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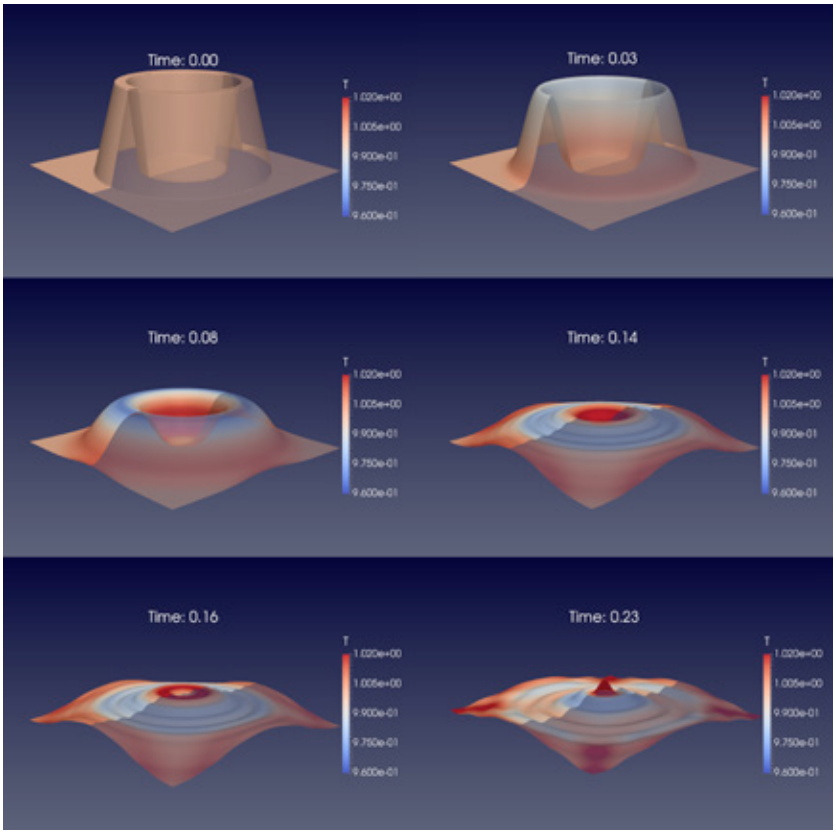

Computational Science and Engineering (CSE)

Annual Report 2014/2015

CSE

Computational Science and Engineering

Annual Report
2014 / 2015

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CSE curricula at ETH Zürich on the internet:

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

Cover:
Rarefied gas in a periodic 2D box.
Velocity DoFs: polynomial degree K = 26, physical DoFs: 65536, total DoFs: 23M,
$\Delta t = 5 \times 1E{-}4$. Elevation: macroscopic density, coloring: temperature.

Groups having contributed to this report

Research Group	Institute	Projects	Publs.
P. Arbenz	Computer Science	34	180
K. Boulouchos	Engines and Combustion Laboratory	37	182
C. Coperet	Inorganic Chemistry	41	183
D. Giardini	Geophysics	45	185
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Introduction

Preface to CSE Report 2015

R. Hiptmair*

December 13, 2015

Editorial

At ETH Zürich D-BSSE stands for "Department of Biosystems Science and Engineering" and this is one of the youngest departments at ETH Zurich and one whose name will leave many an outsider puzzled. It was founded in 2007, is based in Basel and comprises 17 groups and a total of about 300 scientific staff as of autumn 2015. Lecturers from D-BSSE contribute the bulk of the courses to the field of specialization "Biology" in the CSE master program at ETH Zürich. This suggests substantial involvement in CSE of researchers of D-BSSE. With this editorial I intend to shed light on these links. Of course, I was as clueless as many of you, Dear Readers, and so I decided to consult the experts, two professors of D-BSSE that were kind enough to meet me for an interview.

T. Stadler, D-BSSE

Prof. Dr. Tanja Stadler has been an Assistant Professor at D-BSSE since 2014. She studied Applied Mathematics at TU Munich (Germany), the University of Cardiff (UK), and the University of Canterbury (New Zealand). She obtained a Master degree in 2006 and a PhD in 2008 from the Technical University of Munich (with Prof. Anusch Taraz and Prof. Mike Steel). Tanja then joined ETH Zürich as a postdoctoral researcher with Prof. Sebastian Bonhoeffer in the Department of Environmental Systems Sciences, and was promoted to Group Leader in 2011. Her work is at the interface of mathematics, computer science, evolution, ecology and infectious diseases. In particular, she develops phylogenetic tools to address epidemiological and medical questions, as well as questions in the fields of ecology, species evolution, cell differentiation and language evolution. Her honors include the TUM PhD award 2008, the John Maynard Smith prize 2012, the ETH Latsis prize 2013, and the Zonta prize 2013. In 2013, Tanja received an ERC starting grant.

In 2005, **Jörg Stelling** joined D-INFK of ETH Zurich as an assistant professor for Bioinformatics. From 1989 until 1996 he studied Biotechnology at the Technical University Braunschweig, with a stay abroad at the Ecole Normal Superieure d'Agronomie Montpellier. Starting in the end of 1996 he was postgraduate at the Institute for

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Systems Dynamics and Control Engineering of the University Stuttgart, before in mid 1998 he became one of the first collaborators of the newly founded Max-Planck-Institute for Dynamics of Complex Technical Systems. There Jörg Stelling was significantly involved in establishing the division "Systems Biology". In this field he received his PhD in 2004 on the analysis of robustness of complex biological networks at the Faculty of Mechanical Engineering, Stuttgart University. In Mai 2008 he became professor of Computational Systems Biology at D-BSSE. His research interests are in the fields of analysis and synthesis of biological networks with the help of - and by further development of - methods from systems theory and computer science.

J. Stelling, D-BSSE

I had conversations with both in the grand setting of the ETH faculty club in the main building and asked them a few questions. Let me now give you a summary of their answers.

1. What is "Biosystems Science and Engineering"?

   T.S.: Our emphasis is on the system and process view on the level of cells, tissues, organs, and organisms. We are not content with mere descriptions and qualitative understanding, but aim for quantitative models with predictive power. This entails a deep understanding of relationships and feedback loops connecting the constituent parts of biological systems. It also entails deep analysis of experimental data.

   J.S.: There is also distinct "engineering flavor" to the research activities at D-BSSE. This means that many groups, beside experimental and theoretical characterization, pursue the design and control of biological systems. We want to use our insights to make biological agents serve certain purposes, not mainly for treating diseases as at D-HEST (health science and technology), but also with an eye on advancing technology. The engineering activities at D-BSSE are also focused on new methods for measurement and data acquisition. All this requires a truly interdisciplinary effort drawing on techniques from biology, engineering, computer science, and mathematics.

2. What kind of methods from mathematics, computer science, and physics are crucial for your work?

   T.S.: of course, my research in phylogenetics needs graph theory, but also heavily relies on stochastic methods, both for modeling and parameter identification from genetic data. Bayesian statistics and maximum likelihood techniques are key tools. So are stochastic processes and (population) dynamic models with ordinary (stochastic) differential equations.

   J.S.: Dynamic network models are crucial for my research. Since I have to build them from data, techniques for parameter estimation and model selection are important. Data are inevitably affected by errors and therefore I have to deal with many

sources of uncertainty. This has rendered uncertainty quantification an indispensable tool in my work. In my group we actually extend and develop mathematical methods, invariably driven by the needs of concrete applications.

3. What is the role of algorithms and simulation in your work?

   T.S.: For data analysis and parameter analysis I make heavy use of methods from optimization, which involve massive numerical computations. We usually test ideas in the R programming language and, whenever necessary, run the big analyses in Java or C. Stochastic simulations also play a big role in my research, as well as graph algorithms (tree space analysis).

   J.S.: For dynamic simulations we employ numerical integrators for ordinary differential equations. Parameter identification is often done with tools from numerical optimization, continuous and discrete. Development of numerical codes is not our main concern, but sometimes conducted as part of a project.

4. What is the role of HPC in your work and at D-BSSE?

   T.S.: We do massive simulations on the Euler cluster to validate and calibrate models and generate synthetic data. Since it is usually Monte-Carlo type algorithms, parallelization is easy. Numerical stability can be a challenge however, as likelihood calculations may produce very small numbers easily tainted by numerical noise. In addition, many of the algorithms and implementations are probably not optimal and increasing their performance would be greatly appreciated.

   J.S.: For me HPC is merely a tool and not a research focus. It is important, of course, because stochastic simulations, image analysis and large-scale optimization could not be tackled without parallel computing. Most groups at D-BSSE rely on massive computations as part of their research, though none would claim to do research in the field of HPC.

5. What is the relationship of simulation and experiments in your work?

   T.S.: Both can never be separated in my field. We need experimental data for model calibration and validation. On the one hand simulations are motivated by surprising observations made in experiments. On the other hand, simulations tell experimenters what to look for and how to design their experiments. There is a close connection nowadays. My group currently uses a lot of data from clinical settings to understand infectious disease evolution and epidemic spread.

   J.S.: My current research is based on both simulations and "wet lab" experiments. Observations and data are the starting point, of course. However, often insights can be gleaned only through simulation, since direct observation of processes inside living cells may not be possible.

6. What kind of computational skills do you expect from graduate students?

   T.S.: I greatly value algorithmic skills, both in terms of knowledge about computational methods and as a way of approaching problems. More concretely, it is desirable that graduate students are proficient in programming languages. We code our algorithms mainly in R and Java, but I believe that a good algorithmic

understanding enables students to quickly become familiar with these languages. I would like to point out the central role of stochastics and statistical methods in my field.

J.S.: In my group I have got a mix of students with backgrounds in mathematics, computer science, and biology. The latter usually take care of the experiments. Ideally, I would like to hire graduate students that know everything, mathematics, computer science, and biology. Of course, this remains a dream. More realistically, when modeling and simulation is the focus of a project I prefer candidates with a strong background in applied mathematics and computer science.

Zürich, December 15, 2015

Ralf Hiptmair,

Director of Studies CSE, member of the CSE Committee

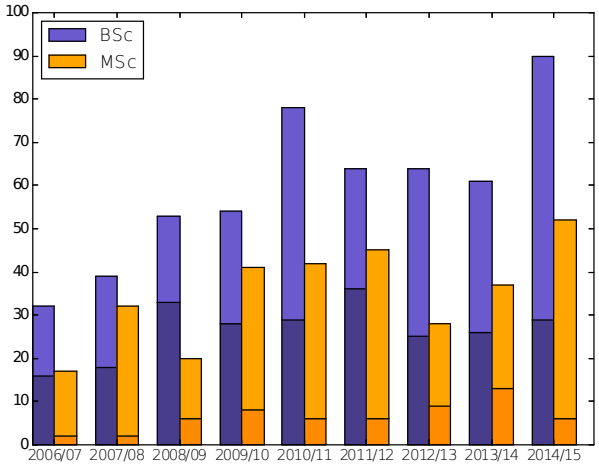
2

Education

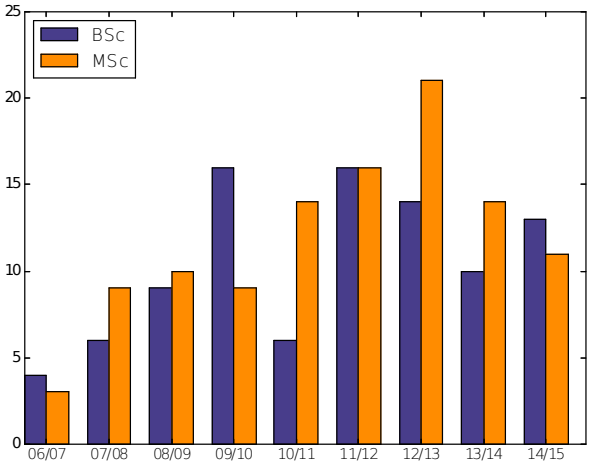
In September 2014, 29 new students started their CSE Bachelor studies, 16 in the first semester and 13 in the third semester. From outside ETH 6 students entered the CSE Master curriculum.

The total number of CSE students enrolled at the end of the academic year 2014/2015 was 142 (90 in the BSc program and 52 in the MSc program).

In the past academic year 24 students have successfully finished a CSE curriculum, 13 Bachelor students and 11 Master students, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/Master thesis and the name and the department of the advisor. Included are also some theses from the previous academic year, not mentioned in the report 2013/14.



Number of CSE students in the curriculum; dark = number of new students



Number of CSE graduates

Bachelor Theses

Roman Cattaneo	Worm Percolation (Hans Jürgen Herrmann, D-BAUG)
Estefani Carvalhais	Compartment-Based Stochastic Reaction-Diffusion Simulations (Petros Koumoutsakos, D-MAVT)
Rodic Donjan	OpenMPI User Level Failure Mitigation in Boost::MPI (Matthias Troyer, D-PHYS)
Simon Etter	FFT-based Ridgelets for Radiative Transport (Philipp Grohs, D-MATH)
Matthias Frey	Parallelization of a Differential Algebra Framework (Andreas Adelmann, D-INFK)
Maurice Gonzenbach	Visual Tracking of the RodBot Micro-robot (Bradley J. Nelson, D-MAVT)
Thomas Häner	Numerical Solution of a Coefficient Identification Problem for the Poisson Equation (Ralf Hiptmair, D-MATH)
Samuel Keusch	Finite-Element Analysis of Waveguide Modes (Christian Hafner, D-ITET)
Fabio Luchsinger	Implementing a Flexible Optical Depth Calculation in Radiation Hydrodynamics (Lucio Mayer, D-PHYS)
Lionel Miserez	A Fast Discrete Pseudo-Polar Ridgelet Transform (Philipp Grohs, D-MATH)
Lukas Mosimann	An Energy Balance Tool (Martin Wild, D-ENV)
Dominic Stemmler	Gravitational N-Body Simulations (Ben Moore, ICS, UZH)
Ann-Christine Straw	A Framework for Comparing Otimizers for NP-Hard Problems (Matthias Troyer, D-PHYS)

Master Theses

Kushagra Alankar	Video Registration using Alignment of Intermediate 3D Reconstruction (Luc Van Gool, D-ITET)
Nicolas Andrey-Sterner	Picewise Affine System Modeling of RC Race Cars (John Lygeros, D-ITET)
Andrea Arteaga	Case Studies on Bit-Reproductibility and Portability of High-Performance Applications (Torsten Hoefler, D-INFK)
Stefano Battaglia	Implementation of the Relativistic Four-Component DMRG Approach in MAQUIS (Markus Reiher, D-CHAB)
Martina Beer	Conservative Formulation of an Isentropic Model (Chrisoph Schär, D-ENV)
Daniele Casati	Hierarchical Population Generation in Transportation Modelling (Kay Axhausen, D-BAUG)
Rodic Donjan	Ginzburg-Landau 3D Simulation of Superconductors: Cooper Pair Density, Vortices, Fields (Matthias Troyer, D-PHYS)
Leonardo Echeverria	Numerical Modeling of Human Population Dynamics (Anthony Patt, D-ENV)
Simon Etter	Parallel Tensor-Formatted Numerics for the Chemical Master Equation (Christoph Schwab, D-MATH)
Matthias Frey	Matched Distributions in Cyclotrons with Higher Order Moments of the Charge Distribution (Andreas Adelmann, D-INFK)
Maria Han Veiga	Task-driven Information Valuation in web Communities (Thomas Hofmann, D-INFK)
Sharan Jagathrakshakan	A Generic Parallel C++ Library for the Multilevel Monte Carlo Method (Peter Arbenz, D-INFK)
Vineet Mohan	Grouped Regression in High Dimensional Statistics (Sara van de Geer, D-MATH)

Sander Schaffner	Using Trilinos to Solve Large Scale Eigenvalue Problem in Amorphous Materials (Peter Arbenz, D-INFK)
Arthur Schwaninger	Variations of the Replica Exchange Method for Free Energy Computations (Sereina Riniker D-CHAB)
Philipp Wissmann	Implementation of a Staggered Grid Finite Difference Mode Solver and Application to Plasmonic Waveguides (Qiuting Huang, D-ITET)

Term Papers

Matthias Frey	Matched Distributions in Cyclotrons (Andreas Adelmann, D-INFK)
Maurice Gonzenbach	Prediction of Epileptic Seizures using EEG Data (Gabor Szekely, D-ITET)
Thomas Häner	qhardware: A Quantum Computer Emulation Library featuring Compile-time Gate Substitution (Matthias Troyer, D-PHYS)
Stefan Hegglin	An Efficient Implementation of Time Evolution Operators and Quantum Gates for spin-1/2-systems (Mathias Troyer, D-PHYS)
Marc Maetz	Implementation of Discrete Time Path Integral Quantum Monte Carlo of an Ising Model in CUDA (Matthias Troyer, D-PHYS)
Lionel Miserez	Porting WaveBlocksND Matrix Potential Functionality to C++ (Vasile Gradinaru, D-MATH)
An Phi Nguyen	Dense MultiBody Motion Segmentation and 3D Reconstruction from Perspective Views (Davide Scaramuzza, UZH)
Sander Schaffner	Price of Stability in the Global Connection Game with Three Players in Undirected Graphs (Peter Widmayer, D-INFK)
Sandro Sgier	Matlab Implementation of Affine Multi-factor Option Pricing Models (Walter Farkas, D-MATH)

Kelly Steich	RoboCup: Dynamic Role Assignment within the B-Human Framework (John Lygeros, D-ITET)
Roger Walt	Brute-force TSP Solver on FPGAs: A theoretical Estimate (Matthias Troyer, D-PHYS)
Dzmitry Zhyhadla	Depth Reconstruction from Multiple Landscape Photos Markus Gross (D-INFK)

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

Zürich, November 4, 2015
Vasile Gradinaru,
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.cse.ethz.ch

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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 HS14

18.09.14	Tapio Schneider, Climate Dynamics Simulating Clouds and their Response to Climate Change
25.09.14	Oliver Rain, Robert Bosch GmbH, Stuttgart Fast Boundary Element Methods in Industrial Applications
09.10.14	Roger Käppeli, Seminar for Applied Mathematics (SAM) Computational Astrophysics: The Explosion Mechanism of Massive Stars
30.10.14	Miriam Mehl, Parallel and Distributed Systems, University of Stuttgart Iterative Solvers for Multiphysics Simulations
13.11.14	John Lygeros, Automatic Control Laboratory Modeling, Analysis and Control of Cell Populations
04.12.14	Hossein Gorji, Fluid Dynamics Variance Reduction for Gas Flow Simulations Based on Stochastic Molecular Models
18.12.14	Peter Arbenz, Computer Science Bone Structure Analysis with Multi-GPGPUs

Case Studies Seminar FS15

19.02.15	Jörn Sesterhenn, Computational Fluid Dynamics, TU Berlin Direct and Adjoint Methods for the Investigation of High Speed Jets and Volcanic Eruptions
26.02.15	Benjamin Stamm, Université de Pierre et Marie Curie, Paris VI Towards High Performance Polarizable Molecular Dynamics Simulations
12.03.15	Ulrike Lohmann, Atmospheric and Climate Science Numerical Modelling of Climate
26.03.15	Nicolai Meinshausen, Seminar for Statistics High-Dimensional Data Analysis
23.04.15	Andreas Fichtner, Earth Sciences Computational Seismology - A Tour from Seismic Imaging to Tsunami Warnings
07.05.15	Riko Jacob, Theoretical Computer Science, ITU Copenhagen Cache Optimized Hierarchization of Sparse Grids: I/O-model, Implementations and Experiments

4

Computational Highlight

Computational Highlight: A Parallel Spectral Boltzmann Solver

R. Hiptmair and S. Pintarelli *

December 9, 2015

1 The Boltzmann Equation

The Boltzmann equation

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{kn} Q(f,f)(\mathbf{v}), \qquad (\mathbf{x},\mathbf{v}) \in \Omega = D \times \mathbb{R}^d, \tag{1}$$

provides a fundamental mesoscopic model for the dynamics of rarefied gases. Its primary unknown is the *distribution function* $f = f(\mathbf{x},\mathbf{v},t)$ sought on the $2d$-dimensional phase space $\Omega = D \times \mathbb{R}^d$, where $D \subset \mathbb{R}^d$ denotes a bounded spatial domain with piecewise smooth boundary, and $\mathbb{R}^d$ stands for the space of velocities. Interactions of gas molecules are taken into account by the *collision operator* Q represented by the $2d-1$-dimensional integral

$$Q(f,h)(\mathbf{v}) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} B(\|\mathbf{v}-\mathbf{v}_\star\|, \cos\theta)(h(\mathbf{v}'_\star)f(\mathbf{v}') - h(\mathbf{v}_\star)f(\mathbf{v}))\,\mathrm{d}\sigma\,\mathrm{d}\mathbf{v}_\star, \tag{2}$$

where B is the so-called collision kernel, and a prime tags post-collisional velocities, see [1] for details. In (1) kn stands for the dimensionless Knudsen number essentially linked to the mean free path length in the gas model.

Equation (1) has to be supplemented with an initial distribution

$$f(\mathbf{x},\mathbf{v},t=0) = f_0(\mathbf{x},\mathbf{v}), \tag{3}$$

and boundary conditions. For instance, Dirichlet boundary conditions can be imposed on the inflow boundary

$$\Gamma^- := \{(\mathbf{x},\mathbf{v}) : \mathbf{x} \in \partial D \wedge \mathbf{v}\cdot\mathbf{n} \le 0\}, \tag{4}$$

but other choices like specular or diffusive reflective walls are possible, see [3, Sect. 5].

The computational challenge posed by the Boltzmann equation is twofold:

(i) we face a moderately high-dimensional problem, since f is defined on a 4-($d=2$) or 6-dimensional ($d=3$) domain,

(ii) the collision operator is non-linear and non-local in velocity $\mathbf{v}$.

Moreover, the exact evolution conserves mass, momentum, and energy, and so should a viable numerical model.

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2 Discretization

We aim for a deterministic and asymptotically exact Petrov-Galerkin discretization of a suitable variational formulations of boundary value problems for (1). This sets our approach apart from stochastic Monte-Carlo-type methods as well as Fourier spectral discretization in velocity for which aliasing foils asymptotic exactness.

We restrict the discussion to $d = 2$. As trial space we use a *tensor product* space $S_h := X_N \times V_K$ comprised of the following component spaces:

- In velocity we use Gaussian weighted space of tensor product polynomials of total degree K, see [3, Sect. 2] and [6]. In the so-called polar Laguerre representation it can be written as

$$V_N := \operatorname{Span}\left\{\{\Psi^{\cos}_{k,j} : j = 0, \dots, \lfloor \tfrac{k}{2} \rfloor\} \cup \{\Psi^{\sin}_{k,j} : j = 1 - (k \mod 2), \dots, \lceil \tfrac{k}{2} \rceil\}\right\},$$

$$\Psi^F_{k,j}(\varphi, r) := \begin{cases} F(2j\varphi)\, r^{2j} L^{(2j)}_{\frac{k}{2}-j}(r^2) e^{-r^2/2}, & k \in 2\mathbb{N} \\ F((2j+1)\varphi)\, r^{2j+1} L^{(2j+1)}_{\frac{k-1}{2}-j}(r^2) e^{-r^2/2}, & k \in 2\mathbb{N}+1 \end{cases}, \quad F \in \{\sin, \cos\},$$

  where $L^{(\alpha)}_n$ are the associated Laguerre polynomials. The functions $\Psi_{k,j}$ are $L^2(\mathbb{R}^2)$-orthogonal.

- For approximation in the spatial direction $\mathbf{x}$ we rely on spaces VX_N piecewise bi-linear continuous finite element functions on quadrilateral meshes of D.

Since $\dim S_h = \dim X_N \cdot \dim V_K$, the dimension of S_h will be huge even for moderate resolutions in space and velocity. A basis for S_h is obtained by attaching the same basis of V_K to every node of the mesh.

An $L^2(\mathbb{R}^d)$ Galerkin discretization of the collision operator Q in V_K yields a three-dimensional tensor with N^3 entries, $N = \frac{1}{2}K(K+1)$. The product structure in radial and angular direction of the polar Laguerre basis allows to exploit rotation invariance properties of the collision tensor and to reduce the number of nonzero entries from $\mathcal{O}(K^6)$ to $\mathcal{O}(K^5)$. This will also be the asymptotic cost for evaluating the discrete collision tensor. Refer to [3, Sect. 3] for more information.

Discretization of (1) in time will employ operator splitting: (1) is split into the advection operator

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = 0, \tag{5}$$

and the collision part

$$\partial_t f = \frac{1}{kn} Q(f, f). \tag{6}$$

The latter is tackled by an explicit Euler scheme. In order to conserve mass, momentum, and energy we employ the Lagrange multiplier method proposed in [2]. For the discretization of the advection part we first replace $\partial_t f$ by its backward difference quotient. Then, for the sake of stabilization, we opt for a least squares approach, which amounts to minimization of the functional [3, Sect. 4]

$$J(f^{(n)}; f^{(n-1)}) := \left\| \frac{1}{\Delta t}\left(f^{(n)} - f^{(n-1)}\right) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f^{(n)} \right\|^2_{L^2(\Omega)}. \tag{7}$$

After inclusion of the inflow boundary conditions the corresponding bilinear form is no longer symmetric. Therefore, as an iterative solver we use the (preconditioned) GMRES method.

3 (Parallel) Implementation

An extensive simulation framework for the transient spatially inhomogeneous Boltzmann equation (1) has been implemented in `C++` and parallelized with MPI. Special attention has been paid to a highly modular software design. This makes it possible to plug in different discretization methods in the physical and spatial domain easily. For the finite element module, we use the `deal.II 8.3` finite element library [7]. Since the collision operator is independent of $\mathbf{x}$, it is trivial to parallelize via domain decomposition in the spatial domain. The degrees of freedom living on the spatial mesh can be distributed with the standard tools offered by METIS [5]. In order to reduce fill-in in the preconditioner the Cuthill-McKee algorithm is applied first. The velocity degrees of freedom describing functions in V_K are then associated with each single spatial DoF.

Efficiency of an implementation hinges on farming out computations to a prior setup phase and reuse of information: This is clear for the collision tensor, which is the same for every spatial DoF and does not change with time. Also the large sparse system matrix arising from the advection problem is assembled once and then reused in every time step. The contributions of the boundary conditions are evaluated on-the-fly, which can be done in $\mathcal{O}(K^3)$ compared to direct assembly into the system matrix which results in dense sub-blocks in the velocity degrees of freedom and involves cost of $\mathcal{O}(K^4)$ for the matrix-vector product. The fast evaluation of the boundary conditions is achieved by temporarily switching to a Lagrange basis located at the Gauss-Hermite quadrature nodes. For the solution of the advection problem we use the GMRES solver and ILU preconditioner with zero fill-in offered by Trilinos `12.2.1` [4]. The preconditioned GMRES solver converges typically in less than 10 iterations. No increase of the iteration count has been observed when ignoring the boundary conditions in the preconditioner. In order to avoid additional communication imposed by the preconditioner, we use a block-diagonal variant of ILU. The number of iterations required by the iterative solver does not depend on the number of processors.

The simulations are carried out on the Euler cluster of ETH Zürich. In the case of a physical mesh with $35k$ unknowns and polynomial degree $K = 30$ in velocity, which amounts to a total number $28.9M$ of unknowns, the code scales well up to 480 processors. Timings are reported in Table 1. Due to the operator splitting communication is required for the advection problem only. IO is done with the help of the parallel HDF5 library.

4 Mach Three Flow in a Wind Tunnel

We show numerical results for the famous Mach 3 wind tunnel experiment [8]. The computational domain describes a wind tunnel with a forward facing step at position $x = 0.6$ and of height 0.2. The gas is initially at equilibrium with temperature T_0=1, $\mathbf{v}$=[3, 0], $\rho = 1.4$. At $x\equiv$0 inflow boundary conditions with T=1, $\mathbf{v}$=[3, 0] are posed and outflow (zero inflow) boundary conditions at $x\equiv$3, the remaining walls are specularly reflective.

P	$t_A[ms]$	$t_S[ms]$	E
48	1,586	3,169	1
96	799	1,566	1.01
120	648	1,353	0.95
144	543	1,122	0.95
288	286	565	0.93
360	242	458	0.91
480	184	352	0.89

(a) K=30

P	$t_A[ms]$	$t_S[ms]$	E
24	1,316	912	1
48	662	454	1
96	341	236	0.96
120	277	187	0.96
144	230	158	0.96
288	129	84	0.87
360	112	68	0.83
480	83	51	0.83

(b) K=20

Table 1: Strong scaling for the Mach 3 wind tunnel experiment with $35k$ physical DoFs. P: number of processsors, t_A: time advection part (GMRES), t_S: time scattering, E: parallel efficiency. We observe a linear speedup in the scattering which dominates for larger values of K. A single node on Euler consists of two 12 core CPUs and 64 GB memory. The parallel efficiency for $K = 20$ was measured against a run on 24 cores. For $K = 30$ the memory requirements exceed the resources on a single node, therefore we have used the timings obtained on 48 cores as reference value. The reported timings were obtained by averaging over 100 repetitions.

The Knudsen number was $kn = 2.5 \times 10^{-3}$ for a Maxwellian gas. In Fig. 1 the pressure is shown at different times $t \in [0, 1]$ with Δt=2.5×10^{-5}. The results qualitatively agree with actual measurements carried out in a wind tunnel, cf. Woodward and Colella [8].

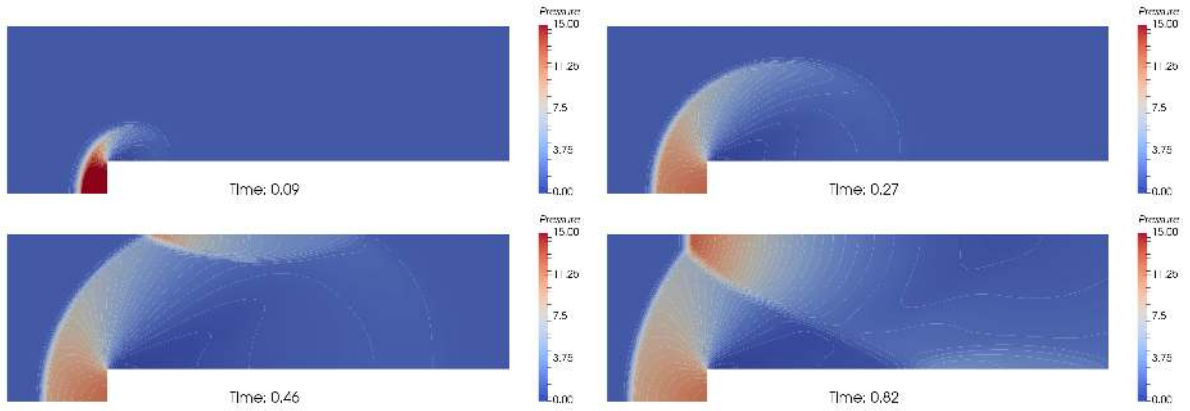
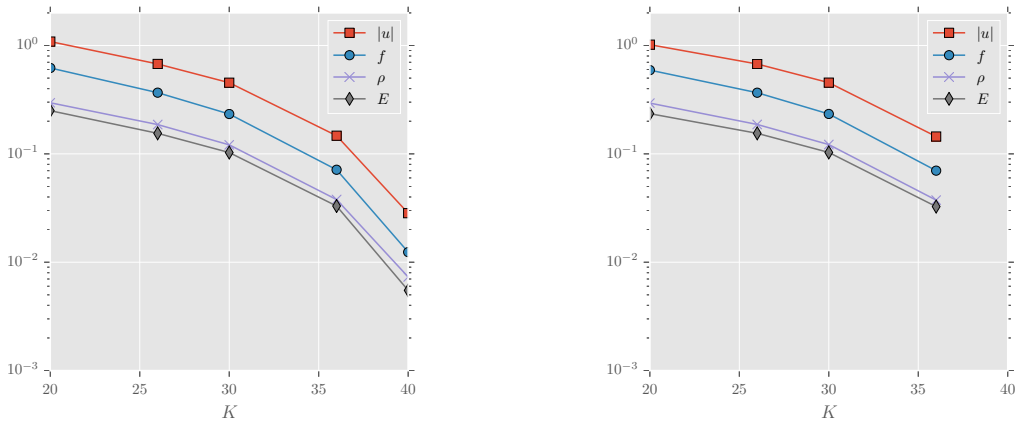


Figure 1: $28.9M$ total DoFs, polynomial degree K=40. Coloring: pressure, contour lines: density. Computations were carried out on the Euler cluster of ETH Zurich (Xeon E5-2697 v2) with 480 cores.



(a) Number of phys. DoFs L=8945

(b) Number of phys. DoFs L=35 297

Figure 2: Relative L_2-errors vs. polynomial degree K for two different physical meshes. The solution on the finer grid with highest polynomial degree K=40 was used as reference. Errors are shown for the velocity distribution function f and the macroscopic observables: mass ρ, momentum $\mathbf{u}$ and energy E. The error is dominated by the polynomial degree K. For simulations with higher Knudsen numbers (rarefied gases) and smooth initial distributions we observe faster convergence and smaller absolute errors.

References

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5

CSE Research Projects

Title: **Fault tolerance in Multilevel Monte Carlo methods**

Researchers: Peter Arbenz[⋆]
Stefan Pauli[⋆]
Christoph Schwab[†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]Seminar für Angewandte Mathematik, ETH Zürich

Description:
In large scale simulations on emerging, massively parallel computing platforms processor failures at runtime are inevitable and occur, in fact, with increasing frequency as the number of processors increases. We investigate a fault tolerant Monte Carlo (FT-MC) and a fault tolerant multi-level Monte Carlo (FT-MLMC) method neither relying on checkpoint/restart nor on recomputation of samples. Instead we propose to use all surviving samples (i.e. samples unaffected by failures) in the computation of the end result, and simply ignore samples affected by a failure. Failures therefore do not lead to an overhead, but potentially lower the quality of the results.

References:

S. Pauli, P. Arbenz: *Determining optimal multilevel Monte Carlo parameters with application to fault tolerance*. Comput. Math. Appl. (2015) doi:10.1016/j.camwa.2015.07.011.

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S. Pauli, M. Kohler, P. Arbenz: *A fault tolerant implementation of multi-level Monte Carlo methods*. Parallel Computing: Accelerating Computational Science and Engineering (CSE). M. Bader et al. (eds.). Parallel Computing: Accelerating Computational Science and Engineering (CSE), Advances in Parallel Computing 25, IOS Press, 2014, pp. 471–480.

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

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

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]ARTORG Center, University of Bern

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 preconditioned GMRES solver. The parallel performance of this algorithm is illustrated by a number of numerical experiments in one and two space dimensions.

References:

D. Hupp, P. Arbenz, and D. Obrist. A parallel Navier–Stokes solver using spectral discretization in time. Int. J. Comput. Fluid Dyn., 2015. submitted.

D. Hupp, D. Obrist, P. Arbenz: *Multigrid preconditioning for time-periodic Navier–Stokes problems*. Proc. Appl. Math. Mech. (PAMM) 15, 595–596 (2015).

P. Arbenz, D. Hupp, D. Obrist: *A parallel solver for the time-periodic Navier–Stokes equations*. In: Parallel Processing and Applied Mathematics (PPAM 13), Part II. R. Wyrzykowski, J. Dongarra, K. Karczewski, J. Waśniewski (eds.). Lecture Notes in Computer Science 8385, pp. 291–300. Springer, Berlin, 2014.

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

Researchers: Peter Arbenz[⋆]
Cyril Flaig[⋆]
Ralph Müller[†]
Patrik Christen[†]

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

Description:

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

References:

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E. Turan, P. Arbenz: *Preconditioning aspects of large scale micro finite element analysis of 3D bone poroelasticity.* Parallel Comput. 40, 239–250 (2014).

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

Title: Investigation of wall heat transfer and thermal stratification under engine-relevant conditions

Institute/ Group: M. Schmitt[1], C.E. Frouzakis[1], Y.M. Wright[1], A.G. Tomboulides[2], K. Boulouchos[1]
[1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]Department of Mechanical Engineering, University of Western Macedonia, 50100 Kozani, Greece

Unsteady wall heat transfer and thermal stratification during the compression stroke under engine relevant conditions were investigated using direct numerical simulations (DNS). In order to avoid artificial initial and boundary conditions the initial conditions were obtained from a separate DNS of the intake stroke involving thermal and composition mixing. The dynamically changing thermodynamic properties were found to strongly affect turbulence and wall heat transfer during the compression stroke. The increasing pressure results in a strongly reduced kinematic viscosity, and thus in significantly reduced length scales in the flow and temperature fields towards the top dead center (TDC). This has a direct impact on wall heat transfer, since reduced length scales lead to increased temperature gradients at the walls. Hence the heat transfer coefficient, which expresses the hydrodynamic influence on the heat transfer, increases by a factor of approximately five during compression. For the simulated conditions, the heat transfer coefficient extracted from the DNS data is found to agree reasonably well with the global correlation by Hohenberg but deviates strongly from the Woschni correlation. The influence of the boundary layers is not limited to the region close to walls, since close to TDC it affects the temperature distribution in the cylinder core. Vortical structures are identified, which transport cold gases from the boundary layer into the inner cylinder indicating that the assumption of an isentropic core temperature in the inner cylinder is not valid.

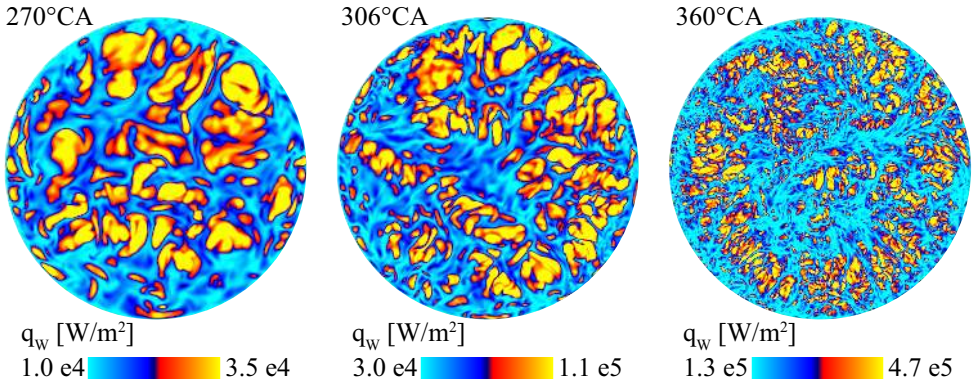


Figure 1: Distribution of wall heat flux on the cylinder head at 270^o, 306^o and 360^o crank angle.

References:

• M. Schmitt, C.E. Frouzakis, Y.M. Wright, A.G. Tomboulides, K. Boulouchos, Investigation of wall heat transfer and thermal stratification under engine-relevant conditions using DNS, Int. J. Eng. Res., 1-13, 2015

Title: Direct numerical simulation of the compression stroke under engine-relevant conditions: Evolution of the velocity and thermal boundary layers

Institute/ Group: M. Schmitt[1], C.E. Frouzakis[1], Y.M. Wright[1], A.G. Tomboulides[2], K. Boulouchos[1]
[1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]Department of Mechanical Engineering, University of Western Macedonia, 50100 Kozani, Greece

The unsteady velocity and thermal boundary layers during the compression stroke under engine-relevant conditions were investigated numerically using realistic initial conditions from a precursor direct numerical simulation (DNS) of the intake stroke. The results show decreasing velocity and thermal boundary-layer thicknesses towards Top Dead Center (TDC) due to decreasing kinematic viscosity. Compared to the fluctuating flow field, the azimuthally-averaged velocities are found to have a minor effect on the boundary-layer profiles and the structures at all engine walls during compression become similar. The averaged velocity and thermal boundary-layer profiles deviate strongly from the law-of-the-wall, the basis for many wall heat transfer models in internal combustion engines. In density wall-normal units, the averaged and the rms boundary-layer profiles for velocity and temperature collapse onto a single curve during the whole compression stroke. Finally, the data showed that between 60% and 80% of the total wall heat losses are attributed to convective transport due to wall-normal velocity fluctuations.

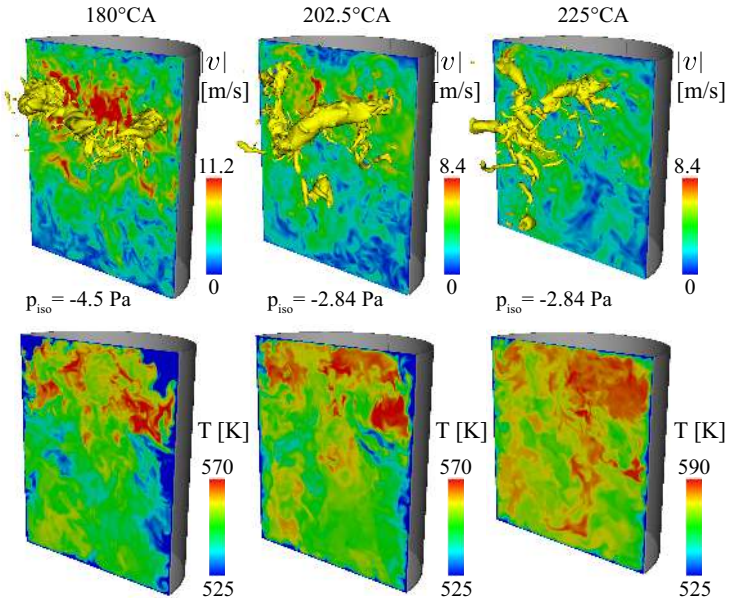


Figure 2: Distribution of velocity magnitude and temperature on axial slices at 180^o, 202.5^o and 225^o crank angle. The yellow pressure isosurfaces show the breakup of the central vortex ring.

