. Millis, A. Rubtsov, M. Troyer, and P. Werner

Continuous-time Monte Carlo methods for quantum impurity models

Rev. Mod. Phys. **83**, 349 (2011)

E. Gull, P. Werner, S. Fuchs, B. Surer, T. Pruschke and M. Troyer
Continuous-time Quantum Monte Carlo impurity solvers
Computer Physics Communications **182**, 1078 (2011)

CSE

Computational Science and Engineering

Annual Report
2010/2011