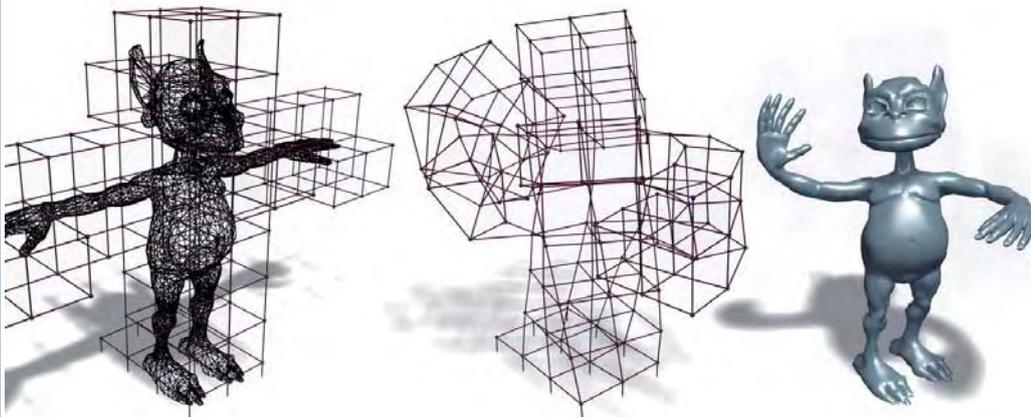


CSE

Computational Science and Engineering

Annual Report
2008/2009



ETH

Eidgenössische Technische Hochschule Zürich
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CSE

Computational Science and Engineering

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Ralf Hiptmair, Kaspar Nipp, Wilfred van Gunsteren
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Prof. Dr. Kaspar Nipp
Seminar for Applied Mathematics
Tel.: 41 44 632 3407
E-mail: nipp@math.ethz.ch

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Cover:

A high-resolution Goblin triangle model is embedded in a coarse simulation mesh (left). In order to achieve a desired pose, the artist defines several constraints on the simulation mesh. A constrained minimization of the elastic energy using the Finite Element Method then fully defines the configuration of the deformed mesh (middle). The resulting C^0 -continuous deformation field is improved by applying a moving least-squares interpolation. The high-resolution triangle model is then deformed using this smooth deformation field (right).

Groups having contributed to this report

Research Group	Institute	Projects	Publs.
P. Arbenz	Scientific Computing	32 - 36	286
J. Blatter	Theoretical Physics	199 - 246	
S. Bonhoeffer	Experimental and Theoretical Biology		288
K. Boulouchos	Engines and Combustion Laboratory	37 - 45	293
W. Fichtner	Integrated Systems Laboratory	46	294
D. Giardini	Geophysics	47 - 59	295
M. Gross	Visual Computing	60 - 63	
D. Helbing	Sociology		298
H. Herrmann	Building Materials	64 - 78	300
R. Hiptmair	Seminar for Applied Mathematics	79 - 81	
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P. Hünenberger	Physical Chemistry	86 - 91	302
A. Jackson	Geophysics	92 - 94	304
R. Jeltsch	Seminar for Applied Mathematics	95	
P. Jenny	Fluid Dynamics	96 - 107	
H. Katzgraber	Theoretical Physics	199 - 246	305
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D. Kressner	Seminar for Applied Mathematics	112	307
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Introduction

As in the years before, this impressive collection of outlines of CSE related research activities documents the central, crucial, and focal role of numerical simulation for research in many groups at ETH Zürich. I would like to thank all those who contributed to this latest volume of the CSE report.

Are we witnessing a turning point in hardware development? For surprisingly many years the chip makers managed to uphold the so-called Moore's law that predicts an exponential increase of processor power over time. Lets wait until computers become powerful enough to solve our problem was an option for large scale scientific computations. Now, it seems, Moore's law finally has to yield to fundamental physical limits and patience alone will no longer pay off in computational science.

Hardware development will not stop, of course: massive concurrency, new processor designs will continue to boost the theoretical performance of supercomputers. However, merely porting codes to these new systems will usually not work, because they will require sophisticated algorithms and data structures in order to harness their potential: the codes will have to cope with slow inter-processor communication, low bandwidth of local memory, likely failure of a computational core and many other peculiarities of these systems, peculiarities often ignored by existing simulation codes.

Bad news? Maybe for scientists and engineers, who dismiss the design and development of simulation codes as a tedious sideshow in their research. But exciting news for those with interest and expertise in CSE techniques. They will see scores of topical and fascinating research question arise. Bright prospects for both researchers and graduates with skills and experience in CSE.

Thus, this CSE report also sends the message that researchers at ETH Zürich are well equipped for the future of high-performance computing.

Zürich, November 16, 2009

Ralf Hiptmair, Head of Student Studies CSE and member of the CSE Committee
SAM, ETH Zürich, CH-8092 Zürich, hiptmair@sam.math.ethz.ch

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Education

In September 2008, 33 new students started their CSE Bachelor studies, 18 in the first semester and 15 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 2008/2009 was 73 (53 in the BSc program and 20 in the MSc program).

Gisela Widmer, a former RW/CSE student (start in 2000) and a PhD student at the Seminar for Applied Mathematics (SAM) of ETH Zürich won the BGCE Student Prize in CSE at the 2009 SIAM conference on Computational Science and Engineering in Miami in March. Congratulations!

In the past academic year 15 students have successfully finished a CSE curriculum, Bachelor and Master, respectively, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/Master thesis and, in parentheses, the name and the department/institute of the advisor.

Bachelor Theses

- | | |
|----------------|---|
| R. Gehrig | Atomistic Molecular Dynamics Simulations of 2-component Newton Black Films
(I. Sbalzarini, Theoretische Informatik) |
| A. Hildebrand | Numerical Simulation of Developing Pipe-Flow with Turbulent Wall Boundary Layer
(L. Kleiser, Fluidodynamik) |
| R. Lingenhag | Cloud-Resolving Simulations of Moist Convection
(C. Schär, Atmosphäre und Klima) |
| M. Moschovitis | Atlantic Hurricanes and European Mirrors: A Correlation Study
(U. Lohmann, Atmosphäre und Klima) |
| D. Murer | Development and Evaluation of a Domain Decomposition Method for the Linear Eddy Model
(K. Boulouchos, Energietechnik) |
| Y. Salathé | Computer-Assisted Feedback-Control-Based Optimization of Multistage Zeeman Acceleration
(F. Merkt, Physikalische Chemie) |
| P. Simmler | A New Model Approach in Coarse Graining Alkanes
(W. van Gunsteren, Physikalische Chemie) |
| S. Wettstein | Inversion Percolation on Fracture Networks
(H. Herrmann, Baustoffe) |

N. Zollinger Parallel Maxwell Solver
(P. Arbenz, Scientific Computing)

Master Theses

C. Bolliger On the Combination of Density Matrix Renormalization Group and
Density Functional Theory
(M. Reiher, Physikalische Chemie)

F. Freitag A New Algorithm for Structure Determination of Biomolecules on X-
Ray Diffraction Data: development, implementation and application
(W. van Gunsteren, Physikalische Chemie)

F. Gaignat CELL / Multicore High Precision Arithmetic
(W. Petersen, Seminar für Angewandte Mathematik)

M. Moschovitis Skeleton Reconstruction
(M. Pollefeys, Visual Computing)

H. Piehl Fluid-structure Interaction in a Pulsating Channel Flow with the Lattice
Boltzmann Method
(L. Kleiser, Fluidodynamik)

B. Popovic Option Pricing Methods for Stochastic Volatility Tentative Models
(C. Schwab, Seminar für Angewandte Mathematik)

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

Term Papers

M. Gloor Refined Wake Models for a Coaxial Rotor Simulation
(P. Jenny, Fluidodynamik)

G. Moll Implementation of the Calculation of Residual Dipolar Coupling into
Gromos
(W. van Gunsteren, Physikalische Chemie)

M. Müller Optimization of Schaback's Adaptive Method of Fundamental Solutions
(L. Kleiser, Fluidodynamik)

D. Murer Data Acquisition Software Development for a Novel Fast Neutron
Detector
(A. Rubbia, Teilchenphysik)

- M. Spreng Real Space Greens Function Solver for Nano Devices
 (A. Schenk, Integrierte Systeme)
- N. Zollinger Function Development
 (R. Jeltsch, Seminar für Angewandte Mathematik)

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 (containing articles from, e.g., Nature, Science, Scientific American, etc.). These presentations help the students to practise giving talks. Students are also asked to give talks on their term papers and voluntarily on their Master theses (if there are free time slots).