References:

• M. Schmitt, C.E. Frouzakis, Y.M. Wright, A.G. Tomboulides, K. Boulouchos, Direct numerical simulation of the compression stroke under engine-relevant conditions: Evolution of the velocity and thermal boundary layers, Int. J. Heat Mass Transfer, 91, 948-960, 2015

Title: Comparison of Direct and Large Eddy Simulations of the Turbulent Flow in a Valve/Piston Assembly

Institute/ Group: Andrea Montorfano[1], Federico Piscaglia[1], Martin Schmitt[2], Yuri M. Wright[2], Christos E. Frouzakis[2], Ananias G. Tomboulides[3], Konstantinos Boulouchos[2], Angelo Onorati[1] [1] Energy Department, Politecnico di Milano, Milano, Italy
[2]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[3]Department of Mechanical Engineering, University of Western Macedonia, 50100 Kozani, Greece

The dynamics and evolution of the turbulent flow inside an experimentally investigated engine-like geometry consisting of a flat-top cylinder head with a fixed, axis-centered valve and low-speed piston were studied numerically by means of Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES), with a particular focus on Cycle-to-Cycle Variability (CCV). DNS was performed by the spectral element code nek5000 on a 58M points grid, whereas LES was carried out by the finite volume software OpenFOAM on a 4.6M hexahedral mesh. Results obtained by DNS and LES are compared with respect to the velocity means and fluctuations, as well with other derived quantities, showing good agreement between simulations and experiments. The cyclic variability and complex unsteady flow features like the laminar-to-turbulent transition and the evolution of the tumble vortices were studied by time-resolved analysis and Proper Orthogonal Decomposition (POD). Simulations show that during the first half of the intake stroke the flow field is dominated by the dynamics of the incoming jet and the vortex rings it creates. With decreasing piston speed, the large central ring becomes the dominant flow feature until the top dead center. The flow field at the end of the previous cycle is found to have a strong effect on the jet breakup process and the dynamics of the vortex ring below the valve of the subsequent cycle as well as on the observed significant cyclic variations.

References:

• A. Montorfano, F. Piscaglia, M. Schmitt, Y. M. Wright, C.E. Frouzakis, A.G. Tomboulides, K. Boulouchos, A. Onorati, Comparison of Direct and Large Eddy Simulations of the Turbulent Flow in a Valve/Piston Assembly *Flow, Turb. Combust.* 95(2), 461-480, 2015

Title:	n-Heptane/air combustion in perfectly stirred reactors: Dynamics, bifurcations and dominant reactions at critical conditions
Institute/ Group:	Mahdi Kooshkbaghi, Christos E. Frouzakis, Ilya V. Karlin, Konstantinos Boulouchos Aerothermochemistry and Combustion Systems Laboratory, ETHZ

The dynamics of n-heptane/air mixtures in perfectly stirred reactors (PSR) was investigated systematically using bifurcation and stability analysis and time integration. A skeletal mechanism of n-heptane constructed by entropy production analysis was employed, which was extensively validated for different conditions with respect to the ignition delay time, laminar flame speed, and the typical hysteretic behavior observed in PSRs. The significantly reduced size of the skeletal mechanism, enables the extension of the bifurcation analysis to multiple parameters. In addition to residence time, the effect of equivalence ratio, volumetric heat loss and the simultaneous variation of residence time and inlet temperature on the reactor state were investigated using one- and two-parameter continuations. Multiple ignition and extinction turning points leading to steady state multiplicity and oscillatory behavior of both the strongly burning and the cool flames were found, which can lead to oscillatory (dynamic) extinction. The two-parameter continuations revealed isolas and codimension-two bifurcations (cusp, BogdanovTakens, and double Hopf). Computational Singular Perturbation (CSP) and entropy production analysis were used to probe the complex kinetics at interesting points of the bifurcation diagrams.

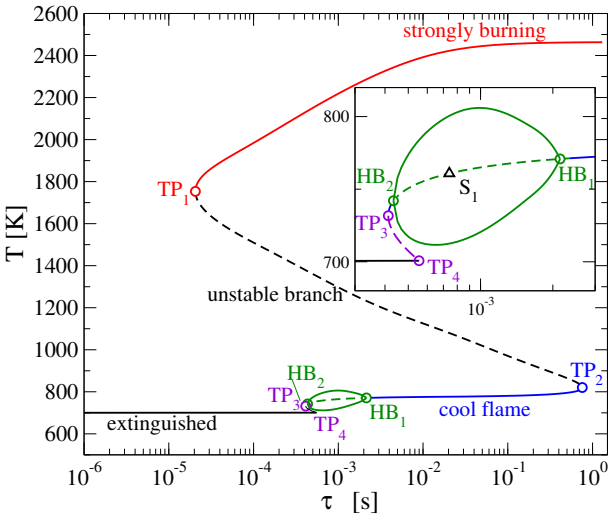


Figure 3: Reactor temperature as a function of residence time for a stoichiometric n-heptane/air mixture ($p = 1$ atm, $T_0 = 700$ K) in an adiabatic PSR. Solid (dashed) lines indicate stable (unstable) states, while the solid curves between the Hopf bifurcation points HB1 and HB2 of the expanded inset show the maximum and minimum reactor temperatures during the oscillations.

References:

• M. Kooshkbaghi, C.E. Frouzakis, I. Karlin, K. Boulouchos, n-Heptane/air combustion in perfectly stirred reactors: Dynamics, bifurcations and dominant reactions at critical conditions *Combust. Flame*, 161, 2692–2707, 2015

Group of Prof. C. Copéret and Dr. A. Comas-Vives (SNF Ambizione)
Laboratory of Inorganic Chemistry
ETH Zürich

www.coperetgroup.ethz.ch

Area(s) of Research: Computational Chemistry Surface Chemistry Heterogeneous Catalysis

Keywords:
DFT Calculations NMR Reaction Mechanisms Molecular Dynamics

Research Projects

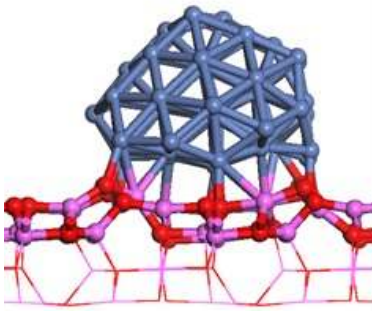
Title: Support Effects in Catalysis: The Case of Dry Reforming (SNF Ambizione Fellowship PZ00P2_148059).

Researchers: Lucas Foppa, Màrius-Christian Silaghi, Christophe Copéret, Aleix Comas-Vives

Institute/Group: Laboratory of Inorganic Chemistry/Copéret Group

Description:

Ni is the most used metal-based catalyst for dry reforming because of economic reasons although noble metals present better performances and are less prone to coke formation. Oxides such as Al_2O_3 are typically used in industry since it is stable at high temperatures and in the presence of steam. Despite all the studies devoted to understand the mechanism of dry reforming the evaluation of the whole reaction mechanism has been just partially addressed and needs further investigation on more realistic metal/support systems. For example, Al_2O_3 is able to adsorb CO_2, it can provide OH groups, it is "strongly interacting" with metallic particles and it is even able to activate CH_4. Also, the role of the metal/support interface is unclear. In this sense, some studies have proposed that the metallic atoms near the metal-support perimeter determine the catalytic activity, stressing the role of the metal/support interface. The aim of this research project is to study by means of *ab initio* calculations the dry reforming reaction occurring on Ni and Pt metallic nanoparticles supported on Al_2O_3 and SiO_2. The specific aims of this research project include the evaluation of the adsorption of reactants and products on the metallic particles and the supports, the optimization of Ni and Pt nanoparticles, the construction of the supported nanoparticles on SiO_2 and Al_2O_3 and the mechanistic evaluation of dry reforming on such systems. The current study will provide a better understanding of dry reforming from an atomistic point of view of "real" metal/support systems.



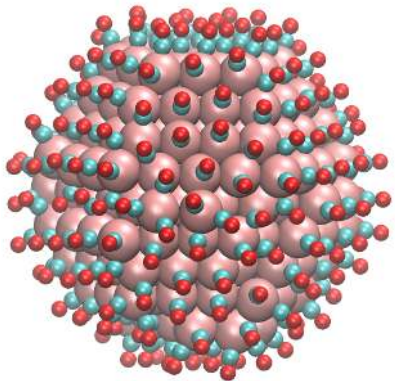
Title: Understanding Interfaces in Fischer-Tropsch Catalysts: An *Ab Initio* Approach (ETH Research Grant ETH-42 14-1)

Researchers: Lucas Foppa, Christophe Copéret, Aleix Comas-Vives

Institute/Group: Laboratory of Inorganic Chemistry / Copéret Group

Description

The gas-to-liquid technologies convert syngas (CO + H_2) to hydrocarbons via the Fischer-Tropsch reaction. This reaction, widely used in chemical and energy related industries, is catalyzed by metallic nanoparticles supported on oxides. Among the metals active in the Fischer-Tropsch reaction, Ru is the most active and selective one towards long-chain of hydrocarbons. However, not only the nature of the metallic particles but also the support can drastically affect the reactivity. When Ru nanoparticles are supported on modified SiO_2, in which $OSiMe_3$ (TMS) groups have substituted the OH ones, important changes on the selectivity and activity of the methanation reaction occur.[1] The aim of this project is to investigate by means of *ab initio* calculations the CO and H_2 chemisorption on the Ru nanoparticles supported on SiO_2 and on TMS-modified SiO_2 to achieve a better understanding at atomistic level of these systems. We are evaluating the CO and H_2 adsorption on Ru model surfaces and nanoparticles,[2] and the study of the metal/support interactions and the CO and H_2 chemisorption on the Ru/SiO_2 and Ru/SiO_2-TMS systems. For these purposes, static and dynamic *ab initio* simulations are being performed using state-of-the-art computational codes. Finally, the CO activation step with and without H_2 assistance is being evaluated on the Ru nanoparticle by means of metadynamics simulations, which are rather challenging calculations for heterogeneous catalyst.
The results of this investigation will shed light on the knowledge at molecular level of these industrially relevant catalysts, a key step for a rational design of more active, selective and efficient catalysts for fuel production.



References

1. Furman, K.; Baudouin, D.; Margossian, T.; Sabnis, K. D.; Cui, Y.; Ribeiro, F. H.; Copéret, C., *J. Catal.* **2015,** *324*, 9-13.

2. Comas-Vives, A.; Furman, F.; Gajan, D.; Akatay, M. C.; Lesage, A.; Ribeiro, F. H.; Copéret, C., *submitted.*

Title: Understanding active sites of single-site, zeolite and metal oxide supports

Researchers: Màrius Christian Silaghi, Kim Larmier, Erwin Lam, Aleix Comas-Vives and Christophe Copéret

Institute/Group: Laboratory of Inorganic Chemistry / Copéret Group

Description:

This research project focuses on the characterization of the active sites in several heterogeneous catalysts and the evaluation of their reactivity by means of DFT calculations. *Ab Initio* simulations are very useful in order to assign the experimental signals obtained by IR, NMR or EPR spectroscopy. In the recent years, we have been working on the characterization of single-sites on silica surfaces, such as Cr^{3+} sites active in ethylene polymerization and propane dehydrogenation and on the evaluation of their reactivity by means of DFT calculations.[1,2] In parallel, we are also working on developing more realistic periodic models of highly dehydroxylated silica, a widely used support in heterogeneous catalysis. We have also assigned the most likely active sites of Sn-β catalysts by means of *ab initio* simulations of ^{119}Sn NMR characterization tools in order to determine which is the nature of the active sites under aqueous media.[3] The reactivity of metal oxides such as γ-alumina surfaces has been another subject of interest. We have recently found that highly acidic Al_{III} sites present on the 110 termination of γ-Al_2O_3 are able to promote the formation of carbon-carbon bonds from C_1 compounds such as CH_3F or CH_3OCH_3.[4,5]

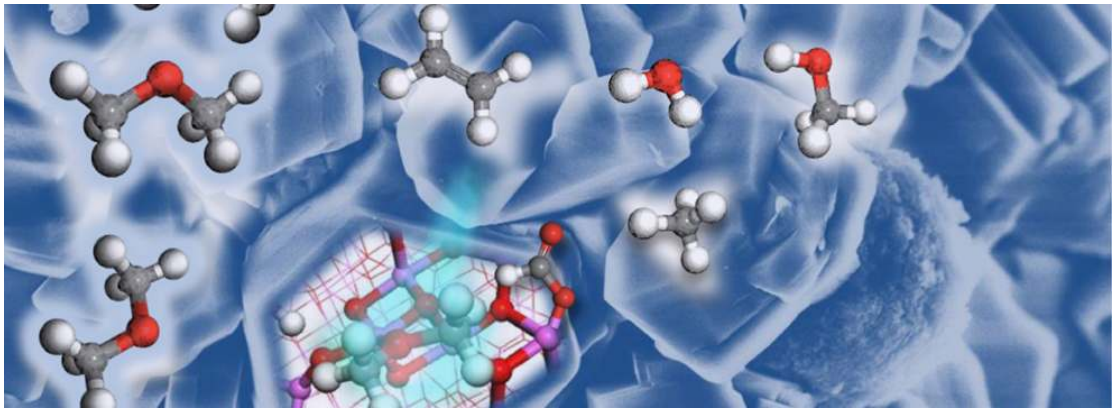


Figure. Methanol/Dimethyl Ether Conversion to Fuels on the γ-Al_2O_3 surface.

References:

1. Delley, M. F.; Núñez-Zarur, F.; Conley, M. P.; Comas-Vives, A.; Siddiqi, G.; Norsic, S.; Monteil, V.; Safonova, O. V.; Copéret, C., *PNAS*, **2014,** *111*, 11624-11629.
2. Conley, M. P.; Delley, M. F.; Núñez-Zarur, F.; Comas-Vives, A.; Copéret, C., *Inorg. Chem.* **2015**, *54*, 5065-5078.
3 Wolf, P.; Valla, M.; Rossini, A. J.; Comas-Vives, A.; Núñez-Zarur, F.; Malaman, B.; Lesage, A.; Emsley, L.; Copéret, C.; Hermans, I., *Angew. Chem. Int. Ed.* **2014**, *53*, 10179-10183.
4. Comas-Vives, A.; Schwarzwälder, M.; Copéret, C.; Sautet, P., *J. Phys. Chem. C* **2015**, *119*, 7156-7163.
5. Comas-Vives, A.; Valla, M.; Copéret, C.; Sautet, P., *ACS Cent. Sci.* **2015**, *1*, 313-319.

Group of D. Giardini

Title: Waveform-based images of seismic velocity variations underneath Europe embedded in a global model: a hybrid approach

Researchers: Ludwig Auer, Lapo Boschi, Simon Stähler, Kasra Hosseini, Martin van Driel, Tarje Nissen-Meyer, Domenico Giardini

Institute of Geophysics, Department of Earth Sciences

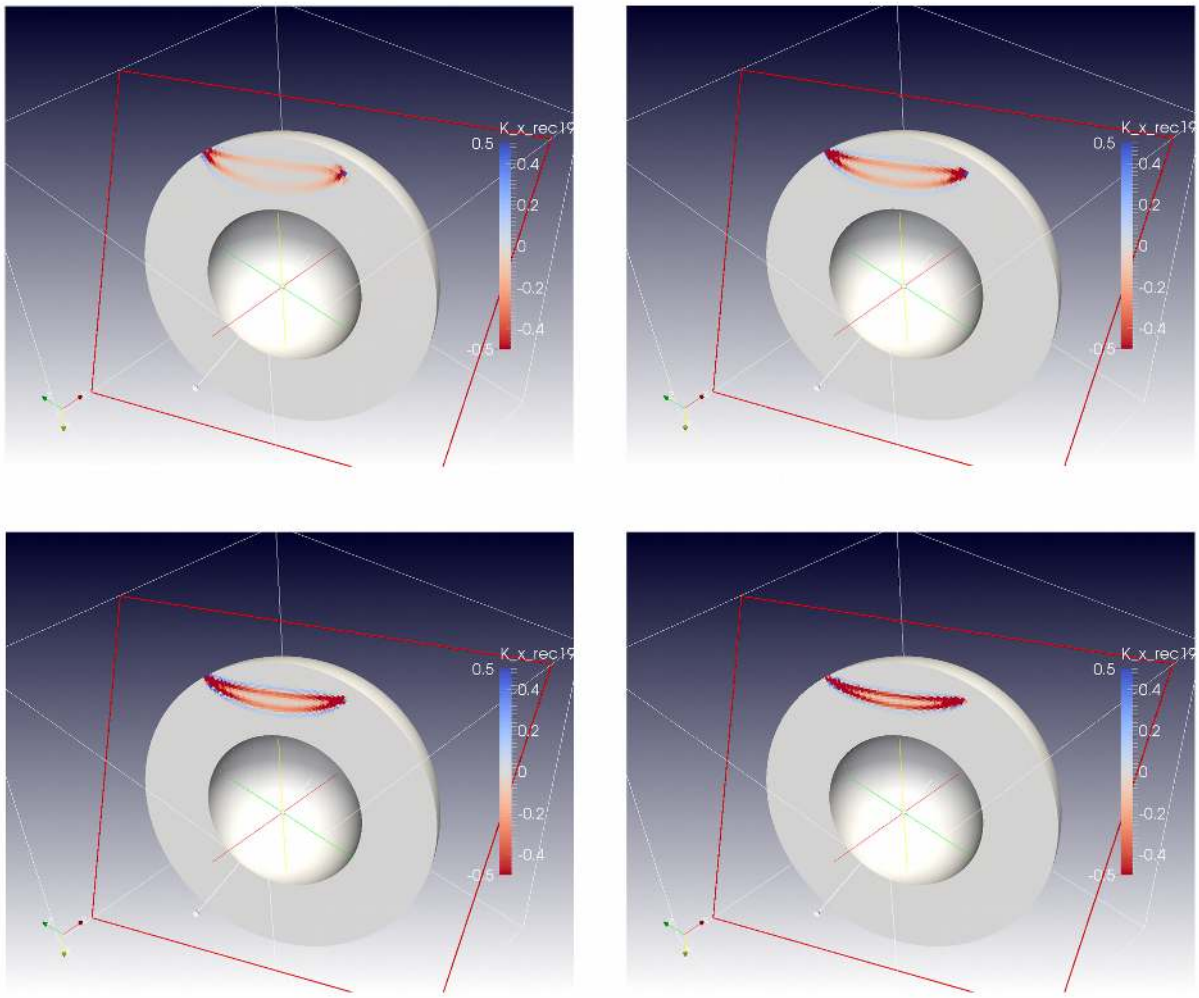
Description:

In a recent study (Auer et al., 2014) we have devised a novel tomography approach to image radially anisotropic velocity variations in the Earth's mantle. By applying our tomography toolbox to a comprehensive compilation of surface-wave phase delays from fundamental modes up to the 6th overtone and cross-correlation traveltimes of major body-wave phases, we derived the multi-resolution tomography model SAVANI, which is one of the first whole-mantle models of radial S-wave anisotropy. In the endeavour to develop the second iteration of our model we have added P-wave constraints and define Europe and the surrounding regions as the target area for a higher-resolution regional revision of our initial model. Importantly, regional waveform observations will be interpreted using Fréchet sensitivity kernels computed with AxiSEM (Nissen-Meyer et al., 2014), which is an efficient visco-elastic spectral element solver for axisymmetric background models. The main idea behind our new model is to keep semi-approximate (ray) theory where appropriate (global long-wavelength structure, surface wave dispersion), but to revert to a full-waveform interpretation where necessary (regional scale, non-geometrical wave phenomena). Our hybrid approach to waveform inversion has multi-scale capabilities and is essentially equivalent to the first iteration step of a Gauss-Newton type inverse problem, thus allowing full access to the model resolution matrix. The set of algorithms we are developing represent a straightforward manner to stepwise improve upon a global background model by updating the tomographic system whenever new data becomes available. Computing Fréchet sensitivity functions is computationally challangening, since they involve an expensive interpolation upon inversion grids and require the availability of high-resolution global wavefields. We perform kernel quadrature using a Monte-Carlo Integration approach, implemented in a novel software package, parallelized using a Master-Slave communication, that we run on the CSCS cluster Mönch on up to 1000 cores. Preliminary estimates indicate computational costs of around 1 CPU/hr per kernel, rendering the problem of global waveform inversions with a few millions of kernels at high frequency tractable.

References:

Auer, L., Boschi , L., Becker, T. W., Nissen-Meyer, T. and Giardini, D.: Savani: a variable-resolution whole-mantle model of anisotropic shear-velocity variations based on multiple datasets. J. Geophys. Res., 2014. doi:10.1002/2013JB010773

Nissen-Meyer, T., van Driel, M., Stähler, S., Hosseini, K., Hempel, S., Auer, L., Colombi, A., and A. Fournier.: AxiSEM: Broadband 3D seismic wavefields in axisymmetric media. Solid Earth Discuss., 2014. doi:10.5194/sed-6-265-2014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Title: Large High-frequency Green's Function Databases for the Mars InSight Mission

Researchers: Martin van Driel, Amir Khan, Maren Boese, John Clinton, Domenico Giardini

Institute of Geophysics, Department of Earth Sciences

Description: The upcoming NASA-lead Mars InSight mission, to be launched in March 2016 and scheduled to
land September 2016, will deploy a seismometer on Mars. This will be the first extra-terrestrial seismic mission since the Apollo lunar landings (1969--1972) and Mars Viking missions (1975) with the goal of investigating the interior structure of a planet other than Earth.

In this project we analyze a number of seismic models of Mars for seismic response to gain understanding for which seismic experiments within the framework of the InSight mission will be able to address questions concerning interior structure, origin and evolution of Mars.

To compute the seismic response of Mars, we rely on AxiSEM, which is a parallelized spectral-element method that efficiently computes the full seismic wavefield on planetary scales.

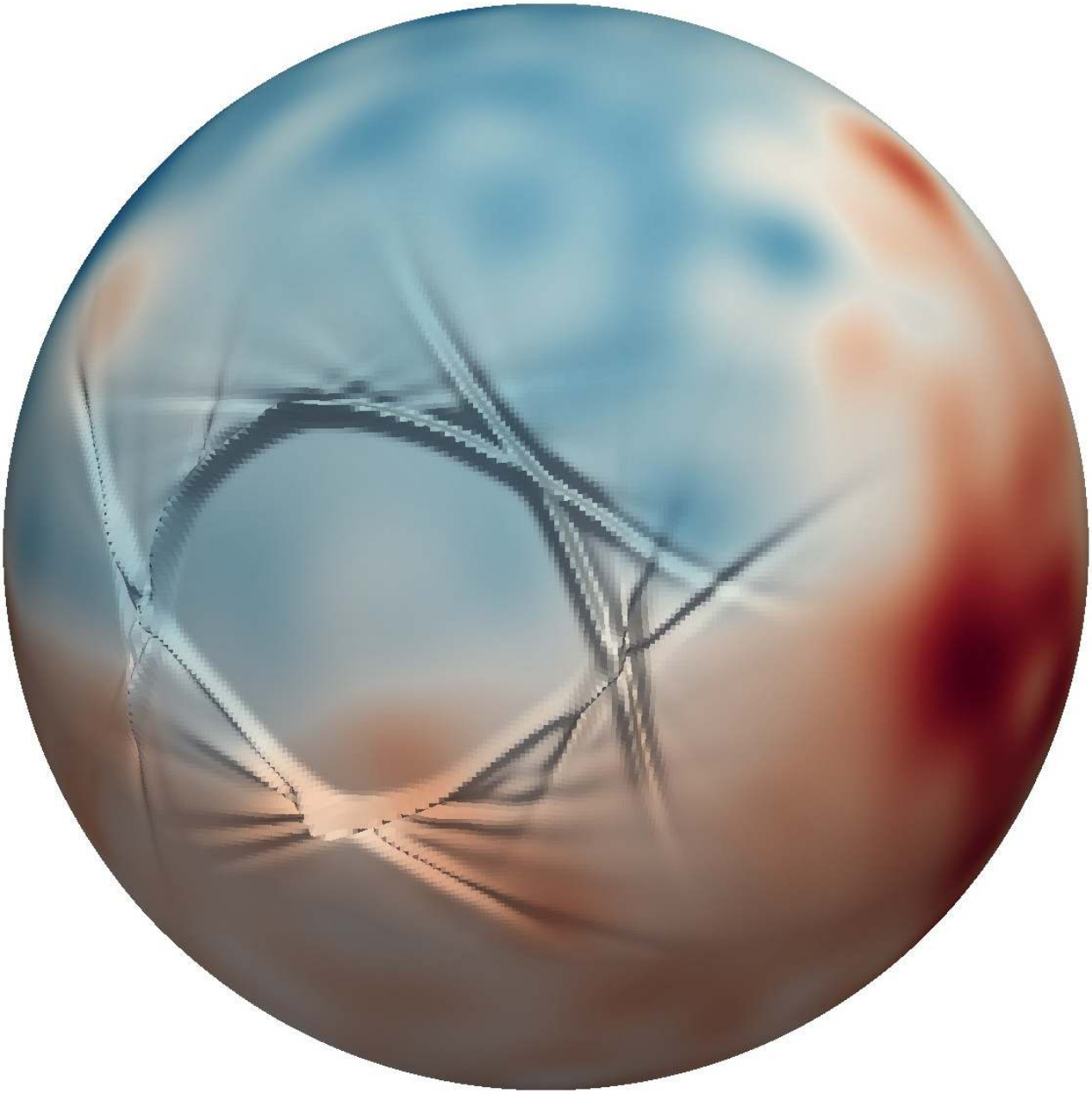
The Figure shows a visualization of seismic surface waves on Mars close to refocussing on the antipode. The background colorscale indicates phase velocity perturbations due to crustal thickness variations.

References:

van Driel, Martin, L. Krischer, S. C. Stähler, K. Hosseini, and T. Nissen-Meyer. 2015. “Instaseis: Instant Global Seismograms Based on a Broadband Waveform Database.” Solid Earth 6 (2): 701–717. doi:10.5194/se-6-701-2015.

A. Khan, M. Bose, M. van Driel, J. Clinton, D. Giardini. 2015. "Single-station probabilistic marsquake location and inversion for structure using synthetic martian seismograms, surface-wave dispersion data, and body-wave travel times", to be submitted to Physics of the Earth and Planetary Interiors.

Nissen-Meyer, T., Martin van Driel, S. C. Stähler, K. Hosseini, S. Hempel, L. Auer, A. Colombi, and A. Fournier. 2014. “AxiSEM: Broadband 3-D Seismic Wavefields in Axisymmetric Media.” Solid Earth 5 (1) (June 4): 425–445. doi:10.5194/se-5-425-2014.



Title: Design and optimization of electromagnetic structures and devices

Researchers: Jürg Leuthold
Christian Hafner
Sascha Schnepp
Jens Niegemann
Nikolay Komarevsky
Alexandros Emboras
Mustafa Boyvat
Alexander Dorodnyy
Sahar Sargheini
Pegah Souzanghar
Uli Koch
Christian Haffner

Institute Institute of Electromagnetic Fields

Description:

We develop various numerical methods and software packages for computational electromagnetics and optimal design with applications ranging from very low up to optical frequencies. These codes, free software (freeFEM++, NGsolve, Concepts) and commercial packages (Comsol, CST, HFSS, etc.) are applied to 1) metamaterials for magnetic field shielding, radar absorption, thermal protection, and efficient solar cells; 2) photonic crystals, dielectric and plasmonic waveguide structures for optical frequencies and for fast interconnects in the mm wave range; 3) ultra-compact plasmonic devices for optical communication such as modulators, switches, etc., 4) design of antenna structures ranging from radio frequencies up to optical frequencies, e.g., plasmonic nano antennas for bio sensing; 5) analysis and design of scanning probe tips for microwaves, optics, and electron emission; etc.
Currently we develop and combine various field solvers based on boundary discretization methods such as the Multiple Multipole Program (MMP) as well as domain discretization methods in frequency and time domain, namely Finite Elements Methods (FEM), Discontinuous Galerkin (DG), Fourier Modal Method (FMM), etc.
Our MMP and FDTD codes are contained in the OpenMaXwell platform, which is an OpenSource project (see http://openmax.ethz.ch/).
We link our electromagnetic field simulation codes with other software, e.g., for handling quantum effects and for optimizing structures and devices. We use freely available optimizers but we also develop our own codes for increasing the efficiency.

References:
From fall 2014 till fall 2015, 12 papers on various topics of computational electromagnetics were published in reviewed journals.

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

Description:

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

Understanding social systems from fundamental principles is one of the most important scientific challenges of the modern area. The main objective of the simulation of sophisticated interacting agents is to show how other-regarding human behavior (characterizing a "homo socialis") can be the result of competition and the co-evolution of social mechanisms. Our models will not assume that actors are equipped with certain social institutions already at the outset of the evolutionary process. We want to demonstrate that, for example, social cooperation and social norms are not static features of societies, but rather emergent outcomes of repeated and multifaceted interactions between many individuals. Rather than *implementing* "homophily", cooperation, norms, inequality, conflict etc. as features of our simulated model societies, we want to understand them as outcomes of a co-evolutionary process in which individual behaviors, social interactions, learning processes and their interplay evolve over time. We study how for example meritocracy can lead to pro-social behavior.

This year we made progress on several of the proposal's main themes, in particular in explaining the emergence of cooperation and co-evolutionary processes. Our results span theoretic, simulation and experimental techniques.

References:

D. Helbing, and H. Gintis. (2015). Homo Socialis: An Analytical Core for Sociological Theory. Review of Behavioral Economics, 2 (1-2): 1-59.
[The entire Review of Behavioral Economics, 2 (1-2), is dedicated as a double-special issue to this target article (edited by J. Barkley Rosser, Jr.)

H. H. Nax, M. Perc, A. Szolnoki, D. Helbing. (2015). Stability of cooperation under image scoring in group interactions. Scientific Reports 5: 12145.

C. Efferson, C. P. Roca, S. Vogt & D. Helbing (2015). Sustained cooperation by running away from bad behavior. Evolution and Human Behavior

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

Description:

Nervousnet: (www.nervousnet.ch)

The planetary nervous system is a large-scale distributed research platform that provides real-time social sensing services as a public good. Existing Big Data systems threaten social cohesion as they are designed to be closed, proprietary, privacy-intrusive and discriminatory. In contrast, the Planetary Nervous System is an open, privacy-preserving and participatory platform designed to be collectively built by citizens and for citizens.

The planetary nervous system is enabled by Internet of Things technologies and aims at seamlessly interconnecting a large number of different pervasive devices, e.g. mobile phones, smart sensors, etc. For this purpose, several universal state-of-the-art protocols and communication means are introduced. A novel social sensing paradigm shift is engineered: Users are provided with freedom and incentives to share, collect and, at the same time, protect data of their digital environment in real-time. In this way, socialsensing turns into a knowledge extraction service of public good.

The social sensing services of the planetary nervous system can be publicly used for building novel innovative applications. Whether you would like to detect an earthquake, perform a secure evacuation or discover the hot spots of a visited city, the Planetary Nervous system makes this possible by collectively sensing social activity of participatory citizens.

SwarmPulse: (www.swarmpulse.net)

The SwarmPulse service allows for collective visualization and sharing of mobile sensor data, messages, media files and website links. The "SwarmPulse" service is built on top of the Nervousnet research platform, a large-scale distributed research platform that provides real-time social sensing services as a public good. Existing Big Data systems threaten social cohesion as they are designed to be closed, proprietary, privacy-intrusive and discriminatory. In contrast, the Planetary Nervous System is an open, privacy-preserving and participatory platform designed to be collectively built by citizens and for citizens.
The SwarmPulse mobile app allows the user to share mobile sensor data and text messages from their mobile phone and to see a collective visualization on the SwarmPulse website (www.swarmpulse.net).

References:

- D. Helbing and E. Pournaras, "Build a digital nervous system", Nature, Vol. 527, pp 33-34, Nov. 2015
- F. Giannotti, D. Pedreschi, P. Lukowicz, D. Kossmann, J. Crowley and D. Helbing (2013). A planetary nervous system for social mining and collective awareness. arXiv preprint arXiv:1304.3700.
- D. Helbing (2013). New Ways to Promote Sustainability and Social Well-Being in a Complex, Strongly Interdependent World: The FuturICT Approach. arXiv preprint arXiv:1310.3498.
- D. Helbing (2011). FuturICT-New science and technology to manage our complex, strongly connected world. arXiv preprint arXiv:1108.6131.

Title: Rayleigh-Bénard instability in graphene

Researchers: O. Furtmaier
M. Mendoza
I. Karlin
Prof. H. J. Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

Motivated by the observation that electrons in graphene, in the hydrodynamic regime of transport, can be treated as a two-dimensional ultrarelativistic gas with very low shear viscosity, we examine the existence of the Rayleigh-Bnard instability in a massless electron-hole plasma. First, we perform a linear stability analysis, derive the leading contributions to the relativistic Rayleigh number, and calculate the critical value above which the instability develops. By replacing typical values for graphene, such as thermal conductivity, shear viscosity, temperature, and sample sizes, we find that the instability might be experimentally observed in the near future. Additionally, we have performed simulations for vanishing reduced chemical potential and compare the measured critical Rayleigh number with the theoretical prediction, finding good agreement.

References:

[1] O. Furtmaier, M. Mendoza, I. Karlin, S. Succi, and H. J. Herrmann, Rayleigh-Bénard instability in graphene, Phys. Rev. B 91, 085401 (2015).

Title: Simulation of magnetoviscous effect in a ferromagnetic colloid

Researchers: D. Zablotsky
E. Blums
Prof. H. J. Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

The emerging applications of ferromagnetic colloids in biomedicine - in magnetic drug targeting, magnetic hyperthermia or imaging - require the understanding of the rheology of these materials in the conditions of the simultaneous influence of shear flow and magnetic field. It is known from previous studies that the ferrocolloids show strong magnetoviscous effect the dependence of their viscosity on the magnetic field. The presence of relatively minor amount of magnetic nanoparticles can lead to a dramatic increase of shear viscosity by up to several orders of magnitude [1-3].

We use numerical simulations to study the structure and rheology of ferromagnetic colloids in the presence of magnetic field. Using molecular dynamics and stochastic rotation dynamics we observe the assembly of suspended magnetic nanoparticles in linear chains (see figure) due to strong dipole-dipole interaction and the eventual destruction of chains under shear flow. We are able to determine the shear viscosity of the colloid, which shows significant shear thinning owing to the change of internal structure.

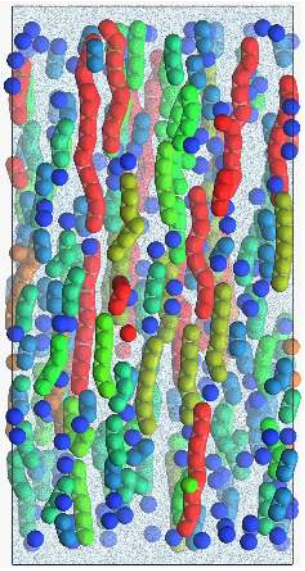


Figure 1: Simulation snapshot: structure of the ferrocolloid under shear and vertical magnetic field. Particles colored by cluster size.

References:

[1] J. Nowak et al., JMMM 354, 98 (2014).

[2] M. T. Lopez-Lopez et al., Langmuir 28, 6232 (2012).

[3] D. I. Santiago-Quinonez et al., Soft Matter 8, 5327 (2012).

Title: Orthotropic rotation-free thin shell elements

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

Institute: Institute for Building Materials
ETH Zürich

Description:

We propose a method to simulate orthotropic behaviour in thin shell finite elements. The approach is based on the transformation of shape function derivatives, resulting in a new orthogonal basis aligned to a specified preferred direction for all elements. This transformation is carried out solely in the undeformed state leaving minimal additional impact on the computational effort expended to simulate orthotropic materials compared to isotropic, resulting in a straightforward and highly efficient implementation. This method is implemented for rotation-free triangular shells using the finite element framework built on the KirchhoffLove theory employing subdivision surfaces. To showcase the efficiency of this implementation, the wrinkling of orthotropic sheets under shear displacement is analyzed (see figure). It is found that orthotropic subdivision shells are able to capture the wrinkling behavior of sheets accurately for coarse meshes without the use of an additional wrinkling model. Further work is being performed on the buckling of orthotropic spherical shells under external loading.

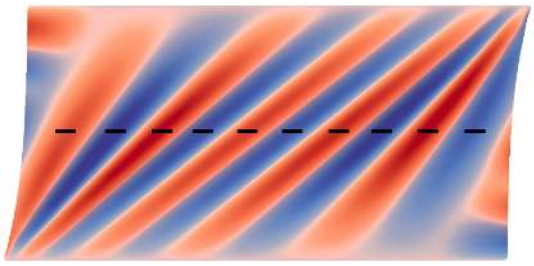


Figure 1: Wrinkling of an orthotropic sheet due to shear displacement.

References:

[1] G. Munglani, R. Vetter, F.K. Wittel, H.J. Herrmann, Orthotropic rotation-free thin shell elements, Computational Mechanics, Computational Mechanics 08/2015; DOI:10.1007/s00466-015-1202-x (2015).

Title: Continuous Fiber Reinforcement for Jammed Granular Architecture

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

Institute: Institute for Building Materials
ETH Zürich

Description:

The mechanical behavior of continuous fiber reinforced granular columns is simulated by means of a Discrete Element Model. Spherical particles are randomly deposited simultaneously with wire, that is deployed along different patterns inside of a flexible cylinder for triaxial compression testing. For three different configurations we quantify the effect of fiber deployment patterns on the failure envelope, represented by Mohr-Coulomb cones.

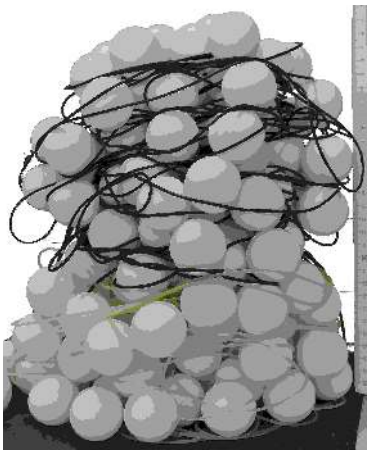


Figure 1: Free standing column of table tennis balls with continuous reinforcement.

Title: Predicting bearing states in three dimensions

Researchers: D. Stäger
N. A. M. Araújo
H. J. Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

Bichromatic bearings have an infinite number of sliding-free states, so called bearing states. For three-dimensional bichromatic bearings whose bearing states have four degrees of freedom, we show how the bearing state can be analytically predicted from the initial state without any information about the nature of the contact forces. We provide a systematic way of constructing such bearings and also show how the bearing state is modified by blocking a single sphere and that any bearing state can be induced by controlling the angular velocities of only two spheres. Furthermore, we show that it is possible to determine the total mass and the center of mass of the bearing by analyzing its response to changes of the angular velocities of at most two spheres.

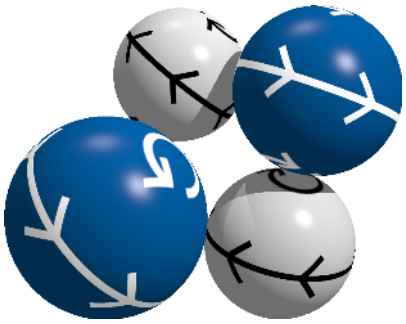


Figure 1: A single loop of four spheres whose centres do not lie in a common plane has a four dimensional set of possible slip-free states of rotation. By solely controlling the rotation of two spheres one can impose any of the possible slip-free states.

Title: Crumpling Damaged Graphene

Researchers: I. Giordanelli
M. Mendoza
J. S. Andrade
M. A. F. Gomes
H. J. Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

Through molecular mechanics we find that non-covalent interactions modify the fractality of crumpled damaged graphene. Pristine graphene membranes are damaged by adding random vacancies and carbon-hydrogen bonds. Crumpled membranes exhibit a fractal dimension of 2.71 ± 0.02 when all interactions between carbon atoms are considered, and 2.30 ± 0.05 when non-covalent interactions are suppressed. The transition between these two values, obtained by switching on/off the non-covalent interactions of equilibrium configurations, is shown to be reversible and independent on thermalisation. In order to explain this transition, we propose a theoretical model that is compatible with our numerical findings. Finally, we also compare damaged graphene membranes with other crumpled structures, as for instance, polymerised membranes and paper sheets, that share similar scaling properties.

Title: High Resolution Simulation Tool for Power Devices

Researchers: Raffael Casagrande
Dr. Christoph Winkelmann
Dr. Joerg Ostrowski
Prof. Dr. Ralf Hiptmair

Institute: Seminar for Applied Mathematics, ETH Zürich
ABB Corporate Research, Baden-Dättwil

Description:

The project has two main goals:

1. Enable arc-simulations of circuit breakers on hybrid, moving meshes, and
2. resolve the skin-effect in electromagnetic devices on coarse meshes.