Zürich, October 30, 2009

Kaspar Nipp,

Advisor of Student Studies CSE and member of the CSE Committee

(Fachberater RW und Mitglied des Ausschusses Rechnergestützte Wissenschaften)

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

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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 HS08

- | | |
|----------|--|
| 25.09.08 | B. Auchmann, CERN, Genf
Magnetic field simulation for superconducting accelerator magnets at CERN: Coupled FE-BE methods for eddy-current problems in a differential-form framework |
| 02.10.08 | J. Stelling, Computational Systems Biology
Geometries and dynamics of cellular networks |
| 09.10.08 | I. Sbalzarini, Computational Biophysics
Simulating diffusion in complex geometries using particle methods: application to intracellular protein transport |
| 23.10.08 | M. Müller, Solianis Monitoring AG, Zürich
Data processing for non-invasive continuous glucose monitoring with a multi-sensor monitoring device |
| 30.10.08 | S. Goedecker, Computational Physics, Uni Basel
Global structure optimization of clusters and nanostructures: Finding the global energy minimum out of zillions of local minima |
| 06.11.08 | D. Folini, Centre de la Recherche d'Astrophysique Lyon /
Institut für Atmosphäre und Klima
From the stars to the telescope: modeling the way of the photons |
| 20.11.08 | A. Voigt, Wissenschaftliches Rechnen, TU Dresden
Atomistic phase field modeling in materials science |
| 04.12.08 | B. Rembold / K. Lanzenberger, ABB Turbo Systems AG, Baden
Simulationen in der Turboladerentwicklung bei ABB Turbo Systems: von der Komponente bis zum Gesamtsystem |

Case Studies Seminar FS09

- 26.02.09 B. Ruhstaller, Computational Physics, ZHAW Winterthur
Optoelectronic simulation of organic semiconductor devices for displays, lighting and photovoltaics
- 05.03.09 Symposium "Twelve years of computational science and engineering education at ETH: where do we go?"
(chair Wilfred van Gunsteren, D-CHAB, ETH)
- 14.15 – 14.30 <Welcome>
Heidi Wunderli-Allenspach (Rektorin ETH Zürich)
Hans Rudolf Künsch (Chairman D-MATH)
- 14.30 – 14.55 <Numerical methods for computer animation>
Markus Gross (D-INFK, ETH)
- 15.00 – 15.25 <On the combination of density matrix renormalization group and density functional theory>
Christine Bolliger (RW/CSE master thesis student at D-CHAB, ETH)
- 15.30 – 15.55 <Computational Engineering at ABB>
Jörg Ostrowski (ABB Schweiz)
- 16.30 – 16.55 <Numerical weather prediction: fighting the chaos with supercomputers>
Daniel Leuenberger (RW/CSE alumnus, Meteo Swiss)
- 17.00 – 17.25 <Geomorphical simulations>
Hans Herrmann (D-BAUG, ETH)
- 12.03.09 H. Nordborg, CADFEM AG, Aadorf
Numerical Simulations, virtual Product Design and Innovation -- how CSE is changing the world!
- 26.03.09 V. Gradinaru, Applied Mathematics
Numerical methos in quantum molecular dynamics
- 09.04.09 P. Ledger, Civil and Computational Engineering, Swansea University
Eddy Current Simulations: Medical Applications and Efficient Computation
- 23.04.09 G. Widmer, Applied Mathematics
Breaking the complexity of radiation for circuit breaker simulations
- 07.05.09 K. Wagner, EPCOS AG, München
Computational Methods for the Development of Innovative Microacoustic Components

4

Computational Highlight

FEM for Modeling and Computer Animation

Sebastian Martin, Peter Kaufmann, Markus Gross

October 13, 2009

Abstract

The Finite Element Method (FEM) has become an indispensable tool in computer graphics. Typical applications range from computer games, special effects and feature films to virtual surgery training simulators. In the field of geometric modeling, the FEM can help in creating realistic and physically plausible deformations with the user only having to specify a low number of constraints. Using the FEM to set up an equation of motion and integrating the equation in time, convincing animations of deformable objects can be produced that would be difficult to create manually. In this report, we present an FEM-based modeling approach, which produces a smooth deformation field through moving least-squares. To simulate cutting and fracturing of deformable objects, we further present two approaches for the animation of topological changes in the FEM mesh. As our methods are able to simulate arbitrary polyhedral elements, they can circumvent the cumbersome remeshing step that would otherwise be necessary when performing topological changes.

1 Introduction

Thanks to its versatility and rigorous mathematical foundation, the Finite Element Method has become tremendously important in computer graphics. Geometric modeling constitutes one particular domain of problems to which the FEM has been successfully applied. In short terms, a central goal in geometric modeling is the design of tools for intuitive shape deformations with a simple and easy-to-use interaction metaphor. Click-and-drag interfaces are particularly popular, since they allow direct manipulation of a geometric object by specifying a few constraints on the surface of the model. The algorithm then computes a deformation function that warps the shape to satisfy the user constraints as closely as possible. In addition, the computed warp should meet the user's expectation of an intuitive shape deformation. Recent methods have approached this goal using physically inspired shape deformations, which are modeled by applying the FEM to simplified elastic energy formulations. This leads to an intuitive editing behavior that is in agreement with our everyday experience of how shapes deform in the physical world. The surface geometry to deform is typically given as a highly detailed triangle mesh. Creating a finite element mesh by discretizing the volume enclosed by the surface is usually not practical as it would lead to a prohibitively large number of elements. Instead, one typically performs the simulation on a much coarser element mesh that fully contains the surface geometry, and then deforms the surface according to the deformation field resulting from the FEM simulation. When using simple elements such as tetrahedra or hexahedra, the resulting deformation field is not C^1 continuous, leading to visible artifacts in the deformed geometry. In Section 3, we present a method to compute a smooth deformation field even for very coarse simulation meshes.

Another domain of applications deals with the animation of scenes showing "real-world" behavior, such as virtual reality applications, surgery simulations, or computer animations for feature films. In this context, FEM simulations in computer graphics traditionally rely on strictly tetrahedral or hexahedral meshes, which simplifies the finite element approximation and significantly speeds up the involved computations. However, allowing only a single element shape can be too restrictive, since it requires complex remeshing in case of topological changes, for instance due to cutting, fracturing,

or adaptive refinement. An interesting alternative is the approach of Wicke et al. [WBG07]: They directly support more general convex polyhedral elements in finite element simulations by employing mean-value coordinates as a generalization of linear barycentric FEM shape functions. We therefore propose two approaches for how to extend the FEM to arbitrary convex and non-convex polyhedral elements using either 1) harmonic coordinates [JMD⁺07] as FEM basis functions or 2) the discontinuous Galerkin (DG) method, which modifies the problem’s weak form. Harmonic basis functions naturally generalize linear basis functions for tetrahedral elements and trilinear basis functions for hexahedral elements, and therefore seamlessly integrate into existing FEM frameworks. The DG formulation on the other hand relaxes the continuity requirements of the solution and enforces them only in a weak sense, allowing arbitrary non-conforming basis functions to be used in the individual elements. This allows for the simulation of arbitrarily complex polyhedral elements with a fixed budget of degrees of freedom.

2 FEM for Linear Elasticity

In the following we consider a 3D object with material coordinates $\mathbf{x} = (x, y, z)^T \in \Omega$, which is to be deformed by a displacement vector field $\mathbf{u} : \Omega \rightarrow \mathbb{R}^3$. A detailed derivation of CG FEM for linear elasticity can be found in many textbooks (e.g., [Hug00]) and also in the recent survey [NMK⁺06]. Hence, we refer the reader to the literature for details, and only give the equations required for the two approaches presented in Section 4.

We measure local deformations of the material using the linear Cauchy strain

$$\boldsymbol{\epsilon}(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T),$$

which under the assumption of a Hookean material is linearly related to the stress

$$\boldsymbol{\sigma}(\mathbf{u}) = \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{u}) \tag{1}$$

through a symmetric 4-tensor \mathbf{C} containing material parameters. The colon operator “:” denotes the tensor product between two matrices \mathbf{A} and \mathbf{B} or between a matrix \mathbf{A} and a 4-tensor \mathbf{C} . The dot operator “·” denotes vector dot products $\mathbf{u} \cdot \mathbf{v}$ or matrix-vector products $\mathbf{A} \cdot \mathbf{v}$ and $\mathbf{v} \cdot \mathbf{A}$.

In static equilibrium the internal forces have to be in balance with the external forces \mathbf{f} , which is expressed by

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) = \mathbf{f}. \tag{2}$$

Equations (1) and (2), in combination with suitable boundary constraints on $\partial\Omega$, constitute the strong form of elastostatics. Multiplying them by test functions, integrating by parts over Ω , and combining the resulting equations yields the weak form of CG FEM:

$$a_{\text{CG}}(\mathbf{u}, \mathbf{v}) := \int_{\Omega} \boldsymbol{\epsilon}(\mathbf{v}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{u}) = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}. \tag{3}$$

In order to discretize (3) the domain Ω is partitioned into finite elements $K \in \mathcal{T}$. On top of this tessellation a set of basis functions $\{N_1, \dots, N_n\}$ is defined and used to approximate \mathbf{u} as

$$\mathbf{u}(\mathbf{x}) \approx \sum_{i=1}^n \mathbf{u}_i N_i(\mathbf{x}) \quad \text{with} \quad \mathbf{u}_i \in \mathbb{R}^3. \tag{4}$$

For a weak form containing m ’th partial derivatives, standard FEM requires basis functions N_i from the Sobolev space $H^m(\Omega)$. This in particular restricts the basis functions to be *conforming*, i.e., C^m continuous within and C^{m-1} continuous across elements [Hug00]. For the weak form (3) the N_i therefore have to be C^0 *continuous* across elements.

Approximating both \mathbf{u} and \mathbf{v} by the shape functions N_i and exploiting the bilinearity of $a_{\text{CG}}(\cdot, \cdot)$ finally leads to the linear system

$$\mathbf{KU} = \mathbf{F}, \tag{5}$$

where $\mathbf{K}_{ij} = a_{CG}(N_i, N_j) \cdot \mathbf{I}_3 \in \mathbb{R}^{3 \times 3}$, $\mathbf{U}_i = \mathbf{u}_i \in \mathbb{R}^3$, $\mathbf{F}_i = \int_{\Omega} \mathbf{f} N_i \in \mathbb{R}^3$ and \mathbf{I}_3 denotes the (3×3) identity matrix.

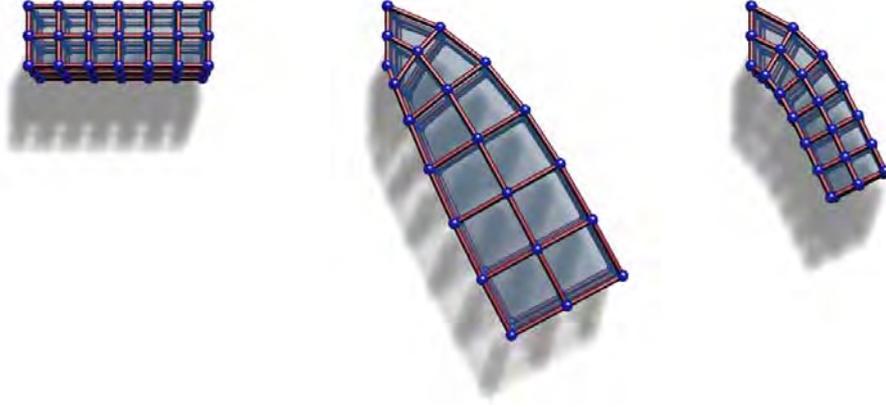


Figure 1: Exposing a clamped bar (left) to gravity, the resulting rotational deformations lead to artifacts in the linear model (middle). The co-rotational approach compensates for rotations and produces the expected result (right).