The first part of the project was successfully completed by the end of 2014 [1] whereas the second part is research in progress: In order to resolve the skin layer on coarse meshes we use a-priori knowledge about the skin effect; For example on flat surfaces of conductors it is well known that the electric field strength decreases exponentially towards the interior. The idea is now to enrich the classical finite element space with such exponential basis functions, thus enabling the resolution of the exponential behavior on coarse meshes (see Fig. 1).

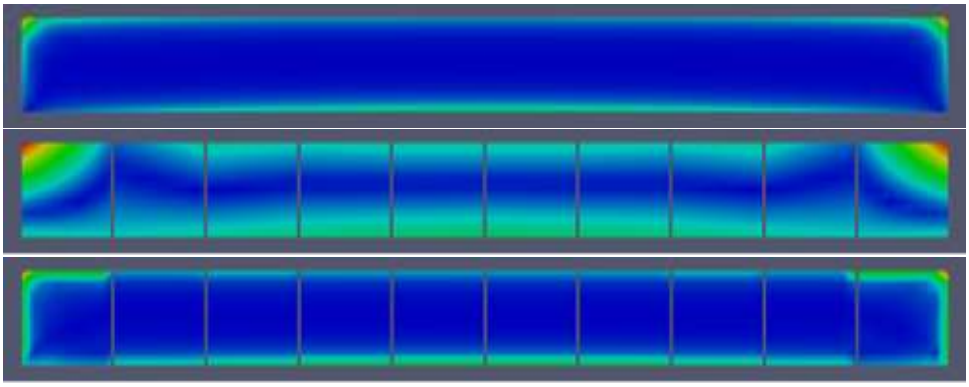


Figure 1: Top: distribution of the current density in a box-shaped conductor (excitation current is external and not shown).
Middle: Solution with first order edge elements on a coarse mesh.
Bottom: Solution with exponential basis functions on the same coarse mesh.

References

[1] R. Casagrande, C. Winkelmann, R. Hiptmair, and J. Ostrowski, *DG Treatment of Non-Conforming Interfaces in 3D Curl-Curl Problems*, SAM Report 32, ETH Zürich, 2014.

Title: **Shape optimization of microlenses**

Researchers: Alberto Paganini[2]
Sahar Sargheini[1,2]
Prof. Ralf Hiptmair[1]
Christian Hafner[2]

Institute: [1] Seminar for Applied Mathematics, ETH Zürich
[2] Institute of Electromagnetic Fields, ETH

Funding: partly ETH Grant CH1-02 11-1

Description: Microlenses are highly attractive for optical applications such as super resolution and photonic nanojets, but their design is more demanding than the one of larger lenses because resonance effects play an important role, which forces one to perform a full wave analysis. Although mostly spherical microlenses were studied in the past, they may have various shapes and their optimization is highly demanding, especially, when the shape is described with many parameters. We employ the shape optimization algorithm described in [1] and optimize the shape microlenses starting from different reasonable elliptical and semi-circular shapes. We show that strong increases of the performance of the lenses may be obtained for any reasonable value of the refraction index [2].

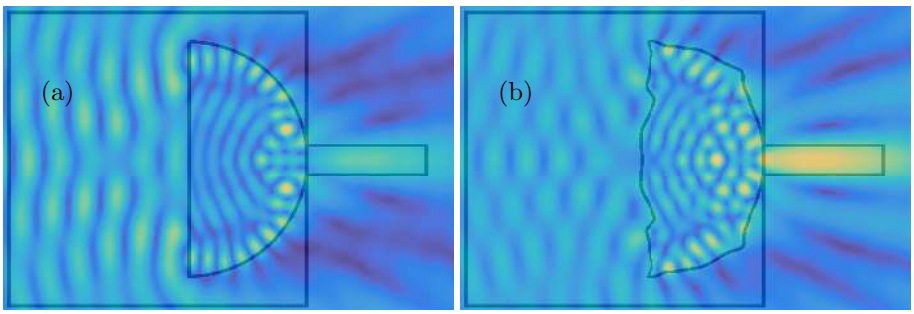


Figure 1: An incoming plane wave hits (from the left) a cylindrical lens with semi-circular cross section (a). The shape of the lens is optimized to maximize the focused light in the thing rectangle on the backside of the lens (b).

References

[1] R. Hiptmair and A. Paganini, *Shape optimization by pursuing diffeomorphisms*, Comput. Methods Appl. Math., 15 (2015), pp. 291–305.

[2] A. Paganini, S. Sargheini, R. Hiptmair, and C. Hafner, *Shape optimization of microlenses*, Opt. Express, 23 (2015), pp. 13099–13107.

Title: Auxiliary Space Preconditioners for DG Discretizations of H(curl)-elliptic Problems with Discontinuous Coefficients

Researchers: Cecilia Pagliantini (SAM, ETH Zürich)
Prof. Ralf Hiptmair (SAM, ETH Zürich)
Prof. Blanca Ayuso de Dios (Università di Bologna, Italy)

Institute: Seminar for Applied Mathematics, ETH Zürich

Funding: Swiss NSF Grant No. 146355.

Description: Second order H($\mathbf{curl}, \Omega$)-elliptic equations with discontinuous coefficients are ubiquitous in interface problems in electromagnetism or in time domain eddy current simulations with implicit time stepping.

We propose a family of preconditioners for linear systems of equations arising from a piecewise polynomial symmetric Interior Penalty Discontinuous Galerkin (DG) discretization of H($\mathbf{curl}, \Omega$)-elliptic boundary value problems on conforming meshes. The design and analysis of the proposed solvers relies on the auxiliary space method (ASM): The preconditioners are obtained for the non-conforming DG approximation by using an auxiliary space of H($\mathbf{curl}, \Omega$)-conforming finite elements together with a relaxation technique (local smoothing).

On simplicial meshes, the proposed preconditioners enjoy asymptotic optimality with respect to mesh refinement. Moreover, we address the influence on the asymptotic performance of the preconditioners of possible discontinuities in the coefficients α and β in the second and zero-th order parts of the operator respectively. Asymptotic optimality and robustness with respect to jumps in the coefficients can be shown, except when both coefficients are discontinuous and the problem is curl-dominated in some regions and reaction dominated in others.

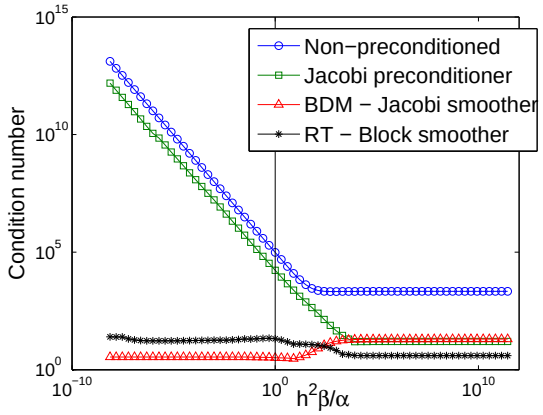


Figure 1: Condition number vs ratio $h^2\beta/\alpha$ for a fixed mesh size h: non-preconditioned system (blue), pointwise Jacobi preconditioner (green), ASM based on rotated $\mathcal{BDM}_1$ elements with pointwise Jacobi smoother (red) and ASM based on rotated $\mathcal{RT}_0$ elements with overlapping Schwarz smoother (black). Discretization: discontinuous lowest order rotated $\mathcal{BDM}_1$ elements.

References

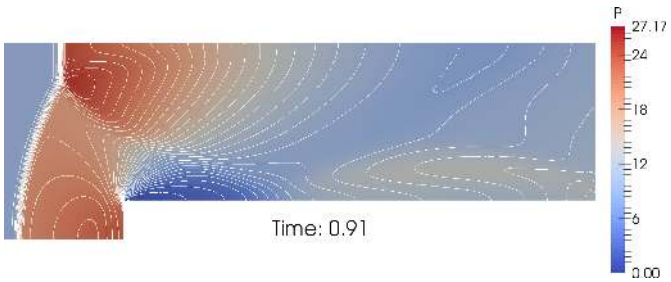
[1] B. Ayuso de Dios, R. Hiptmair and C. Pagliantini, *Auxiliary Space Preconditioners for SIP-DG Discretizations of H($\mathbf{curl}, \Omega$)-elliptic Problems with Discontinuous Coefficients*, Technical Report 2015-14, SAM, ETH Zürich, 2015.

Title: Numerical simulation of the time-dependent and spatially-inhomogeneous Boltzmann equation

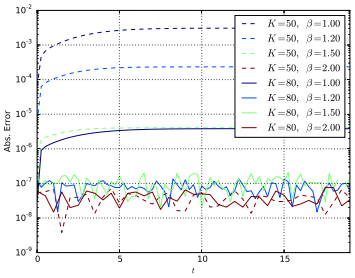
Researchers: Simon Pintarelli
Prof. Philipp Grohs
Prof. Ralf Hiptmair

Institute: Seminar for Applied Mathematics, ETH Zürich
Funding: SNF grant 200020_146356/1

Description: The time-dependent and spatially-inhomogeneous Boltzmann equation is considered. We use a least squares formulation to discretize the advection problem and combine it with a first order splitting method to solve the transient Boltzmann equation. The velocity distribution function is discretized based on Laguerre polynomials. In our scheme, the 3-dimensional scattering tensor can be precomputed, with the advantage that highly accurate quadrature is feasible. For this, previous work from [1] has been extended to obtain a conservative polar spectral discretization with good approximation properties across varying temperatures. We have developped an MPI-parallelized `C++` code , which is running on the Euler cluster of ETH. In future work rigdelets will be included into the existing simulation code.



(a) Mach-3 CFD benchmark problem. Inflow on left boundary, specular reflective wall, outflow boundary condition on the right. 820 DoFs in velocity, $35K$ DoFs on physical grid. Total: 28.7×10^6 DoFs, $40K$ timesteps. Plot shows the scalar pressure with the density as contour lines.



(b) L^2-errors vs. time. Spatially homogeneous case with analytically known solution. β-values correspond to conforming and non-conforming temperatures. K: max. polynomial degree in one direction.

Publications

[1] E. Fonn, P. Grohs, and R. Hiptmair, *Polar spectral scheme for the spatially homogeneous boltzmann equation*, Tech. Rep. 2014-13, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2014.

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

Description:

We consider time harmonic electromagnetic scattering at an object which has piecewise constant permittivity and assume that all homogeneous parts of the scatterer are curvilinear polygonal Lipschitz. We focus on the corresponding electric field integral equation. Since we have to cope with unbounded domains, boundary element approaches are a convenient tool for numerical treatment. Classical first-kind approaches are ill-conditioned and there is no suitable preconditioner available.

We establish a well-conditioned second-kind boundary element approach which uses $H_{\mathbf{t}}^{\delta}$ as test space for a fixed δ, $0 < \delta < \frac{1}{2}$. Here, $H_{\mathbf{t}}^{\delta}$ is the space of tangential vector fields of Sobolev regularity H^{δ}. As trial space we use its dual space $H_{\mathbf{t}}^{-\delta}$, $L_{\mathbf{t}}$ playing the role of the pivot space. This setting allows us to use discontinuous vector fields to approximate the unknown boundary data in a Galerkin discretisation. We take the boundary element space of piecewise constant tangential vector fields on each element of the mesh to discretise the new formulation.

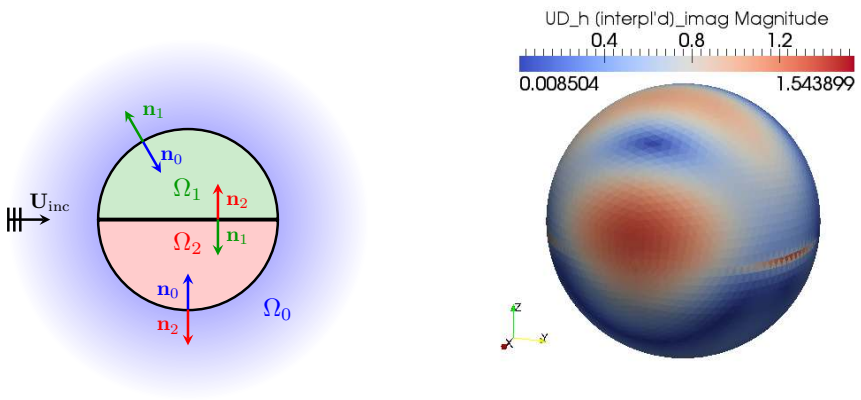


Figure 1: Left figure: the geometry of the model problem is sketched. It should be seen as a 2D-cut through the scatterer. Each domain Ω_0, Ω_1 and Ω_2 is charactarized by a constant wave number κ_i. We take $\kappa_0 = 6$, $\kappa_1 = 9$, $\kappa_2 = 3$. The incident field $\mathbf{U}_{\text{inc}}$ is given by the plane wave with direction of propagation $\mathbf{d} = (1, 0, 0)^{\top}$ and polarization $\mathbf{p} = (0, 1, 0)^{\top}$. The complete scatterer in 3D is given in the figure on the right hand side. It shows the magnitude of the imaginary part of the tangential trace of the solution to the model problem.

Implementations of both approaches have been done based on the C++ Boundary Element Template Library (BETL2) by Lars Kielhorn. The geometry of the model problem for which we show the numerical results is depicted in Fig. 1. The results show competitive accuracy of the new second-kind approach (see Fig. 2), bounded condition

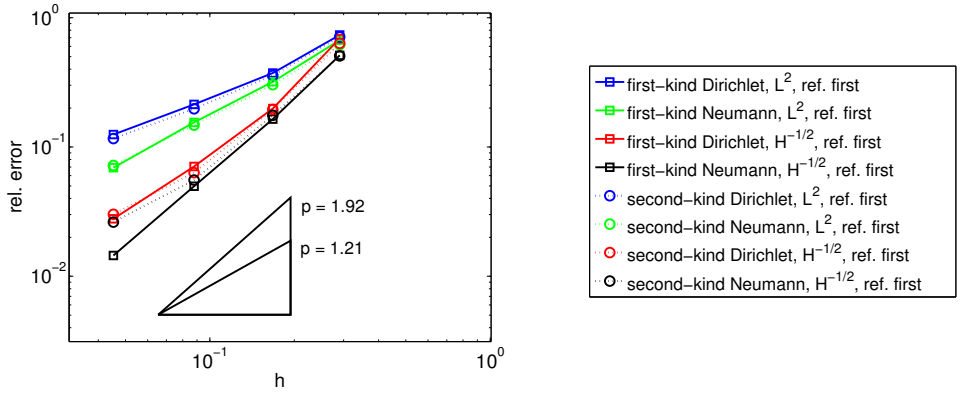
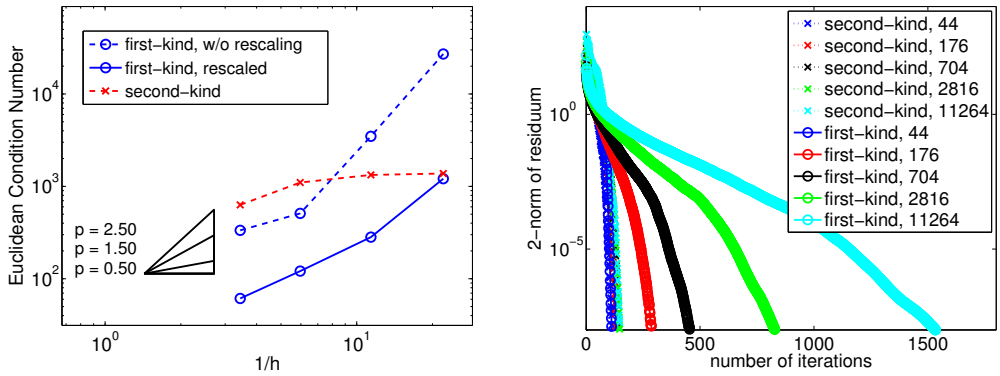


Figure 2: Error convergence studies of the Dirichlet and Neumann data of the solution to the model problem in L^2 and $H^{-\frac{1}{2}}$-norm. The reference solution is taken to be the highest resolution of the first-kind approximation.



(a) Condition Numbers of Galerkin matrices (b) Performance GMRES

Figure 3: Left figure: Euclidean condition numbers of the (diagonally rescaled) Galerkin matrices for a sequence meshes plotted wrt. mesh size. Right figure: the performance of GMRES when solving the corresponding linear system. The numbers given in the legend correspond to the number of elements of the mesh.

numbers of the Galerkin matrices with respect to the mesh size and superior convergence of GMRES (see Fig. 3).

Publications:

[1] X. Claeys, and R. Hiptmair, and E. Spindler, *Second-Kind Boundary Integral Equations for Scattering at Composite Partly Impenetrable Objects*, Technical Report No. 19, ETH Zürich, 2015.

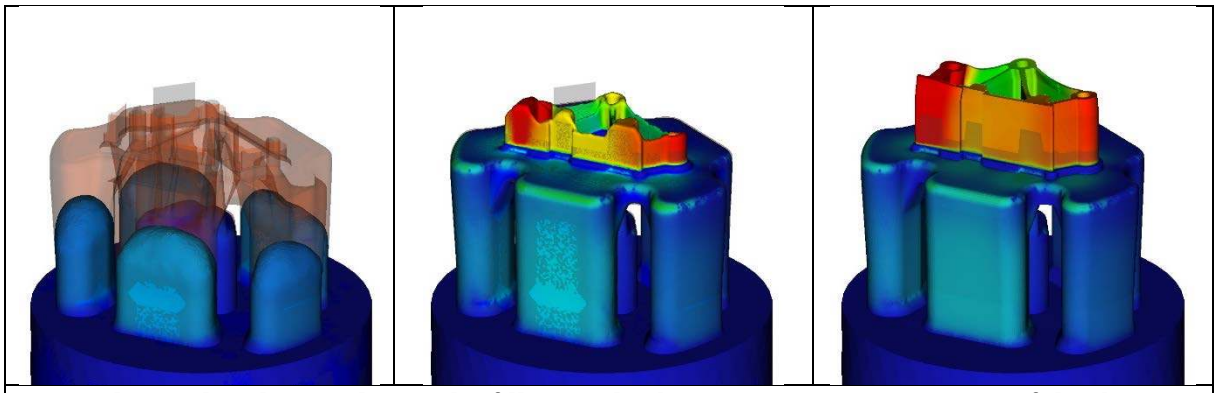
[2] X. Claeys, and R. Hiptmair, *Electromagnetic scattering at composite objects: A novel multi-trace boundary integral formulation.*, ESAIM: Mathematical Modelling and Numerical Analysis, 46(06):1421-1445, 2012.

Title: Innovative finite element method for extrusion processes

Researchers: L. Tong
D. Hora
C. Becker
P. Hora

Institute/ Group: Institute of Virtual Manufacturing

Description:
The simulation of Al-extrusion processes with industrial complexity has been challenging under many different aspects. The correct description of contact conditions, the accurate prediction of the complex flow conditions during the chambers filling stage, the adequate description of the material flow around sharp edges and last but not least under the very high computation time have until today prevented a widespread industrial application of numerical approaches. The presented novel method, specially developed for extrusion processes, successfully overcomes virtually all of the mentioned difficulties. Up to now two different simulation techniques and programs are used to simulate the filling process (UL) of the die and the subsequent extrusion process (ALE). Due to the coupling of the material flow and the mesh in filling simulations, mesh distortion at edges is a common problem treated by remeshing operations. Small time increments and high simulation time are the result. The extrusion process is commonly simulated by ALE-technique that requires a filled tool and by that, a mapping of the deformation and the temperature field on the new mesh from the filling simulation. The new developed technique uses a pre-meshed filled tool, with deactivated elements in the beginning of the simulation. Due to the material flow and the velocity distribution, the filled elements are activated and smoothed by surface tracking. After the filling process is completed, the extrusion process is activated and is proceeded by the ALE method [1]. Due to the computation of the stream line field by means of the velocity distribution of the material flow inside the tool, the welding position of the single feed streams can be predicted, too.



Velocity distribution during the filling and subsequent extrusion process of the die.

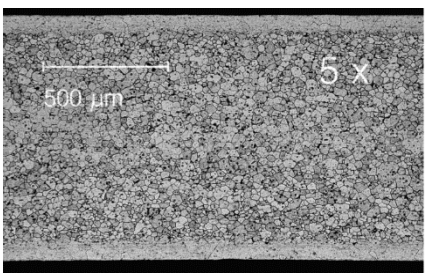
[1] Hora P., Becker C., Tong L., Maier J., Müller S.: Advanced frictional models for extrusion application, Key Engineering Materials Vol. 585, pp. 41-48, 2014.

Title	Effect of through Thickness Strain Distribution on Shear Fracture Hazard and its Mitigation by using Multilayer Aluminum Sheets
Researchers:	M. Gorji, B. Berisha, N. Manopulo, P. Hora
Institute / Group:	Institute of virtual manufacturing

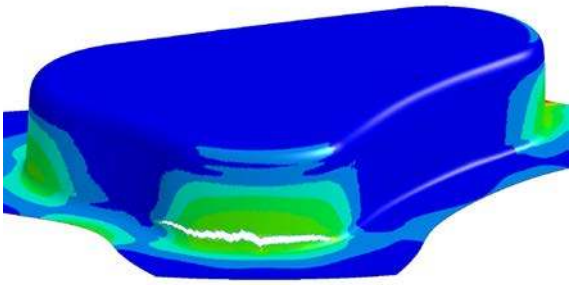
Description:

The formability of sheet metal is generally accepted to be limited by the so-called forming limit curve (FLC). This is valid for a majority of operations, given that localization immediately precedes fracture. For the characterization of the latter, a microscopy based new method is applied in this research. A newly designed triangle shape deep drawing part is also used in the framework of this work to validate the constitutive and failure models. In addition, fracture concept in studied aluminum alloy AA6016 sheet sample is investigated by using different well-known fracture criteria: Constant equivalent fracture strain, Johnson-Cook (JC), shear stress based and new linear fracture line (in principal strains space). The measured principal fracture strains are then implemented in the FE-code to predict rupture. It has been displayed that considering the equivalent strain and shear stress based as a fracture criterion is not proper to define the crack initiation in such a complex deep drawing processes. Whereas, both linear fracture line and JC models deliver similar results for the triangular shape deep drawing process. The linear fracture criterion has a better agreement with experimental results, especially in the equi-biaxial loading range. Moreover, initiation and propagation of cracks in multi-layer aluminum alloys are studied. It is highlighted that the multilayer material shows better forming behavior, compared to the monolithic material in bending and deep drawing experiments.

[Left] Exemplary failed monolithic AA6016 and [Right] multilayer material



Microscopic picture of multilayer material, showing the thickness distribution of core material (thickness=0.88mm) and clad material (thickness=0.06mm)



Simulated deep drawing experiment of studied aluminum alloy by applying new linear fracture line

Title: Development of an intelligent planning- and an on-line process monitoring system for optimal design and monitoring of the metal spinning process

Researchers: B. Rentsch

P. Hora

Institute: Institute of Virtual Manufacturing

Description:

A new class of forming processes known as Incremental sheet forming (ISF) has raised a lot of attention in the last two decades. These processes are characterized by the fact that at any time only a small part of the product is actually being formed and this area of local deformation is moving over the entire product. A particular incremental sheet metal forming process is metal spinning, used for the manufacturing of rotational parts in low to medium series [1].
Plenty of research has been done in this field, however the use of numerical simulation techniques in the design of the process remains very limited. The rapidly changing contact states complicate the application of implicit FEM solvers. For this reason, explicit solvers with very small time steps are applied [2]. This method is bound to restrictive computational times. An optimization of the tool path, which perhaps may require the tracing of several hundred variants, is hardly feasible due to time constraints.
In the scope of the project a simplified model of the metal spinning process is developed, aiming to map an optimized initial design of the intermediate stages with reduced requirements in computational time. Concurrently sophisticated material models and failure criteria, which properly reflect the material behaviour in incremental sheet forming are implemented in the commercial FE code *LS-DYNA* through user subroutines.
In a later stage, experiments will be conducted on a CNC lathe and the resulting data compared to the output of *LS-DYNA Explicit solver* (Figure 1).

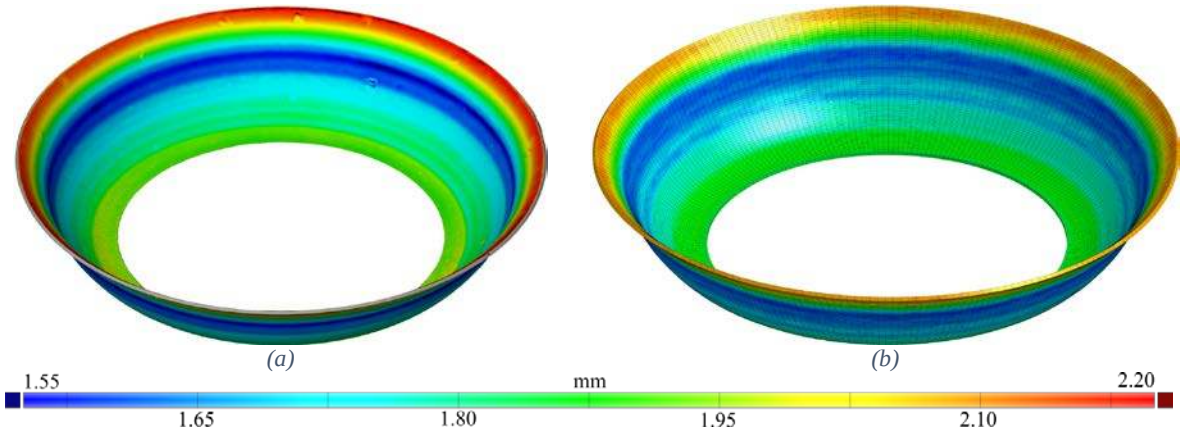


Figure 1: Thickness distribution of experimental data (a) and output of LS-DYNA Explicit solver (b)

References

[1] W. C. Emmens, G. Sebastiani und A. H. Van den Boogard, «The technology of Incremental Sheet Forming - A brief review of the history,» *Journal of Materials Processing Technology*, Bd. 210, pp. 981-997, 2010.

[2] J. Li, P. Geng und J. Shen, «Numerical simulation and experimental investigation of multistage incremental sheet forming,» *International Journal of Advanced Manufacturing Technology*, Nr. 68, pp. 2637-2644, 2013.

Title: On the ambiguity of conformational states: A B&S-LEUS simulation study of the helical conformations of decaalanine in water.

Researchers: N.S. Bieler*
P.H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Estimating the relative stabilities of different conformational states of a (bio)molecule using molecular dynamics simulations involves two challenging problems: the conceptual problem of how to define the states of interest and the technical problem of how to properly sample these states, along with achieving a sufficient number of interconversion transitions. In this study, the two issues are addressed in the context of a decaalanine peptide in water, by considering the 3_{10}-, α- and π-helical states. The simulations rely on the ball-and-stick local-elevation umbrella-sampling (B&S-LEUS) method. In this scheme, the states are defined as hyperspheres (balls) in a (possibly high dimensional) collective-coordinate space, and connected by hypercylinders (sticks) to ensure transitions. A new object, the pipe, is also introduced here to handle curvilinear pathways. Optimal sampling within the so-defined space is ensured by confinement and (one-dimensional) memory-based biasing potentials associated with the different objects. The simulation results are then analysed in terms of free energies using reweighting, relying on two possibly distinct sets for the collective coordinates and for the state definitions. The four possible choices for these sets are Cartesian coordinates, hydrogen-bond distances, backbone dihedral angles, or pairwise sums of successive backbone dihedral angles. The results concerning decaalanine underline that the concept of conformational state may be extremely ambiguous, and that its tentative absolute definition as a free-energy basin remains subordinated to the choice of a specific analysis space. For example, within the force-field employed and depending on the analysis coordinates selected, the 3_{10}-helical state may refer to weakly overlapping collections of conformations, differing by as much as $25\,\mathrm{kJ\,mol^{-1}}$ in terms of free energy. As another example, the π-helical state appears to correspond to a free-energy basin for three choices of analysis coordinates, but to be unstable with the fourth one. The problem of conformational-state definition may become even more intricate when comparison with experiment is involved, where the state definition relies on spectroscopic or functional observables.

References: N.S. Bieler & P.H. Hünenberger.
J. Chem. Phys. **142** (2015) 165102/1-165102/17.

Title: Multistate λ-local-elevation umbrella-sampling (MS-λ-LEUS): Method and application to the complexation of cations by crown ethers.

Researchers: N.S. Bieler*
J.P. Tschopp*
P.H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

An extension of the λ-local-elevation umbrella-sampling (λ-LEUS) scheme [Bieler *et al.*, *J. Chem. Theory Comput.* **10** (2014) 3006] is proposed to handle the multistate (MS) situation, *i.e.* the calculation of the relative free energies of multiple physical states based on a single simulation. The key element of the MS-λ-LEUS approach is to use a single coupling variable Λ controlling successive pairwise mutations between the states of interest in a cyclic fashion. The Λ variable is propagated dynamically as an extended-system variable, using a coordinate transformation with plateaus and a memory-based biasing potential as in λ-LEUS. Compared to other available MS schemes (one-step perturbation, enveloping distribution sampling and conventional λ-dynamics) the proposed method presents a number important advantages, namely: (*i*) the physical states are visited explicitly and over finite time periods; (*ii*) the extent of unphysical space required to ensure transitions is kept minimal and, in particular, one-dimensional; (*iii*) the setup protocol solely requires the topologies of the physical states; (*iv*) the method only requires limited modifications in a simulation code capable of handling two-state mutations. As an initial application, the absolute binding free energies of five alkali cations to three crown ethers in three different solvents are calculated. The results are found to reproduce qualitatively the main experimental trends, and in particular the experimental selectivity of 18C6 for K^+ in water and methanol, which is interpreted in terms of opposing trends between the solvation free energy of the cation and the direct electrostatic interactions within the complex along the cation series.

References: N.S. Bieler, J.P. Tschopp & P.H. Hünenberger.
J. Chem. Theory. Comput. **11** (2015) 2575-2588.

Title: Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI *vs.* λ-LEUS.

Researchers: N.S. Bieler*
P.H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

In a recent article [Bieler *et al.*, *J. Chem. Theory Comput.* **10** (2014) 3006], we introduced a combination of λ-dynamics and local-elevation umbrella-sampling termed λ-LEUS to calculate free-energy changes associated with alchemical processes using molecular dynamics simulations. This method was suggested to be more efficient than thermodynamic integration (TI), because the dynamical variation of the alchemical variable λ opens up pathways to circumvent barriers in the orthogonal space, which is defined by the $N-1$ degrees of freedom that are not subjected to the sampling enhancement, a feature λ-LEUS shares with Hamiltonian replica-exchange (HR) approaches. However, the mutation considered, hydroquinone to benzene in water, was no real challenge in terms of orthogonal-space properties, which were restricted to solvent-relaxation processes. In the present article, we revisit the comparison between TI and λ-LEUS considering non-trivial mutations of the central residue X of a KXK tripeptide in water (with X = G, E, K, S, F or Y). Side-chain interactions that may include salt bridges, hydrogen bonds or steric clashes lead to slow relaxation in the orthogonal space, mainly in the two-dimensional subspace spanned by the central φ and ψ dihedral angles of the peptide. The efficiency enhancement afforded by λ-LEUS is confirmed in this more complex test system, and can be attributed explicitly to the improved sampling of the orthogonal space. The sensitivity of the results to the non-trivial choices of a mass parameter and of a thermostat coupling time for the alchemical variable is also investigated, resulting in recommended ranges of 50 to 100 u nm^2 and 0.2 to 0.5 ps, respectively.

References: N.S. Bieler & P.H. Hünenberger.
J. Comput. Chem. **36** (2015) 1686-1697.

Title: Revision of the GROMOS 56A6$_{CARBO}$ force field for hexopyranose-based carbohydrates: Improving the description of ring-conformational equilibria in oligo- and polysaccharide chains.

Researchers: W. Plazinski*
A. Lonardi*
P.H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

This article describes a revised version 56A6$_{CARBO_R}$ of the GROMOS 56A6$_{CARBO}$ force field for hexopyranose-based carbohydrates. The revision involves a modification of two Lennard-Jones exceptions and one torsional potential for residues involving an alkylated or glycosylated anomeric oxygen atom. The simulated properties of unfunctionalized hexopyranoses are unaltered with respect to 56A6$_{CARBO}$, and the $^4C_1$ chair is the most stable conformation for all D-hexopyranoses except α-idose, in agreement with experiment. For O_1-alkylated hexopyranoses, the revision stabilizes the regular $^4C_1$ chair for α-anomers (with the opposite effect for β-anomers), and the $^4C_1$ chair is the most stable conformation for all methyl-D-hexopyranosides in 56A6$_{CARBO_R}$. In the context of oligosaccharides, the revision has qualitatively the same effect, and alleviates spurious ring inversions observed in $\alpha(1\rightarrow4)$-linked chains when using the original 56A6$_{CARBO}$ force field. The $^4C_1$ chair is now also the most stable conformation for all D-hexopyranose residues in 56A6$_{CARBO_R}$, irrespective of the linkage type and anomery, and of the position of the residue along the chain. The results obtained using the revised force field also reveal two interesting effects. First, the methylation of a D-hexopyranose leads to a systematic shift in the ring-inversion free energy ($^4C_1$ to $^1C_4$) by 7-8 kJ mol^{-1}, positive for the α-anomers and negative for the β-anomers, which is qualitatively compatible with the expected enhancement of the anomeric effect upon methylation at O_1. Second, the ring-inversion free energies for residues within chains are typically smaller in magnitude compared to those of the monomers, and correlate rather poorly with the latter. This suggests that the crowding of ring substituents upon chain formation significantly alters (generally enhances) the ring flexibility in a non-systematic fashion. Consequently, inferring ring-conformational properties for residues within chains based on experimental or theoretical information concerning monomers may be unreliable. In general, the description of carbohydrate chains afforded by 56A6$_{CARBO_R}$ suggests a significant extent of ring flexibility, *i.e.* small but often non-negligible equilibrium populations of inverted chairs, and challenges the textbook picture of conformationally-locked carbohydrate rings.

References: W. Plazinski, A. Lonardi & P.H. Hünenberger.
J. Comput. Chem. (2015) submitted.

Title: Large-scale 3D modelling and inversion of magnetotelluric data using adaptive finite element method

Researchers: A. Grayver [(1)]
A. Kuvshinov [(1)]
T. Kolev [(2)]

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) Lawrence Livermore National Laboratory, Livermore, California, USA

Description:

Geo-electromagnetic (EM) methods is one of the few techniques to study interior structure of the Earth by inferring electrical conductivity distribution at depths. Recently, we have investigated the use of the adaptive high-order finite-element method (FEM) for EM modelling (Grayver and Kolev, 2015). Because high-order FEM is challenging from the numerical and computational points of view, most published FEM studies in geoelectromagnetics use the lowest order FEM. We have developed a fully parallel and distributed robust and scalable linear solver. To get accurate solutions at reduced computational cost, we have implemented goal-oriented adaptive mesh refinement. The numerical tests indicated that the high-order FEM in combination with the goal-oriented local mesh refinement required less computational time and DoFs than the conventionally used lowest order FEM.

This modelling engine was used in the inversion scheme described in Grayver (2015). The key novel aspect of the algorithm is the use of automatic mesh refinement techniques for both forward and inverse modelling. This alleviates tedious and subjective procedure of choosing a suitable model parametrization. For further efficiency gain, EM fields for each frequency were calculated using independent meshes in order to account for substantially different spatial behaviour of the fields over a wide range of frequencies. An automatic approach for efficient initial mesh design in inverse problems based on linearized model resolution matrix was developed. The developed algorithm for adaptive inverse mesh refinement is capable to deliver meshes suitable to resolve features on multiple scales. Overall, the use of automatic adaptive schemes results in significant computational savings and enables us to consider problems which were previously thought to be too expensive.

Our current work concentrates on two aspects: (i) application of these numerical methods to real-world magnetotelluric data and (ii) developments of approaches to quantify uncertainty of the models in non-linear inverse problems using stochastic methods (Grayver and Kuvshinov, 2015). The research outlined above involves extensive use of HPC resources. We anticipate that aforementioned directions will require approximately 200,000 CPU hours during the next year.

References:

Grayver A.V., and Kolev, T. V., 2015, Large-scale 3D geo-electromagnetic modeling using parallel adaptive high-order finite element method, Geophysics, 80(6), pp. 277-291.

Grayver A.V., 2015, Parallel 3D magnetotelluric inversion using adaptive finite-element method. Part I: theory and synthetic study, Geophysical Journal International, 202(1), pp. 584-603.

Grayver A.V., and Kuvshinov, A. V., 2015, Exploring equivalence domain in non-linear inverse problems using Covariance Matrix Adaption Evolution Strategy and random sampling, submitted.

Title: The novel high-performance and scalable 3D MT forward solver
Researchers: A. Geraskin (1)
M. Kruglyakov (2)
A. Kuvshinov (1)

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) Lomonosov Moscow State University, Moscow, Russia

Description:

Magnetotellurics (MT) is a frequency-domain electromagnetic (EM) method aimed at studying the electrical conductivity distribution inside the Earth. During an MT survey, naturally-occurring variations of the electric and the magnetic field are measured which furthermore - via appropriate interpretation tool - are translated into a map of the subsurface conductivity. To date, MT method is widely used at local, regional and even continental scales for a large variety of academic and applied problems, including detecting hydrocarbon and geothermal reservoirs. Starting with 1-D and 2-D MT interpretations, nowadays 3-D MT analysis becomes a common practice. However, still, 3-D MT forward modelling - core element of any 3-D interpretation - with realistic levels of complexity, accuracy and spatial detail remain challenging from the computational point of view.
This project is aimed to developing new high-performance (HP) and scalable code (solver) for 3D MT forward simulations. Forward solution (in other words, numerical solution of Maxwells equations) is based on an integral equation (IE) approach with contracting kernel (cf. Pankratov and Kuvshinov, 2015). Most of the code is written in C#, some performance-critical parts and wrappers for native libraries are implemented using C. The software is designed to be cross platform (it was already tested on Windows 7, 8 and on a variety of linux-based OSes, including CentOs and Cray linux). The program can efficiently run on personal computers and laptops (for small to moderate models). However, in order to deal with large-scale models, the HP clusters (HPC) are used, and the program can be easily scaled (both by memory and by CPU time) to match the problems complexity. In particular our computational experiments performed at different platforms ranging from modern laptops to HPC Piz Daint demonstrate practically linear scalability of the code up to thousands of nodes.
The code has highly-modular architecture, which allows for optimization at each individual platform (e.g. using different fft and math libraries and various MPI implementations). In addition it allows for implementing different parallelization strategies, not compromising the integrity of the program.

References:

Pankratov O. and A. Kuvshinov, 2015. Applied mathematics in EM studies with special emphasis on an uncertainty quantification and 3-D IE modelling. Survey in Geophysics, in press.
Geraskin A., M. Kruglyakov and A. Kuvshinov, 2015. Novel robust and scalable 3-D EM forward solver based on contracting integral equation method and modern programming techniques, Computers and Geosciences, submitted.

Title: 3-D analysis and interpretation of magnetotelluric data from the Aluto-Langano geothermal field, Ethiopia

Researchers: F. Samrock (1)
A. Kuvshinov (1)
J. Bakker (1)

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland

Description:

The magnetotelluric (MT) method is a technique, which uses naturally occurring time-varying electromagnetic (EM) fields, to study the Earths interior. Based on MT data it is possible to recover the subsurface electrical resistivity distribution down to depths of hundred kilometers. In geothermal reservoir exploration electrical resistivity is a crucial geophysical parameter as hydrothermal and magmatic reservoirs are typically related to low resistive zones, which can be easily sensed by MT. Thus by mapping the electrical resistivity one can identify and analyze geothermal reservoirs with respect to their temperature, extent and potential for energy production.
In early 2012 we conducted an MT survey at the Aluto-Langano geothermal field, Ethiopia, which is known to be actively deforming with reoccurring periods of uplift and setting (Biggs et al., 2011). In order to get a 3-D model of the geothermal system we inverted the observed data using the ModEM-code (Egbert & Kelbert, 2012; Kelbert et al., 2014). This modular system comprises forward and inversion schemes for frequency-domain EM geophysical data. The 3-D forward scheme is based on finite differences and the inverse scheme exploits the non-linear conjugate gradient method. ModEM is parallelized with respect to frequency and source field polarization. In our case we achieved the minimum computing time by distributing the inverse problem to 83 processors.
Our recovered 3-D model revealed a subsurface resistivity structure, which is typical for high enthalpy geothermal reservoirs. The resistive upflow zone and hottest part of the reservoir below 2km depth and the low resistive clay cap at shallower depths could be clearly identified in the model (Samrock, 2015a; Samrock et al., 2015b). An important outcome of our study is that we found no evidence for an active magmatic system under Aluto-Langano. This implies that the deforming source is most likely situated within the shallow hydrothermal system of the geothermal field.