Co-Rotational Formulation. Under large rotational deformations, linear FEM shows artifacts such as an unrealistic increase in volume as depicted in Fig. 1. To avoid the cost of a full nonlinear simulation but still get physically plausible deformations in these cases, a corotated formulation can be employed, which computes elastic forces in a rotated coordinate frame defined for each element [MG04, HS04].

In linear CG FEM, the forces acting on the nodes of an element K are computed from nodal displacements \mathbf{U} and the element stiffness matrix \mathbf{K}_K as follows:

$$\mathbf{F}_K = \mathbf{K}_K \mathbf{U} = \mathbf{K}_K (\mathbf{X} - \mathbf{X}^0), \quad (6)$$

with \mathbf{X} and \mathbf{X}^0 denoting the deformed and undeformed nodal positions, respectively. In order to avoid the aforementioned rotational artifacts, the *corotational*, or *warped stiffness* approach [MG04, HS04] first reverts the element's rotation, computes displacements and forces in the un-rotated state, and re-rotates the resulting forces:

$$\mathbf{F}_K = \mathbf{R}_K \mathbf{K}_K (\mathbf{R}_K^T \mathbf{X} - \mathbf{X}^0), \quad (7)$$

where \mathbf{R}_K is a block-diagonal matrix containing the 3×3 rotation matrix of element K on its diagonal.

Applications. The method described above can be directly applied to the implementation of geometric modeling tools. A simple way to realize such a modeling framework is by considering the static elasticity equation (5). The user then first defines a set of handles at which the deformation of the object is fixed to a user-defined value. Interpreting those handles as Dirichlet boundary conditions of the elasticity equation, an artist can manipulate the handles in order to model the geometry at his gusto.

The derivation shown above can also be used to realistically animate elastic objects over time. To this end, the discrete equations of motion can be formulated as

$$\mathbf{M} \ddot{\mathbf{U}} + \mathbf{C} \dot{\mathbf{U}} + \mathbf{K} \mathbf{U} = \mathbf{F}, \quad (8)$$

where \mathbf{M} is the mass matrix computed as $\mathbf{M}_{ij} = \int_V \rho N_i N_j dx$ and \mathbf{C} is a diagonal damping matrix. Note that in this case \mathbf{U} is a function of time and applying a suitable time integration scheme to Eq. (8) leads to the dynamic simulation of the object.

3 MLS-Based Surface Embedding

When it comes to the simulation of complex models, a common approach for keeping computation costs low is to embed a high resolution surface mesh into a lower resolution simulation mesh. The latter can be simulated efficiently, and its displacement field $\mathbf{u}(\mathbf{x})$ is used to deform the surface mesh (see, e.g., [FvdPT97]).

The nodal displacements have to be interpolated within elements in order to deform the embedded mesh. For tetrahedral or hexahedral elements this amounts to simple linear or trilinear interpolation, respectively. For more general convex or non-convex polyhedra, mean value coordinates [FKR05] or harmonic coordinates [JMD⁺07] can be employed. All these methods, however, correspond to a non-smooth, generalized barycentric C^0 interpolation.

[BPWG07] employ globally supported radial basis functions for high quality interpolation, but the involved dense linear systems are prohibitive for complex simulation meshes. To overcome these limitations, and inspired by meshless methods [MKN⁺04], we propose a smooth embedding based on moving-least-squares (MLS) interpolation.

If we denote by \mathbf{x}_i the nodes of the undeformed simulation mesh and by $\tilde{\mathbf{u}}_i$ their displacements, then the displacement at a material point \mathbf{x} is computed by fitting an affine transformation, which amounts to minimizing the weighted least square error

$$\sum_i \theta(\|\mathbf{x} - \mathbf{x}_i\|) \left\| \mathbf{a}(\mathbf{x})^T \mathbf{p}(\mathbf{x}_i) - \tilde{\mathbf{u}}_i \right\|^2, \quad (9)$$

with $\mathbf{p}(x, y, z) = (1, x, y, z)^T$ and $\theta(x)$ a (truncated) Gaussian weight function. Solving a 4×4 linear system $\mathbf{A}(\mathbf{x}) \mathbf{a}(\mathbf{x}) = \mathbf{b}(\mathbf{x})$ yields the coefficients $\mathbf{a}(\mathbf{x})$ for the interpolated displacement $\tilde{\mathbf{u}}(\mathbf{x}) = \mathbf{a}(\mathbf{x})^T \mathbf{p}(\mathbf{x})$ at the position \mathbf{x} . This MLS-based embedding has several interesting properties, such as the exact reproduction of linear displacements \mathbf{u} , i.e., in particular of rigid motions. We note that an accurate approximation of higher order polynomial displacements \mathbf{u} only requires to add more samples ($\mathbf{x}_i^0, \tilde{\mathbf{u}}_i$) to (9), such as edge, face, or element midpoints. Fig. 2 shows an example of a triangle mesh embedded in a coarse hexahedral mesh using the interpolation described above.

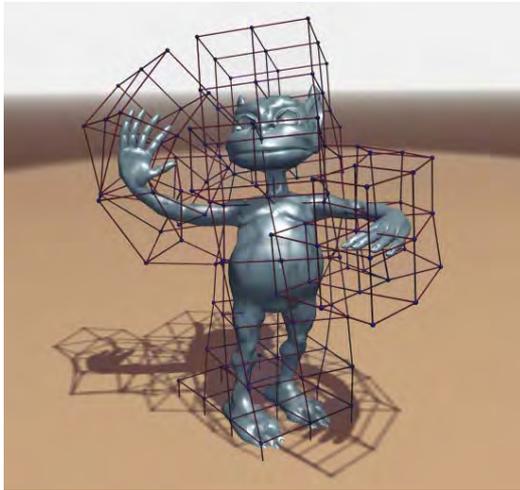


Figure 2: A Goblin triangle model (5411 triangles) embedded in a coarse simulation mesh consisting of only 58 elements. The MLS interpolation deforms the embedded mesh in a smooth way, despite the FEM basis function being only C^0 continuous.

4 Cutting and Fracturing

To realistically model the behavior of real-world objects, it is important to also capture the failure of material under high stresses (fracturing) or due to external manipulations such as cutting. In order to simulate the effects of the induced material discontinuities, the underlying simulation mesh needs to be updated accordingly. Usually, this comes with a change of the mesh topology and requires a cumbersome remeshing step which generally produces ill-shaped elements, leading to numerical problems when solving the resulting linear system. The remeshing requirement, however, stems from the simple element types used in these simulations and could be omitted if more general element types could be employed instead. In the following, we present two different approaches for how the classic FEM can be extended to arbitrary convex and non-convex polyhedral elements.

In the first approach, we propose the use of harmonic coordinates for the interpolation inside polyhedral elements. We show that these coordinates generalize classic linear basis functions and we present an efficient numerical scheme for their computation. The second approach employs a modified weak form of the problem, known as the discontinuous Galerkin method, which allows the use of non-conforming elements. Both of these approaches can handle arbitrarily shaped elements and lead to significant advantages when it comes to cutting, fracturing and adaptive simulations.

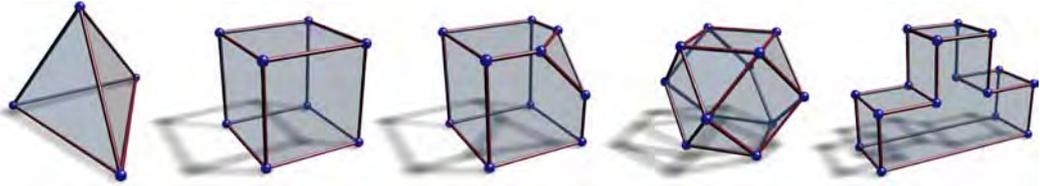


Figure 3: The methods presented here are able to simulate arbitrary polyhedral elements, from simple tetrahedra to non-convex polyhedra.

4.1 Harmonic FEM

Harmonic Basis Functions. We propose to use harmonic basis functions as a generalization of linear barycentric basis functions to general polyhedral elements. A shape function $N_i^e : e \rightarrow \mathbb{R}$ is *harmonic* if its Laplacian vanishes in element e , in which case it is uniquely determined by Dirichlet boundary constraints $b(\mathbf{x})$ on ∂e :

$$\Delta N_i^e(\mathbf{x}) = 0, \quad \text{for } \mathbf{x} \in e, \quad (10)$$

$$N_i^e(\mathbf{x}) = b_i(\mathbf{x}), \quad \text{for } \mathbf{x} \in \partial e. \quad (11)$$

For a finite element simulation we need nodal basis functions N_i^e for interpolating quantities within each element e . If these functions are chosen to be harmonic, they are fully determined by the values $b_i(\mathbf{x})$ on the element boundary ∂e , which we set up following [JMD⁺07]: First, in order to interpolate nodal quantities, the basis function N_i^e of node i has to equal 1 at the node \mathbf{x}_i and 0 at all others, i.e.,

$$N_i^e(\mathbf{x}_j) = \delta_{ij} \quad \forall i, j = 1, \dots, k. \quad (12)$$

Additionally, in order to ensure continuity across element boundaries, the values of the basis function for node i defined in neighboring elements e_1 and e_2 should coincide on the face or edge shared by the two elements:

$$N_i^{e_1}(\mathbf{x}) = N_i^{e_2}(\mathbf{x}) \quad \text{for } \mathbf{x} \in e_1 \cap e_2. \quad (13)$$

This can be guaranteed by choosing the values on the faces of a d -dimensional element to be $(d - 1)$ -dimensional harmonic coordinates. For a trivariate harmonic basis function N_i^e on a 3D element e the boundary conditions are bivariate harmonic coordinates on its faces, which themselves

are determined by univariate harmonic (i.e., linear) interpolation of the nodal values $N_i^e(\mathbf{x}_j) = \delta_{ij}$ along the edges.

It follows from these recursively defined boundary constraints and the uniqueness of harmonic functions for fixed Dirichlet constraints, that harmonic shape functions reproduce linear triangles and bilinear quads in 2D, as well as linear tetrahedra and trilinear hexahedra in 3D. Harmonic basis functions satisfy all requirements for admissible FEM basis functions [MKB⁺08]. The harmonic basis for a more complex 2D element along with the numerical computation primitives next are shown in Fig. 4.

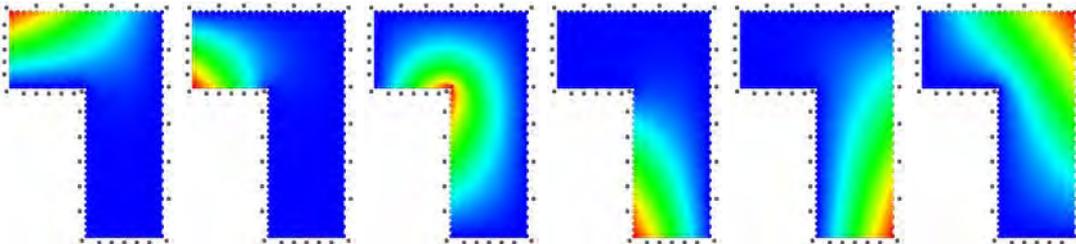


Figure 4: Harmonic basis functions for the six nodes of a non-convex 2D element. The constraint collocation points \mathbf{c}_i are visualized as small spheres along the element boundary, the kernel centers \mathbf{k}_i are shifted slightly outside and are shown in gray.

Numerical Approximation. Closed form expressions for harmonic basis functions exist for simple element shapes only, such as tetrahedra or hexahedra. For more general elements, harmonic basis functions N_i^e have to be computed numerically as the solution of (10), (11). While there exist numerous possibilities how to solve such PDEs numerically we found the method of fundamental solutions (MFS) [FK98] to be a flexible, easy-to-implement and sufficiently accurate choice.

A shape function $N_i^e(\mathbf{x})$, simply denoted by $N(\mathbf{x})$ in the following, is represented in the following form:

$$N(\mathbf{x}) = \sum_{j=1}^n w_j \cdot \psi(\|\mathbf{x} - \mathbf{k}_j\|) + \mathbf{a}_1^T \mathbf{x} + a_0, \quad (14)$$

where the first part is a superposition of n weighted radial basis functions ψ (RBFs), centered at \mathbf{k}_j , and the second part is a linear polynomial in \mathbf{x} . The kernel function ψ is chosen as fundamental solution of the Laplace PDE, which is $\psi(r) = \log r$ in 2D and $\psi(r) = 1/r$ in 3D. As a consequence, the function (14) is harmonic by construction [Duc77], in the whole domain except at the kernels' singularities \mathbf{k}_j .

Hence, the kernel \mathbf{k}_j have to be placed outside the element. A standard method is to first sample the boundary and to move the kernels outward in (interpolated) normal direction. For non-convex elements one additionally has to take care that this simple offsetting does not generate centers in the element's interior.

The function (14) satisfies (10) by construction, thus we solve for the best approximation of the Dirichlet constraints (11). To this end, we approximate the L^2 error on the boundary by a sum of m collocation points \mathbf{c}_i :

$$\int_{\partial e} |N(\mathbf{x}) - b(\mathbf{x})|^2 \approx \frac{1}{m} \sum_{i=1}^m |N(\mathbf{c}_i) - b(\mathbf{c}_i)|^2 \rightarrow \min. \quad (15)$$

These collocation points $\mathbf{c}_i \in \partial e$ are generated equivalently to the samples \mathbf{k}_j , but at a higher resolution and without any offset from the element boundary. Given the kernel centers \mathbf{k}_i , the minimization of the L^2 error (15) amounts to solving an overdetermined linear least squares system for the coefficients of (14).

Results. Supporting general polyhedra in FEM simulations effectively avoids the need for complex remeshing during cutting and thus considerably simplifies the implementation. The harmonic basis functions seamlessly integrate into both tetrahedral and hexahedral simulations, which has the big advantage that only the cut elements have to be computed as harmonic polyhedral elements (see Fig. 5).

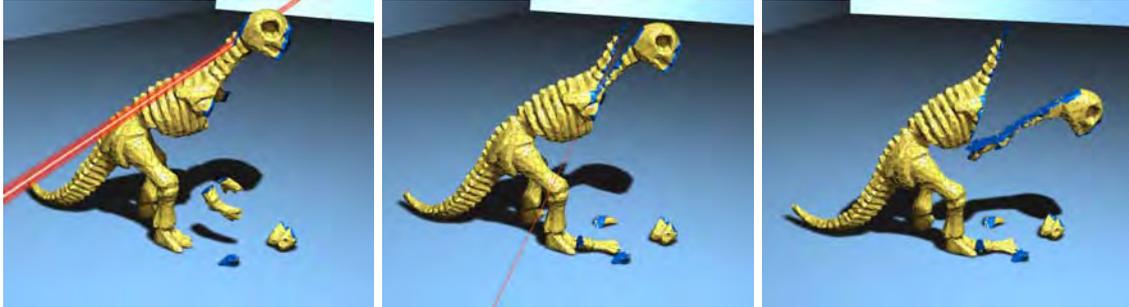


Figure 5: The dinosaur model is cut with a laser beam. Simple tetrahedral elements are colored in yellow, more complex elements occurring at the interface during cutting are colored in blue.

4.2 DG FEM

The Discontinuous Galerkin Finite Element Method (DG FEM) differs from standard FEM in that basis functions are no longer required to be continuous across element boundaries, leading to discontinuous approximations of \mathbf{u} . Each element is represented by its own set of basis functions, and continuity between elements (i.e. preventing the mesh from falling apart) is achieved by introducing additional terms into the weak form that “glue” the elements together. In other words, continuity across elements is only enforced in a weak sense. Using per-element basis functions gives us two very desirable properties: First, the basis functions no longer have to be nodal, and we can choose simple basis functions such as polynomials up to third order, which can be integrated very efficiently over the element. Second, we are not limited to simple tetrahedral or hexahedral elements but we can use arbitrary polyhedral elements instead. The basic idea of DG FEM, i.e., employing discontinuous shape functions and weakly enforcing boundary constraints and inter-element continuity through penalty forces, is rather old (see, e.g., [BZ73, DD76]). In the last decade, however, DG FEM regained increasing attention in applied mathematics [ABCM01, Coc03].

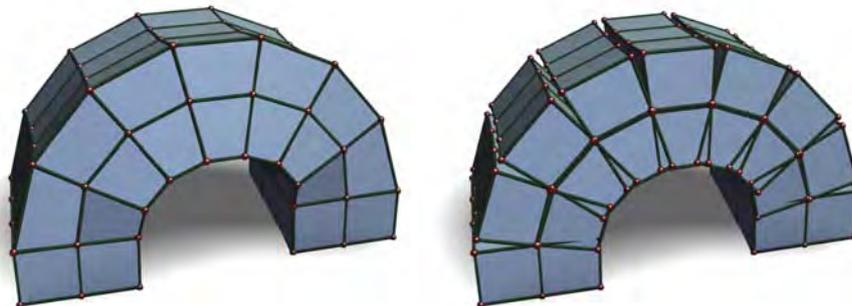


Figure 6: While continuous FEM (left) only allows for the elements to deform, DG FEM (right) additionally allows the elements to separate and the C^0 continuity of the deformation field is only enforced in a weak sense.

DG Weak Form. Analogous to CG FEM, equations (1) and (2) are multiplied by test functions and integrated over the domain $\Omega = \cup_{K \in \mathcal{T}} K$, formulated as a sum of integrals over elements $K \in \mathcal{T}$. Integration by parts over these K leads to additional integrals over all element boundaries $\Gamma = \cup_K \partial K$, which due to the discontinuities of \mathbf{u} and $\boldsymbol{\sigma}$ do *not* cancel out as in CG FEM. In order to “glue” the discontinuities, the functions \mathbf{u} and $\boldsymbol{\sigma}$ are replaced by their so-called *numerical fluxes* on the element boundaries Γ . The various DG methods differ in exactly these fluxes, a detailed overview and classification of which can be found in [ABCM01]. In the resulting DG weak form they show up as penalty terms punishing discontinuities, thereby weakly enforcing continuity.