References:

Biggs, J., Bastow, I., Keir, D. & Lewi, E., 2011. Pulses of deformation reveal frequently recurring shallow magmatic activity beneath the Main Ethiopian Rift, Geochem. Geophys. Geosyst., 12(9).
Egbert, G.D. & Kelbert, A., 2012. Computational recipes for electromagnetic inverse problems, Geophys. J. Int., 189(1), 251267.
Kelbert, A., Meqbel, N., Egbert, G. & Tandon, K., 2014. ModEM: A modular system for inversion of electromagnetic geophysical data, Comput. Geosci., 66, 4053.
Samrock, F. (2015a). Constraints on the source of unrest at the Aluto-Langano geothermal field, Ethiopia, inferred from 3-D interpretation of MT measurements (Doctoral dissertation, ETH Zürich, Nr. 22357).
Samrock, F., Kuvshinov, A., Bakker, J., Jackson, A., & Fisseha, S. (2015b). 3-D analysis and interpretation of magnetotelluric data from the Aluto-Langano geothermal field, Ethiopia. Geophys. J. Int., 202(3), 1923-1948.

Title: Torsional Waves in Earth's core
Researchers: Elisabeth Canet [(1)]
Nicolas Gillet [(2)]
Dominique Jault [(2)]

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) University Grenoble Alpes, ISTerre, Grenoble, France

Description:

Torsional waves in Earth's core are due to the geostrophic zonal flow. A differential rotation shears the component of the magnetic field perpendicular to the rotation axis and propagates in the direction perpendicular to the rotation axis as an Alfven torsional wave. The propagation velocity of these waves gives an insight into the shape and strength of the magnetic field within the core.
The aim of our research is to better understand the emergence of a period of about 6 years in the system, which has also been observed in core flow inversion and in length of day variations.
In this context, we do numerical simulations of Alfven torsional waves in a deep shell. The excitation mechanism is stochastic and takes place in the volume of the system. The forcing space and timescales are deduced from and should represent our partial knowledge of the nonlinear interaction between the non-zonal flow and the magnetic field at secular variation timescales in the quasi-geostrophic approximation.
We find that discrete frequencies, which corresponds to the Alfven wave period and its harmonics, are brought up inherently by the system and depend on the shape and strength of the magnetic field that enters the wave equation, that is, the average over a geostrophic cylinder of the component perpendicular to the rotation axis, $\frac{1}{4\pi sH} \oint \int_{-h}^{h} sB_s^2(s,\phi,z) d\phi dz$, with (s,ϕ,z) the cylindrical coordinates.
Moreover the response at timescales longer than the rotation timescale is independent of the frequency which corresponds to our perception of the Taylor state where inertia is absent from the momentum equation.
The question of the explanation of apparent absence of reflection of the torsional waves at the core-mantle boundary is currently under investigation.

References:

Paper in preparation.

Title: Dynamos driven by precession and libration
Researchers: S. Vantieghem [(1)]
Y. Lin [(1)]
A. Jackson [(1)]

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
Description:

The aim of our research is to understand the dynamics of planetary core flows and their ability to generate and sustain magnetic fields. It is commonly assumed that thermochemical convection is the power source that drives today's Earth's dynamo. It has been argued, however, that the energy provided by convection may not be sufficient to drive or have driven the dynamos of other planets and moons (ancient Earth & Moon, Ganymede, ...).
This motivates us to investigate dynamo models whereby core turbulence and magnetic fields are generated by variations in the rotation rate of the mantle of a planet, such as precession and libration. One can distinguish between three different coupling mechanisms that allow to transfer the precessing and librating motion of the mantle to the core and its dynamo. For the study of viscous and electromagnetic coupling mechanisms, we use a highly parallell pseudo-spectral code (Marti, 2012) that is based on expansions in spherical harmonics. This allows to reach ultra-low viscosity regimes; typical CPU times associated with models at an Ekman number (which quantifies the effect of viscosity) of 10^{-5} are of the order of 100,000 CPUh (Lin et al.). Our eventual aim is to perform simulations in which the coupling is purely electromagnetic (as viscous coupling is believed to be negligible in planetary context).
We also have developed a parallel unstructured finite-volume code (Vantieghem et al., 2015) that allows taking into account topographic effects (i.e. the departure of spherical symmetry of a planetary core). This tool has been used to perform simulations of precession-driven dynamos in spheroidal enclosures with and without inner core; a typical computational budget is of the order of 5,000 CPUh per model.

References:

P. Marti. Convection and boundary driven flows in a sphere. PhD thesis, ETH Zurich, 2012.
Y. Lin, S. Vantieghem and A. Jackson, Numerical study of precession-driven dynamos driven by electromagnetic, viscous and topographic coupling, in preparation.
S. Vantieghem, A. Sheyko, A. Jackson. Applications of a finite-volume algorithm for incompressible MHD problems. Geophysical Journal International, under review.

Title: Optimal dynamo action by steady flows confined in a cube

Researchers: L. Chen [(1)]
W. Herreman [(2)]
A. Jackson [(1)]

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) University Paris Sud 11, LIMSI-CNRS, Orsay, France

Description:

The Earth's magnetic field is spontaneously generated in the outer core via dynamo action. To better understand such phenomena, it is useful to excite dynamos in the lab under controlled conditions, but the replication of such mechanism in the lab is often challenging. We search for the optimal initial conditions for dynamo action in a confined space, which could be potentially useful for lowering the threshold for dynamo experiments. The model we use is the kinematic dynamo model, where the flow is prescribed and no back reaction from the magnetic field is considered.
The optimization procedure is carried out via computer simulations. We use the Lagrangian method from Willis (2012) and search a huge class of stationary and incompressible flows that are confined in a cube. We demand that the magnetic field satisfies either superconducting (T) or pseudovacuum (N) boundary conditions on opposite pairs of walls of the cube, which results in four different combinations. For each of these setups, we find the optimal flow and its corresponding magnetic eigenmodes. We also find its corresponding minimal lower bound for dynamo action. Numerically it is observed that swapping the magnetic boundary from T to N leaves the magnetic energy growth nearly unchanged, and the same fluid moving in both positive and negative directions are optimal flows for these different but complementary setups. This can be related to work by Favier & Proctor (2013).

References:

Optimal dynamo action by steady flows confined in a cube. Journal of fluid mechanics (accepted).
Willis, Ashley P. Optimization of the Magnetic Dynamo. Physical review letters 109.25, 2012.
Favier, B. and M. R. E. Proctor. Growth rate degeneracies in kinematic dynamos. Physical Review E 88.3, 2013.

Title: Reversing dynamos in a rapidly rotating spherical shell with slip-free boundaries
Researchers: A.A. Sheyko [(1)]
C.C. Finlay [(2)]
A. Jackson [(1)]

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) Division of Geomagnetism, DTU Space, Technical University of Denmark

Description:

Generation of magnetic fields by turbulent flows of conducting media is a common phenomenon in planetary and astro- physics. In the solar system large rotating bodies such as the Sun itself and the Earth's outer core generate magnetic fields by a process called dynamo action. These magnetic fields have strong dipolar components and both exhibit flipping polarities. However Sun's magnetic field is reversing very regularly in an 11-year cycle, whereas the Earth's magnetic reversals are unsystematic and to date it is not possible to predict them.
In our studies we investigate convection driven dynamos reversing quasi-periodically. We use rapid rotation and low viscosity ($E = 10^{-6}$), and a small ratio of magnetic to viscous diffusivities ($P_m = 5 \cdot 10^{-2}$) so that we are as close to the Earth's core parameters as is feasible computationally. The region of parameters is inconvenient in the sense that large computing resources are necessary and it is therefore scarcely investigated. The set of incompressible magnetohydrodynamic equations is solved in the spherical shell with an Earth-like ratio of inner and outer radii using a parallelized spectral code (Willis et al., 2007). The employed resolution is similar to 528x256x256 (radial points, harmonic degrees, orders). The consumption of computing resources ranges from 0.1 up to 1.5 million core-hours per one magnetic diffusion time (magnetic dipole decay time) subject to the parameters used. In the set of simulations the driving force and the ratio of diffusivities P_m are varied.
Initial states of the flow and magnetic field were obtained from our previous studies, where we have discovered the set-up where the dipole moment starts to change its direction quasi-periodically after a long stage of single polarity. The aim of the study is to understand if our dynamos are the consequence of the Parker dynamo wave mechanism (Parker, 1955) or have some other underlying operating principles, whether this dynamo mechanism can persist for a long time and whether it is feasible in the geodynamo context.

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Willis, A. P., Sreenivasan, B., and Gubbins, D. Thermal core-mantle interaction: Exploring regimes for locked dynamo action. Physics of the Earth and Planetary Interiors, (165), 8392, 2007.

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

Institute/ Group: (1) EPM, Institut für Geophysik, ETH Zürich, Switzerland
(2) School of Earth and Environment, University of Leeds, UK

Description:

This study is concerned with a very special kind of magnetohydrodynamical (MHD) system, known as the Taylor state dynamo. Earth's dynamo system is heavily influenced by her rapid rotation, which results from the force balance between the Coriolis and Lorentz forces in Earth's core; thus in this regime the inertial force and the viscous force are negligible. This extreme parameter regime is far beyond the reach of modern high-performance computing power, hence, an alternative approach is required if one wishes to study the dynamics of the geodynamo system in this regime.
Taylor (1963) invented an inertia-free and viscous-free model as the asymptotic limit of such a rapidly rotating system. In this theoretical limit, the velocity and the magnetic field organize themselves in a special manner, such that, the Lorentz torque acting on a geostrophic cylinder has to tend to zero as the inertial force and the viscous force tend to zero. Moreover, as these two forces vanish entirely, the flow is instantaneously and uniquely determined by the magnetic field and its averaged Lorentz torque. The flow consists of two components, 1) the magnetostrophic part and 2) the geostrophic part, where the former one is the unique solution of the Navier-Stokes equation up to an arbitrary geostrophic component and via the induction process both components acting together on the magnetic field results in a vanishing Lorentz torque averaged on the geostrophic cylinder. This sophisticated flow-magnetic interaction in space and time leads to a longstanding problem for modeling this system and over the last decades, little progress has been made in this field.
We propose an entirely new approach for solving this system based upon the concept of optimal control theory and the further development of our variational data assimilation for MHD system (Li et al., 2014). In this approach, the Lorentz torque is treated as the target function to be minimized at each time step and we seek the optimal geostrophic flow, such that, the Lorentz torque remains arbitrarily small at the future time step. Testing this approach on an illustrative model, i.e., a 2D MHD system driven by a prescribed α-effect, we successfully find a dynamo solution in the Taylor state.

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Title: Flow and transport in porous and fractured media

Researchers: Davide Cortinovis
Rajdeep Deb
Amir Delgoshaie
Karim Khayrat
Florian Müller
Daniel Meyer
Patrick Jenny

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

General description:

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

Multi-scale modeling:

One of the major challenges in the numerical simulation of large-scale subsurface flow and transport phenomena is the correct treatment of complex permeability distributions involving multiple length scales and strong contrasts. In the past decade multiscale methods have become a promising alternative to classical iterative methods (e.g. AMG). More recently, enriched coarse-space approaches were introduced in the multiscale methodology in order to handle high permeability contrasts in an appropriate way.

In collaboration with Dr. Seong Lee (Chevron) we have developed an extension of the multiscale finite-volume method (MSFV). In the presence of high permeability contrast, our new iterative Galerkin-enriched MSFV (i-Ge-MSFV) method is more robust than earlier MSFV variants, retains the capabilities of the existing MSFV method, but provides significantly higher convergence speeds [1].

Currently, a more general version of the i-Ge-MSFV method is being investigated. The method introduces a new coarse-space enrichment strategy which is more flexible and computationally efficient than the previously adopted one.

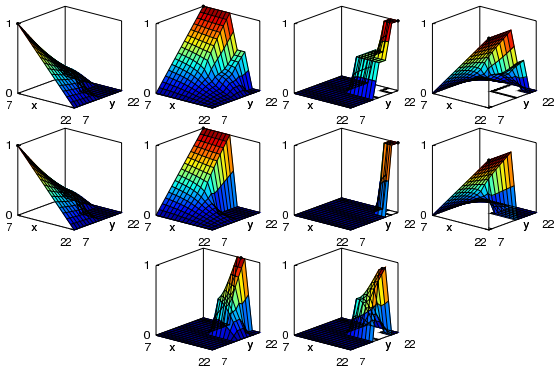


Figure: Nodal basis functions of the standard MSFV method (top figures). Nodal basis functions (4 center figures) after the insertion of two additional degrees of freedom. The corresponding enrichment functions are shown in the bottom figures.

Hierarchical model of fractured reservoirs:
In the context of geothermal power production, the coupling of fluid flow, rock mechanics and heat transport is important. Due to the very large number of fractures in a typical geothermal reservoir, we apply a description where only large fractures are resolved. The cloud of small unresolved fractures is treated by effective permeabilities.

Our recent research is focused on the seismicity and the feedback of rock mechanics on the flow or more precisely the porosity and permeability of the fractured reservoir. To this end, we employ a finite volume description together with special basis functions for displacement discontinuities to account for shear and tensile failures of fractures. The quantification of the magnitude of micro-seismic events such as shear failures is important when assessing risks involved in geothermal projects.

Uncertainty assessment of flow and transport in porous media:
This is a collaboration with Prof. Christoph Schwab, Prof. Siddhartha Mishra (both SAM, ETHZ), Prof. Peter Arbenz (D-INF, ETHZ) and Prof. Hamdi Tchelepi (Stanford University). The transport of chemical substances in the subsurface is relevant in many different applications. For example, for the management of groundwater aquifers or oil reservoirs predictive methods are needed. These tools have to account for the uncertainty in the soil parameters that are hard to measure.

One of our goals is the development of a simulation framework for flow and transport that provides probabilistic information about local tracer concentrations or oil saturations. A probability density function (PDF) method was proposed that is applicable for highly heterogeneous porous media thanks to newly-developed Markovian velocity processes (MVPs). Recently, we have reevaluated the applicability of the Markovian hypothesis [2] and have validated our method for a realistic setup similar to the MADE tracer dispersion benchmark study [3]. Moreover in the context of two-phase flow, e.g., in oil reservoirs, we have proposed an efficient method that enables the quantification of water or oil saturation uncertainties through a direct mapping based on flows statistics [4]. This greatly reduces the number of transport solutions that have to be computed.

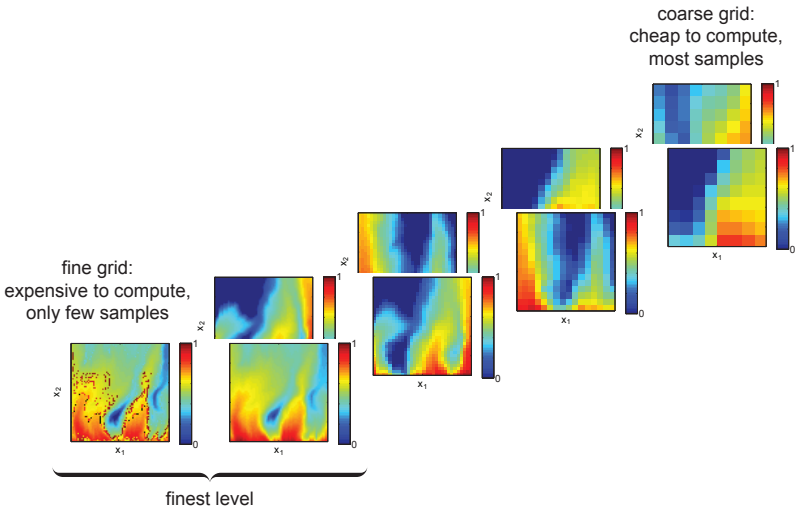


Figure: Multi-grid hierarchy typically applied in multi-level Monte Carlo (MLMC) sampling.

In addition, a novel multi-level Monte Carlo (MLMC) method has been developed. It allows to combine expensive high fidelity methods with cheap approximate solvers into an approximation hierarchy (classical multi-grid hierarchy see figure) to achieve output statistics more efficiently [5]. Recently, we have devised an MLMC method that balances sampling and discretization errors to achieve an optimal total work vs. total error convergence [6].

Prediction of non-equilibrium multi-phase flow:
Currently, storing CO_2 in geological subsurface formations seems to be one of the most promising feasible technologies to stabilize the CO_2 concentration in the Earth's atmosphere. The prime objective of our research is to improve our understanding of how the physics and dynamics at the pore scale is linked to the macro-scale description that is used for predictions at the formation scale.

To this end, we have devised new model equations for sub-phase saturations [7]. The resulting equation set is able to model hysteric effects. It requires, however, empirical constitutive relations that are calibrated by means of pore network simulations. Moreover, in connection with pore network simulations, we have developed a multi-scale pore network model that couples pore-scale sub-networks with a meso-scale description to simulate large pore networks at a small computational cost (see below figure). Effective conductances between the sub-networks are computed based on the sub-network two-phase configuration using the MSFV method. The fluid interface in each sub-network is then evolved in time, either by a full dynamic simulation or a quasi-static simulation depending on the capillary number. Our multi-scale model can account for both viscous and capillary effects.

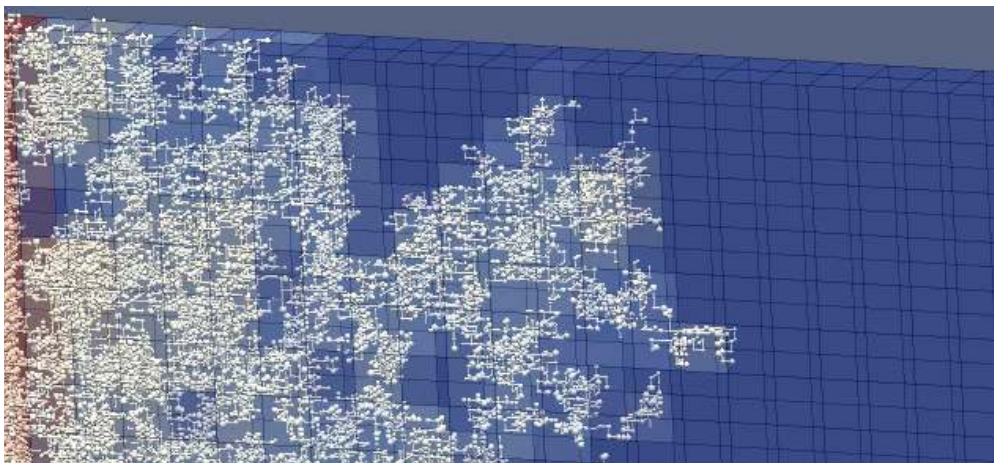


Figure: Simulation of viscous fingering for viscosity ratio 10 using the multi-scale pore network model. Grid cells encapsulate different coupled subnetworks. Shown in white are subnetwork tubes that are filled with invading non-wetting fluid. The meso-scale saturation of non-wetting fluid is shown in color (red 0.74, blue 0).

Non-equilibrium effects result from density differences between CO_2-saturated brine and pure brine. With the non-wetting CO_2 phase typically sitting on top of the wetting brine phase, so-called gravity fingers form at the phase interface with CO_2 diffusing into the brine and increasing the brine density (see below figure). The resulting finger-like structures are much

smaller than the formation scale and therefore cannot be resolved numerically. In our recent research, we have developed a scale analysis that implies opportunities for different modeling approaches [8]. These approaches do not require the resolution of the underlying fine-scale structures.

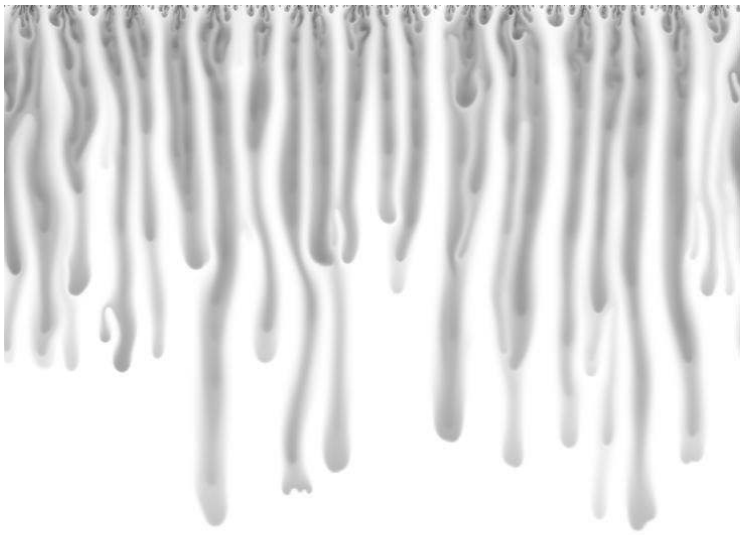


Figure: Gravity fingering simulation with CO_2 interface at the top boundary and CO_2 diffusing into the rectangular computational domain filled with brine. Plotted is the concentration of dissolved CO_2 (Rayleigh number is 80k).

Non-local Darcy formulation:

For the description of flow and transport in natural porous media, network models provide suitable descriptions of the underlying physical processes. For example at the pore scale, pore networks are applied to determine the pressure distribution and flow in tubes that connect different pores. Pore network simulations provide, on one hand, detailed information about the flow, but become computationally expensive when large sample volumes are considered. A continuum description like Darcy's law, on the other hand, enables the simulation of large samples, but cannot account for non-local mesoscale pressure effects. Recently, we have formulated a continuum description that can represent mesoscale effects and reduces in the limit of large samples to Darcy's law [9].

Title:	Fluid dynamics in biological systems and biomedical optics
Researchers:	Thomas Kummer Adrien Lücker Franca Schmid Patrick Jenny
Institute/Group:	Institute of Fluid Dynamics/Prof. Patrick Jenny

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

Dynamics of flow with particles (erythrocytes) in capillary networks:
This is a collaboration with Dr. Dominik Obrist (ARTORG Center, University of Bern), 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 simulation framework was developed in which the erythrocytes are resolved. At bifurcations the RBCs follow the path of the steepest (local) pressure gradient. The application of the bifurcation rule and RBC-dependent resistance has a strong impact on the flow and transport processes within the capillary network. 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.

Assigning boundary conditions constitutes a major challenge in simulating realistic cerebral networks. We developed and validated a hierarchical approach to assign pressure boundary conditions at the capillary level (see figure). Our results in artificial and realistic networks show that the presence of RBCs increases the number of bifurcations with similar bulk flow velocities in the outflow branches (well-balanced bifurcations). We postulate that those bifurcations are ideal locations to locally alter the distribution of RBCs [10].

Currently, we focus on analyzing pathways of individual RBCs through the capillary bed. This will enable us to explain effects such as capillary transit time heterogeneity, which for example directly influences RBC oxygen saturation.

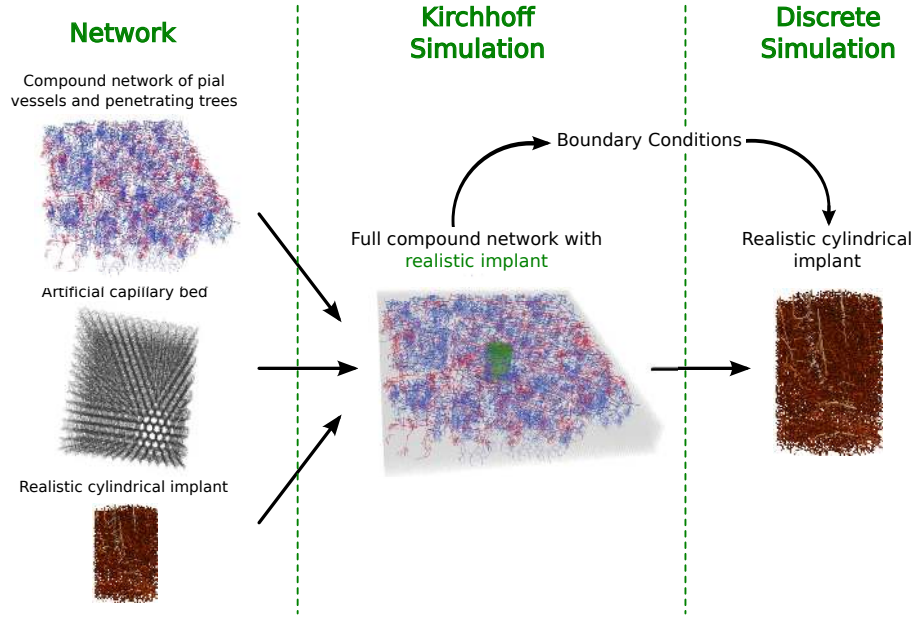


Figure: Approach to define appropriate boundary conditions.

Oxygen transport in the microcirculation:

The most fundamental function of the blood circulation is oxygen transport to tissue. Gas and nutrient exchange mostly occurs at the capillary level due to their large total surface area. In organs such as the brain or in muscles, oxygen supply is a dynamic process that is strongly linked to metabolism. The mechanisms involved in this coupling are only partly understood, especially at the capillary level, but are of fundamental importance. A correct interpretation of functional magnetic resonance imaging requires a sound understanding of the link between neuronal activity and cerebral blood flow (known as neurovascular coupling). Besides, disorders such as Alzheimer's disease are often related to abnormalities in the microcirculation. However, these phenomena are very difficult to observe experimentally due to the small size of capillaries and the challenges of in vivo experimentation.

In collaboration with Prof. Bruno Weber (University of Zürich), a new model for oxygen transport from capillaries to tissue has been developed. The presence of individual moving red blood cells in this model allows us to capture the spatial and temporal heterogeneity of blood flow and its influence on tissue oxygenation. After a successful comparison with recent oxygen measurements in the rodent brain, we have developed a multi-scale model that couples oxygen transport with the discrete red blood cell transport model developed at the Institute of Fluid Dynamics [11]. This new model was applied to quantitatively assess the influence of capillary dilations on tissue oxygenation. Capillary diameters can be altered by changing the tone of contractile cells called pericytes. We found that capillary dilations can cause a local increase of up to 2.5mmHg in oxygen partial pressure in the tissue, away from capillaries. This can help compensate a local increase in metabolic rate of oxygen consumption, but the dilation of a single capillary segment is not sufficient to offset a large increase in oxygen consumption. Therefore, capillary dilations are a candidate mechanism that could locally support arteriolar dilations during functional hyperaemia.

We will next investigate how dilations of multiple capillaries can affect tissue oxygenation in realistic capillary networks. Additionally, we have started investigating how capillary transit time heterogeneity translates into heterogeneity of blood oxygen content on the venous side of capillary beds.

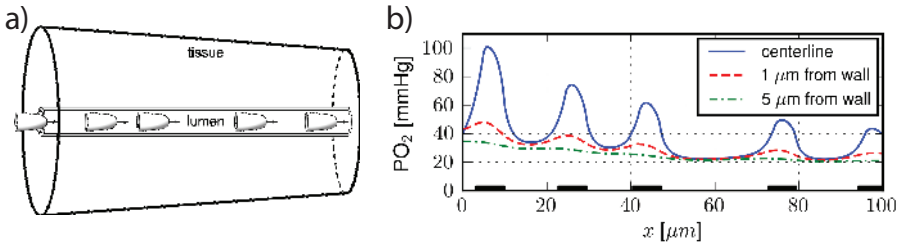


Figure: a) Computational domain with a fixed tissue region and red blood cells moving in a capillary. b) Longitudinal partial oxygen pressure profiles at three radial positions. The thick lines indicate the red blood cell locations.

Computational model for the design of heart assist devices

Designing and optimizing heart assist devices is complicated by a lack of parameter data and limited experimental capabilities. Here, computational models can provide a better understanding of underlying fluid and structure mechanics.

In this context our research effort is focused on developing a fluid-structure-interaction model, which allows for testing and optimization of medical devices. The structure of the heart is represented by a finite element model, whereas the blood circulation is simulated by a hydraulic circuit. The finite element model contains both the electrophysiology as well as the structure mechanics. The electrophysiology is included in such a way that heart fibers only begin to contract when the electrical signal has reached them, thus yielding a more physiological contraction pattern. By imposing boundary conditions on the pericardium we can then investigate how assist devices influence the contraction and cardiac output of insufficiently working hearts.

Our model is mainly intended for the development of assist devices, which directly act on the heart's surface. However, other applications are conceivable as well.

Title:	Turbulence modeling and turbulent reactive flow
Researchers:	Valentin Giddey
	Daniel Meyer
	Heng Xiao (now AP TT at Virginia Tech)
	Patrick Jenny
Institute/Group:	Institute of Fluid Dynamics/Prof. Patrick Jenny

General description:
Most flows involving human made devices or flows in the environment are turbulent and involve a large range of length and time scales. Consequently such flows are expensive to solve numerically. To reduce the computational burden, methods are applied that solve only for a fraction of these scales but require turbulence models to incorporate effects that result from neglected scales. Most important are Reynolds-averaged Navier-Stokes (RANS) models, large eddy simulation (LES) and probability density function (PDF) methods.

Worldwide, more than 80% of the consumed energy is converted by burning fossil fuels. Therefore, improving emission rates and efficiency of combustion devices automatically has a significant impact on our environment and is of crucial importance. To achieve such improvements, however, the capability of accurately predicting the governing physical processes (which involve turbulence-reaction interaction) is essential.

Modeling of group effect in turbulent spray combustion:
The combustion of fuel sprays plays a role, for example, in aircraft turbines and Diesel combustion engines. Despite the importance of these devices, the formation and combustion of droplet groups is not yet well understood. Our research in this area is focused on direct numerical simulation (DNS) of the underlying processes to gain a better understanding of the governing physiochemical effects. In a second step, we plan to formulate improved models to accurately account for group combustion effects in PDF method simulations. Recently, we validated particle or droplet collision statistics stemming from a synthetic turbulence model with high-fidelity DNS [12].

Hybrid LES/RANS modeling framework:
While LES is a very powerful approach to model turbulent flows, it entails high computational costs, which are 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, we have proposed and successfully tested an improved resolution evaluation criterion [13]. This criterion is applied in hybrid RANS/LES simulations to determine the RANS and LES regions in the computational domain.

Title: Rarefied gas kinetics

Researchers: Nemanja Andric
Hossein Gorji
Stephan Küchlin
Patrick Jenny

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

General description:

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

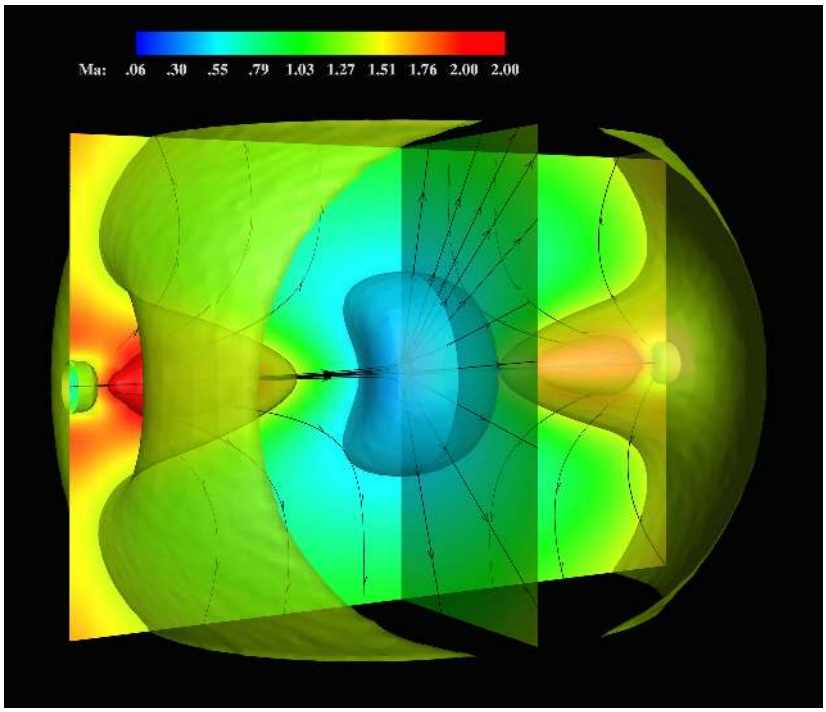


Figure: Mach contour surfaces and streamlines of source-source interaction in the vacuum space, using the hybrid FP-DSMC solution method. Note that the distance between the two sources is one mean free path and the inflows are initially at Mach zero.

General purpose algorithm for rarefied gas flows:

Current advances in engineering fields ranging from aerospace to micro-nano devices drive an ever increasing demand for accurate simulations of fluid flows characterized by a mean free path that is significant compared to flow length scales. In this so called rarefied regime, the conventional Navier-Stokes-Fourier system is no longer a valid description, necessitating stochastic simulation algorithms directly based on the Boltzmann equation. While the conventional Direct Simulation Monte Carlo (DSMC) technique introduced by Bird enjoys widespread success, its computational cost becomes prohibitive in the near continuum regime,

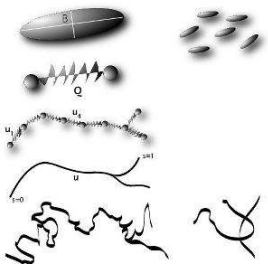
where the Knudsen number (Kn)–characterizing the degree of rarefaction–becomes small. The Fokker-Planck (FP) based particle Monte Carlo scheme introduced by Jenny et al. and further developed by Gorji et al. [14], allows for the computationally efficient simulation of rarefied gas flows in the low Kn regime. Here, instead of performing binary collisions employed by the DSMC method, continuous stochastic processes for the phase space evolution are integrated in time. This allows for time step and grid cell sizes larger than the respective collisional scales required by DSMC. Recently, a hybrid algorithm combining the FP and DSMC schemes was introduced and successfully applied to flows covering the whole Kn range [15]. The hybrid algorithm combines the efficiency of FP for small to moderate Kn with the accuracy of DSMC for large Kn. Currently, we are developing a general, efficient and flexible implementation of this method and are applying it to problems of practical relevance.

Investigation of non-equilibrium phenomena for separation mechanisms:
The separation of gas mixtures lies in the heart of many different industries with applications ranging from natural gas treatment, CO_2 capturing, hydrogen separation for fuel cells and oxygen enrichment for oxyfuel combustion. The goal of this study is towards understanding the influence of gas-surface and gas-gas interactions on species separation at high Knudsen numbers. Accordingly, our objective is threefold: First, computational studies of time dependent rarefied gas flow into the vacuum were conducted. Flow simulations were performed using DSMC consisting of a high pressure chamber connected via a small pipe to the outflow. Therefore, the influence of gas-surface interaction on the mass flow rate and gas separation is analyzed. Second, different possibilities for a separation scheme based on the electromagnetic excitation of internal energy modes proposed by Gorji & Jenny [16] are further investigated. The main idea here is that the energy transfer between internal and translational modes in successive collisions would cause the excited species to attain higher velocities and thus discharge at a faster rate compared to the unexcited one. Third, the effect of adding a heavy inert gas, such as Xenon, into the mixture is considered. It is investigated how this novel approach could alter the requirement on the Knudsen number in order to achieve and maintain thermal non-equilibrium between excited and unexcited species and thus influence the performance of the separation mechanism.

Variance-reduction for Monte-Carlo simulations:
We tackle the issue of statistical errors, which is common in Monte-Carlo techniques, with a suitable variance reduction method. It is shown by Gorji et al. [17] that introducing auxiliary stochastic processes with known solutions can substantially reduce the noise of the FP-based particle simulations. The method employs an equilibrium stochastic process, which evolves parallel to the main Langevin process. The correlation between the two processes allows to reduce the statistical error. Note that the proposed scheme is consistent, i.e. no new model assumptions are introduced. Further, in contrast to the deviational schemes for FP equations, such as the two-weight method, the proposed low variance method is free from instabilities. This is a crucial feature, since otherwise the method is not suitable for simulations of low Mach flows. Using the introduced parallel correlated processes, counter Fourier heat fluxes can be investigated in low Mach rarefied gas flows. Following this methodology for the low Mach lid-driven cavity flow, we found out that the dominant contribution in the heat flux

evolution equation comes through the deviatoric part of the fourth order velocity moment. Note that the corresponding contribution is zero in the hydrodynamic approximation and thus it is absent in Fouriers law. On the contrary by using e.g. Grads closure, the mentioned contribution is replaced by the gradient of the stress tensor which leads to the counter Fourier heat flux in lid-driven cavity flow simulations using the R-13 set of equations. In order to further examine the origin of this departure from the Fourier law, different scenarios including rarefied gas flow through a thin slit and rotating flow inside a cylinder are investigated. In both cases, similar to the lid-driven cavity flow counter Fourier heat fluxes are present. Accordingly, budgets of different contributions in the heat transport are evaluated using the low variance Fokker-Planck solution algorithm, where the role of the fourth order deviatoric velocity moment is carefully assessed.

Title: Multiscale modeling of polymers, dendronized polymers, actin filaments, entanglements, endocytosis



Researchers: Prof. Martin Kröger [1]
Prof. Avraham Halperin [2]
Prof. Andreas Bausch [3]
Prof. Nic Spencer [4]
Prof. Wing Kam Liu [5]

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

Description:

Computational Polymer Physics @ ETH recently focused its attention on the simulation of the nanotribology of coarse-grained polymer brushes [1], the internal organization of macromonomers and dendronized polymers based on thiophene dendrons via atomistic simulation [2,3], the endocytosis of PEGylated nanoparticles and the structural changes of grafted polyethylene glycols [4], the effect of polymer chain length on the mechanical properties of triblock copolymer gels [5], the microscopic origin of the non-Newtonian viscosity of semiflexible polymer solutions in the semidilute regime [6], accurate approximants of the inverse Langevin and Brillouin functions, relevant for strong polymer deformations and flows [7], and primitive-path statistics of entangled polymers in an attempt to map multi-chain simulations onto single-chain mean-field models [8]. Details available at www.complexfluids.ethz.ch

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Title: *Ab-initio* Transmission Calculations for a Carbon Nanotube Transistor

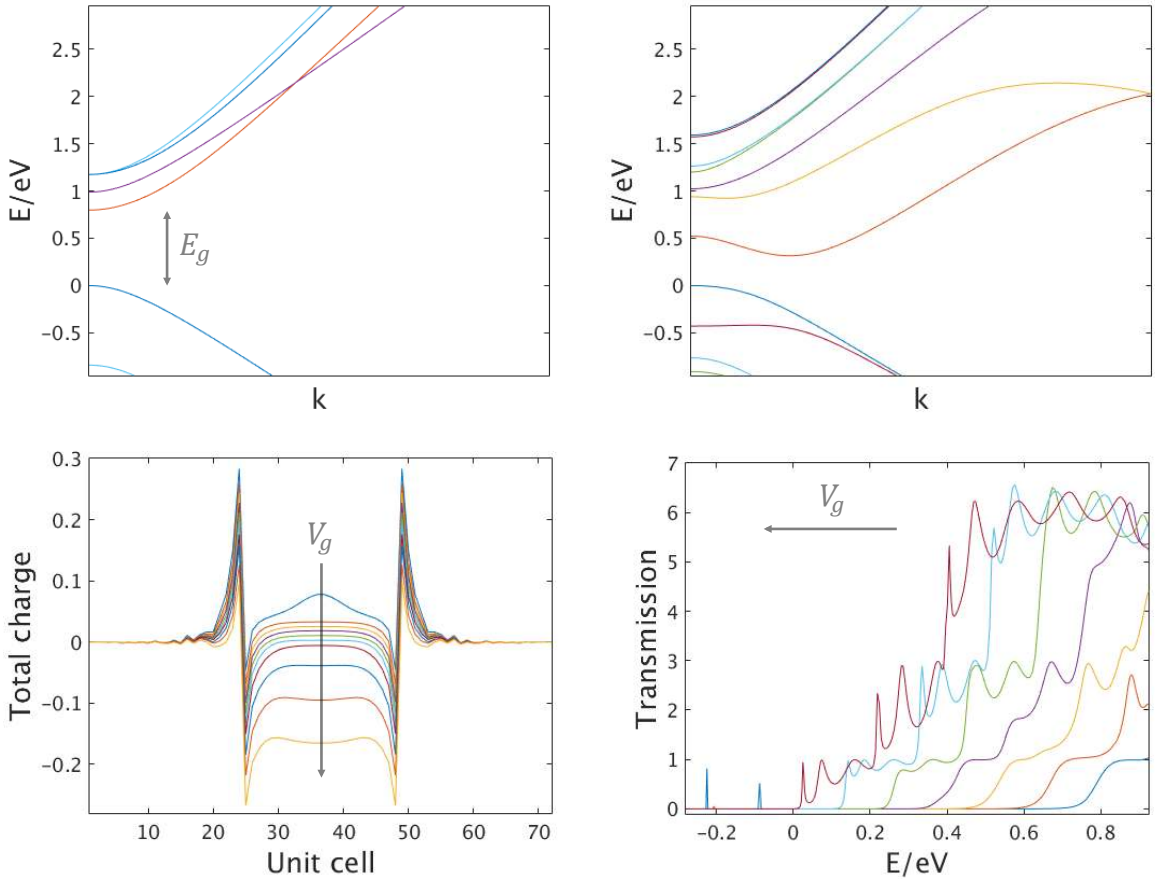
Researchers: Sascha Brück
Mathieu Luisier

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

Description:

Nanowire field-effect transistors with small diameters require considering the effects of individual atoms. In the case of heavily doped leads, for example, the change of the band structure may be considerable. In order to compute quantum transport properties for such devices with *ab-initio* methods, the gate voltage around the channel must be fixed in the Poisson equation. The density can then be computed with the resulting potential by filling the electronic states of the total system up to the Fermi level, thus keeping the leads neutral. After self-consistency is established for each gate voltage, the transmission profile at equilibrium can be determined.