To formalize this we introduce the *jump* operator $[[\cdot]]$ for the vector-valued functions \mathbf{u} on an element boundary. If we denote by \mathbf{u}^\pm functions evaluated on either side of the element boundary and by $\mathbf{u} \otimes \mathbf{n} = \mathbf{u} \mathbf{n}^T$ the outer product, then this operator is defined as

$$[[\mathbf{u}]] := \mathbf{u}^- \otimes \mathbf{n}^- + \mathbf{u}^+ \otimes \mathbf{n}^+.$$

A straightforward approach is to minimize the squared jump $[[\mathbf{u}]] : [[\mathbf{u}]] = \|\mathbf{u}^- - \mathbf{u}^+\|^2$. This corresponds to the method of Babuška and Zlámal [BZ73], denoted by BZ, whose weak form uses a_{BZ} instead of a_{CG} in (3):

$$a_{\text{BZ}}(\mathbf{u}, \mathbf{v}) := \int_{\Omega} \boldsymbol{\epsilon}(\mathbf{v}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{u}) + \int_{\Gamma} \eta_f [[\mathbf{u}]] : [[\mathbf{v}]] . \quad (16)$$

Note that the BZ weak form (16) differs from the CG weak form (3) in the Γ -integral only, which punishes the jump $[[\mathbf{u}]]$ weighted by a penalty parameter per face f [HL02]

$$\eta_f = \eta \cdot \text{area}(f) \cdot \left(\frac{1}{\text{vol}(K^-)} + \frac{1}{\text{vol}(K^+)} \right) , \quad (17)$$

using a global penalty parameter $\eta > 0$ typically being in the order of 10^1 – 10^2 in all our experiments. The internal elastic energy of the deformed object can then be written as

$$a_{\text{BZ}}(\mathbf{u}, \mathbf{u}) = \int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\epsilon}(\mathbf{u}) + \int_{\Gamma} \eta_f \|\mathbf{u}^- - \mathbf{u}^+\|^2 .$$

The BZ method is geometrically intuitive and easy to implement. It is *stable* in the sense that the stiffness matrix \mathbf{K} is positive definite for any $\eta > 0$. However, as detailed in [ABCM01], the method is *not consistent*: A continuous solution \mathbf{u} of the problem might not satisfy the BZ weak form (16). Consequently, the approximate solution \mathbf{u} does in general not converge toward the exact solution under element refinement. Our experiments have shown that the BZ method is very well suited for applications aiming at *physically plausible* deformations only. However, if physical accuracy is important, other DG methods should be chosen such as the interior penalty (IP) method further described in [KMBG08].

Results. Similar to the harmonic basis function approach, the DG method allows for the simple handling of arbitrarily shaped elements. In contrast to the harmonic approach, there is no need to compute element-specific basis functions and low order polynomials can be used instead. Fig. 7 shows two examples where an elastic material is cut into pieces. Each of these pieces, independently of its geometric complexity, can easily be handled at more or less constant cost.

For such complex examples, the DG approach outperforms the harmonic basis function approach in terms of speed and stability. On the other hand, the discontinuity of the solution makes it not straightforwardly applicable to the representation of embedded visualization geometry. Therefore an additional interpolation step using MLS (Section 3) needs to be performed.

5 Conclusion

We have presented an interpolation approach based on moving-least-squares that allows for the embedding of detailed geometry in very coarse simulation meshes. While a naïve embedding using

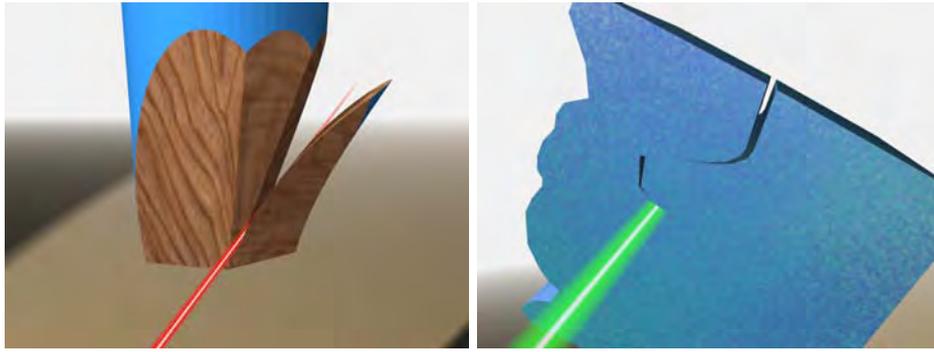


Figure 7: Sharpening a pencil consisting of a single convex element (left). Cutting a bunny out of a cube (right).

the FEM basis functions would lead to visible artifacts at the element boundaries, our MLS-based approach produces a smooth interpolation field suitable for arbitrary embedding.

Furthermore, we have introduced two FEM frameworks for the simulation of arbitrary polyhedral elements. Being able to use polyhedral elements in FEM simulations considerably simplifies topological changes of the simulation domain during the simulation of adaptive refinement, fracturing and progressive cutting. While conventional methods based on tetrahedral or hexahedral elements require a cumbersome remeshing step that can lead to numerical problems, our approaches avoid remeshing during cutting by simulating the resulting polyhedral elements directly. Of the two methods we presented, the approach based on harmonic basis functions generalizes the shape functions of tetrahedral and hexahedral elements and can thus be easily integrated into an existing FEM framework. Only the elements directly affected by the cut need to be simulated using harmonic basis functions, while all other elements can still be simulated as tetrahedral or hexahedral elements respectively. While the second method based on discontinuous Galerkin FEM cannot as easily be integrated into an existing FEM framework, it excels in the case of highly complex elements, because its basis functions are not required to be nodal. We note that although the two approaches were demonstrated in the context of corotated linear elasticity, they can as well be used with nonlinear strain measures and nonlinear material behavior, which constitutes an interesting direction for future work.

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5

CSE Research Projects

Title: Multi-level μ -Finite Element Analysis for Human Bone Structures

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

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

Description:

The recent advances in microarchitectural bone imaging are disclosing the possibility to assess both the apparent density and the trabecular microstructure of intact bones in a single measurement. Coupling this with microstructural finite element (μ FE) offers a powerful tool to improve strength assessment and individual fracture risk prediction.

In order to be effectively solved quickly and reliably on state-of-the-art parallel computers, the resulting μ FE models require advanced solution techniques. We investigate the solution of the resulting systems of linear equations by the conjugate gradient algorithm, preconditioned using aggregation-based multigrid methods. We introduce a variant of aggregation preconditioner that can be used with the matrix-free solvers that commonly arise in the solution of bone structures when linear elasticity models are adopted. The preconditioner works directly on the contributions from individual elements, and it has modest memory requirements, while being at the same time robust and scalable.

Using the proposed methods, we have solved a model of trabecular bone composed by 247'734'272 elements, leading to a matrix with 1'178'736'360 rows, in less than 10 minutes using 1024 CRAY XT3 processors. We expect our μ FE solver to help us improve our understanding of the influence of densitometric, morphological and loading factors in the etiology of spontaneous fractures of the hip and the spine.

Web sites:

Project homepage: <http://people.inf.ethz.ch/arbenz/projects/bone.html>
Software: <http://parfe.sourceforge.net/>

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Title: **Resonant Lossy Electromagnetic Structures**

Researchers: Peter Arbenz*
 Hua Guo*
 Benedikt Oswald†

Institute/ *Chair of Computational Science, ETH Zürich
Group: †Paul Scherrer Institut, Villigen

Description:

Resonant electromagnetic cavity structures are used in virtually all types of particle accelerators. The X-ray free electron laser currently under study at the Paul Scherrer Institut, is no exception and will consist of a large variety of radio frequency (RF) structures for guiding and accelerating electrons from the photo-cathode through the linear accelerator section, see LEG-Web-Site.

The numerical computation of eigenfrequencies and corresponding eigenmodal fields of large accelerator cavities, based on full-wave, three-dimensional models, has attracted considerable interest in the recent past.

Much work has been invested to compute electromagnetic eigenmodes. In many cases the eigenproblem has been modeled without electromagnetic loss mechanisms. This is a justifiable approximation, especially when saving computational expense is an issue or when the cavity becomes large in terms of the dominant wavelength.

However, the eigenmodal solution is affected considerably by loss. Traditionally, loss has been integrated into the model by computing the quality factor Q . The electromagnetic power dissipated in the cavity boundary is calculated with a perturbation approach using the magnetic field B after the eigenmodes have been computed. While this allows for estimating that important cavity parameter it does not model the effect of loss onto the resonance frequency which is one of the most important cavity parameters. Only if losses are integrated into the eigenvalue problem a priori can we extract thereby affected resonance frequencies from the eigensolution.

We intend to model different loss mechanisms:

1. Lossy dielectric and/or magnetic materials;
2. Larger or smaller apertures in the boundary of the resonating structure. These significantly change the character of the eigenvalue problem by introducing loss caused by electromagnetic fields radiating away part of the energy stored in the field;
3. Finite conductivity cavity wall by the inclusion of a surface impedance boundary condition.

We intend to use the finite element (FE) method because modern cavity designs typically exhibit delicate and detailed geometrical features that must be considered for obtaining accurate results.

There is some work into this direction. We note that often the approaches are relatively small with only a few thousand unknowns, or, losses, introduced either by holes in the aperture or cavity walls with a finite conductivity, are not addressed. Today's accelerator cavities require a computational mesh with tens of millions of unknowns and, ultimately, in the region of 108 unknowns.

We plan to extend an available parallel Jacobi-Davidson-type solver for large-scale real symmetric eigenvalue problems, see Ref [1] into a solver of complex symmetric eigenvalue problems.

Web site:

Project homepage: <http://people.inf.ethz.ch/arbenz/projects/lossy.html>

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Title: Dynamics of premixed flames in inert and catalytic channels and ducts

Researchers: G. Pizza^{1,2}, C.E. Frouzakis¹, J. Mantzaras², A. Tomboulides³, V.N. Kurdyumov³, K. Boulouchos¹

Institute/ ¹Aerothermochemistry and Combustion Systems Laboratory

Group: ²Paul Scherrer Institute, Villigen PSI

³University of Western Macedonia, Kozani, Greece

⁴CIEMAT, Department of Energy, Madrid, Spain

Combustion at the micro- (sub-millimeter range) and meso-scale (millimeter range) has attracted increased interest during the last few years in attempts to harness the high specific energy of fuels in miniaturized devices for portable power generation. Progress in the fundamental knowledge of combustion at these scales and in the understanding of reactor thermal management is essential for the further development of such systems.

Dynamics of lean premixed hydrogen flames was studied using the full system of conservation equations for reactive flows with detailed kinetics and transport as well as a simplified model within the realm of the thermo-diffusive approximation in two- and three-dimensional geometries. The possibility to suppress the instabilities by covering the walls with a predetermined catalyst load was also addressed.

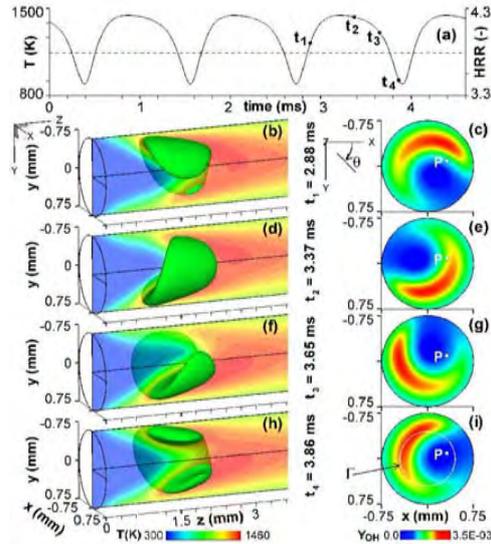


Figure 1: Clockwise spinning flame at $U_{IN} = 150$ cm/s in a $d = 1.5$ mm tube: (a) time history of temperature (solid line) at the reference point $P = (0.3, 0.1, 2.06)$ mm, and integral heat release rate HRR (dashed line); (b, d, f, h) iso-surfaces of OH mass fraction $Y_{OH} = 1.7 \cdot 10^{-3}$, and temperature iso-contours on the $y - z$ plane at the four times t_1 to t_4 ; (c, e, g, i) iso-contours of Y_{OH} on the $x - y$ plane at $z = 1.5$ mm at t_1 to t_4 .

In 3-D tubes, and depending of the tube diameter, axisymmetric and non-axisymmetric,

steady and unsteady combustion modes are observed in the narrow tube. As the inflow velocity of the incoming mixture is increased, these modes include steady mild combustion, oscillatory ignition/extinction, steady closed and open axisymmetric flames, steady non-axisymmetric flames, and azimuthally spinning flames. Some of the modes are found to co-exist of extended ranges of inflow velocities.

The effect of channel height, inflow velocity and wall temperature on the dynamics and stability of unity Lewis number premixed flames in channels with specified wall temperature was investigated with steady and transient numerical simulations using a two-dimensional thermo-diffusive model. The simplified model was capable of capturing many of the transitions and the combustion modes observed experimentally and in direct numerical simulations in micro- and meso-scale channels, indicating that the thermal flame/wall interaction was the mechanism leading to the observed flame instabilities.

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Title: Three-dimensional simulations of cellular non-premixed jet flames

Researchers: A.L. Valär¹, C.E. Frouzakis¹, P. Papas², A.G. Tomboulides³, K. Boulouchos¹

Institute/Group: ¹Aerothermochemistry and Combustion Systems Laboratory
²Division of Engineering, Colorado School of Mines, Golden, U.S.A.
³University of Western Macedonia, Kozani, Greece

The formation, dynamics and structure of cellular flames in circular non-premixed jets are examined with three-dimensional numerical simulations incorporating detailed descriptions of chemistry and transport. Similar to past experiments reported in the literature, CO₂-diluted hydrogen in diluted or pure oxygen co-flowing streams in the proximity of the extinction limit are considered. As in the experiments, several preferred cellular states are found to co-exist with the particular state realized depending on initial conditions as well as on the jet characteristics. The simulations provide additionally the temporal transitions to different stationary or rotating cellular flames, their detailed structure, and the dependence of the scaling of the realized number of cells with the vorticity thickness.

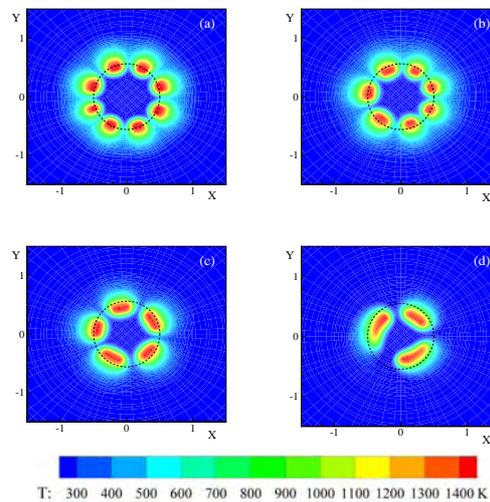


Figure 2: (a) to (d): Temperature iso-contours on the plane $0.5d_j$ above the nozzle for the inlet velocity profiles P_1 to P_4 , respectively. (Jet: $u_j = 37.7$ cm/s, $X_{H_2} = 0.19$; co-flow: $u_c = 4.66$ cm/s, $X_{O_2} = 1.0$). Nozzle location marked by the dashed circle.

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A.L. Valär, C.E. Frouzakis, P. Papas, A.G. Tomboulides, K. Boulouchos, Three-dimensional simulations of cellular non-premixed jet flames, *Combust. Flame*, (accepted)

Title: An experimental and numerical study of the structure and stability of laminar opposed-jet flows

Researchers: A. Ciani¹, W. Kreutner^{1,2}, C.E. Frouzakis², K. Lust³, G. Koppola⁴, K. Boulouchos²

**Institute/
Group:** ¹Paul Scherrer Institute, Villigen PSI
²Aerothermochemistry and Combustion Systems Laboratory
³Mathematics Dept., K.U.Leuven, Celestijnenlaan 200B, 3001 Heverlee, Belgium
⁴Yale Center for Combustion Studies, Department of Mechanical Engineering, Yale University, New Haven, CT 06511, USA

Experiments, simulations, and numerical bifurcation analysis are used to study the incompressible flow between two opposed tubes with disks mounted at their exits. The experiments in this axisymmetric geometry show that for low and equal Reynolds numbers, Re , at both nozzles, the flow remains symmetric about the plane halfway through the nozzle exits and the stagnation plane is located halfway between the two jets. When Re is increased past a critical value, asymmetric flow fields are obtained even when the momentum fluxes of the two opposed streams are equal. For unequal Re at the jet exits, when the fixed velocity (and the corresponding Reynolds number, Re_1) of one stream is low, the stagnation plane location, SPL, changes smoothly with the Re_2 . For high enough Re_1 , a hysteretic jump of SPL is observed. Particle Image Velocimetry and flow visualization demonstrate that within the hysteretic range, the two stable flow fields are anti-symmetric. The experimental setup is also studied with transient incompressible flow simulations using a spectral element solver. It is found that to accurately model the flow, we either need to extend the domain into the nozzles, or impose experimental velocity profiles at the nozzle exits. As in the experiments asymmetric flows are obtained past a critical Re . Finally, bifurcation analysis using a NewtonPicard method shows that the transition from symmetric to asymmetric flows results from the loss of stability of the symmetric flows at a pitchfork bifurcation.

References:

- A. Ciani, W. Kreutner, C.E. Frouzakis, K. Lust, G. Coppola and K. Boulouchos, An experimental and numerical study of the structure and stability of laminar opposed-jet flows, *Comp. Fluids*, (in press)

Title: Lattices for the lattice Boltzmann method

Researchers: Shyam S. Chikatamarla, Ilya V. Karlin

**Institute/
Group:** Aerothermochemistry and Combustion Systems Laboratory, IET, D-
MAVT, ETH Zurich

A recently introduced theory of higher-order lattice Boltzmann models [Chikatamarla and Karlin, *Phys. Rev. Lett.* 97, 190601 (2006)] is elaborated in detail. A general theory of the construction of lattice Boltzmann models as an approximation to the Boltzmann equation is presented. New lattices are found in all three dimensions and are classified according to their accuracy degree of approximation of the Boltzmann equation. The numerical stability of these lattices is argued based on the entropy principle. The efficiency and accuracy of many new lattices are demonstrated via simulations in all three dimensions.

References:

S.S. Chikatamarla and I.V. Karlin, *Phys. Rev. E* 79, 046701 (2009).

Title: Generalized Maxwell state and H theorem for computing fluid flows using the lattice Boltzmann method

Researchers: I.V. Karlin and P. Asinari

**Institute/
Group:** Aerothermochemistry and Combustion Systems Laboratory, IET,
D-MAVT, ETH Zurich

Generalized Maxwell distribution function is derived analytically for the lattice Boltzmann (LB) method. All the previously introduced equilibria for LB are found as special cases of the generalized Maxwellian. The generalized Maxwellian is used to derive a different class of multiple relaxation-time LB models and prove the H theorem for them.

References:

P. Asinari and I.V. Karlin, *Phys. Rev. E* 79, 036703 (2009).

Title: Combustion simulation via lattice Boltzmann and reduced chemical kinetics

Researchers: E. Chiavazzo, I.V. Karlin, A.N. Gorban and K. Boulouchos

**Institute/
Group:** Aerothermochemistry and Combustion Systems Laboratory, IET, D-MAVT, ETH Zurich

In this work, we present and validate a methodology for coupling reduced models of detailed combustion mechanisms within the lattice Boltzmann framework. A detailed mechanism (9 species, 21 elementary reactions) for modeling reacting mixtures of air and hydrogen is considered and reduced using the method of invariant grids (MIG). In particular, a 2D quasi-equilibrium grid is constructed, further refined via the MIG method, stored in the form of tables and used to simulate a 1D flame propagating freely through a homogeneous premixed mixture. Comparisons between the detailed and reduced models show that the technique presented enables one to achieve a remarkable speedup in the computations with excellent accuracy.