Below, the results are shown for a 30 nm carbon nanotube consisting of 72 unit cells. In the leads, two of the 32 carbon atoms per unit cell have been replaced by nitrogen dopants. The gate voltage induces charge carriers inside the channel, which shifts the transmission curve to lower energies and increases the current. As conduction and valence electrons are treated on the same footing, resonant tunneling peaks for low gate voltages are automatically captured.



Top Left: Band structure of the semiconducting carbon nanotube channel.
Top Right: Band structure of the heavily doped carbon nanotube leads.
Bottom Left: Total charge per unit cell for different gate voltages.
Bottom Right: Transmission profile for different gate voltages.

Title: Scaling Quantum Electron Transport Calculations to Tens of Thousands of Atoms on Hybrid Computing Nodes

Researchers: Mauro Calderara
Sascha Brück
Mathieu Luisier

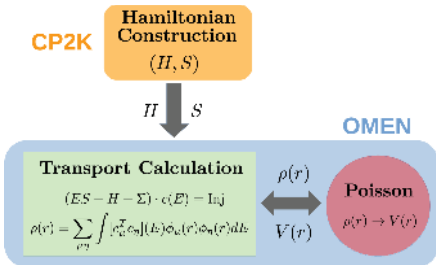
Institute/ Group: Integrated Systems Laboratory/ Nano-TCAD Group

Description:

Simulation of materials at an atomistic level is a well established field relevant for a variety of scientific domains and engineering applications. Many simulations from first principles, however, do not attempt to investigate the behavior of materials under applied external voltages due to the significant computational effort required to do so. Yet these simulations are needed to investigate nanotransistors, batteries, and other switching devices.

By coupling the density-functional theory community code CP2K with our quantum transport solver, OMEN, and by developing algorithms optimized for both the specific physical problem and accelerator based computing platforms, we have been able to simulate structures containing more than 50'000 atoms and extract their current vs. voltage characteristics. The code scales efficiently up to 18'500 hybrid nodes, reaching a sustained performance of 15 PFlop/s on the Titan supercomputer.

a)



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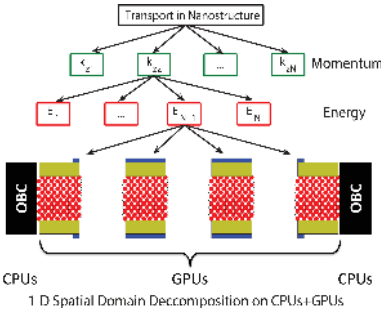
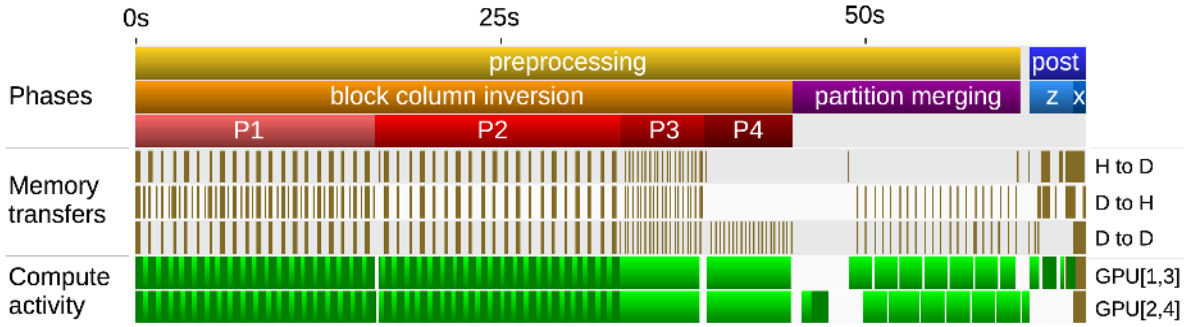
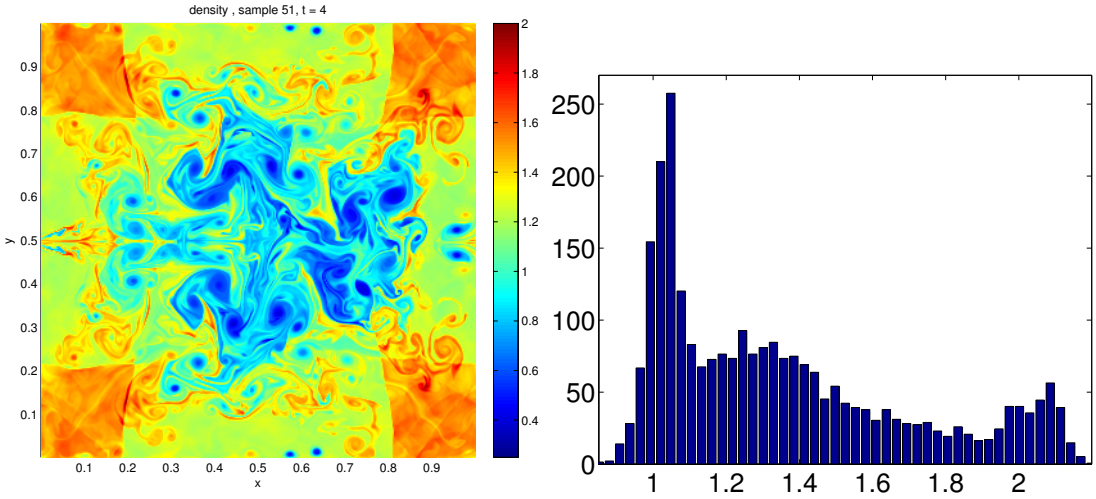


c)



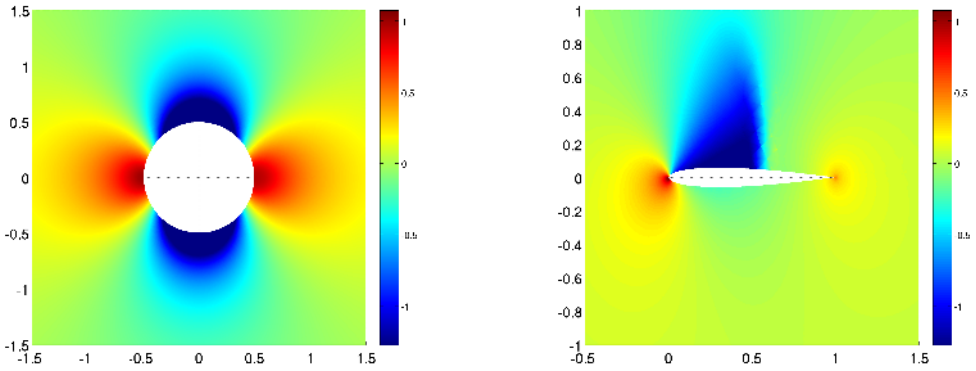
a) Schematic view of the coupling between CP2K (ab-initio structure generation) and OMEN (transport calculation). b) Levels of parallelism in ballistic transport calculations. Only the lowest level is not embarrassingly parallel. c) GPU utilization for 4 GPUs working on one quadrature point (lowest level in b).



Title: Computation of measure valued and statistical solutions of the equations of inviscid fluid dynamics.

Insitute: SAM.
Researchers: S. Mishra, R. Käppeli, F. Leonardi, K. Lye, F. Weber, U. S. Fjordholm (NTNU, Trondheim, Norway).
Description: Measure valued solutions are a new paradigm in CFD that appear to be promising as the appropriate solution framework of both the incompressible as well as compressible Euler equations of fluid dynamics. These solutions are space-time parametrized probability measures that represent (weak) limit of approximation schemes, such as numerical methods. A new ensemble based sampling algorithm is proposed to approximate measure valued solutions and is shown to converge as the mesh parameters tend to zero. Statistical quantities of interest, such as the mean, variance, pdfs and multi-point correlation functions can be computed in a convergent manner. Statistical solutions are a novel concept that include information on the correlation structure of the equations of fluid dynamics.
Publications:

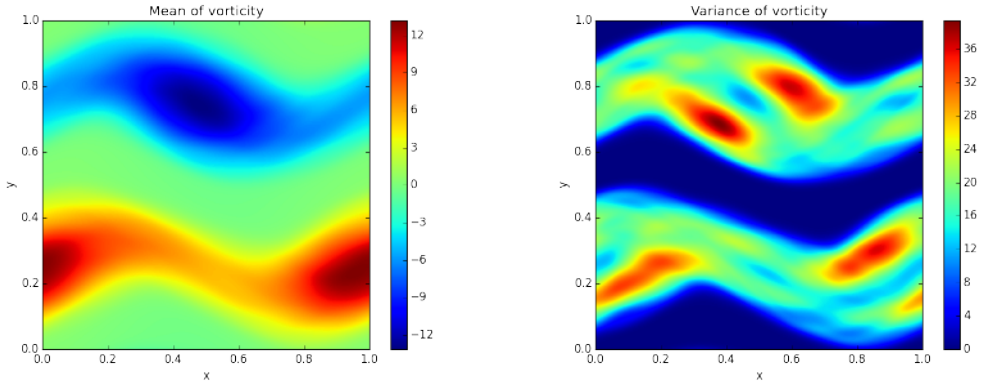
- U. S. Fjordholm, R. Käppeli, S. Mishra and E. Tadmor, Construction of approximate entropy measure valued solutions for hyperbolic systems of conservation laws. *Preprint*, available as arXiv:1402.0909 [math.NA].
- S. Lanthaler and S. Mishra, Computation of measure valued solutions of the incompressible Euler equations, *Math. Models Methods Appl. Sci.*, 25 (2015), 11, 2043-2088.



Title: High resolution entropy stable finite volume and space-time Discontinuous Galerkin methods for approximating compressible Euler and Navier-Stokes equations on unstructured grids.

Insitute: SAM.
Researchers: S. Mishra, A. Hiltebrand, S. May, D. Ray and P. Chandrasekher (TIFR Bangalore, India), U. S. Fjordholm (NTNU, Norway).
Description: We design entropy stable high-resolution finite volume schemes for the Euler and Navier-Stokes equations, based on a judicious combination of entropy conservative fluxes, numerical diffusion operators and sign preserving limiters. Similarly, space-time shock capturing DG methods are also designed to be entropy stable. Both sets of methods are designed on unstructured grids to approximate realistic flows on domains with complex geometry.
Publications:

- P. Chandrasekhar, U. S. Fjordholm, S. Mishra and D. Ray, Entropy stable schemes on two-dimensional unstructured grids, preprint 2014.
- A. Hiltebrand and S. Mishra, Efficient computation of all speed flows using an entropy stable shock-capturing space-time discontinuous Galerkin method, *Research report 2014-17,* SAM ETH Zurich.
- A. Hiltebrand and S. Mishra, Efficient pre conditioners for a shock capturing space-time discontinuous Galerkin method for systems of conservation laws, *Commun. Comput. Phys.,* 17 (2015), 1, 83-98.



Title: Multi-level Monte Carlo methods for computing statistical solutions of incompressible Navier-Stokes equations.

Insitute: SAM.
Researchers: S. Mishra, C. Schwab, F. Leonardi
Description: Multi-level Monte Carlo (MLMC) methods are developed and employed to efficiently compute uncertainty in the solutions of the incompressible Navier-Stokes equations, in the context of statistical solutions. These solutions are time parametrized probability measures on the function space and the MLMC method has been adapted to compute statistical quantities of interest with respect to these measures on infinite dimensional spaces.

Publications:

- F. Leonardi, S. Mishra, Ch. Schwab Numerical approximation of statistical solutions for incompressible flow, *Research report 2015-27*, SAM ETH Zurich.

Title: Large-scale microstructural simulation of load-adaptive bone remodelling in whole human vertebrae

Researchers: Sandro D. Badilatti
Patrik Christen
Ralph Müller

Institute/ Group: Institute for Biomechanics
Laboratory for Bone Biomechanics

Description:

The weakening of bone due to osteoporotic bone loss increases the risk of fractures in elderly people leading to pain and increased morbidity and mortality. While preventive approaches with medication and exercise can help maintain bone quality, the key to successfully controlling fracture numbers is to identify the individuals at risk and provide them with focused preventive treatment. The current practice for estimating fracture risk is at best to assess bone mass but not accounting for the bone microstructure although this is the major determinate of bone strength. Additionally, assessments are static and thus do not capture the dynamic nature of bone. In the process referred to as bone remodelling, bone is continuously renewed and the internal microstructure adapted to meet the needs of the bone's load-bearing function. Fracture risk assessment should therefore not only take a snapshot of the present microstructure, but also predict its onset and implications for the future mechanical stability.
Computer simulations using predictive models of bone remodelling could forecast the development of a bone's microstructure and describe the mechanical stability at a later time point if combined with micro-finite element (μFE) models that allow calculating bone mechanical properties. In such simulations, volumes were so far limited to either small animal bones or subregions of whole bones. The calculation of failure, however, ideally includes the whole bone and its microstructure. Bone remodelling simulations for the evaluation of bone strength at a future time point should therefore represent the whole bone microstructure. While studies have been performed in animals, human studies are still lacking, mostly due to the high computational costs associated with these analyses and limitation of the in vivo image acquisition in humans. Another limitation is that boundary conditions are unknown and if non-physiological conditions are applied, they might lead to unnatural bone remodelling.
To address these limitations, we combined our previously developed bone remodelling algorithm with the highly scalable octree-based μFE solver ParOSol and a bone loading estimation method to determine physiological boundary conditions in a unifying computational framework for large-scale bone remodelling simulations. Running μFE analyses on the Cray XE6 at CSCS with ParOSol allowed solving models of human vertebrae as derived from micro-CT images within hours and therefore addressed the computation time limitation. Loading estimates led to realistic bone remodelling over a simulated period of 10 years and thus addressed the boundary conditions limitation. In contrast, this was not achieved with simplified boundary conditions. The presented framework therefore allows large-scale bone remodelling simulations of whole human vertebrae at a spatial resolution not reached before. Newest imaging technology enables high-resolution imaging in patients and thus our framework may be used to improve fracture prediction in patients.

References: S. D. Badilatti et al., Biomech. Model. Mechanobiol., Epub 2015 Aug 9, 2015.

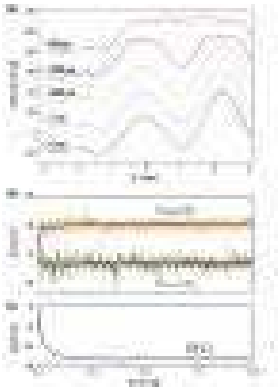
Title: Variational Approach to Enhanced Sampling and Free Energy Calculations

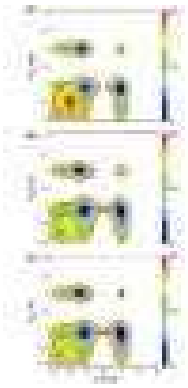
Researchers: O. Valsson[1]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8006 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, CH-6900 Lugano, Switzerland

Description:

The ability of widely used sampling methods, such as molecular dynamics or Monte Carlo simulations, to explore complex free energy landscapes is severely hampered by the presence of kinetic bottlenecks. A large number of solutions have been proposed to alleviate this problem. Many are based on the introduction of a bias potential which is a function of a small number of collective variables. However constructing such a bias is not simple. Here we introduce a functional of the bias potential and an associated variational principle. The bias that minimizes the functional relates in a simple way to the free energy surface. This variational principle can be turned into a practical, efficient, and flexible sampling method. A number of numerical examples are presented which include the determination of a three-dimensional free energy surface. We argue that, beside being numerically advantageous, our variational approach provides a convenient and novel standpoint for looking at the sampling problem.





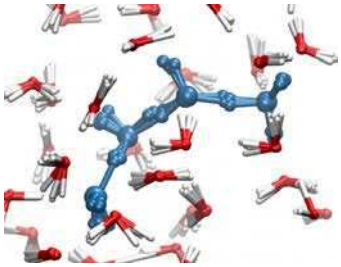
References: *Phys. Rev. Lett*. 113, 090601
DOI: 10.1103/PhysRevLett.113.090601

Title: The Role of Quantum Effects on Structural and Electronic Gluctuations in Neat and Charged Water

Researchers: F. Giberti[1]
A. A. Hassanali[2]
M. Ceriotti[3]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8006 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, CH-6900 Lugano, Switzerland
[2] The Abdus Salaam International Center for Theoretical Physics, Condensed Matter Physics Section, I-34151 Trieste, Italy
[3] Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Description:



In this work, we revisit the role of nuclear quantum effects on the structural and electronic properties of the excess proton in bulk liquid water using advanced molecular dynamics techniques. The hydronium ion is known to be a weak acceptor of a hydrogen bond which gives it some hydrophobic character. Quantum effects reduce the degree of this hydrophobicity which facilitates the fluctuations of the protons along the wires compared to the classical proton. Although the Eigen and Zundel species still appear to be dominant *motifs*, quantum fluctuations result in rather drastic events where both transient autoionization and delocalization over extended proton wires can simultaneously occur. These wild fluctuations also result in a significant change of the electronic properties of the system such as the broadening of the electronic density of states. An analysis of the Wannier functions indicate that quantum fluctuations of neat water molecules result in transient charging with subtle similarities and differences to that of the excess proton.

References: *J. Phys. Chem. B*, 2014, 118 (46), pp 13226–13235
DOI: 10.1021/jp507752e

Title: Insight into the nucleation of urea crystals from the melt

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

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich and Facoltà di Informatica, Instituto di Scienze Computationali, Università della Svizzera Italiana, CH-6900 Lugano, Switzerland
[2] ETH Zurich, Institute of Process Engineering, Soneggstrasse 3, CH-8092 Zurich, Switzerland

Description:

Obtaining molecular-level information regarding nucleation is an essential step towards a thorough comprehension of crystallization processes. In this work we investigate the nucleation of urea at the atomic scale using enhanced sampling Molecular Dynamics simulations. We show that by employing a set of suitably defined collective variables in a Well Tempered Metadynamics scheme it is possible to reversibly drive the system across the solid–liquid phase transition and to recover the associated free energy surface. Our study reveals the presence of an undiscovered metastable ordered structure competing with the experimental one during crystal nucleation, suggesting a non-classical mechanism for this process.

References: *Chemical Engineering Science*, 121, (2015), Pages 51–59
DOI: 10.1016/j.ces.2014.08.032

Title: Kinetics of protein-ligand unbinding: Predicting pathways, rates, and rate-limiting steps

Researchers: P. Tiwary[1]
V. Limongelli[1,2]
M. Salvalaglio[1,3]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano Switzerland
[2] Department of Pharmacy, University of Naples Federico II, I-80131 Naples, Italy
[3] Institute of Process Engineering, Eidgenössische Technische Hochschule Zürich, 8006 Zurich, Switzerland

Description:

The ability to predict the mechanisms and the associated rate constants of protein–ligand unbinding is of great practical importance in drug design. In this work we demonstrate how a recently introduced metadynamics-based approach allows exploration of the unbinding pathways, estimation of the rates, and determination of the rate-limiting steps in the paradigmatic case of the trypsin–benzamidine system. Protein, ligand, and solvent are described with full atomic resolution. Using metadynamics, multiple unbinding trajectories that start with the ligand in the crystallographic binding pose and end with the ligand in the fully solvated state are generated. The unbinding rate k_{off} is computed from the mean residence time of the ligand. Using our previously computed binding affinity we also obtain the binding rate k_{on}. Both rates are in agreement with reported experimental values. We uncover the complex pathways of unbinding trajectories and describe the critical rate-limiting steps with unprecedented detail. Our findings illuminate the role played by the coupling between subtle protein backbone fluctuations and the solvation by water molecules that enter the binding pocket and assist in the breaking of the shielded hydrogen bonds. We expect our approach to be useful in calculating rates for general protein–ligand systems and a valid support for drug design.

References: *PNAS*, 112 (5), 2015, E386–E391
DOI: 10.1073/pnas.1424461112

Title: Molecular-dynamics simulations of urea nucleation from aqueous solution

Researchers: M. Salvalaglio[1,2]
C. Perego[2]
F. Giberti[2]
M. Mazzotti[1]
M. Parrinello[2]

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

Description:

Despite its ubiquitous character and relevance in many branches of science and engineering, nucleation from solution remains elusive. In this framework, molecular simulations represent a powerful tool to provide insight into nucleation at the molecular scale. In this work, we combine theory and molecular simulations to describe urea nucleation from aqueous solution. Taking advantage of well-tempered metadynamics, we compute the free-energy change associated to the phase transition. We find that such a free-energy profile is characterized by significant finite-size effects that can, however, be accounted for. The description of the nucleation process emerging from our analysis differs from classical nucleation theory. Nucleation of crystal-like clusters is in fact preceded by large concentration fluctuations, indicating a predominant two-step process, whereby embryonic crystal nuclei emerge from dense, disordered urea clusters. Furthermore, in the early stages of nucleation, two different polymorphs are seen to compete.

References: *PNAS*, 2015, 10 (4), 112, (1), E6–E14
DOI: 10.1073/pnas.1421192111

Title: Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase

Researchers: E. Formoso[1,3]
V. Limongelli[2]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[2] Department of Pharmacy, University of Naples Federico II, I-80131 Naples, Italy
[3] Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU) and Donostia International Physics Center (DIPC), PK 1072, 20080 Donostia, Euskadi, Spain

Description:

Adenylate Kinase (AK) is a signal transducing protein that regulates cellular energy homeostasis balancing between different conformations. An alteration of its activity can lead to severe pathologies such as heart failure, cancer and neurodegenerative diseases. A comprehensive elucidation of the large-scale conformational motions that rule the functional mechanism of this enzyme is of great value to guide rationally the development of new medications. Here using a metadynamics-based computational protocol we elucidate the thermodynamics and structural properties underlying the AK functional transitions. The free energy estimation of the conformational motions of the enzyme allows characterizing the sequence of events that regulate its action. We reveal the atomistic details of the most relevant enzyme states, identifying residues such as Arg119 and Lys13, which play a key role during the conformational transitions and represent druggable spots to design enzyme inhibitors. Our study offers tools that open new areas of investigation on large-scale motion in proteins.

References: *Scientific Reports* 5, Article number: 8425 (2015)
DOI: 10.1038/srep08425

Title: Combustion Chemistry via Metadynamics: Benzyl Decomposition Revisited

Researchers: D. Polino
M. Parrinello

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

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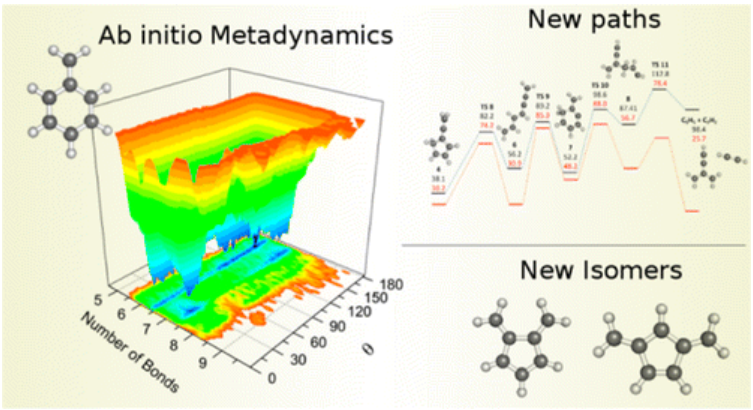


Large polycyclic aromatic hydrocarbons (PAHs) are thought to be responsible for the formation of soot particles in combustion processes. However, there are still uncertainties on the course that leads small molecules to form PAHs. This is largely due to the high number of reactions and intermediates involved. Metadynamics combined with ab initio molecular dynamics can provide a very precious contribution because offers the possibility to explore new possible pathways and suggest new mechanisms. Here, we adopt this method to investigate the chemical evolution of the benzyl radical, whose role is very important in PAHs growth. This species has been intensely studied, and though most of its chemistry is known, there are still open questions regarding its decomposition. The simulation reproduces the most commonly accepted decomposition pathway and it suggests also a new one which can explain recent experimental data that are in contradiction with the old mechanism. In addition, quantitative free energy evaluation of some key reaction steps sheds light on the role of entropy.

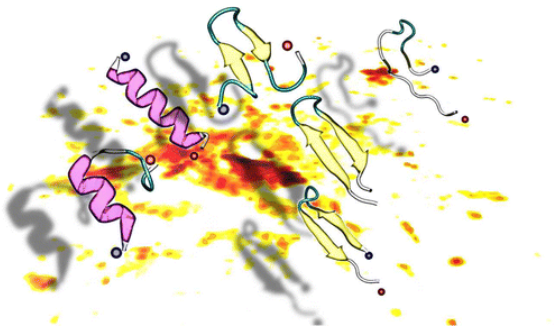
References: *J. Phys. Chem. A*, 2015, 119 (6), pp 978–989
DOI: 10.1021/jp504920s

Title: Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map

Researchers: A. A. Ardevol[1]
G.A. Tribello[2]
M. Ceriotti[3]
M. Parrinello

Institute/Group: [1] Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich, USI-Campus, 6900 Lugano, Switzerland
[2] Atomistic Simulation Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, United Kingdom
[3] Laboratory of Computational Science and Modelling, EPFL, CH-1015 Lausanne, Switzerland

Description:



This work examines the conformational ensemble involved in β-hairpin folding by means of advanced molecular dynamics simulations and dimensionality reduction. A fully atomistic description of the protein and the surrounding solvent molecules is used, and this complex energy landscape is sampled by means of parallel tempering metadynamics simulations. The ensemble of configurations explored is analyzed using the recently proposed sketch-map algorithm. Further simulations allow us to probe how mutations affect the structures adopted by this protein. We find that many of the configurations adopted by a mutant are the same as those adopted by the wild-type protein. Furthermore, certain mutations destabilize secondary-structure-containing configurations by preventing the formation of hydrogen bonds or by promoting the formation of new intramolecular contacts. Our analysis demonstrates that machine-learning techniques can be used to study the energy landscapes of complex molecules and that the visualizations that are generated in this way provide a natural basis for examining how the stabilities of particular configurations of the molecule are affected by factors such as temperature or structural mutations.

References: *J. Chem. Theory Comput.*, 2015, 11 (3), pp 1086–1093
DOI: 10.1021/ct500950z

Title: Metadynamics Studies of Crystal Nucleation

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

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule (ETH) Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[2] ETH Zurich, Institute of Process Engineering, Soneggstrasse 3, CH-8092 Zurich, Switzerland

Description:

Crystallization processes are characterized by activated events and long timescales. These characteristics prevent standard molecular dynamics techniques from being efficiently used for the direct investigation of processes such as nucleation. This short review provides an overview on the use of metadynamics, a state-of-the-art enhanced sampling technique, for the simulation of phase transitions involving the production of a crystalline solid. In particular the principles of metadynamics are outlined, several order parameters are described that have been or could be used in conjunction with metadynamics to sample nucleation events and then an overview is given of recent metadynamics results in the field of crystal nucleation.

References: *IUCrJ*, 2015, 2, part 2, 256 - 266
DOI: 10.1107/S2052252514027626

Title: Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations

Researchers: G. C. Sosso[1,2]
M. Salvalaglio[1,3]
J. Behler[4]
M. Bernasconi[5]
M. Parrinello[1,2]

Institute/Group: [1] ETH Zurich, Department of Chemistry and Applied Biosciences, Via Giuseppe Buffi 13, USI Campus, 6900 Lugano, Switzerland
[2] Faculty of Informatics, Università della Svizzera Italiana, Via G. Buffi 13, CH-6900 Lugano, Switzerland
[3] Institute of Process Engineering, ETH Zurich, Sonneggstrasse 3, CH-8092 Zurich, Switzerland
[4] Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Universitätsstrasse 150, D-44780 Bochum, Germany
[5] Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 55, I-20125 Milano, Italy

Description:

Phase change materials are the active compounds in optical disks and in nonvolatile phase change memory devices. These applications rest on the fast and reversible switching between the amorphous and the crystalline phases, which takes place in the nano domain in both the time and the length scales. The fast crystallization is a key feature for the applications of phase change materials. In this work, we have investigated by means of large scale molecular dynamics simulations the crystal growth of the prototypical phase change compound GeTe at the interface between the crystalline and the supercooled liquid reached in the device upon heating the amorphous phase. A neural network interatomic potential, markedly faster with respect to first-principles methods, allowed us to consider high-symmetry crystalline surfaces as well as polycrystalline models that are very close to the actual geometry of the memory devices. We have found that the crystal growth from the interface is dominant at high temperatures while it is competing with homogeneous crystallization in the melt at lower temperatures. The crystal growth velocity markedly depends on the crystallographic plane exposed at the interface, the (100) surface being kinetically dominant with respect to the (111) surface. Polycrystalline interfaces, representative of realistic conditions in phase change memory devices, grow at significantly slower pace because of the presence of grain boundaries.

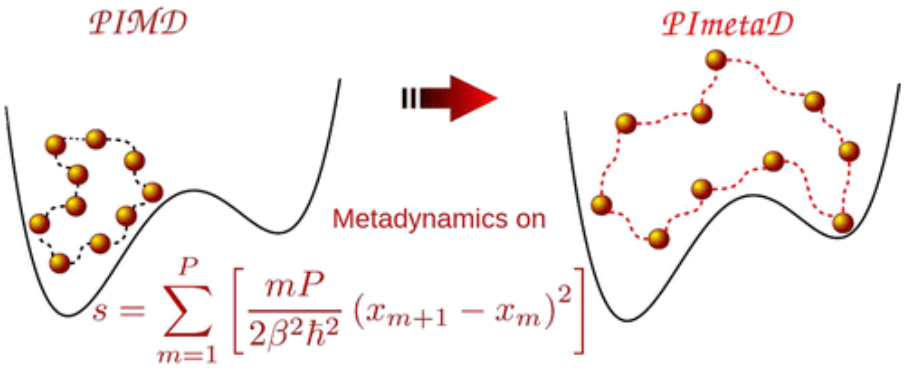
References: *J. Phys. Chem. C*, 2015, 119 (11), pp 6428–6434
DOI: 10.1021/acs.jpcc.5b00296

Title: Path Integral Matadynamics

Researchers: R. Quhe[1,2]
M. Nava[1]
P. Tiwary[1]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via G. Buffi 13, 6900 Lugano, Switzerland
[2] State Key Laboratory of Mesoscopic Physics, Department of Physics and Academy for Advanced Interdisciplinary Studies, Peking University, Beijing 100871, P. R. China

Description:



We develop a new efficient approach for the simulation of static properties of quantum systems using path integral molecular dynamics in combination with metadynamics. We use the isomorphism between a quantum system and a classical one in which a quantum particle is mapped into a ring polymer. A history dependent biasing potential is built as a function of the elastic energy of the isomorphic polymer. This enhances fluctuations in the shape and size of the necklace in a controllable manner and allows escaping deep energy minima in a limited computer time. In this way, we are able to sample high free energy regions and cross barriers, which would otherwise be insurmountable with unbiased methods. This substantially improves the ability of finding the global free energy minimum as well as exploring other metastable states. The performance of the new technique is demonstrated by illustrative applications on model potentials of varying complexity.

References: *J. Chem. Theory Comput.*, 2015, 11 (4), pp 1383–1388
DOI: 10.1021/ct501002a

Title: Molecular dynamics simulations of solutions at constant chemical potential

Researchers: C. Perego[1]
M. Salvalaglio[2]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule (ETH) Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[2] Institute of Process Engineering, ETH Zurich, Sonneggstrasse 3, CH-8092 Zurich, Switzerland

Description:

Molecular dynamics studies of chemical processes in solution are of great value in a wide spectrum of applications, which range from nano-technology to pharmaceutical chemistry. However, these calculations are affected by severe finite-size effects, such as the solution being depleted as the chemical process proceeds, which influence the outcome of the simulations. To overcome these limitations, one must allow the system to exchange molecules with a macroscopic reservoir, thus sampling a grand-canonical ensemble. Despite the fact that different remedies have been proposed, this still represents a key challenge in molecular simulations. In the present work, we propose the Constant Chemical Potential Molecular Dynamics (CμMD) method, which introduces an external force that controls the environment of the chemical process of interest. This external force, drawing molecules from a finite reservoir, maintains the chemical potential constant in the region where the process takes place. We have applied the Cμ MD method to the paradigmatic case of urea crystallization in aqueous solution. As a result, we have been able to study crystal growth dynamics under constant supersaturation conditions and to extract growth rates and free-energy barriers.

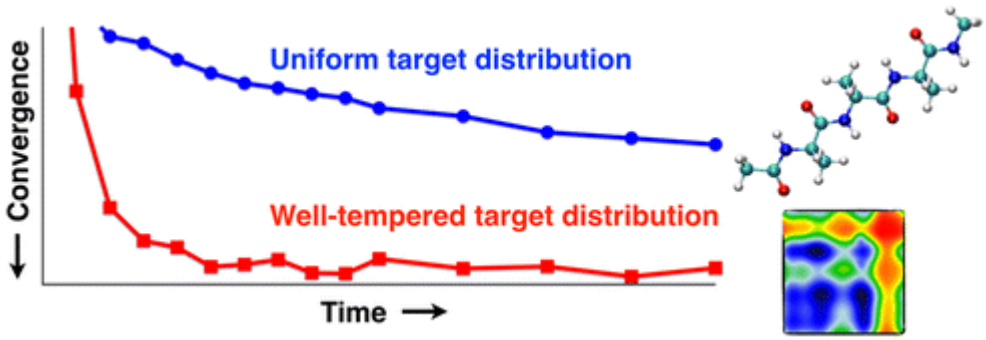
References: *J. Chem. Phys*. 142, 144113 (2015);
DOI: 10.1063/1.4917200

Title: Well-Tempered Variational Approach to Enhanced Sampling

Researchers: O. Valsson[1,2]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule (ETH) Zürich, CH-8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, 6900 Lugano, Switzerland
[2] Facoltà di Informatica, Instituto di Scienze Computationali, and National Center for Computational Design and Discovery of Novel Materials MARVEL, Università della Svizzera italiana, Via Giuseppe Buffi 13, 6900, Lugano, Switzerland

Description:



We propose a simple yet effective iterative scheme that allows us to employ the well-tempered distribution as a target distribution for the collective variables in our recently introduced variational approach to enhanced sampling and free energy calculations [Valsson and Parrinello *Phys. Rev. Lett.* 2014, *113*, 090601]. The performance of the scheme is evaluated for the three-dimensional free energy surface of alanine tetrapeptide where the convergence can be rather poor when employing the uniform target distribution. Using the well-tempered target distribution on the other hand results in a significant improvement in convergence. The results observed in this paper indicate that the well-tempered distribution is in most cases the preferred and recommended choice for the target distribution in the variational approach.

References: *J. Chem. Theory Comput.*, 2015, 11 (5), pp 1996–2002
DOI: 10.1021/acs.jctc.5b00076

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

Researchers: M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We discuss certain sequences of numbers involving 240, in particular, also in a more general number theoretical context, where simple superstructures arise from the detailed mathematical structures. We then relate this to statistical consideration in molecular spectra and molecular dynamics which finally result in simple superstructures as the Pauli Master equation and the second law of thermodynamics.

References:
M. Quack, Adv. Chem. Phys., 2014, 157, 97-116.

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

Researchers: M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We review the question of homochirality as a quasi-fossil of the evolution of life. We discuss how this question is closely linked to fundamental symmetries of physics C, P, T and their violation. There are several fundamentally different hypotheses for the origin of homochirality, but we do not know which one, if any, is correct. We show, which type of observation either in the laboratory or in astrobiological investigations would provide information. We summarize the current status of our investigations on molecular parity violation resulting in a small "parity violating" energy difference between the enantiomers of chiral molecules. The theory for this phenomenon has been substantially revised by us in 1995 leading to about one to two orders of magnitude larger values than anticipated previously and is now well established. However, experimental confirmation (or refutation) is still missing, but we have made progress on this question. We conclude by a discussion of what the consequences of parity violation might be for future studies of the evolution of homochirality, as well as some cosmological speculations.

References:
M. Quack, Adv. Chem. Phys., 2014, 157, 249-290

Title: Survey of the High Resolution Infrared Spectrum of Methane ($^{12}CH_4$ and $^{13}CH_4$): Partial Vibrational Assignment Extended Towards 12000 cm^{-1}

Researchers: O. N. Ulenikov*/**
E. S. Bekhtereva*/**
S. Albert*/***
S. Bauerecker*/****
H.-M. Niederer*
M. Quack*

Institute/Group:
* Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland
** Institute of Physics and Technology, National Research Tomsk Polytechnic University, RU-634050 Tomsk, Russia
*** Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
**** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, DE-38106 Braunschweig, Germany

Description:
We have recorded the complete infrared spectrum of methane $^{12}CH_4$ and its second most abundant isotopomer $^{13}CH_4$ extending from the fundamental range starting at 1000 cm^{-1} up to the overtone region near 12'000 cm^{-1} in the near infrared at the limit towards the visible range, at temperatures of about 80 K and also at 298 K with Doppler limited resolution in the gas phase by means of interferometric Fourier transform spectroscopy using the Bruker IFS 125 HR prototype (ZP 2001) of the ETH Zürich laboratory. This provides the so far most complete data set on methane spectra in this range at high resolution. In the present work we report in particular those results, where the partial rovibrational analysis allows for the direct assignment of pure (J = 0) vibrational levels including high excitation. These results substantially extend the accurate knowledge of vibrational band centers to higher energies and provide a benchmark for both the comparison with theoretical results on the one hand and atmospheric spectroscopy on the other hand. We also present a simple effective Hamiltonian analysis, which is discussed in terms of vibrational level assignments and ^{13}C isotope effects. The analysis uses extensive numerical simulations.

References:
O. N. Ulenikov, E. S. Bekhtereva, S. Albert, S. Bauerecker, H. M. Niederer, and M. Quack *J. Chem. Phys.*, **2014**, *141*, 234302.

Title: Fixierte Konstanten (Zur Definition des Mols (mol), der Masseneinheit (kg) und zur Avogadroschen Konstanten N_A)

Researchers: J. Stohner*
M. Quack**

Institute/Group: * ZHAW
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We discuss the background of the definitions of the various systems of quantities and units and current possibilities of redefining the kg and the mole within a new SI (système international).

References:
1. J. Stohner, M. Quack, Nachrichten aus der Chemie, **63**, 515–521 (2015)
2. E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. Thor
   Quantities, Units and Symbols in Physical Chemistry, Third Edition, IUPAC and Royal Society of Chemistry, RSC, Cambridge (2007)
   (Book with 250 pages, ISBN 978-0-85404-433-7)
   second revised printing 2008, third printing 2011
3. E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. Thor
   Quantities, Units and Symbols in Physical Chemistry, Japanese Translation,
   IUPAC and National Metrology Institute, National Institute of Advanced Industrial Science and Technology and the Chemical Society of Japan (2009)
   (Book with 258 pages, ISBN 978-4-06-154359-1)
4. E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. Thor
   Grandeurs, unités et symboles de la chimie physique
   Recommandations de l'Union internationale de chimie pure et appliquée (IUPAC)
   Traduction de la 3^{e} édition anglaise par Roberto Marquardt, Monique Mottet, Françoise Rouquérol, Jean Toullec
   De Boeck, Bruxelles, 2012, ISBN: 978-2-8041-7207-7
5. J. Stohner, M. Quack, A Concise Summary of Quantities, Units and Symbols in Physical Chemistry, IUPAC & Royal Society of Chemistry, Cambridge, 2009, ISBN 978-1-84973-039-6.

Title: Computation of Molecular Parity Violation Using the Coupled Cluster Linear Response Approach

Researchers: L. Horný,
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We report the implementation of a coupled-cluster linear response approach for the computation of molecular parity violation (in the framework of the PSI3 code, in particular). The approach is applied first to molecules such as hydrogen peroxide (HOOH), hydrogen disulfide (HSSH) and dichlorinedioxide (ClOOCl), which have been studied previously. The importance of including correlation is demonstrated for these examples, also including selected variations of geometry providing parity violation as a function of torsional angles. For the substituted allenes, 1,3-difluoroallene (CHF=C=CHF), 1,fluoro,3-chloroallene (CHF=C=CHCl) and 1,3-dichloroallene (CHCl=C=CHCl), we find that in particular the last molecule may be a suitable candidate for the experimental study of molecular parity violation.