References:

E. Chiavazzo, I.V. Karlin, A.N. Gorban and K. Boulouchos *J. Stat. Mech.*, P06013 (2009).

Title: Method of invariant grid for model reduction of hydrogen combustion

Researchers: E. Chiavazzo, I.V. Karlin, Ch.E. Frouzakis and K. Boulouchos

**Institute/
Groups:** Aerothermochemistry and Combustion Systems Laboratory, IET, D-MAVT, ETH Zurich

The Method of Invariant Grid (MIG) is a model reduction technique based on the concept of slow invariant manifold (SIM). The MIG approximates the SIM by a set of nodes in the concentration space (invariant grid). In the present work., the MIG is applied to a realistic combustion system: an adiabatic constant volume reactor with H₂-air at stoichiometric proportions. By considering the thermodynamic Lyapunov function of the detailed kinetic system, the notion of the quasi-equilibrium manifold (QEM) is adopted as an initial approximation to the SIM. One- and two-dimensional discrete approximations of the QEM (quasi-equilibrium grids) are constructed and refined via MIG to obtain the corresponding invariant grids. The invariant grids are tabulated and used to integrate the reduced system. Excellent agreement between the reduced and detailed kinetics is demonstrated.

References:

E. Chiavazzo, I.V. Karlin, C.E. Frouzakis and K. Boulouchos *Proc. Combustion Inst.* 32, 519-526 (2009).

Title: Lattice Boltzmann method with restored Galilean invariance

Researchers: N.I. Prasianakis and I.V. Karlin, J. Mantzaras and K. Boulouchos

**Institute/
Groups:** Aerothermochemistry and Combustion Systems Laboratory, IET, D-MAVT, ETH Zurich

An isothermal model on the standard two-dimension nine-velocity lattice (D2Q9) is proposed and analyzed. It originates from the thermal model with energy conservation introduced by N. I. Prasianakis and I. V. Karlin [Phys. Rev. E 76, 016702 (2007)]. The isothermal and the thermal equivalent models are tested through the simulation of the decay of a shear wave and of a temperature wave. Both are shown to be Galilean invariant, reference temperature independent, and rotational isotropic through the measurement of the transport coefficients on a rotated moving frame of reference.

References:

N.I. Prasianakis, I.V. Karlin, J. Mantzaras and K. Boulouchos, *Phys. Rev. E* 79, 066702 (2009).

Title: Computational Solid State Electronics

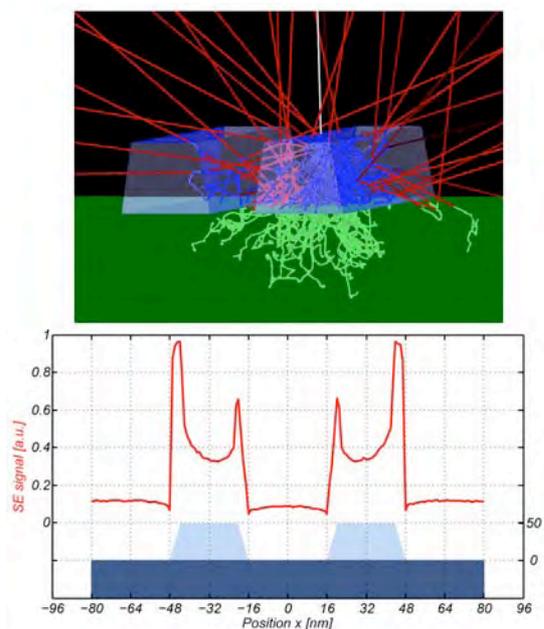
Researchers: Wolfgang Fichtner
Andreas Schenk
Alex Koschik
Martin Frey
Kilian Vollenweider
Dölf Aemmer

Institute/ Integrated Systems Laboratory/
Group: Technology Computer Aided Design (TCAD) Group

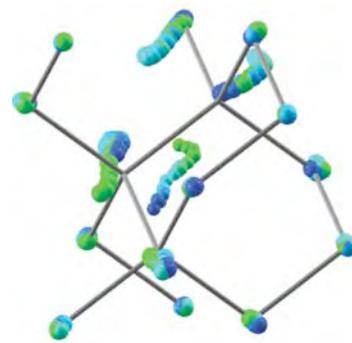
Description:

For the development of novel nano-electronic processes and devices, the use of advanced numerical simulation tools has become indispensable. With the continuing advances in semiconductor technology, and the trend to further scaling of the active device dimensions, computational solid state electronics has reached an extremely high level of physical and numerical sophistication. For nanoscale dimensions (devices in the range of 15 nm with structures down to 1 nm) effects at the atomistic or quantum-mechanical level are becoming dominant.

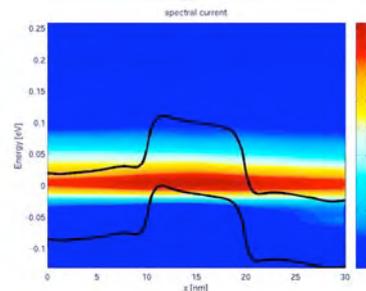
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulation tools for molecular dynamics studies in material diffusion, electron beams for metrology and lithography, novel devices such as nanowire transistors, and quantum devices. For all of our projects, the main emphasis lies in the exploration how accurate physical models can be combined with advanced numerical algorithms including massive parallelization. These simulations were carried out on high-end compute-servers of our laboratory and on the Cray XT5 at CSCS Manno in a *Large User Project*. The following pictures illustrate some of our activities:



Reconstruction of Scanning Electron Microscopy SEM Images by Monte Carlo Simulation.
Top: MC simulation of electron trajectories in SiO₂ lines on Si substrate.
Bottom: Corresponding simulated SE signal.



Molecular Dynamics Simulations of Diffusion of Fluorine in Silicon. The diffusion mechanism of FI: The different steps of the event are chronologically colored from green to blue.



Simulation of Phonon Scattering in Silicon Nanowires. The spectral current of a triple gate silicon nanowire FET: channel length = 30 nm, gate length = 10 nm.

Title: High-performance computing in global seismology: the Earth's power-spectrum determined from a stochastic analysis of global seismic delay-time data

Researchers: PhD candidate S. Della Mora (ETHZ)
Dr. L. Boschi (ETHZ)
Prof. T. W. Becker (University of Southern California)
Prof. D. Giardini (ETHZ)

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

Description:

The wavelength of mantle heterogeneity reflects the nature of the planet's dynamics, and constraining it on the basis of seismic data helps us to evaluate the likelihood of different proposed models of mantle convection. We neglect the geographic distribution of mantle heterogeneity, inverting global delay-time data to determine directly the heterogeneity spectrum of the Earth. Inverting for the spectrum is in principle (fewer unknowns) much cheaper and robust than inverting for the three-dimensional (3D) structure of a planet: as a result, this approach should ultimately help us to constrain the properties of planetary structure at wavelengths shorter than those of current 3D models. It is also going to allow us to conduct a fully nonlinear search of the solution space, with no ray-theory-type approximations: such a procedure is extremely expensive but feasible for the problem in consideration, while it is still way too expensive for classical 3-D tomography. At this point we are exploring a simplified version of the problem, employing a linearized algorithm based on the work of Gudmundsson and co-workers in the early 1990s: seismic rays starting at close sources and arriving at close receivers are collected, and the variance of the associated delay times is calculated; this exercise is repeated for a range of values of maximum distance between close sources and between close receivers. The dependence of calculated variance on the inter-source and inter-receiver distance can then be linked to the heterogeneity spectrum of the planet via a linearized least-squares inversion. For the time being, we limit ourselves to a two-dimensional problem, analyzing surface-wave dispersion in the membrane-wave approximation. Besides inverting global seismic data, we have conducted a number of synthetic tests to evaluate the resolution power of the method and its robustness, and the dependence of inversion results on the amount of inverted data and on the level of complexity that we allow for. Resolution turns out to be low in comparison with “classical” global tomography, suggesting that the simplifications required to linearize the problem compromise accuracy. We infer that a fully nonlinear, computationally intensive search of the solution space might be necessary to directly constrain the Earth’s spectrum up to relatively high harmonic degrees.

References:

L. Boschi, J.-P. Ampuero, D. Peter, P. M. Mai, G. Soldati, D. Giardini
Petascale computing and resolution in global seismic tomography
Phys. Earth Planet. Int., **163** (2007), 245-250.

S. Della Mora, L. Boschi, and T. W. Becker
Heterogeneity spectrum inversion from a stochastic analysis of global surface-wave delay-time data
Geophys. J. Int., in preparation, 2009.

Title: Mutually consistent tomographic models of crust, upper mantle and the lithosphere-asthenosphere boundary region underneath Europe and the Mediterranean Basin

Researchers: PhD candidate J. Schaefer (ETHZ)
Dr. L. Boschi (ETHZ)
Prof. E. Kissling (ETHZ)

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

Description:

We develop an adaptive-grid algorithm for global multi-resolution tomography of surface wave phase anomaly data. An adaptive grid is one whose spacing changes locally depending on the local data coverage and thus the resolution power. We use a pixel size between 1.25° and 5° , and 9 vertical layers of equal thickness; we account for radial anisotropy by defining two independent parameters at each grid point. Our algorithm first identifies the coefficient matrix for the smallest pixel size, which corresponds to 31,808 pixels and 32 GB of memory; these figures are then iteratively reduced as the optimal adaptive grid is derived from the highest-resolution one. Computational difficulties also arise from the need of regularizing the inverse problem via roughness damping (minimization of gradient). It is not straightforward to define a roughness-minimization operator associated to an adaptive grid: we derive it from the corresponding operator defined in the spherical harmonic domain, which requires the calculation of the spherical harmonic coefficients of each pixel. To reach a sufficient representation of each pixel we need a harmonic expansion up to degree 899, which results in 810,000 coefficients (6.2MB for each pixel, about 800pixels/hour). These large matrix sizes can be reduced by taking advantage of the inherent matrix symmetries. Large matrix manipulations are also sped up via parallel computing on the Brutus cluster. In this endeavour, it is necessary to use as much RAM as possible to store a large portion of the matrix for the multiplication since the same columns are needed repeatedly and reading data from memory is extremely time-consuming. Parallel computations on Brutus are also limited in time, and we are sometimes forced to run “smaller” jobs than possible and can not always use the whole computational power. This results unfortunately in a larger total computation time (~70 jobs with a total run-time of up to 8h). We are currently working on strategies to reduce the amount of required computation time and RAM. Since our ultimate goal is European upper mantle tomography, we can maintain our adaptive grid in Europe while replacing it with a uniform, coarse parameterization elsewhere over the globe. The total number of pixels decreases from 12,743 to 3866 pixels per layer (matrix ~9GB).