References:
L. Horný, M. Quack, Mol. Phys., **113**, 1768-1779 (2015)

Title: High-resolution rovibrational spectroscopy of fluorobenzene, C_6H_5F: analysis of the B_1 fundamentals v_4, v_{10b}, v_{17b}, the B_2 fundamental v_{15} and assignment of the A_1 levels v_{12}, $2v_{16a}$ and $2v_{18b}$

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

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland
** Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Description:
We report the rovibrational analysis of the highly resolved (instrumental bandwidth $\Delta\tilde{\nu}$ = 0.0008–0.0018 cm^{-1} full width at half maximum [FWHM]) Fourier transform infrared (FTIR) spectrum of fluorobenzene measured with our Zurich Fourier transform interferometric spectrometer prototype (Bruker IFS 125 HR ZP 2001) in the range 600–1300 cm^{-1}. The analysis comprised initially three B_1 bands and led to an identification of Coriolis resonances and a new assignment of three A_1 bands in the region 790–850 cm^{-1}. In detail, three B_1 fundamentals, ν_4 ($\tilde{\nu}_0$ = 685.206397 (10) cm^{-1}), ν_{10b} ($\tilde{\nu}_0$ = 754.903635 (11) $cm^{-}1$) and ν_{17b} ($\tilde{\nu}_0$ = 894.970254 (14) cm^{-1}) have been analysed using an effective Hamiltonian. A perturbation of the B_2 fundamental ν_{15} ($\tilde{\nu}_0$ = 1066.300590 (12) cm^{-1}) was detected and the interaction is interpreted as a crossing Coriolis resonance between the states ν_{15} and a dark state assigned as $\nu_4 + \nu_{18b}$. The Coriolis parameter ξ_x was determined to be 0.00345 cm^{-1}. The rovibrational analysis of the region between 790 and 850 cm^{-1} revealed three A_1 bands assigned to ν_{12} ($\tilde{\nu}_0$ = 807.548687 (44) cm^{-1}), $2\nu_{18b}$ ($\tilde{\nu}_0$ = 810.331870 (83) cm^{-1}) and $2\nu_{16a}$ ($\tilde{\nu}_0$ = 825.869616 (40) cm^{-1}). A Coriolis resonance between the states $2\nu_{16a}$ and a dark state assigned as ν_{10a} ($\tilde{\nu}_0$ = 819.74 (30) cm^{-1}, A_2 symmetry) was identified and the Coriolis coupling constant ξ_z was determined to be 0.0145 cm^{-1}. The root mean square deviation d_{rms} is in the range 0.0002 − 0.0003 cm^{-1} (6–9 MHz) for the adjustment of the model to almost 17000 assigned rovibrational absorption line positions. This indicates an excellent representation of the data by the model. The analysis is carried out using extensive numerical simulations

References:
S. Albert, K. Keppler, M. Quack, Mol. Phys., **113**, 2267–2289 (2015)

Title: Line shape of amplitude or frequency-modulated spectral profiles including resonator distortions

Researchers: M. Suter
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We report experiments and an improved method of analysis for any harmonics of frequency-modulated spectral line shapes allowing for very precise determinations of the resonance frequency of single absorption lines for gigahertz spectroscopy in the gas phase. Resonator perturbations are implemented into the formalism of modulation spectroscopy by means of a full complex transmission function being able to model the asymmetrically distorted absorption line shapes for arbitrary modulation depths, modulation frequencies, and resonator reflectivities. Exact equations of the in-phase and the quadrature modulation signal, taking into account a full resonator transmission function, are simultaneously adjusted to two-channel lock-in measurements performed in the gigahertz regime to obtain the spectral line position. The determination of the absorption line position of the rotational transition $J'=7\leftarrow J''=6$ of $^{16}O^{12}C^{32}S$ in the vibrational ground state is investigated while changing the resonator distortions. The results are subjected to the approach proposed here and compared to standard methods known from the literature.

References:
M. Suter, M. Quack, Applied Optics, **54**, 4417 – 4421 (2015)

Title: Synchrotron based highest resolution FTIR spectroscopy of chlorobenzene

Researchers: S. Albert*/**
K. Keppler*
P. Lerch,**
M. Quack*
A. Wokaun**

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland
** Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Description:
We report the Fourier Transform Infrared (FTIR) spectrum of chlorobenzene (C_6H_5Cl) measured using synchrotron radiation and the ETH-SLS 2009 prototype spectrometer at the Swiss Light Source (SLS). The maximum optical path difference of these measurements was 11.8 m leading to a resolution of better than 0.0008 cm^{-1}. The spectra were taken at room temperature in the range 600–900 cm^{-1}. It was possible to analyze the in-plane mode ν_{12} of A_1 symmetry ($\tilde{\nu}_0$ = 706.6686 cm^{-1}) and the out-of-plane mode ν_{10b} of B_1 symmetry ($\tilde{\nu}_0$ = 741.2240 cm^{-1}) of $C_6H_5{}^{35}Cl$. In addition, the ground state constant D_K of $C_6H_5{}^{35}Cl$ has been readjusted using combination differences (CD).

References:
S. Albert, K. Keppler, P. Lerch, M. Quack, A. Wokaun, J. of Mol. Spectr. **315**, 92–101 (2015)

Title: Investigation of the $\nu_2 + 2\nu_3$ subband in the overtone icosad of $^{13}CH_4$ by pulsed supersonic jet and diode laser cavity ring-down spectroscopy: partial rovibrational analysis and nuclear spin symmetry conservation,

Researchers: Z. Bjelobrk,
C. Manca Tanner
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We have investigated the $\nu_2 + 2\nu_3$ combination band of methane $^{13}CH_4$ centered at 7493.15918 cm^{-1} within the icosad of the overtone absorption. The jet-CRD setup combining supersonic jet expansions and cavity ring-down spectroscopy which was already used for the reinvestigation of the same spectral region for the main isotope of methane ($^{12}CH_4$) has been used to record spectra of the Q and R branches at room temperature as well as at very low temperatures (down to 4 K). Based on our previous temperature-dependent investigations and the present results, we provide a careful analysis and the assignment for lines involving angular momentum quantum numbers up to $J = 4$. The analysis of the relative intensities in spectra taken at various rotational and effective translational temperatures demonstrate conservation of nuclear spin symmetry for $^{13}CH_4$ upon supersonic jet expansion, similar to our previous results regarding $^{12}CH_4$ and also to further results using other techniques and covering other spectral ranges. This is in agreement with theoretical expectation regarding very slow nuclear spin symmetry relaxation under these conditions in supersonic jet expansions.

References:
Z. Bjelobrk, C. Manca Tanner, M. Quack, Z. Phys. Chemie, **229**, 1575–1607 (2015)

Title: Tunneling and Parity Violation in Trisulfane (HSSSH): An Almost Ideal Molecule for Detecting Parity Violation in Chiral Molecules

Researchers: C. Fábri
Ľ. Horný
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
Measuring the parity-violating energy difference $\Delta_{pv}E$ between the enantiomers of chiral molecules is a major challenge of current physical-chemical stereochemistry. An important step towards this goal is to identify suitable molecules for such experiments by means of theory. This step has been made by calculations for the complex dynamics of tunneling and electroweak quantum chemistry of parity violation in the "classic" molecule trisulfane HSSSH, which satisfies the relevant conditions for experiments almost ideally, as the molecule is comparatively simple and parity violation clearly dominates over tunneling in the ground state. At the same time the barrier for stereomutation is easily overcome by the S-H infrared chromophore.

References:
C. Fábri, Ľ. Horný, M. Quack, ChemPhysChem., **16**, 3584–3589 (2015)

Title: Wavepacket Dynamics of the Axially Chiral Molecule Cl-O-O-Cl under Coherent Radiative Excitation and Including Electroweak Parity Violation

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

Institute/Group:
* Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland
** Chair for Philosophy, ETH Zürich, CH-8092 Zürich, Switzerland
*** Institute for Chemistry and Biological Chemistry, Zürich University for Applied Sciences, Campus Reidbach, CH-8840 Wädenswil, Switzerland
**** Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Description:

We report detailed theoretical calculations of the quantum wavepacket dynamics of Cl-O-O-Cl which serves as prototype molecule for the stereomutation dynamics of an axially chiral molecule. We include both the effects from electroweak parity violation and from the interaction with a coherent monochromatic laser field. We use the quasiadiabatic channel Reaction Path Hamiltonian approach to approximately solve the six-dimensional Schrödinger equation describing the vibrational motion, including rotation by an effective Hamiltonian. We calculate time-dependent wave-functions based on the time-dependent Schrödinger equation. We study stereomutation dynamics due to tunneling motion and laser induced population transfer and show results on efficient methods for selectively populating single molecular states in chiral molecules by frequency modulated laser pulses. We also discuss laser induced stereomutation (LISM) and a process which may be called Resonance Raman induced stereomutation (RRISM). The results are discussed in relation to current experimental attempts to measure the parity violating energy difference $\Delta_{pv}E$ between the enantiomers of chiral molecules. Furthermore, we show detailed quantitative simulations of a selection of well-defined parity levels in chiral molecules ("parity isomers") which form the basis of a possible measurement of $\Delta_{pv}E$ by the time evolution of parity.

References:

R. Prentner, M. Quack, J. Stohner, M. Willeke, J. Phys. Chem. A., 000, 000–000 (2015) (in press), doi: 10.1021/acs.jpca.5b08958.

Title: Infrared Laser Induced Population Transfer and Parity Selection in $^{14}NH_3$: A Proof of Principle Experiment Towards Detecting Parity Violation in Chiral Molecules

Researchers: P. Dietiker
E. Miloglyadov
M. Quack
A. Schneider
G. Seyfang

Institute/Group: Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich, CH-8093 Zurich, Switzerland

Description:
We have set up an experiment for the efficient population transfer by a sequential two photon – absorption and stimulated emission – process in a molecular beam to prepare quantum states of well defined parity and their subsequent sensitive detection. This provides a proof of principle for an experiment which would allow for parity selection and measurement of the time evolution of parity in chiral molecules, resulting in a measurement of the parity violating energy difference $\Delta_{pv}E$ between enantiomers of chiral molecules. Here we present first results on a simple achiral molecule demonstrating efficient population transfer (about 80%) and unperturbed persistence of a selected excited parity level over flight times of about 2 ms in the beam. In agreement with model calculations with and without including nuclear hyperfine structure efficient population transfer can be achieved by a rather simple implementation of the rapid adiabatic passage (RAP) method of Reuss and coworkers and considering also the STIRAP technique of Bergmann and coworkers as an alternative. The preparation step uses two powerful single mode continuous wave optical parametric oscillators (OPO) of high frequency stability and accuracy. The detection uses a sensitive REMPI (resonantly enhanced multiphoton ionization) method after free flight lengths of up to 0.8 m in the molecular beam. Using this technique we were able to also resolve the nuclear hyperfine structure in the rovibrational levels of the ν_1 and ν_3 fundamentals as well as the $2\nu_4$ overtone of $^{14}NH_3$, for which no previous data with hyperfine resolution were available. We present our new results on the quadrupole coupling constants for the ν_1, ν_3 and $2\nu_4$ levels in the context of previously known data for ν_2 and its overtone, as well as ν_4, and the ground state. Thus now ^{14}N quadrupole coupling constants for all fundamentals and some overtones of $^{14}NH_3$ are known and can be used for further theoretical analysis. Extensive numerical simulations are carried out to quantitatively describe the population transfer processes.

References:
P. Dietiker, E. Miloglyadov, M. Quack, A. Schneider, .G. Seyfang, J. Chem. Physics (in press 2015)

Title: Electric transition dipole moment in pre-BornOppenheimer molecular structure theory

Researchers: Benjamin Simmen[1]
Edit Mátyus[2]
Markus Reiher[1]

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

[2]Eövtös University, Institute of Chemistry, P.O. Box 32, H-1518, Budapest 112, Hungary

Description:

In this project the calculation of the electric transition dipole moment in a pre-Born–Oppenheimer framework is presented. Electrons and nuclei are treated equally in terms of the parametrization of the non-relativistic total wave function, which is written as a linear combination of basis functions constructed from explicitly correlated Gaussian functions and the global vector representation. The integrals of the electric transition dipole moment are derived corresponding to these basis functions in both the length and the velocity representation. The calculations are performed in laboratory-fixed Cartesian coordinates without relying on coordinates which separate the center of mass from the translationally invariant degrees of freedom. The effect of the overall motion is eliminated through translationally invariant integral expressions. The electric transition dipole moment is calculated between two rovibronic levels of the H_2 molecule assignable to the lowest rovibrational states of the $X^1\Sigma_g^+$ and $B^1\Sigma_u^+$ electronic states in the clamped-nuclei framework. This is the first evaluation of this quantity in a full quantum mechanical treatment without relying on the BornOppenheimer approximation.

References: Benjamin Simmen, Edit Mátyus and Markus Reiher, *J. Chem. Phys.*, **2014**, 141, 154105.

Title: MetREx: A protein design approach for the exploration of sequence-reactivity relationships in metalloenzymes

Researchers: Martin T. Stiebritz[1]

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

Description:

Metalloenzymes represent a particular challenge for any rational (re)design approach because the modeling of reaction events at their metallic cofactors requires time-consuming quantum mechanical calculations, which cannot easily be reconciled with the fast, knowledge-based approaches commonly applied in protein design studies. An approach for the exploration of sequence-reactivity relationships in metalloenzymes was developed (MetREx) that consists of force field-based screening of mutants that lie energetically between a wild-type sequence and the global minimum energy conformation and which should, therefore, be compatible with a given protein fold. Mutant candidates are subsequently evaluated with a fast and approximate quantum mechanical/molecular mechanical-like procedure that models the influence of the protein environment on the active site by taking partial charges and van der Waals repulsions into account. The feasibility of the procedure was demonstrated for the active site of [FeFe] hydrogenase from *Desulfovibrio desulfuricans*. MetREx allows for the identification of mutants with altered properties, such as inhibitor-coordination energies, and the understanding of the robustness of enzymatic reaction steps with respect to variations in sequence space.

References: M. T. Stiebritz, *J. Comput. Chem.*, **2015**, *36*, 553 – 563.

Title: Polarizable Embedding with a Multiconfiguration Short-Range Density Functional Theory Linear Response Method

Researchers: Erik Donovan Hedegård[1]
Jógvan Magnus Haugaard Olsen[2]
Stefan Knecht[1]
Jacob Kongsted[3]
Hans Jørgen Aagaard Jensen[3]

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

[2]Laboratory of Computational Chemistry and Biochemistry, EPFL, Lausanne

[3]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense

Description:

Computational methods in biology should be efficient, yet accurate, to handle the large, complex structures. This task can be achieved through coupling of methods that can treat large systems, with methods that can treat multiconfigurational systems. We have for the former used the polarizable embedding (PE) method which we have coupled to the recently developed multiconfiguration short-range DFT method (MC-srDFT). The MC-srDFT method can treat multiconfigurational systems with a simultaneous account for dynamical and static correlation effects. Thus, PE-MC-srDFT is designed to combine efficient treatment of complicated electronic structures with inclusion of effects from the surrounding environment. With PE-MC-srDFT it is further possible to calculate molecular properties such as excitation energies and oscillator strengths through response theory. Benchmarking of the PE-MC-srDFT approach against literature data has been carried out with investigations of the low-lying electronic excitations of acetone and uracil. Both molecules were immersed in water solution. The PE-MC-srDFT results turned out to be consistent and accurate, both in terms of the calculated solvent shift and, unlike regular PE-MCSCF, also with respect to the individual absolute excitation energies.
The PE-MC-srDFT method has also been applied for more multiconfigurational systems, namely the retinylidene Schiff base chromophore. The chromophore is embedded in the channelrhodopsin protein: The PE-MC-srDFT approach yields excitation energies comparable in quality to CASSCF/CASPT2 benchmarks.

References: Erik Donovan Hedegård, Jógvan Magnus Haugaard Olsen, Stefan Knecht, Jacob Kongsted, Hans Jørgen Aagaard Jensen, *J. Chem. Phys.*, **2015**, 142, 114113.

Title: Density matrix renormalization group with efficient dynamical electron correlation through range separation

Researchers: Erik Donovan Hedegård[1]
Stefan Knecht[1]
Jesper Skau Kielberg[2]
Hans Jørgen Aagaard Jensen[2]
Markus Reiher[1]

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

[2]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense

Description:

One of the most challenging task of quantum chemistry is to account for dynamical correlation in multiconfigurational systems. Today, this is often done with perturbation-based methods, which are of limited use due to their computational cost. The study entitled "Density matrix renormalization group with efficient dynamical electron correlation through range separation" investigates a new multiconfigurational method based on the concept of range-separation. The multiconfigurational method in question combines the density matrix renormalization group (DMRG) approach with density functional theory (DFT) and is dubbed DMRG short-range DFT (DMRG–srDFT). In the study, the working equations for DMRG–srDFT have been derived and implemented in the quantum chemical computer program DALTON, allowing accurate calculations on molecular systems with multiconfigurational electronic structures.
Calculations on small moleculer systems with DMRG–srDFT revealed that the major part of dynamical correlation is assigned to the short-range DFT part, as was the aim from the outset. The method was further used to investigate more challenging problems, namely the dissociation energies of ligands from transition metal complexes. This study revealed the true potential of the DMRG–srDFT approach. Very promising results were obtained for such relative energies that are known to be difficult to obtain with standard density functionals. Hence, including dynamical correlation through a short-range density functional is a viable option to preserve the efficiency of DMRG calculations by avoiding standard perturbation-theory-based approaches.

References: Erik Donovan Hedegård, Stefan Knecht, Jesper Skau Kielberg, Hans Jørgen Aagaard Jensen, Markus Reiher, *J. Chem. Phys.*, **2015**, 142, 224108.

Title: Systematic dependence of transition-metal coordination energies on density-functional parametrizations

Researchers: Thomas Weymuth[1]
Markus Reiher[1]

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

Description:

In recent years, the calibration of parameters in approximate exchange-correlation density functionals was intensified by the proposition of diverse and increasingly unbiased reference datasets. It is, however, not obvious how sensitive the accuracy of a given functional is with respect to a small change of its parameters. Knowledge about this sensitivity would be desirable for the assessment of the general accuracy that can be expected for the calculation of a given observableespecially for notorious cases as found, for instance, in coordination chemistry. At the example of the well-known BP86 exchange-correlation functional, we investigate the dependence of the coordination energies in the WCCR10 reference set [Weymuth et al., J. Chem. Theory Comput. 2014, 10, 3092] on the empirical parameters of this density functional. The WCCR10 reactions were found to be a true challenge for contemporary density functionals. In this project we find that the parameter dependence is qualitatively the same for all reactions. This observation is important in view of the fact that the BP86 functional was never parametrized against transition-metal data. Still, within the parameter intervals investigated, the individual reaction energies vary significantly, which seems to suggest a reoptimization of the empirical parameters. However, it turns out that the overall description of all 10 reactions can be improved by only 9.5 kJ/mol, and therefore, such a reoptimization is not advisable.

References: Thomas Weymuth and Markus Reiher, *Int. J. Quantum Chem.*, **2015**, 115, 90–98.

Title: Carotenoids and light-harvesting: from DFT/MRCI to the Tamm-Dancoff approximation

Researchers: Oliviero Andreussi[1]
Stefan Knecht[2]
Christel Maria Marian[3]
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Benedetta Mennucci[1]

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[2]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich / Reiher Group

[3] Institute of Theoretical and Computational Chemistry, University of Düsseldorf, 40225 Düsseldorf

[4]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense

Description:

Carotenoids are known to play a fundamental role in photosynthetic light-harvesting (LH) complexes; however, an accurate quantum-mechanical description of that is still missing. This is due to the multideterminant nature of the involved electronic states combined with an extended conjugation which limits the applicability of many of the most advanced approaches. In this study we applied a multi-reference configuration interaction extension of density functional theory (DFT/MRCI) to describe transition energies and densities as well as the corresponding excitonic couplings, for the three lowest singlet excited states of nine carotenoids present in three different LH complexes of algae and plants. These benchmark results were used to find an approximated computational approach, which could be used to quantitatively reproduce the key quantities at a reduced computational cost. To this end, we tested the Tamm-Dancoff approximation (TDA) to time-dependent density functional theory in combination with different functionals. By analyzing the errors with respect to DFT/MRCI-TDA results for the full set of electronic properties we concluded that TDA-TPSS with small basis sets indeed represents an effective approach to investigate LH processes which involve carotenoids.

References: Oliviero Andreussi, Stefan Knecht, Christel Maria Marian, Jacob Kongsted and Benedetta Mennucci, *J. Chem. Theory Comput.*, **2015**, 11, 655-666.

Title: Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment

Researchers: Thomas Dresselhaus[1]
Johannes Neugebauer[1]
Stefan Knecht[2]
Sebastian Keller[2]
Yingjin Ma[2]
Markus Reiher[2]

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[2]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich / Reiher Group

Description:

In this project we presented the first implementation of a density matrix renormalization group algorithm embedded in an environment described by density functional theory. The frozen density embedding scheme was used with a freeze-and-thaw strategy for a self-consistent polarization of the orbital-optimized wavefunction and the environmental densities with respect to each other.

References: Thomas Dresselhaus, Johannes Neugebauer, Stefan Knecht, Sebastian Keller, Yingjin Ma and Markus Reiher, *J. Chem. Phys.*, **2015**, 142, 044111.

Title: Orbital entanglement and CASSCF analysis of the RuNO bond in a Ruthenium nitrosyl complex

Researchers: Leon Freitag[1]
Stefan Knecht[2]
Sebastian Franz Keller[2]
Mickaël G. Delcey[3]
Francesco Aquilante[3,4]
Thomas Bondo Pedersen[5]
Roland Lindh[6]
Markus Reiher[2]
Leticia González[1]

Institute/Group: [1]Institut für theoretische Chemie, Universität Wien, 1090 Vienna

[2]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich / Reiher Group

[3]Department of Chemistry – Ångström, The Theoretical Chemistry Programme, Uppsala University, 751 20 Uppsala

[4]Dipartimento di Chimica "G. Ciamician", Universitá di Bologna, 40126 Bologna

[5]Centre for Theoretical and Computational Chemistry, Department of Chemistry, University of Oslo, 0315 Oslo

[6]Uppsala Center for Computational Chemistry – UC3, Uppsala University, 751 20 Uppsala

Description:

Complete active space self-consistent field (CASSCF) wavefunctions and an orbital entanglement analysis obtained from a density-matrix renormalisation group (DMRG) calculation were used to understand the electronic structure, and, in particular, the Ru-NO bond of a Ru nitrosyl complex. The analysis of the CASSCF wavefunctions in the electronic singlet ground state and the first triplet state provided a picture of the Ru-NO moiety beyond the standard representation based on formal oxidation states. The electron configuration of Ru is an equally weighted superposition of Ru^{II} and Ru^{III} configurations, with the Ru^{III} configuration originating from charge donation mostly from Cl ligands. However, and contrary to what was typically assumed, the electronic configuration of the NO ligand is best described as electroneutral.

References: Leon Freitag, Stefan Knecht, Sebastian F. Keller, Mickaël G. Delcey, Francesco Aquilante, Thomas Bondo Pedersen, Roland Lindh, Markus Reiher and Leticia González, *Phys. Chem. Chem. Phys.*, **2015**, 17, 14383-14392.

Title: Theoretical study on ThF^+, a prospective system in search of time-reversal violation

Researchers: Malika Denis[1]
Morten Steen Nørby[2]
Hans Jørgen Aagaard Jensen[2]
André Severo Pereira Gomes[3]
Malaya K. Nayak[1,4]
Stefan Knecht[5]
Timo Fleig[1]

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[2]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense

[3]Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), CNRS UMR 8523, Université de Lille, F-59655 Villeneuve d'Ascq

[4]Bhabha Atomic Research Centre, Trombay, Mumbai - 400085

[5]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich / Reiher Group

Description:

The low-lying electronic states of ThF^+, a possible candidate in the search for $\mathcal{P}$- and $\mathcal{T}$-violation, have been studied using high-level correlated relativistic ab initio multi-reference coupled-cluster and configuration interaction approaches. For the $^3\Delta$ state component with $\Omega = 1$ (electron electric dipole moment "science state") we obtained an effective electric field of $E_{\text{eff}} = 35.2$ GV cm^{-1}, a $\mathcal{P}$- and $\mathcal{T}$-odd electron-nucleon interaction constant of $W_{P,T} = 48.4$ kHz, a magnetic hyperfine interaction constant of $A_{\parallel} = 1833$ MHz for ^{229}Th ($I = 5/2$), and a very large molecular dipole moment of 4.03 D. The $\Omega = 1$ state was found to be more than 300 cm^{-1} lower in energy than $\Omega = 0^+$ ($^1\Sigma^+$), challenging the state assignment from an earlier theoretical study on this species (Barker *et al*).

References:

Malika Denis, Morten S. Nørby, Hans Jørgen Aa. Jensen, André Severo Pereira Gomes, Malaya K. Nayak, Stefan Knecht and Timo Fleig, *New J. Phys.*, **2015**, 17, 043005.

Beau J. Barker, Ivan O. Antonov, Michael C. Heaven and Kirk A. Peterson, *J. Chem. Phys.*, **2012**, 136, 104305.

Title: A theoretical benchmark study of the spectroscopic constants of the very heavy rare gas dimers

Researchers: Avijit Shee[1]
Stefan Knecht[2]
Trond Saue[1]

Institute/Group: [1]Laboratoire de Chimie et Physique Quantiques, IRSAMC, CNRS/Université Paul Sabatier Toulouse III, F-31062 Toulouse

[2]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich / Reiher Group

Description:

Spectroscopic constants for the homonuclear dimers of the very heavy rare gases radon (Rn) and eka-radon (Uuo) have been reported. A computational protocol using the eXact 2-Component molecular-mean field Hamiltonian has been established based on extensive calculations of the xenon dimer. We found that reliable results require CCSD(T) calculations at the extrapolated basis set limit. In this limit counterpoise corrected results are closer to experimentally derived values than uncorrected ones. Furthermore, in an attempt to reduce the computational cost while retaining very high accuracy, we studied the performance of range-separated density functional theory. Although we observed a somewhat more favorable basis set convergence and reduced importance of connected triples by range-separated methods compared to pure wave function theory, in practice we had to employ the same computational protocol for obtaining converged results. At the DiracCoulomb level we found an almost fourfold increase of binding energy when going from the radon to the eka-radon dimer, but the inclusion of spin-other orbit interaction reduced the dissociation energy of the heaviest dimer by about 40%.

References: Avijit Shee, Stefan Knecht and Trond Saue, *Phys. Chem. Chem. Phys.*, **2015**, 17, 10978.

Title: Linear interpolation method in ensemble Kohn-Sham and range-separated density-functional approximations for excited states

Researchers: Bruno Senjean[1]
Stefan Knecht[2]
Hans Jørgen Aagaard Jensen[3]
Emmanuel Fromager[1]

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[3]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense

Description:

Gross-Oliveira-Kohn density-functional theory (GOK-DFT) for ensembles is, in principle, very attractive but had so far been hard to use in practice. In this project we discussed a practical model based on GOK-DFT for the calculation of electronic excitation energies. The model relies on two modifications of GOK-DFT: use of range separation and use of the slope of the linearly interpolated ensemble energy, rather than orbital energies. The range-separated approach is appealing, as it enables the rigorous formulation of a multideterminant state-averaged DFT method. In the exact theory, the short-range density functional, which complements the long-range wave-function-based ensemble energy contribution, should vary with the ensemble weights even when the density is held fixed. This weight dependence ensures that the range-separated ensemble energy varies linearly with the ensemble weights. When the (weight-independent) ground-state short-range exchange-correlation functional is used in this context, curvature appears, thus leading to an approximate weight-dependent excitation energy. In order to obtain unambiguous approximate excitation energies, we proposed to interpolate linearly the ensemble energy between equiensembles. It was shown that such a linear interpolation method (LIM) can be rationalized and that it effectively introduces weight dependence effects. As proof of principle, the LIM had been applied to He, Be, and H_2 in both equilibrium and stretched geometries as well as the stretched HeH^+ molecule. Very promising results had been obtained for both single (including charge transfer) and double excitations with spin-independent short-range local and semilocal functionals. Even at the Kohn-Sham ensemble DFT level, which is recovered when the range-separation parameter is set to 0, LIM performed better than standard time-dependent DFT.

References: Bruno Senjean, Stefan Knecht, Hans Jørgen Aa. Jensen, and Emmanuel Fromager, *Phys. Rev. A*, **2015**, 92, 012518.

Title: Mode-Tracking Based Stationary Point Optimization

Researchers: Maike Bergeler[1]
Carmen Herrmann[2]
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Institute/Group: [1]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

[2]Institute of Inorganic and Applied Chemistry, University of Hamburg, 20146 Hamburg

Description:

In this work we present a transition-state optimization protocol based on the Mode-Tracking algorithm [*J. Chem. Phys.*, **2003**, *118*, 1634]. By calculating only the eigenvector of interest instead of diagonalizing the full Hessian matrix and performing an eigenvector following search based on the selectively calculated vector, we can efficiently optimize transition-state structures. The initial guess structures and eigenvectors are either chosen from a linear interpolation between the reactant and product structures, from a nudged-elastic band search, from a constrained-optimization scan, or from the minimum-energy structures. Alternatively, initial guess vectors based on chemical intuition may be defined. We then iteratively refine the selected vectors by the Davidson subspace iteration technique. This procedure accelerates finding transition states for large molecules of a few hundred atoms. It is also beneficial in cases where the starting structure is very different from the transition-state structure or where the desired vector to follow is not the one with lowest eigenvalue. Explorative studies of reaction pathways are feasible by following manually constructed molecular distortions.

References: M. Bergeler, C. Herrmann, M. Reiher, *J. Comput. Chem.*, **2015**, 36, 1429-1438.

Title: A Stable Phosphanyl Phosphaketene and Its Reactivity

Researchers: Zhongshu Li[1,2]
Xiaodan Chen[1]
Maike Bergeler[3]
Markus Reiher[3]
Cheng-Yong Su[2]
Hansjörg Grützmacher[1,2]

Institute/Group: [1]Laboratorium für Anorganische Chemie, ETH Zürich, 8093 Zürich

[2]Lehn Institute of Functional Materials (LIFM), Sun Yat-Sen University, 510275 Guangzhou

[3]Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich

Description:

Sodium phosphaethynolate, Na(OCP), reacts with the bulky P-chloro-diazaphosphole yielding a phosphanyl phosphaketene, which is stable for weeks under an inert atmosphere in the solid state. This compound is best described as a tight ion pair with a remarkably long P-P bond distance (2.44 Å). In solution, this phosphaketene dimerizes under loss of CO to give 1,2,3-triphosphabicyclobutane identified by an X-ray diffraction study. As an intermediate, a five-membered heterocyclic diphosphene was trapped in a Diels–Alder reaction with 2,3-dimethylbutadiene. The formation of this intermediate in a hetero-Cope-rearrangement as well as dimerization/CO loss were computed with various DFT methods which allowed us to understand the reaction mechanisms.

References: Z. Li, X. Chen, M. Bergeler, M. Reiher, C.-Y. Su, H. Grützmacher, *Dalton Trans.*, **2015**, 44, 6431-6438.

Title: Selection of active spaces for multiconfigurational wavefunctions

Researchers: Sebastian Keller[1]
Katharina Boguslawski[1]
Tomasz Janowski[2]
Markus Reiher[1]
Peter Pulay[2]

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

[2]Department of Chemistry and Biochemistry, Fulbright College of Arts and Sciences, University of Arkansas, Fayetteville, Arkansas 72701, USA

Description:

The efficient and accurate description of the electronic structure of strongly correlated systems is still a largely unsolved problem. The usual procedures start with a multiconfigurational (usually a Complete Active Space CAS) wavefunction which accounts for static correlation and add dynamical correlation by perturbation theory configuration interaction or coupled cluster expansion. This procedure requires the correct selection of the active space. Intuitive methods are unreliable for complex systems. The inexpensive black-box unrestricted natural orbital (UNO) criterion postulates that the Unrestricted Hartree-Fock (UHF) charge natural orbitals with fractional occupancy (e.g. between 0.02 and 1.98) constitute the active space. UNOs generally approximate the CAS orbitals so well that the orbital optimization in CAS Self-Consistent Field (CASSCF) may be omitted resulting in the inexpensive UNO-CAS method. A rigorous testing of the UNO criterion requires comparison with approximate full configuration interaction wavefunctions. This became feasible with the advent of Density Matrix Renormalization Group (DMRG) methods which can approximate highly correlated wavefunctions at affordable cost. We have compared active orbital occupancies in UNO-CAS and CASSCF calculations with DMRG in a number of strongly correlated molecules: compounds of electronegative atoms (F2 ozone and NO2) polyenes aromatic molecules (naphthalene azulene anthracene and nitrobenzene) radicals (phenoxy and benzyl) diradicals (o- m- and p-benzyne) and transition metal compounds (nickel-acetylene and Cr2). The UNO criterion works well in these cases. Other symmetry breaking solutions with the possible exception of spatial symmetry do not appear to be essential to generate the correct active space. In the case of multiple UHF solutions the natural orbitals of the average UHF density should be used. The problems of the UNO criterion and their potential solutions are discussed: finding the UHF solutions discontinuities on potential energy surfaces and inclusion of dynamical electron correlation and generalization to excited states.

References: Sebastian Keller, Katharina Boguslawski, Tomasz Janowski, Markus Reiher and Peter Pulay, *J. Chem. Phys.*, **2015**, 142, 244104.

Titel: Structural Effects of Posttranslational Modifications of Polytheonamide B Revealed by Molecular Dynamics Simulations

Researchers: Annick Renevey, Sereina Riniker

Institute/Group: Laboratory of Physical Chemistry, Computational Chemistry Group

Description:
Marine sponges are a unique source for bioactive metabolites, which are of potential interest for the development of new antibiotics. In particular, symbiotic bacteria of the marine sponge *Theonella swinhoei* produce a highly cytotoxic peptide, polytheonamide B (PTB) [1]. PTB consists of 48 amino acids and exerts its cytotoxic function by inserting into membranes to act as a pore. 13 of the 19 different amino acids present in PTB are non-proteinogenic amino acids, generated by posttranslational epimerization, C-methylation, (side chain) N-methylation and hydroxylation [2]. The peptide adopts an uncommon $\beta_{6.3}$-helical fold, which is thought to be due to alternating L- and D-amino acids. In this study, we investigated the effects of the posttranslational modifications (PTMs) on the β-helical structure using molecular dynamics (MD) simulations. Individual PTM or groups of PTMs were reverted to the corresponding natural amino acids in the simulations and the impact on the structure examined. The results indicate that epimerization is necessary but not sufficient for the β-helical structure. A set of N-methylations was found to be crucial for the formation of a hydrogen-bonding network, which stabilizes the fold.

References:
[1] T. Hamada *et al.*, *J. Am. Chem. Soc*., 132, 12941 (2010).
[2] M. F. Freeman *et al*., *Science*, 338, 387 (2012).
[3] Manuscript in preparation for *J. Am. Chem. Soc.*

Titel: Cyclosporin revisited: Conformational landscapes in water and apolar solvents

Researchers: Jagna Witek, Sereina Riniker

Institute/Group: Laboratory of Physical Chemistry, Computational Chemistry Group

Description:
The ability to passively cross cell membranes is crucial for drug absorption in the gastrointestinal tract and thus oral administration. Small peptides have often a low membrane permeability due to their size and high number of hydrogen-bond donors and acceptors. Nevertheless, naturally occurring cyclic peptides such as Cyclosporin A are able to penetrate cell membranes. It is hypothesized that this is due to a conformational change between an "open" structure in water, where the unmethylated backbone amides form hydrogen bonds with the solvent, and a "closed" structure in the membrane interior, where intramolecular hydrogen-bonds shield the polar groups from the apolar environment [1]. However, sampling of the complete conformational space in water and in chloroform using 5-microseconds molecular dynamics (MD) simulations revealed a more complex conformational behavior. The kinetic models build with the simulation data showed in both solvents the existence of multiple metastable conformational states. The "open" state in water and the "closed" state in chloroform exhibited thereby the slowest transition rates of several tens of nanoseconds. Interestingly, other shorter-lived states were observed that occurred in both solvents, thus potentially acting as conformational "transition states" in the permeation process.

References:
[1] T. R. White *et al.*, *Nature Chem. Biol.*, **7**, 810 (2011).
[2] Manuscript in preparation for *Angew. Chem.*

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

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

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

Description:

We are using global and regional atmospheric models on a wide range of temporal and spatial scales. The high-resolution regional modeling uses the COSMO-CLM limited-area atmospheric model. Comprehensive European-scale climate-change scenario simulations were conducted in the framework of the COordinated Regional climate Downscaling Experiment (Euro-CORDEX) at horizontal resolutions of 12 and 50 km covering the period 1950- 2100. Recent work in this context is addressing a standard validation of all models participating in Euro-CORDEX, the calibration of the COSMO-CLM, the analysis of changes in heat-wave, heavy precipitation events and snow cover, the height-dependence of the climate change signals, the representation of aerosol effects, and the quantification of different drivers behind the European summer climate. In parallel, we are further developing a high-resolution climate simulation capability with horizontal resolutions at the km-scale. Both idealized and real-case simulations are conducted. 10 year long simulations for present and future climate conditions for the whole Alpine area were performed at this resolution. They showed especially an improved representation of precipitation on the sub-daily time scale. The long simulations are complemented by detailed analyses of convective processes over mountainous terrain using a combination of satellite data and idealized large-eddy simulations. The main motivation behind this work is the desire to explicitly simulate convective clouds (as opposed to using convective cloud parameterization schemes in lower-resolution models). We have also started using a recent GPU version of the COSMO model (jointly developed in HP2C projects by MeteoSwiss, ETH/C2SM and CSCS). This allows to extend the simulation domain for convection-resolving simulations to the European continent. This configuration is extensively used in the SNF-Sinergia project crClim. The use of the COSMO-CLM is coordinated by Drs. D. Lüthi, L. Schlemmer and S. Kotlarski.

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

References:

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

Title: Sparse Grid, Reduced Basis Bayesian Inversion

Researchers: Dr. Peng Chen
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

This project deals with Bayesian inverse problems constrained by PDEs with distributed uncertain input field, which face considerable challenges due to the curse of dimensionality in sampling the infinite-dimensional uncertain field as well as the large-scale computational cost of solving the PDEs at each of a large samples. To tackle these challenges, we have developed sparse model reduction techniques that feature: (1) effectively breaking the curse of dimensionality by generalized anisotropic sparse grid approximation/sampling, such that the sparse approximation error converges with rate independent of the parameter dimenions; (2) efficiently reducing the computational cost by model order reduction, such that solution of the PDEs depends only on the reduced degrees of freedom and not on the high-fidelity degrees of freedom, bearing in mind that the former is typically several orders of magnitude smaller than the latter.

Both linear and nonlinear, affine and nonaffine parametric operator equations are considered in this project, which cover a large range of engineering problems, including diffusion, heat transfer, structural mechanics, fluid dynamics, electromagnetics, etc.

References:

[1] P. Chen and Ch. Schwab. *Sparse Grid, Reduced Basis Bayesian Inversion*, Computer Methods in Applied Mechanics and Engineering, in press. Technical Report 2014-36, Seminar for Applied Mathematics, ETH Zürich, 2015.

[2] P. Chen and Ch. Schwab. *Adaptive Sparse Grid Model Order Reduction for Fast Bayesian Estimation and Inversion*, Sparse Grid & Application, submitted. Technical Report 2015-08, Seminar for Applied Mathematics, ETH Zürich, 2015.

[3] P. Chen and Ch. Schwab. *Sparse Grid, Reduced Basis Bayesian Inversion: Nonaffine-Parametric Nonlinear Equations*, Journal of Computational Physics, submitted. Technical Report 2015-21, Seminar for Applied Mathematics, ETH Zürich, 2015.

[4] P. Chen and Ch. Schwab. *Model Order Reduction Methods for Computational Uncertainty Quantification*, Handbook of Uncertainty Quantification R. Ghanem et. al. (Eds). , Springer Publ. 2016.

Title: Higher Order Quasi-Monte Carlo for Parametric Partial Differential Equations

Researchers: Robert N. Gantner,
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics (SAM)

Description:

The focus of the project is on the efficient numerical approximation of problems in uncertainty quantification involving parametric partial differential equations. In particular, we are interested in novel quasi-Monte Carlo methods with dimension-independent orders of convergence greater than 1. The main application is to Bayesian inverse problems, which attempt to compute moments of quantities of interest, given perturbed measurements of the system response. The use of parallel algorithms and high-performance computing hardware is central to the practical applicability of the involved methods. Favorable scaling properties have been verified and large simulations carried out on the Swiss Supercomputing Center (CSCS) infrastructure, under project ids s522 and d41.

References:

[1] R.N. Gantner, C. Schillings and Ch. Schwab, *Binned Multilevel Monte Carlo for Bayesian Inverse Problems with Large Data*, Proc. Intl. Conf. Domain Decomposition DD22, (2014) (in print).

[2] R.N. Gantner, Ch. Schwab, *Computational Higher Order Quasi-Monte Carlo Integration*, Proc. MCQMC14, (2014) (in review).

[3] J. Dick and F.Y. Kuo and Q.T. Le Gia and Ch. Schwab, *Fast QMC matrix-vector multiplication*, SAM Report 2015-07 (2015).

[4] J. Dick and Q.T. Le Gia and Ch. Schwab, *Higher order Quasi Monte Carlo integration for holomorphic, parametric operator equations*, SAM Report 2014-23 (2014).

Title: Numerical analysis of stochastic partial differential equations

Researchers: Lukas Herrmann
Christoph Schwab

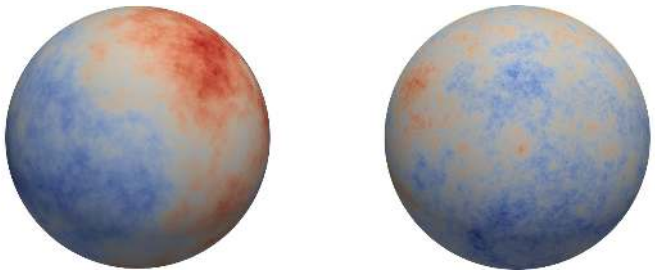
Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Random fields are used to model random quantities that arise in science and engineering in a mathematical way. Isotropic covariance kernels of these fields result in various properties of the random fields.

Isotropic spherical random fields are defined and analyzed, especially isotropic Gaussian spherical random fields. The connection between the angular power spectrum, the path regularity and the integrability of these fields is in particular investigated. One application of this is the discussion of the stochastic heat equation with additive isotropic Q-Wiener noise as well as unique solvability and Hölder regularity of second order, elliptic partial differential equations on the sphere with lognormal isotropic coefficients.

In this project we further focus on the numerical analysis of problems of this kind.



References:

[1] L. Herrmann, *Isotropic random fields on the sphere – regularity of random elliptic PDEs*, Master's thesis, ETH Zürich, 2013

[2] A. Lang and Ch. Schwab, *Isotropic Gaussian random fields on the sphere: regularity, fast simulation, and stochastic partial differential equations*, Ann. Appl. Prob., 2015

[3] L. Herrmann, A. Lang and Ch. Schwab, *tentative title*, in preparation

Title: Low-rank tensor-structured solution of differential equations

Researchers: Vladimir Kazeev, Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The project focuses on the numerical solution of high-dimensional ODEs and PDEs in low-parametric representations known as *tensor decompositions*. Naive FDM or FEM discretizations constructed on extremely fine uniform tensor-product meshes are usually not employed in advanced numerical algorithms due to an excessively large number of degrees of freedom. The key idea of the project is combining such discretizations with non-linear approximations based on the separation of variables, so that the solution, operator and the intermediate data are represented in terms of relatively few parameters. The underlying full discretizations are then not dealt with explicitly; instead, adaptive algorithms of the low-rank tensor recompression extract the "effective" degrees of freedom.

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

The current stage of the project focuses on the solutions of second-order elliptic problems in polygons with straight or, more generally, analytic edges. Such solutions are known to belong to certain countably normed spaces of analytic functions, which may exhibit point singularities at the boundary of the domain. We study the approximation of such functions with a first-order, h-version finite element (FE) method based on uniform tensor-product meshes. Such FE approximations are well known to converge with algebraic rate: generally $1/2$ in terms of the number of degrees of freedom, and even slower in the presence of singularities.

We prove that this apparent inefficiency is eliminated by representing the corresponding FE coefficient vectors in the QTT format. Specifically, we show that continuous first-order FE approximations (constructed on uniform tensor-product meshes in a reference domain) converge exponentially in terms of the effective number N of degrees of freedom involved in the QTT representations: $N = \mathcal{O}(\log^{\kappa} \varepsilon^{-1})$, where $\varepsilon \in (0, 1)$ is the accuracy measured in the energy norm and $\kappa > 1$. This result holds for all functions from the analyticity classes mentioned above.

References:

[1] V. Kazeev, M. Khammash, M. Nip, and C. Schwab, *Direct solution of the Chemical Master Equation using Quantized Tensor Trains*, Technical Report 3, March 2014.

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

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

[4] V. Kazeev, O. Reichmann, and C. Schwab, *Low-rank tensor structure of linear diffusion operators in the TTand QTT formats*, Linear Algebra and its Applications, 438(11):4204–4221, 2013

[5] V. Kazeev and C. Schwab, *Tensor approximation of stationary distributions of chemical reaction networks*, SIAM Journal on Matrix Analysis and Applications, 36(3):1221–1247, 2015.

[6] V. Kazeev and C. Schwab, *Approximation of singularities by quantized-tensor FEM*, Research Report 16, Seminar for Applied Mathematics, ETH Zürich, 2015.

[7] V. Kazeev and C. Schwab, *Quantized tensor-structured finite elements for second-order elliptic PDEs in two dimensions*, Research Report 24, Seminar for Applied Mathematics, ETH Zürich, 2015.

[8] V. Kazeev, *Quantized tensor-structured finite elements for second-order elliptic PDEs in two dimensions*, PhD thesis, SAM, ETH Zurich, ETH Dissertation No. 23002.

Title: Finite Elements with mesh refinement for linear, second-order hyperbolic PDEs on polygons and polyhedra.

Researchers: Fabian L. Müller
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

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

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

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

References:

[1] F. Müller and Ch. Schwab, *Finite Elements with mesh refinement for wave equations in polygons*, Journal for Computational and Applied Mathematics, 2015.

[2] F. Müller and Ch. Schwab, *Finite Elements with mesh refinement for elastic wave propagation in polygons*, Mathematical Models in the Applied Sciences, 2025.

Title: Compositional layering within the large low shear-wave velocity provinces in the lower mantle

Researchers: M. D. Ballmer, V. Lekic, G. Ito, L. Schumacher, and C. Thomas

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

Description:
Seismic tomography reveals two antipodal LLSVPs in the Earth's mantle, each extending from the core-mantle boundary (CMB) up to ~1000 km depth. The LLSVPs are thought to host primitive mantle materials that bear witness of early-Earth processes, and/or subducted basalt that has cumulated in the mantle over billions of years. A compositional distinction between the LLSVPs and the ambient mantle is supported by anti-correlation of bulk-sound and shear-wave velocity (Vs) anomalies as well as abrupt lateral gradients in Vs along LLSVP margins. Both of these observations, however, are mainly restricted to the LLSVP bottom domains (2300~2900 km depth). Comparison of seismic observations with mineral-physics data suggests that these bottom domains are more likely to be composed of primitive mantle than of basaltic material. On the other hand, the seismic signature of the LLSVP shallow domains (1000~2300 km depth) is consistent with a basaltic composition, though a purely thermal origin cannot be ruled out.
Here, we explore the dynamical, seismological, and geochemical implications of the hypothesis that the LLSVPs are compositionally layered with a primitive bottom domain and a basaltic shallow domain (see Fig.). We test this hypothesis using 2D thermochemical mantle-convection models. Depending on the density difference between primitive and basaltic materials, the materials either mix or remain separate as they join to form thermochemical piles in the deep mantle. Separation of both materials within the piles provides an explanation for LLSVP seismic properties, including substantial internal vertical gradients in Vs observed at 400-700 km height above the CMB. Geodynamic models predict short-lived "secondary" plumelets to rise from the roofs of these compositionally layered piles while entraining basaltic material that has evolved in the lower mantle. Long-lived "primary" plumes rise from LLSVP margins and entrain a mix of materials, including small fractions of primitive mantle material. These predictions address the geochemical and geochronological record of intraplate hotspot volcanism on the Pacific plate. LLSVP compositional layering has indeed important implications for our understanding of heat and material fluxes through mantle reservoirs, as well as bulk Earth chemistry and evolution.

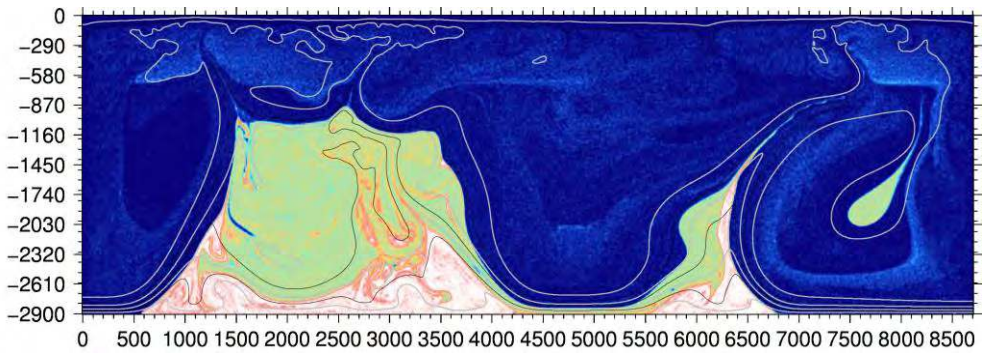


Figure: Predictions of temperature (contours) and compostion (colors) of example numerical model. Dark blue, light green, and white colors represent pyrolytic ambient mantle, basaltic and primitive materials, respectively.

Title: Compositional mantle layering revealed by slab stagnation at ~1,000 km depth

Researchers: M. D. Ballmer, N. C. Schmerr, T. Nakagawa, and J. Ritsema

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

Description:
Improved constraints on lower-mantle composition are fundamental to understand the accretion, differentiation and thermochemical evolution of our planet. Whereas cosmochemical arguments indicate that lower-mantle rocks may be enriched in Si relative to upper-mantle pyrolite, seismic tomography images suggest whole-mantle convection and efficient mantle mixing. This study reconciles cosmochemical and geophysical constraints using the stagnation of some slab segments at ~1,000 km depth as the key observation. Whereas slab stagnation at ~660 km depth is well explained by the effects of the spinel-perovskite endothermic phase transition, flattening of slabs in the uppermost lower mantle remains poorly understood. Through numerical modeling of subduction, we show that enrichment of the lower mantle in intrinsically dense basaltic heterogeneity can render slabs neutrally buoyant at ~1,000 km depth. Slab stagnation (at ~660 and ~1,000 km depth) as well as unimpeded slab sinking to great depths can only coexist as three different modes of slab sinking behavior on Earth if the basalt fraction is ~8% higher in the lower than in the upper mantle, equivalent to a lower-mantle Mg/Si of ~1.18. Geodynamic models demonstrate that such a moderate compositional gradient can be sustained by compositional filtering of both slabs and plumes as they cross the transition zone, and thus persist over billions of years of whole-mantle convection. Whereas basaltic heterogeneity tends to get trapped in the transition zone and ultimately sink into the lower mantle, harzburgitic heterogeneity tends to rise into the uppermost mantle.

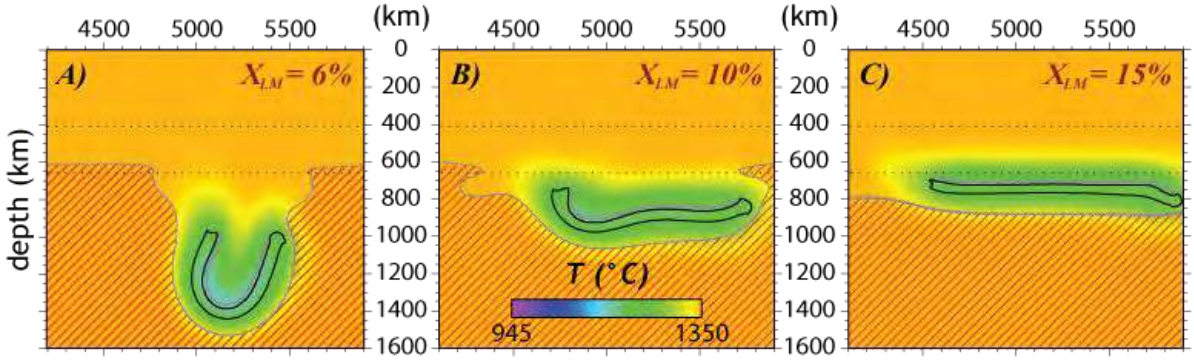


Figure: Three regimes of slab sinking behavior through the mantle as manifested for different lower-mantle excess basalt fraction X_{LM}. (**A**-**C**) Colors denote potential temperature in snapshots at 150 Myr. The 5% iso-contours of harzburgite (black) and basalt fraction (grey) are labeled. Domains with $X_{LM} > 0$ (specific values labeled) are shown with dark-red hatching. Slab sinking behavior varies as a function X_{LM} between cases shown.

Reference: Ballmer, M. D., N. C. Schmerr, T. Nakagawa, and J. Ritsema: Compositional mantle layering revealed by slab stagnation at ~1,000 km depth, *Science Adv.*, in press

Title: Crystallization and Cooling of a Deep Silicate Magma Ocean

Researchers: Dan J. Bower* and Aaron S. Wolf**

Institute/ Group: *Institute of Geophysics, GFD, D-ERDW, ETH Zürich
**Earth and Environmental Sciences, University of Michigan, USA

Description:

Impact and accretion simulations of terrestrial planet formation suggest that giant impacts are both common and expected to produce extensive melting. The moon-forming impact, for example, likely melted the majority of Earth's mantle to produce a global magma ocean that subsequently cooled and crystallized. Understanding the cooling process is critical to determining magma ocean lifetimes and recognizing possible remnant signatures of the magma ocean in present-day mantle heterogeneities. Modeling this evolution is challenging, however, due to the vastly different timescales and lengthscales associated with turbulent convection (magma ocean) and viscous creep (present-day mantle), in addition to uncertainties in material properties and chemical partitioning.

We consider a simplified spherically symmetric (1-D) magma ocean to investigate both its evolving structure and cooling timescale. Mixing-length theory is employed to determine convective heat transport, producing a high-resolution model that captures the ultra-thin boundary layer (few cms) at the surface of the magma ocean. The thermodynamics of mantle melting are represented using a pseudo-one-component model, which retains the simplicity of a standard one-component model while introducing a finite temperature interval for melting (important for multi-component systems). We derive a new high P-T equation of state (EOS) formulation designed to capture the energetics and physical properties of the partially molten system using parameters that are readily interpreted in the context of magma ocean crystallization. This model is used to determine the cooling timescale for a variety of plausible thermodynamic models, with special emphasis on comparing the center-outwards vs bottom-up cooling scenarios that arise from the assumed EOS.

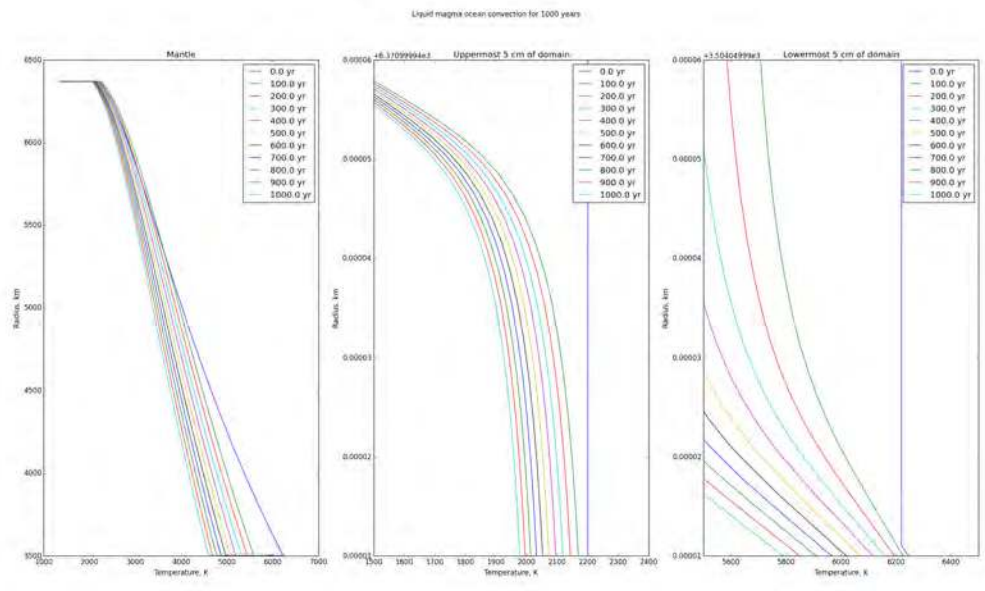


Figure. Cooling of a liquid magma ocean from an initial adiabat with potential temperature 2200 K (rightmost blue line). The middle and rightmost panel show the ultra-thin thermal boundary layer at the top and bottom, respectively.

Title: Numerical modelling of subduction zones

Researchers: Taras Gerya, Robert Herrendoerfer, Liang Zheng, David May

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

Group: Geophysical Fluid Dynamics

Description:
Various aspects of subduction zones dynamics, seismicity, magmatic activities, fluid regimes and geochemical transport 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 by mantle plumes (Fig. 1) (Gerya et al., 2015)
- Seismicity of subduction zones (Herrendoerfer et al., 2014)
- Material transportation and fluid-melt activity in the subduction channel (Li et al., 2015)

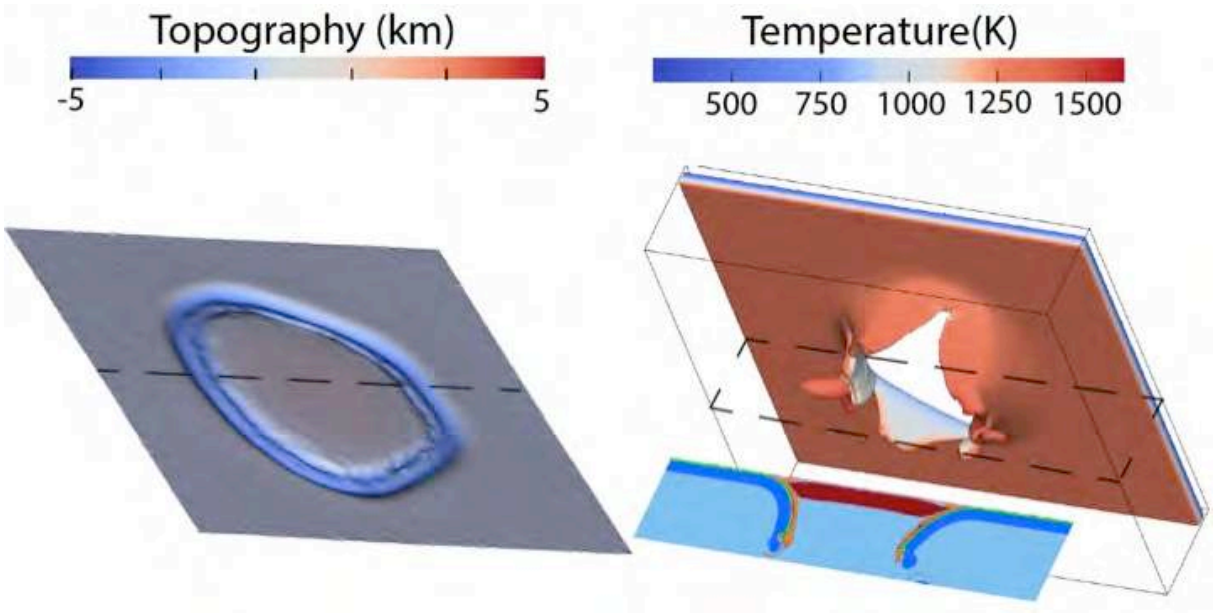


Fig. 1. Plume-induced subduction initiation (Gerya et al., 2014).

References:

Gerya, T.V., Stern, R.J., Baes, M., Sobolev, S.V., Whattam, S.A. (2015) Plate tectonics on the Earth triggered by plume-induced subduction initiation. Nature, 528.

Herrendoerfer, R., van Dinther, Y., Gerya, T., Dalguer, L.A. (2015) Earthquake supercycle in subduction zones controlled by the width of the seismogenic zone. Nature Geoscience, 8, 471-U73.

Li, Z.H., Liu, M.Q. Gerya, T. (2015) Material transportation and fluid-melt activity in the subduction channel: Numerical modeling. Science China-Earth Sciences, 58, 1251-1268.

Title: Numerical modelling of Precambrian geodynamics

Researchers: Taras Gerya, Ria Fisher, Antoine Rosel

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

Group: Geophysical Fluid Dynamics

Description:
Styles of Precambrian geodynamics and continental crust formation are modelled in 2D (Fig. 2) 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:

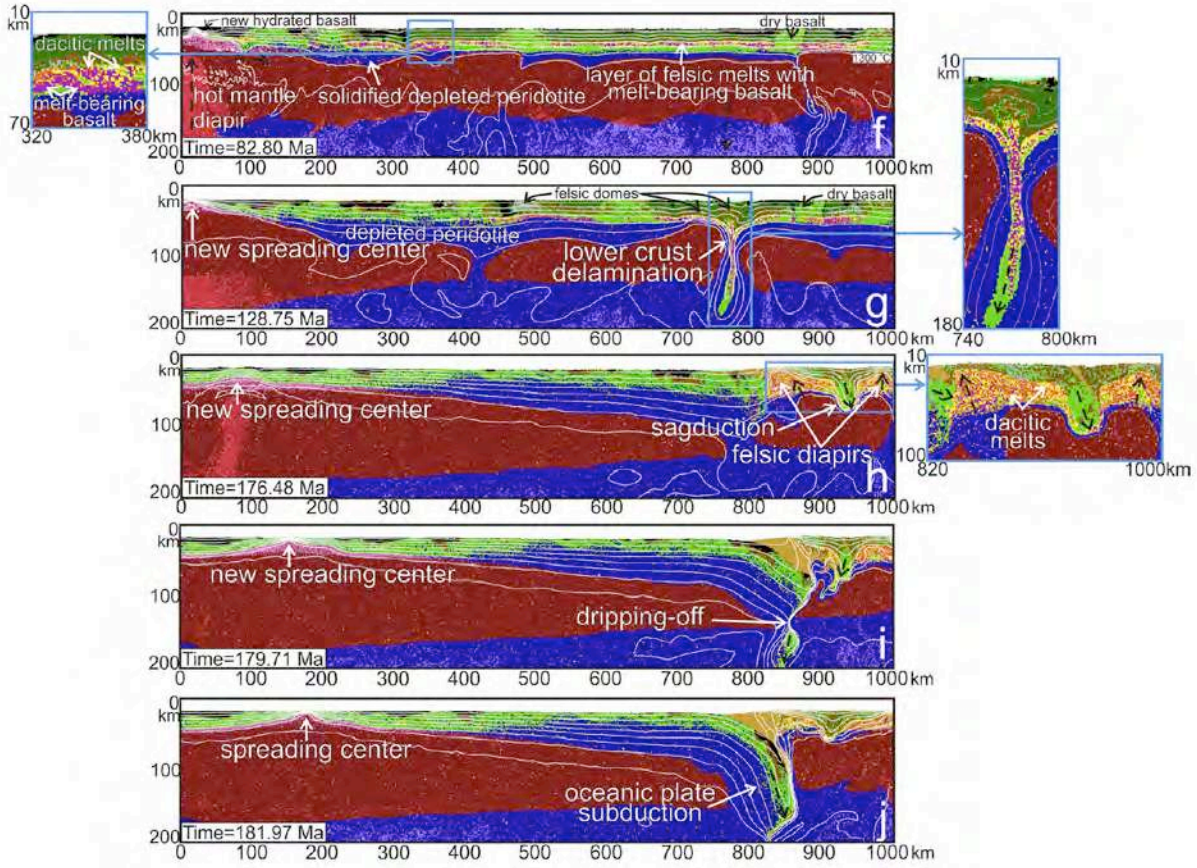


Fig. 2. Precambrian tectono-magmatic processes in 2D models (Sizova et al., 2014).

References:
Sizova, E., Gerya, T., Stüwe, K., Brown, M. (2015) Generation of felsic crust in the Archean: A geodynamic modeling perspective. Precambrian Research, 271, 198–224.

Zakharov, V.S.; Perchuk, A.L.; Zav'yalov, S.P. Sineva, T.A.; Gerya, T.V. (2015) Supercomputer simulation of continental collisions in Precambrian: the effect of lithosphere thickness. Moscow University Geology Bulletin, 70, 77-83.

Title: Numerical modelling of continental collision zones

Researchers: Taras Gerya, Jie Liao, Ria Fischer

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

Group: Geophysical Fluid Dynamics

Description:
Various aspects of continental collision zones are modelled in 2D and 3D (Fig. 3) 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:

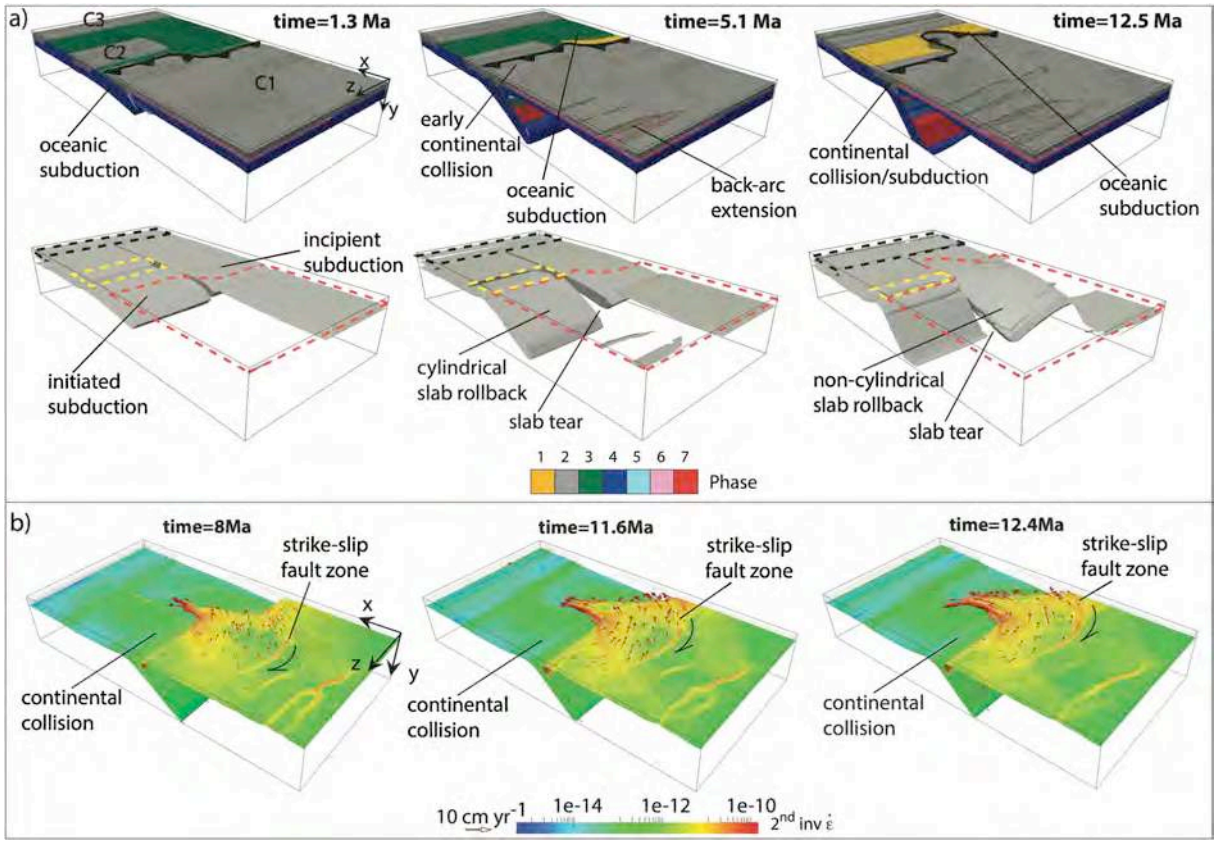


Fig. 3. Evolution of 3D structure of laterally variable collision zone (Sternai et al., 2014).

References:

Labrousse, L. Duretz, T., Gerya, T. (2015) H2O-fluid-saturated melting of subducted continental crust facilitates exhumation of ultrahigh-pressure rocks in continental subduction zones. Earth and Planetary Science Letters, 428, 151-161.

Sternai, P., Jolivet, L., Menant, A., Gerya, T. (2014) Driving the upper plate surface deformation by slab rollback and mantle flow. Earth and Planetary Science Letters, 405, 110-118.

Title: Numerical modelling of lithospheric extension and faulting processes

Researchers: Taras Gerya, Jie Liao, Kosuke Ueda, Noel Ammann

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

Group: Geophysical Fluid Dynamics

Description:
Various aspects of passive and active 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:

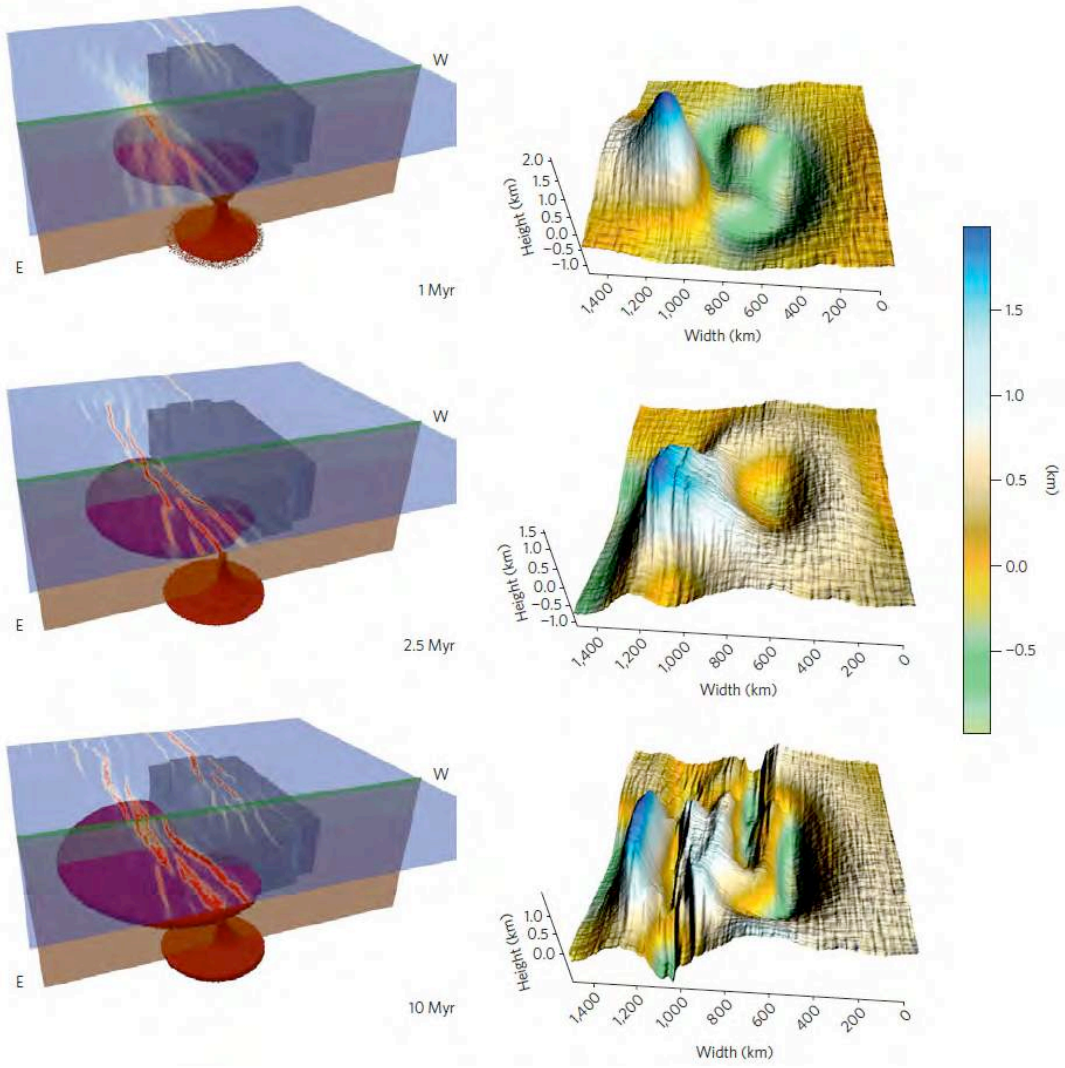


Fig. 4. Plume-assisted continental breakup (Koptev et al., 2015)

References:

Koptev, A., Calais, E., Burov, E., Leroy, S., Gerya, T. (2015) Dual continental rift systems generated by plume-lithosphere interaction. Nature Geoscience, 8, 388-392.

Liao, J., Gerya, T. (2015) From continental rifting to seafloor spreading: Insight from 3D thermo-mechanical modeling. Gondwana Research, 28, 1329-1343.

Title: Development of new numerical geodynamic modeling techniques

Researchers: Taras Gerya, Dave May, Kosuke Ueda, Dzmitry Zhyhadla, Claudio Petrini

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

Group: Geophysical Fluid Dynamics

Description:
Further development of numerical modeling approaches for geodynamic problems by including surface processes (erosion, sedimentation, river pattern development) into thermomechanical models (Fig.5).

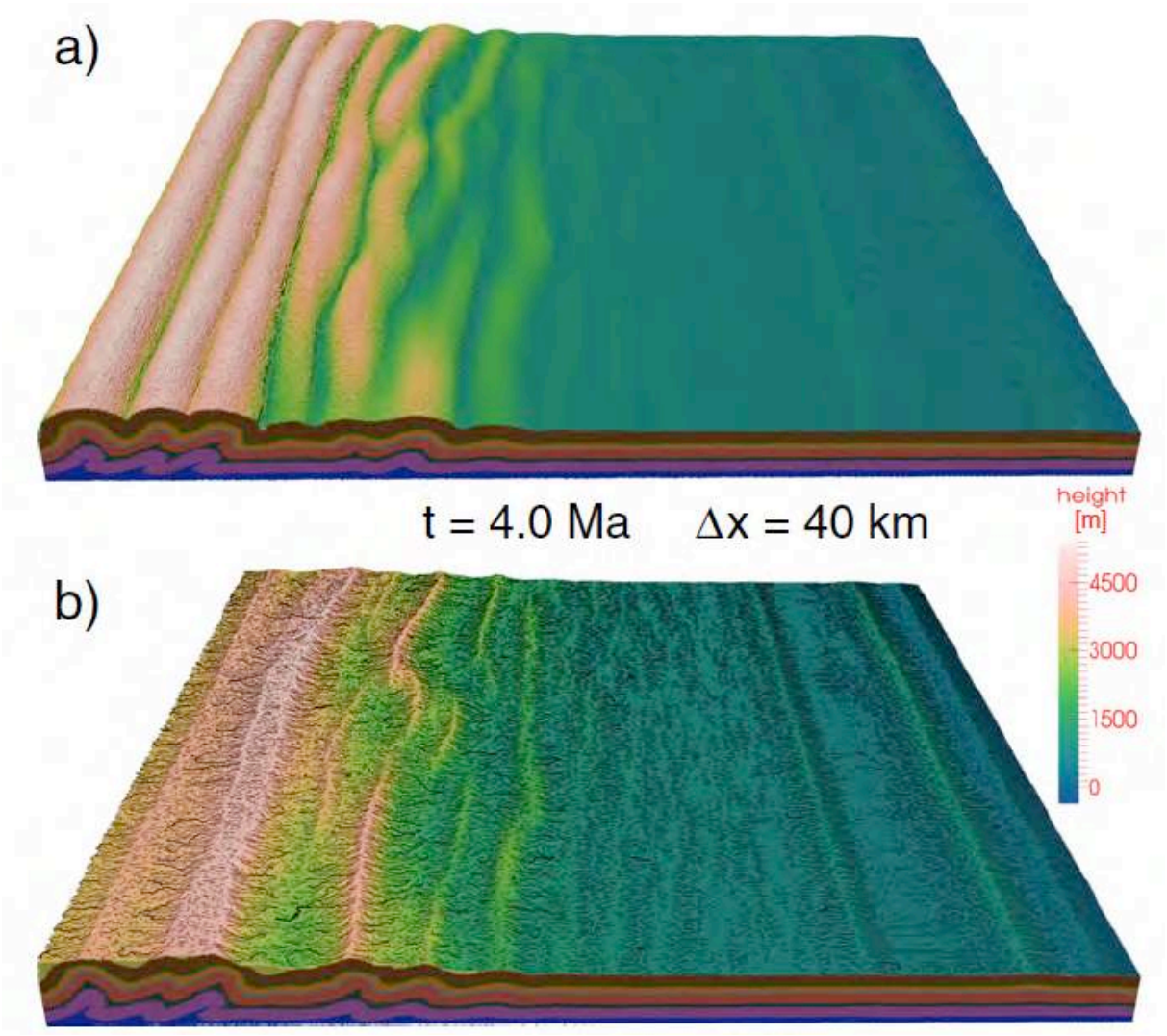


Fig. 5. Influence of erosion on the development of accretionary wedges (Uedaet al., 2013)

References:

Ueda, K., Willett, S.D., Gerya, T., Ruh, J. (2015) Geomorphological–thermo-mechanical modeling: Application to orogenic wedge dynamics. Tectonophysics, 659, 12-30.

Title: Melting-induced crustal production helps plate tectonics on Earth-like planets

Researchers: D. Lourenco, A. Rozel, P. J. Tackley

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

Description:

Within our Solar System, Earth is the only planet to be in a mobile-lid regime. It is generally accepted that the other terrestrial planets are currently in a stagnant-lid regime, with the possible exception of Venus that may be in an episodic-lid regime. In this study, we use numerical simulations to address the question of whether melting-induced crustal production changes the critical yield stress needed to obtain mobile-lid behaviour (plate tectonics). Our results show that melting-induced crustal production strongly influences plate tectonics on Earth-like planets by strongly enhancing the mobility of the lid, replacing a stagnant lid with an episodic lid, or greatly extending the time in which a smoothly evolving mobile lid is present in a planet. Finally, we show that our results are consistent with analytically predicted critical yield stress obtained with boundary layer theory, whether melting-induced crustal production is considered or not.

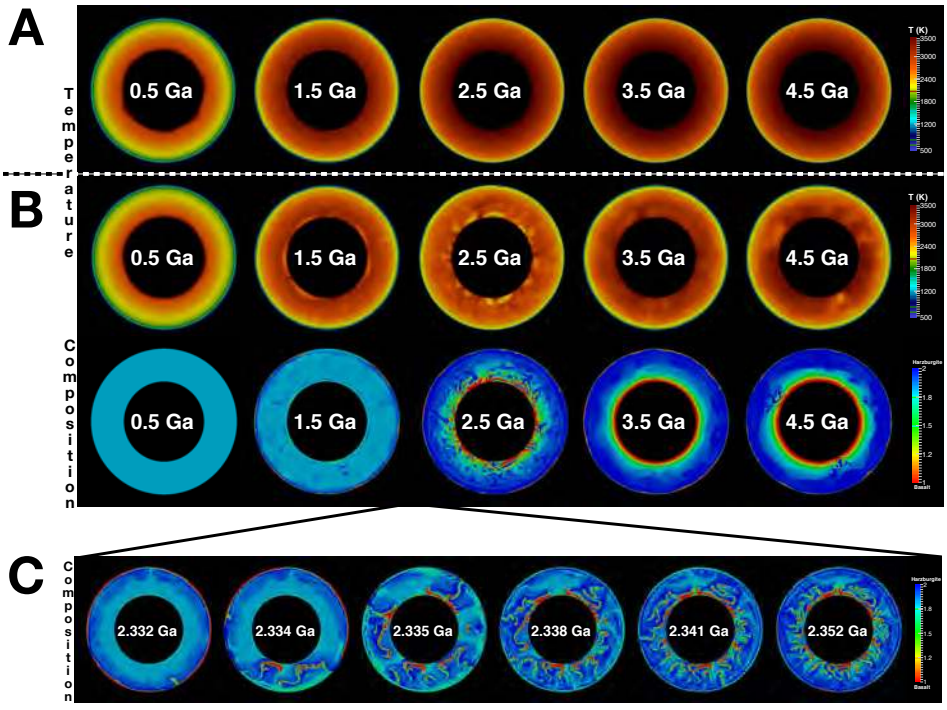


Figure. Comparison of simulations without (A) and with (B) melting-induced crustal production. Crustal production facilitates episodic plate tectonics; without it a stagnant lid is obtained. (C) shows a zoom-in of an episodic plate tectonics event.

Title: A spectral element discretization on unstructured simplex meshes for elastodynamics

Researchers: Dave A. May

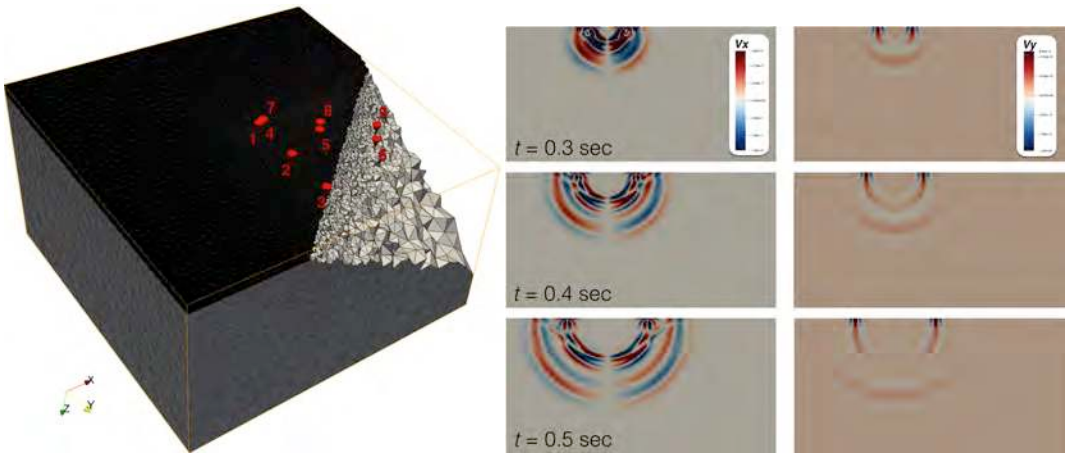
Institute/ Group: Geophysical Fluid Dynamics
Department of Earth Sciences

Description:

Spectral finite element methods (SEM) defined over quadrilateral and hexahedral element geometries have proven to be a fast, accurate and scalable approach to study wave propagation phenomena. In the context of regional scale seismology and or simulations incorporating finite earthquake sources, the geometric restrictions associated with hexahedral elements limit the applicability of the classical SEM.

I have extended the SEM methodology to triangular and tetrahedral element geometries. Due to the lack of a natural tensor product basis and sufficiently accurate collocated quadrature rule, the spectral method applied on simplices does not result in a diagonal mass matrix. Consequently, I have developed highly efficient matrix-free SpMV kernels exploiting DGEMM and an iterative sub-structuring preconditioner to solve mass matrix systems. The implementation is massively parallel and is being utilized on Euler.

A number of benchmark studies and comparisons with analytic solutions has been undertaken. Spectral accuracy is observed in all test cases. Preliminary results also indicate the spectral implementation permits very aggressive spatial coarsening or refinement without introducing artifacts in the wave field. Exploring the applicability of using implicit time integration schemes together with aggressive local mesh refinement is underway.



Reference:

D. A. May, A.-A. Gabriel & J. Brown, A spectral element discretization on unstructured simplex meshes for elastodynamics, Geophysical Journal International (2015) [in prep]

Title: Influence of plate tectonic mode on the coupled thermochemical evolution of Earth's mantle and core

Researchers: T. Nakagawa, P. J. Tackley

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

Description:

We investigate the influence of tectonic mode on the thermochemical evolution of mantle convection coupled to a parameterized core cooling model. The tectonic mode is controlled by varying the friction coefficient for brittle behavior, producing the three tectonic modes: mobile lid (plate tectonics), stagnant lid, and episodic lid. The resulting compositional structure of the deep mantle is strongly dependent on tectonic mode, with episodic lid resulting in a thick layer of subducted basalt in the deep mantle, whereas mobile lid produces only isolated piles and stagnant lid no basaltic layering. The tectonic mode is established early on, with subduction initiating at around 60 Myr from the initial state in mobile and episodic cases, triggered by the arrival of plumes at the base of the lithosphere. Crustal production assists subduction initiation, increasing the critical friction coefficient. The tectonic mode has a strong effect on core evolution via its influence on deep mantle structure; episodic cases in which a thick layer of basalt builds up experience less core heat flow and cooling and a failed geodynamo. Thus, a continuous mobile-lid mode existing from early times matches Earth's mantle structure and core evolution better than an episodic mode.

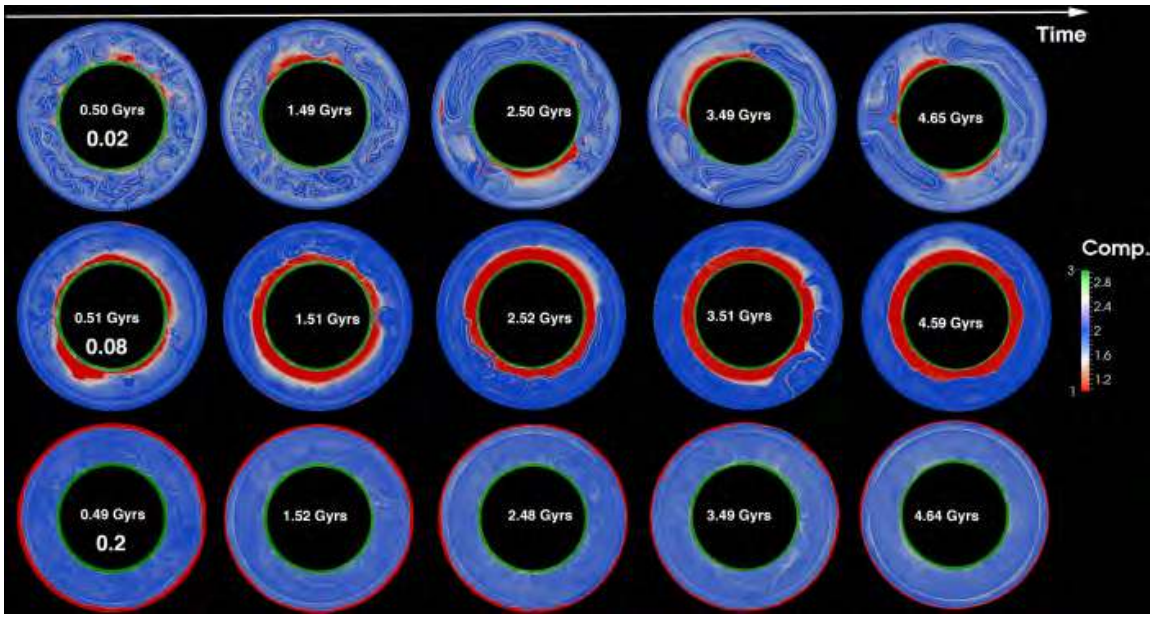


Figure. Evolution of the compositional structure for three cases with (top row) plate tectonics, (middle row) episodic plate tectonics and (bottom row) a stagnant lid.

References. Nakagawa, T. and P. J. Tackley (2015) Influence of plate tectonic mode on the coupled thermochemical evolution of Earth's mantle and core, Geochem. Geophys. Geosyst. 16, doi:10.1002/2015GC005996.

Title: Grain size evolution in the mantle of terrestrial planets

Researchers: A. Rozel, M. Thielmann, G. Golabek, T. Gerya, P.J. Tackley

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

Description:

We have developed a semi analytical model of mantle convection able to predict the grain size profile of the present day Earth. Grain size evolution has been studied with increasing interest over the last decades but its behavior in both mantle and lithosphere remains largely misunderstood due to its non-linearity. Several recent studies suggest that it might play a fundamental role in localization of deformation in the lithosphere but we focus here on the mantle in which we also observe important processes.

We work on a 1D compressible thermal convection model based on the equality of advective heat flux and the integral of viscous dissipation in the whole domain. Imposing mass conservation, our model is able to predict all rheological parameters able to produce both present day average surface velocity and lower mantle viscosity. Composite rheologies involving dislocation creep and grain size dependent diffusion creep are considered. The effect of phase transitions on the grain size is also explicitely taken into account. We present the family of solutions for the activation volume and the viscosity jump at the 660 discontinuity according to any initial choice of activation energy. The scaling laws for rheological parameters obtained are compared to self-consistent evolutionary simulations of mantle convection considering grain size dependent diffusion creep in 2D spherical annulus geometry.

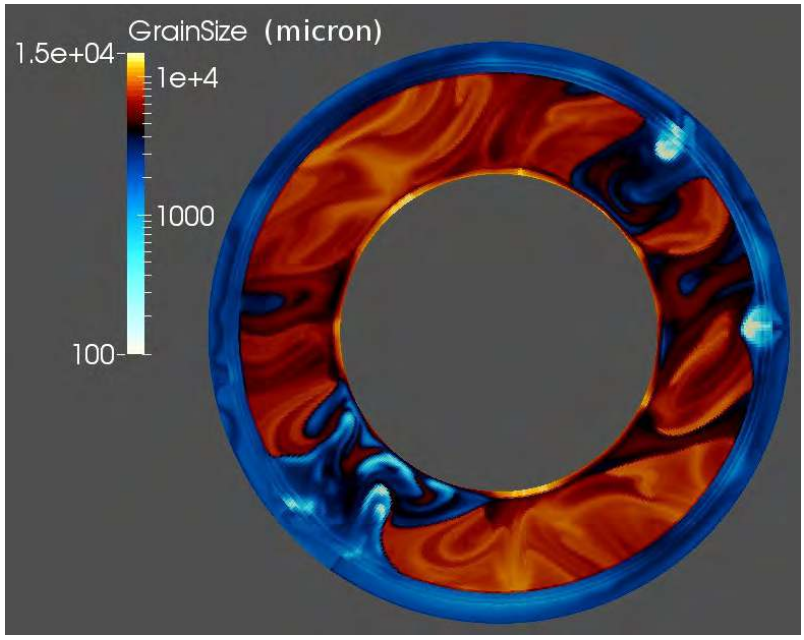


Figure. An example of grain size field obtained for present day Earth.

Title: Tracking of the conditions of TTG rocks formation in the archean through large scale numerical modeling of mantle thermochemical convection

Researchers: A. Rozel, G. Golabek, C. Jain, T. Gerya, P.J. Tackley

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

Description:

We use a new version of the convection code StagYY which is now tracking for PT conditions for TTG rocks creation. Starting from a very warm state, representing the mantle of the Earth just after magma ocean crystallization, we investigate the impact of melting and oceanic crust formation on the temperature profile of the lithosphere. We use various partitioning between intrusion and extrusion of molten rocks and different friction coefficient in the lithosphere.

Our results clearly show that only simulations with large intrusion fractions, between 70 and 100%, are able to produce a steep enough temperature profile in the lithosphere to produce a significant amount a TTG rocks, as is reported in the literature. Moreover, 3 types of TTG rocks (corresponding to 3 pressure ranges) have been reported with different volume ratios at the archean: 20% of low pressure TTG, 20% of high pressure TTG and 60% of intermediate pressure TTG. The figure below shows the ratio of volumes of (Intermediate pressure)/(low pressure + high pressure) TTG rocks tracked in our simulations. The expected value is 1.5. Only high intrusion fraction are able to reach the expected value for this ratio, whatever the value of the friction coefficient.

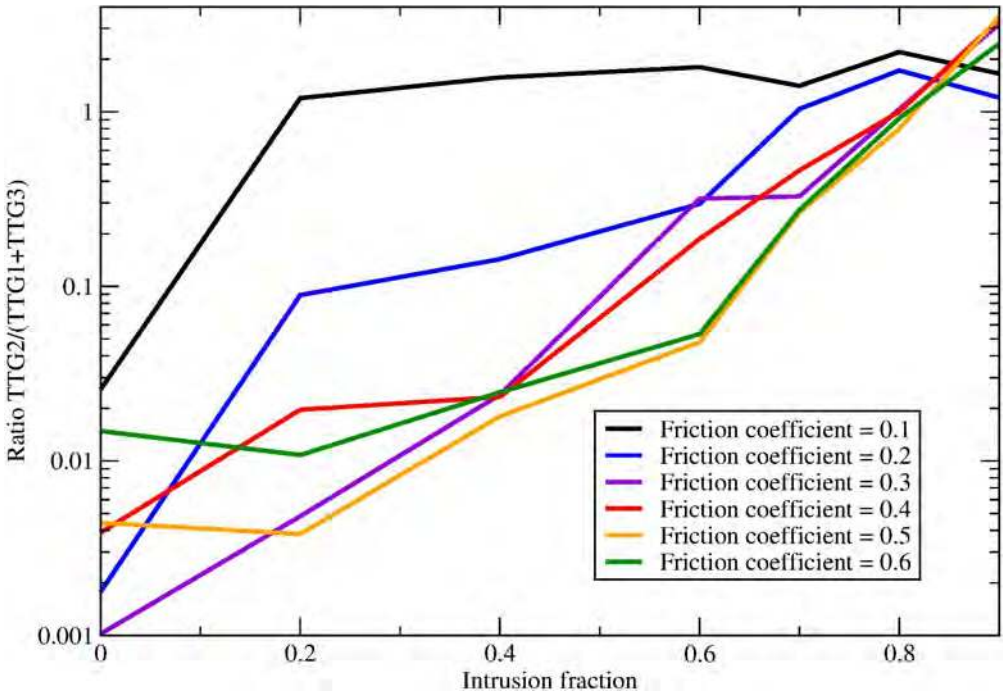


Figure. Ratio of volumes of (Intermediate pressure)/(low pressure + high pressure) TTG rocks tracked in our simulations

Title: Development of a method to model magma ocean evolution into long-term solid-state convection

Researchers: P. J. Tackley, D. Lourenco

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

Description:

The Earth and other large rocky planets likely started off molten due to energy release during their formation, which involved giant impacts during its final phase. Cooling and solidification of this molten "magma ocean" state was likely quite rapid, and transitioned into long-term mantle convection and plate tectonics in the (mostly) solid state. We are developing a numerical treatment that allows us to model this key phase, which is very important because any compositional layering that developed would have a strong influence on subsequent evolution over billions of years. This is challenging because the viscosity changes by ~18 orders of magnitude as rock goes from liquid to solid. Our model parameterizes turbulent convection in the liquid state using mixing-length theory while fully resolving processes in the solid state. Melt-solid separation is treated using Darcy's law, a radiative boundary condition is applied at the surface, and a parameterized core cooling model is used. In this way, we can simulate Earth evolution from a 100% molten state to the present day.

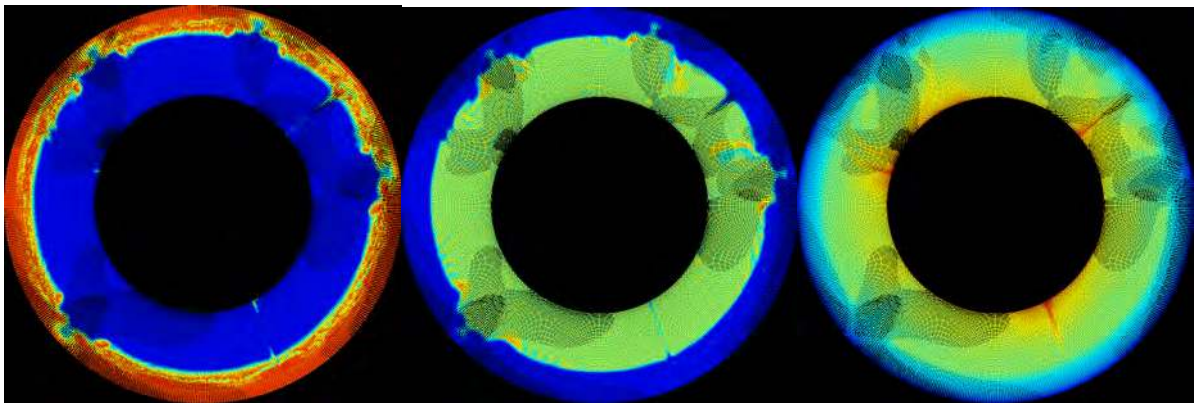


Figure. Melt fraction (left), Composition (centre) and Temperature (right) during a simulation. At this point a magma ocean still exists in the upper part of the mantle but the lower mantle has solidified.

Title: Interior—atmosphere co-evolution of terrestrial planets

Researchers: F. W. Wagner*, J. Mendonca**, P. J. Tackley*, K. Heng**

Institute/Group: *ETHZ, Institute of Geophysics/Geophysical Fluid Dynamics
**Uni Bern, Centre for Space & Habitability/Exoplanets & Exoclimes

Description:

The climate evolution and habitability of terrestrial planets is governed by both insolation and atmospheric composition. The latter may change substantially over time if greenhouse gasses such as water vapour and carbon dioxide are released into the atmosphere as a consequence of volcanic degassing. Higher concentrations of greenhouse gasses lead to an increase in surface temperature, which in turn affects melt production and volcanic activity of the planetary body. This study focuses on the complex interplay between interior dynamics and climate evolution. To model the thermo-chemical evolution of the interior we rely on StagYY. The numerical code is already capable of tracking compositional variations within the convecting mantle. Therefore, the calculation of volatile fluxes from the interior into the atmosphere can be done in a straightforward way. To determine surface temperature conditions with respect to time-varying concentrations of greenhouse gasses, we are currently developing a one-dimensional, two-stream model of radiative-convection equilibrium that treats the transport of thermal radiation in an evolving atmosphere. In particular for the planet Venus, a microphysical model for H_2SO_4-rich clouds has been implemented into the climate simulation platform. First results are consistent with literature and indicate that under Venus-like conditions the increase of either H_2O or SO_2 in the atmosphere yields thicker cloud layers due to a higher cloud production rate. Furthermore, thicker clouds increase the optical depth of the atmosphere, thereby strongly affecting surface temperature. After completion of the climate model, we will couple it with StagYY to study possible interior-atmosphere feedback mechanisms controlling the long-term habitability of terrestrial planets.

Title: Calibration of the mixing-length theory for highly viscous fluids

Researchers: F. W. Wagner*, A.-C. Plesa**

Institute/Group: *ETHZ, Institute of Geophysics/Geophysical Fluid Dynamics
**DLR, Institute of Planetary Research/Planetary Physics

Description:

The internal dynamics and thermal evolution of terrestrial planets is mainly governed by the efficiency of convective heat transfer through the mantle. Since it is computationally challenging to investigate a large parameter space while precisely modelling the full convective heat flux, parameterised descriptions of thermal convection are essential. A simple method to calculate quickly the convective heat transport is known as the mixing-length theory. In this study, we present a calibration of the mixing-length parameter in the local mixing-length theory. The parameterisation is derived from a comparison between sophisticated three-dimensional (3-D) numerical experiments and the one-dimensional (1-D) mixing-length theory with a varying mixing length. We find that the mixing length depends strongly on the viscosity contrast of the convective system. Furthermore, simple scaling relationships for the mixing length have been obtained and correspond to different convective regimes (see Figure). For mobile-lid convection at small to intermediate viscosity contrasts, mixing length has to be larger than the conventional formulation as distance to the nearest thermal boundary. However, magnitude of the mixing length decreases toward higher viscosity contrasts, in particular for the so-called transitional regime characterised by an intermediate viscosity contrast. For stagnant-lid convection at large viscosity contrasts, mixing length is adequately described by its conventional formulation. The new calibration will help to establish the mixing-length theory as simple 1-D approach for describing thermal convection inside of rocky planets.

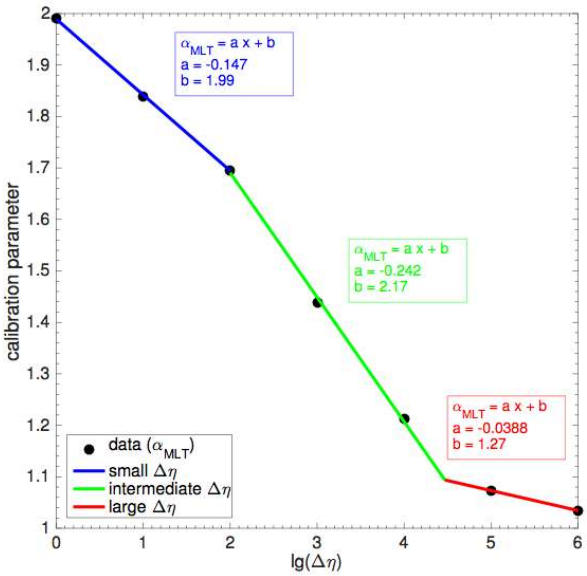


Figure: Calibration parameter as a function of viscosity contrast. The inlays show appropriate fits to data.

Group of W.F. van Gunsteren

Title: GROMOS polarizable charge-on-spring models for liquid urea: COS/U and COS/U2

Researchers: Z. Lin
S.J. Bachmann
W.F. van Gunsteren

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

Description:

Two one-site polarizable urea models, COS/U and COS/U2, based on the charge-on-spring model are proposed. The models are parametrized against thermodynamic properties of urea-water mixtures in combination with the polarizable COS/G2 and COS/D2 models for liquid water, respectively, and are compatible with the GROMOS biomolecular force field. Thermodynamic, dielectric, and dynamic properties of urea-water mixtures simulated using the polarizable models are closer to experimental data than using the non-polarizable models. The COS/U and COS/U2 models could be used in biomolecular simulations of protein denaturation.

References: J. Chem. Phys. 142 (**2015**) 094117, DOI: 10.1063/1.4913955

Title: Polarizable Coarse-Grained Models for Molecular Dynamics Simulation of Liquid Cyclohexane

Researchers: O. Szklarczyk
E. Arvaniti
W.F. van Gunsteren

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

Description:

Force field parameters for polarizable coarse-grained (CG) supra-atomic models of liquid cyclohexane are proposed. Two different bead sizes were investigated, one representing two fine-grained (FG) CH2r united atoms of the cyclohexane ring, and one representing three FG CH2r united atoms. Electronic polarizability is represented by a massless charge-on-spring particle connected to each CG bead. The model parameters were calibrated against the experimental density and heat of vaporization of liquid cyclohexane, and the free energy of cyclohexane hydration. Both models show good agreement with thermodynamic properties of cyclohexane, yet overestimate the self-diffusion. The dielectric properties of the polarizable models agree very well with experiment.

References: J. Comput. Chem. 36 (**2015**) 1311-1321

Title: Effects of Polarizable Solvent Models upon the Relative Stability of an α‑Helical and a β‑Hairpin Structure of an Alanine Deca-Peptide

Researchers: Z. Lin
W.F. van Gunsteren

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

Description:

The free enthalpy of changing a non-polarizable solvent into a polarizable solvent is calculated for an alanine deca-peptide solvated in water, methanol, chloroform, or carbon tetrachloride. Introducing polarizability into a water solvent does not change the relative stability between the α-helix and the β-hairpin, while for methanol and chloroform the α-helix is stabilized by about 1 kJ mol^{-1} per residue and for carbon tetrachloride by about 2 kJ mol^{-1} per residue. These results suggest that the less polar the solvent is, the more the α-helical structure is stabilized with respect to the β-hairpin structure by the use of a polarizable solvent model instead of a non-polarizable one. This highlights that inclusion of polarizability in models for less polar and non-polar solvents or protein environments is as important as, if not more important than, including polarizability in models for liquid water.

References: J. Chem. Theory Comput. 11 (**2015**) 1983-1986

Title: On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations

Researchers: Z. Lin
W.F. van Gunsteren

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

Description:

In a molecular dynamics (MD) simulation, various thermostat algorithms, including Langevin dynamics (LD), Nose-Hoover (NH), and weak-coupling (WC) thermostats, can be used to keep the simulation temperature constant. A canonical ensemble is generated by the use of LD and NH, while the nature of the ensemble produced by WC has not yet been identified. A few years ago, it was shown that when using a WC thermostat with particular values of the temperature coupling time for liquid water at ambient temperature and pressure, the distribution of the potential energy is less wide than the canonical one. This led to an artefact in temperature replica-exchange molecular dynamics (T-REMD) simulations in which the potential energy distributions appear not to be equal to the ones of standard MD simulations. In this paper, we re-investigate this problem. We show that this artefact is probably due to the ensemble generated by WC being incompatible with the T-REMD replica-exchange criterion, which assumes a canonical configurational ensemble. We also show, however, that this artefact can be reduced or even eliminated by particular choices of the temperature coupling time of WC and the replica-exchange time period of T-REMD, i.e., when the temperature coupling time is chosen very close to the MD time step or when the exchange time period is chosen large enough. An attempt to develop a T-REMD replica-exchange criterion which is likely to be more compatible with the WC configurational ensemble is reported. Furthermore, an exchange criterion which is compatible with a micro-canonical ensemble is used in total energy REMD simulations.

References: J. Chem. Phys. 143 (**2015**) 034110, DOI: 10.1063/1.4926937

Title: Supra-Atomic Coarse-Grained GROMOS Force Field for Aliphatic Hydrocarbons in the Liquid Phase

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

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

Description:

A supra-atomic coarse-grained (CG) force field for liquid n-alkanes is presented. The model was calibrated using experimental thermodynamic data and structural as well as energetic properties for 14 n-alkanes as obtained from atomistic fine-grained (FG) simulations of the corresponding hydrocarbons using the GROMOS 45A3 biomolecular force field. A variation of the non-bonded force-field parameters obtained from mapping the FG interactions onto the CG degrees of freedom to fit the density and heat of vaporization to experimental values turned out to be mandatory for a correct reproduction of these data by the CG model, while the bonded force-field parameters for the CG model could be obtained from a Boltzmann-weighted fit with some variations with respect to the corresponding properties from the FG simulations mapped onto the CG degrees of freedom. The model presents 6 different CG bead types, for bead sizes from 2 to 4 distinguishing between terminal and nonterminal beads within an alkane chain (end or middle). It contains different non-bonded Lennard-Jones parameters for the interaction of CG alkanes with CG water. The CG alkane model was further tested by comparing predictions of the excess free energy, the self-diffusion constant, surface tension, isothermal compressibility, heat capacity, thermal expansion coefficient, and shear viscosity for n-alkanes to experimental values. The CG model offers a thermodynamically calibrated basis for the development of CG models of lipids.

References: J. Chem. Theory Comput. 11 (**2015**) 2925-2937, DOI: 10.1021/acs.jctc.5b00295, incl. suppl. mat.

Title: Structural and energetic effects of the use of polarisable water to solvate proteins

Researchers: S.J. Bachmann
W.F. van Gunsteren

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

Description:

Using a non-polarisable model (SPC) for liquid water and two polarisable water models COS/G2, COS/D) the effect of introducing molecular polarisability into the solvent upon protein structure and energetics is investigated for eight proteins, hen egg-white lysozyme (HEWL), major cold shock protein (CspA), protein G (GP), chorismate mutase (CM), the C-terminal domain of the ribosomal protein L7/L12 (RB), the amino terminal domain of phage 434 repressor (GRP), a 12-residue β-hairpin (DNV) and the GCN trigger peptide (GTP), using MD simulation, one 50 ns simulation and four additional 20 ns simulations for each protein and each water model. The differences in overall structural and energetic properties of the proteins induced by the three different water models are small, except for the amino-terminal domain of phage 434 repressor (GRP). The polarisable COS/G2 water model induces a slightly stronger interaction with the proteins modelled using the GROMOS 54A7 force field than the non-polarisable SPC water model, while for the polarisable COS/D water model the opposite effect is observed.

References: Mol. Phys. (**2015**) on-line, DOI: 10.1080/00268976.2015.1042085, incl. suppl. mat.

Title: A comparison of pathway independent and pathway dependent methods in the calculation of conformational free enthalpy differences

Researchers: Z. Lin
W.F. van Gunsteren

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

Description:

The multi-step umbrella sampling method, which belongs to pathway dependent methods to calculate conformational free enthalpy differences, is used to calculate the free enthalpy difference between a right-handed $2.7_{10/12}$-helix and a left-handed 3_{14}-helix of a hexa-β-peptide in methanol solution. The same conformational free enthalpy difference was previously investigated using pathway independent methods such as direct counting and enveloping distribution sampling. Our results show that the pathway dependent simulations are very sensitive to the choice of the pathway and its parameter values. A pathway based on restraining distances of hydrogen-bonding atom pairs shows very poor sampling for two different values of the restraining force constant. Another pathway based on restraining backbone dihedral angles did smoothly sample the transition between the two helical conformations, but only with a proper choice of the restraining force constant. The results illustrate that if, and only if, a proper pathway and proper parameters are chosen, the multi-step umbrella sampling can be almost 50 times more efficient than the pathway independent methods in this case. The analysis illustrates the advantages and pitfalls of the much used multi-step umbrella sampling methodology.

References: Protein Science (**2015**) on-line, DOI: 10.1002/pro.2695

Title: On the Pitfalls of Peer Review

Researchers: W.F. van Gunsteren

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

Description:

The review process of academic, scientific research and its basic tenants is considered, thereby distinguishing between (i) reviewing of manuscripts to be published in the scientific literature, (ii) reviewing of research proposals to be financed by funding agencies, (iii) reviewing of educational or research institutions with respect to their proper functioning, and (iv) reviewing of scientists with the aim of appointing or tenuring faculty.

References: Chimia (**2015**) submitted

Title: Multi-resolution Solvation of Biomolecules: an Algorithm for Spatial Multi-scaling in Molecular Dynamics Simulations

Researchers: O.M. Szklarczyk
N.S. Bieler
P.H. Hünenberger
W.F. van Gunsteren

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

Description:

An algorithm is proposed for performing molecular dynamics (MD) simulation of a biomolecular solute represented at atomistic resolution, surrounded by a surface layer of atomistic fine-grained (FG) solvent molecules within a bulk represented by coarse-grained (CG) solvent beads. The method, called flexible boundaries for multi-resolution solvation (FBMS), is based on: (i) a three-region solvent layering around the solute, involving an FG layer, surrounded by a mixed FG-CG buffer layer, itself surrounded by a bulk CG region; (ii) a definition of the layer boundaries relying on an effective distance to the solute surface and thus, adapted to the shape of the solute and adjusting to its conformational changes. The effective surface distance is defined by inverse-nth power averaging over the distances to all non-hydrogen solute atoms, and the layering is enforced by means of half-harmonic distance restraints, attractive for the FG molecules and repulsive for the CG beads. A restraint-free region at intermediate distances enables the formation of the buffer layer, where the FG and CG solvents can mix freely. The algorithm is tested and validated using the GROMOS force field and the associated FG (SPC) and CG (polarizable CGW) water models. The test systems include pure-water systems, where one FG molecule plays the role of a solute, and a deca-alanine peptide with consideration of two widely different solute shapes, α-helical and fully extended. In particular, as the peptide unfolds, the number of FG molecules required to fill its close-range solvation layer increases, the additional molecules being provided by the buffer layer. Further validation involves simulations of four proteins in multi-resolution FG/CG mixtures. The resulting structural, energetic and solvation properties are found to be similar to those observed in corresponding pure FG simulations.

References: J. Chem. Theory Comput. (**2015**) in press, incl. suppl. mat.

Title: Investigation of the structural preference and flexibility

Researchers: J. Dolenc
B.H. Meier
W.F. van Gunsteren

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

Description: The structural variability of a 16-residue loop (residues 246-261) which is in part disordered and connects two layers of the β-solenoid formed by the prion-form of HET-s and its prion domain HET-s (218-289) is investigated using molecular dynamics computer simulation. A system of three HET-s (218-289) molecules in a β-sheet structure as in the fibril is simulated in aqueous solution. The trajectory structures appear to be consistent with Cα chemical shift data obtained. In order to delineate the influence of the β-sheet core of the fibril upon the structural variability of the loop, the latter is also simulated without the β-sheet core, but with its N- and C-terminal residues restrained at their positions in the fibril. The analysis of the trajectories shows that the structural variability of the loop is restricted by the β-sheet core, least at its N-terminal end and most in the middle of the trimer.

References: Phys. Chem. Chem. Phys. (**2015**) submitted, incl. suppl. mat.

Title: GROMOS Polarizable Model for Acetone

Researchers: V.H. Rusu
S.J. Bachmann
W.F. van Gunsteren

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

Description:

A polarizable model for acetone, COS/A, is proposed that is based on the charge-on-spring (COS) polarization model and is compatible with the polarizable COS/D2 and COS/G2 models for liquid water. A series of acetone-water mixtures at different acetone mole fractions was simulated using the new model in conjunction with the mentioned polarizable and the non-polarizable SPC and SPC/E water models. The model was parameterized to reproduce the following liquid acetone properties: density, heat of vaporization, surface tension, dielectric permittivity, self diffusion and heat capacity. The dynamics of molecules in acetone-water mixtures is slower using the polarizable acetone and water models compared to the non-polarizable KBFF acetone and SPC/E water models. The computational cost of simulating the polarizable acetone-water mixtures is a factor of 3 to 4 higher compared with the non-polarizable models due to the increased number of interaction sites and the multiple iterations required to evaluate self-consistently the positions of the charge-on-spring sites at every simulation step. The COS/A acetone model can be used in biomolecular simulations in conjunction with the mentioned polarizable water models to solvate biomolecules.

References: Mol. Phys. (**2015**) submitted

Title: Going for a PhD: Joys and Pitfalls

Researchers: W.F. van Gunsteren

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

Description:

With the number of students undertaking a PhD increasing and the nature of the working environment for these students changing, opportunities and problems inherent to this particular way of educating students are evolving. Challenges and difficulties that may arise during a PhD are considered and the ways potential problems can be avoided are discussed.

References: Angew. Chem. Int. Ed. (**2015**) submitted

6

High-performance Hardware

Information Technology Services

The IT Services of ETH are currently managing two large Linux clusters called BRUTUS ("Better Reliability and Usability Thanks to Unified System") and EULER (Erweiterbarer, Umweltfreundlicher, Leistungsfähiger ETH Rechner").

Both clusters have been financed and are operated according to a "shareholder" model. Professors, institutes and even whole departments can become shareholders by financing a number of compute nodes in the cluster. In return, they are guaranteed a share of CPU time proportional to their investment. The share financed by the IT Services is made available to the whole scientific community of ETH at no cost.

To make it easier for users to switch back and forth between Brutus and Euler, both clusters use the same operating system (CentOS), batch system (Platform LSF), development tools (GNU, Intel and PGI compilers) and applications.

Brutus

The Brutus cluster has been in operation at ETH since 2008 and has been regularly upgraded and expanded over the years. As a result Brutus is very heterogeneous; there are 10 different types of compute nodes, containing from 4 to 48 cores and between 16 GB and 1024 GB of memory. The cluster's software environment has been designed from the start to hide this complexity and to present Brutus as a monolithic system to its users.

Currently Brutus contains 995 compute nodes with a total of 19,768 processor cores and 34 GPUs, giving it a peak performance of 195 TF.

Two Lustre parallel file systems, with a capacity of 400 TB each, are configured respectively as permanent and non-permanent (scratch) storage for the most data-intensive applications. A Panasas parallel file system with a capacity of 75 TB is configured as medium-term storage for less demanding applications. Lastly, an NFS file system with a capacity of 50 TB, based on four redundant Solaris ZFS servers, is used for home directories and centrally installed applications. This NFS file system is backed up every night to the ETH's central tape archive (TSM).

All compute nodes are connected to the cluster's internal Ethernet network via 1 Gb/s links. The login nodes are connected to this network and to the ETH's network via 10 Gb/s links. The vast majority of the compute nodes are connected to a low-latency 40 Gb/s InfiniBand QDR network.

The two Lustre file systems are attached directly to the cluster's InfiniBand QDR network. The Panasas and NFS file systems, as well as the ETH's central NAS, are connected to the cluster's Ethernet network via 10 Gb/s links.

Euler

Due to lack of space, power and cooling in the computer rooms at ETH in Zurich, the Euler cluster is housed in CSCS's data center in Lugano and managed remotely from Zurich by the IT Services.

Euler does not replace Brutus but complements it. Whereas Brutus was designed primarily for high-throughput computations, Euler is designed for high-performance, which is reflected in the choice of faster processors and networks.

The first phase (Euler I) was commissioned at the end of 2013 and installed in the spring of 2014. It consists of 448 compute nodes (HP BL460c Gen8), each equipped with 24 cores (two 12-core Intel Xeon E5-2697v2 CPUs) and between 64 and 256 GB of memory. All compute nodes are connected to two high-speed networks:

- 56 Gb/s InfiniBand FDR for inter-node communication (typically MPI);
- 10 Gb/s Ethernet for file access and for global communication (system management, monitoring, batch system, etc.).

A second phase (Euler II) was commissioned at the end of 2014 and installed in the beginning of 2015. It consists of 320 compute nodes of a newer generation (HP BL460c Gen9), each equipped with 24 cores (two 12-core Intel Xeon E5-2680v3 CPUs) and 64 GB of memory. These nodes are connected to similar high-speed networks as Euler I.

Euler I and II are operated as a single cluster containing 768 compute nodes, 18,432 processor cores and a peak performance of about 570 TF. Another 452 compute nodes (11,008 cores / 440 TF) will be added at the end of 2015.

Due to the distance (latency) between Zurich and Lugano, it was decided early on that Euler would need its own local storage systems. A Panasas parallel file system with a capacity of 400 TB provides high-performance storage for both permanent and temporary (scratch) data. An NFS file system with a capacity of 200 TB, based on two redundant NetApp servers, provides high-reliability storage for home directories and centrally installed applications, as well as long-term storage for user projects. Like Brutus, the NFS file system of Euler is backed up every night to the ETH's central tape archive (TSM) in Zurich.

A core feature of Euler is the extensive use of virtualization. The cluster's head nodes (login and management nodes) are not physical servers but virtual machines. The underlying virtualization layer, based on VMware, makes it possible to create virtual compute nodes or even offer complete clusters to customers who cannot or do not want to use the Euler cluster in a traditional manner. It also allows Euler to offer "software as a service" (SaaS) to the scientific community of ETH, for programs like CLC Genomics Server and MATLAB.

7

Publications*

*only CSE-related articles
in refereed journals

Group of P. Arbenz

D. Hupp, D. Obrist, P. Arbenz: *Multigrid preconditioning for time-periodic Navier-Stokes problems*. Proc. Appl. Math. Mech. (PAMM) 15, 595–596 (2015).

P. Arbenz, L. Grigori, R. Krause, O. Schenk: "Guest editorial: Special issue on Parallel Matrix Algorithms and Applications (PMAA'14)". Parallel Comput. 49: 99-100 (2015), doi:10.1016/j.parco.2015.10.004.

S. Pauli, P. Arbenz: *Determining optimal multilevel Monte Carlo parameters with application to fault tolerance*. Comput. Math. Appl. (2015) doi:10.1016/j.camwa.2015.07.011.

S. Pauli, P. Arbenz, Ch. Schwab: *Intrinsic fault tolerance of multilevel Monte Carlo methods*. J. Parallel Distrib. Comput. 84: 24-36 (2015), doi:10.1016/j.jpdc.2015.07.005.

S. Pauli, R. Gantner, P. Arbenz, A. Adelmann: *Multilevel Monte Carlo for the Feynman–Kac formula for the Laplace equation*. BIT Numer. Math. (2015), doi:10.1007/s10543-014-0543-8.

S. Pauli: *Fault tolerance in Multilevel Monte Carlo methods*. ETH Zürich, PhD Thesis No. 22404, 2014.

P. Arbenz, C. Flaig, D. Kellenberger: *Bone structure analysis on multiple GPGPUs*. J. Parallel Distrib. Comput. 74, 2941–2950 (2014),

E. Turan, P. Arbenz: *Preconditioning aspects of large scale micro finite element analysis of 3D bone poroelasticity*. Parallel Comput. 40, 239–250 (2014).

S. Pauli, M. Kohler, P. Arbenz: *A fault tolerant implementation of multi-level Monte Carlo methods*. Parallel Computing: Accelerating Computational Science and Engineering (CSE). M. Bader et al. (eds.). Parallel Computing: Accelerating Computational Science and Engineering (CSE), Advances in Parallel Computing 25, IOS Press, 2014, pp. 471–480.

M. Toggweiler, A. Adelmann, P. Arbenz, J. J. Yang: *A novel adaptive time stepping variant of the Boris-Buneman integrator applied to particle accelerator simulation with space charge*. J. Comput. Phys. 273, 255–267 (2014).

Y. Matsuo, H. Guo, P. Arbenz: *Experiments on a Parallel Nonlinear Jacobi–Davidson Algorithm*. Procedia Comput. Sci. 29, 565-575 (2014), Proceedings of the International Conference on Computational Science (ICCS) 2014.

P. Arbenz, D. Hupp, D. Obrist: *A parallel solver for the time-periodic Navier–Stokes equations*. In: Parallel Processing and Applied Mathematics (PPAM 13), Part II. R. Wyrzykowski, J. Dongarra, K. Karczewski, J. Waśniewski (eds.). Lecture Notes in Computer Science 8385, pp. 291–300. Springer, Berlin, 2014.

C. Metzger-Kraus: *A self-consistent particle-in-cell time-domain solver incorporating radiative interaction*. ETH Zürich, PhD Thesis No. 22154, 2014. http://dx.doi.org/10.3929/ethz-a-010261293.

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

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

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

Y. Ineichen, A. Adelmann, C. Bekas, A. Curioni, P. Arbenz: *A fast and scalable low dimensional solver for charged particle dynamics in large particle accelerators*. Comput. Sci. Res. Dev. 28 (2-3): 185–192 (2013).

Group of K. Boulouchos publications

1. M. Schmitt, C.E. Frouzakis, Y.M. Wright, A.G. Tomboulides, K. Boulouchos, Investigation of wall heat transfer and thermal stratification under engine-relevant conditions using DNS, *Int. J. Eng. Res.*, 1-13, 2015

2. M. Schmitt, C.E. Frouzakis, Y.M. Wright, A.G. Tomboulides, K. Boulouchos, Direct numerical simulation of the compression stroke under engine-relevant conditions: Evolution of the velocity and thermal boundary layers, *Int. J. Heat Mass Transfer*, 91, 948-960, 2015

3. A. Montorfano, F. Piscaglia, M. Schmitt, Y. M. Wright, C.E. Frouzakis, A.G. Tomboulides, K. Boulouchos, A. Onorati, Comparison of Direct and Large Eddy Simulations of the Turbulent Flow in a Valve/Piston Assembly *Flow, Turb. Combust.* 95(2), 461-480, 2015

4. M. Kooshkbaghi, C.E. Frouzakis, I. Karlin, K. Boulouchos, n-Heptane/air combustion in perfectly stirred reactors: Dynamics, bifurcations and dominant reactions at critical conditions *Combust. Flame*, 161, 2692–2707, 2015

5. M. Schmitt, C.E. Frouzakis, A. Tomboulides, Y.M. Wright, K. Boulouchos, Direct numerical simulation of the effect of compression on the flow, temperature and composition under engine-like conditions, *Proc. Combust. Inst.*, 35(3), 3069–3077, 2015

6. A. Brambilla, M. Schultze, C.E. Frouzakis, J. Mantzaras, R. Bombach, K. Boulouchos, An experimental and numerical investigation of premixed syngas combustion dynamics in mesoscale channels with controlled wall temperature profiles, *Proc. Combust. Inst.*, 35(3), 3429–3437, 2015

7. C. Altantzis, C.E. Frouzakis, A.G. Tomboulides, K. Boulouchos, Direct numerical simulation of circular expanding premixed flames in a lean quiescent hydrogen-air mixture: Phenomenology and detailed flame front analysis, *Combust. Flame*, 162(2), 331-344, 2015

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