References:

J. Schaefer, L. Boschi, and E. Kissling
European upper mantle tomography: adaptively parameterized models
AGU fall meeting (2009).

Title: Mantle chemical and thermal heterogeneities and anisotropy mapped by nonlinear inversion of global surface wave data

Researchers: Dr. A. Khan (University of Copenhagen/ETHZ)
Dr. L. Boschi (ETHZ)
Dr. J. Connolly (ETHZ)

Institute/Group: Institute of Geophysics, Group of Seismology and Geodynamics (collaboration with Group of Earth and Planetary Magnetism, and Institute of Mineralogy and Petrography, Group of Geochemistry).

Description:

Seismic tomography is a powerful tool to help us understand the dynamics of the Earth and the nature of mantle convection; yet, it suffers from a number of important limitations: adherence to spherically symmetric seismic reference models; limited data sensitivity with respect to all physical properties; the inherent shortcoming of first obtaining profiles of seismic velocities from observations and then interpreting these in terms of mantle composition and temperature. We take advantage of quickly growing computational capabilities to determine composition, temperature, seismic anisotropy and mantle discontinuity (410km, 660km) topography directly from seismic surface-wave data, by means of a computationally intensive stochastic sampling algorithm that does not strictly rely on any a-priori model (i.e., a nonlinear inversion). The algorithm is based on the self-consistent thermodynamic calculation of mineral phase equilibria and their physical properties, predicting radial profiles of seismic velocities and density. At this point, the stochastic exploration of the solution space is conducted on a small linux cluster; the Earth is subdivided in 27 distinct tectonic regions, mantle properties are described by 50 free parameters per tectonic region, and seismic data associated to each region are "inverted" separately on one CPU per region, requiring about two weeks of computation. Improving the computational efficiency of our method is key to the development of higher-resolution, data-based thermochemical maps of the Earth.

References:

A. Khan, L. Boschi, and J. Connolly

On mantle chemical and thermal heterogeneities and anisotropy as mapped by inversion of global surface-wave data

J. Geophys. Res., **114** (2009), B09305, doi:10.1029/2009JB006399

Title: Site-specific numerical simulations of earthquake rupture dynamics and strong ground motion: Application to Swiss NPP's

Researchers: Dr. Luis A. Dalguer (ETHZ)
Prof. Domenico Giardini (ETHZ)
Dr. P. Martin Mai, (KAUST, Saudi Arabia)
Dr. D. Fäh, SED/ETHZ

Description:

We use high performance computing simulation to investigate potential earthquakes and the resulted ground motion in site-specific zones near Swiss Nuclear Power Plants (NPP), to assess the level and variability of near-source ground motion in the zone, for the improvement of seismic safety analysis of future and existing NPP's in Switzerland.

For reliable development of this project, it requires parallelized numerical techniques for multiprocessor execution and highly scalable, enabling high-resolution earthquake simulations. Currently we are running our codes in the Cray XT5 Rosa supercomputer of the Swiss National Supercomputing Centre (CSCS). As show in the figure below, our code (SORD) has been tested to up to 8192 processor, with efficient scalability.

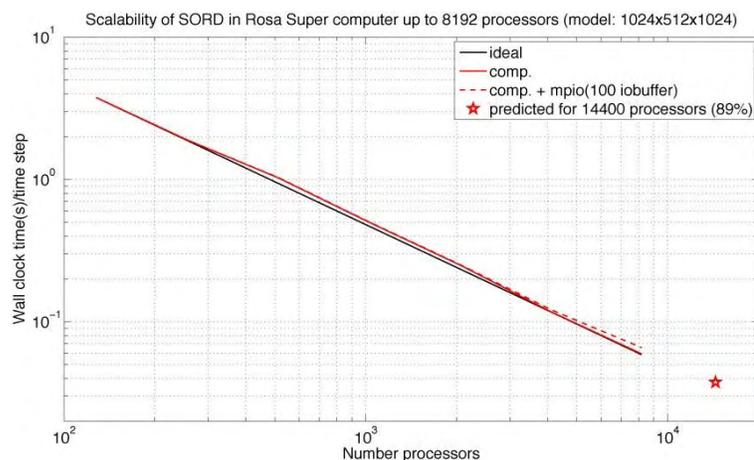


Figure. Scaling of SORD code on the Cray XT5 Rosa supercomputer from CSCS at Manno, Switzerland.

References:

Dalguer L. A. and P. M. Mai

The dynamic rupture and near source ground motion characteristics of thrust, normal and vertical strike slip faults under different tectonic loading regimes
AGU fall meeting (2009)

Title: Rupture Directionality of Dynamic Rupture Propagation at Bimaterial Interface in 3D

Researchers: Dr. Luis A. Dalguer (ETHZ)
Prof. Steven M. Day (SDSU, USA)

Description:

Normal stress perturbations accompany propagating mode II rupture along an interface separating materials of contrasting elastic compliance. We show, by numerical simulations in 3D (see figure below), that purely geometrical effects leading to pulse-like rupture, due to this normal stress perturbation, can induce strong asymmetries (and under very limited conditions can even evolve into strictly unilateral rupture), even when frictional rate dependence is neglected. The effect is studied here in a context that can only apply to strike-slip earthquakes large enough to rupture the entire seismogenic thickness, but the results suggest that other geometrical effects leading to pulse-like rupture will interact with a compliance contrast in a similar manner.

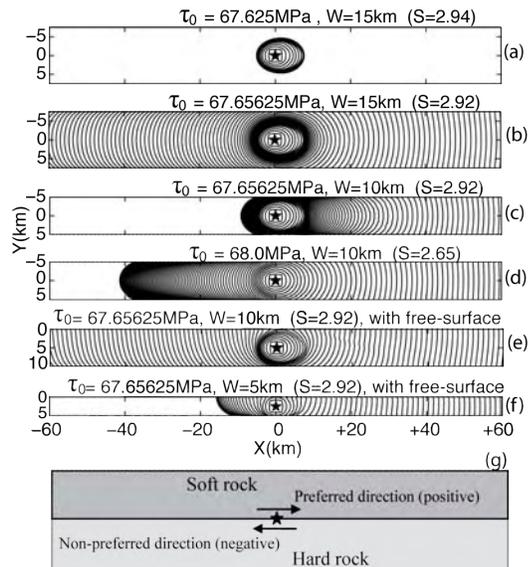


Figure. Rupture-time contours (0.5 sec intervals) for six fault models with fault length 120km. Models in a, b, c and d are embedded (no-freesurface); and models e and f are with free-surface. Figure g (bottom) is a top view of fault model, where preferred (positive) and non-preferred (negative) rupture directions are defined. Star indicates center of nucleation zone.

References:

L. A. Dalguer and P. M. Mai

The dynamic rupture and near source ground motion characteristics of thrust, normal and vertical strike slip faults under different tectonic loading regimes, AGU fall meeting (2009).

Title: Strong Motion Simulation based on Dynamic Rupture Modelling: A case study on the 1999 Düzce Earthquake Modelling

Researchers: Dr. Luis A. Dalguer (ETHZ)
Dr. Gulum Tanircan (Bogazici University, Turkey)

Description:

we investigate the dynamic rupture of the 1999 Duzce earthquake and the ground motion generated, fitting model prediction with observations. Our goal is to understand the underlying physics during this earthquake that ruptured with supershear speed, and the implications in the ground motion. The figure below shows preliminary results of final slip and rupture time for this earthquake.

The computation demand for this work is also very high, because it require highr resolution and large scale simulations to accurately solve the problem . We are currently using a large memory sharing SUN machine with 8 processors and 64 Gbytes.

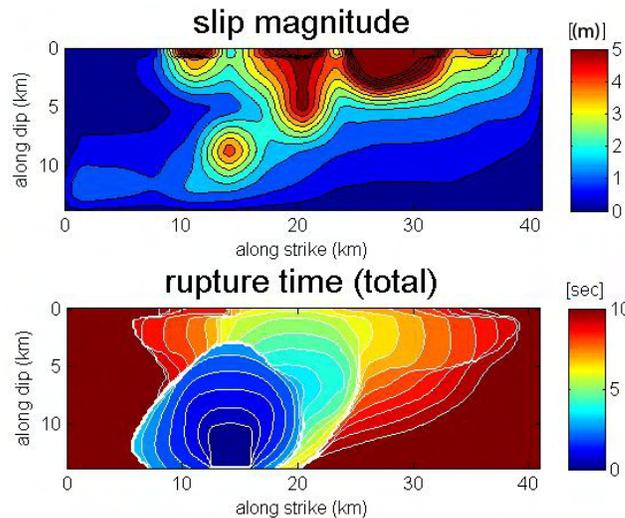


Figure. Final slip and rupture time solutions of dynamic rupture simulation of the 1999 Duzce earthquake.

References:

G. Tanircan and L.A. Dalguer
Strong Motion Simulation based on Dynamic Rupture Modelling: A case study on the 1999 Düzce Earthquake Modelling
10th Canadian Conference on Earthquake Engineering (2010).

Title: Dynamic fault rupture model of the 2008 Iwate-Miyagi Nairiku earthquake, Japan

Researchers: Dr. Luis A. Dalguer (ETHZ)
Dr. Nelson Pulido (NIED, Japan)
Dr. Shin Aoi (NIED, Japan)

Description:

We investigate the physical causes of the extreme ground motion generated by the 2008 Iwate-Miyagi Nairiku earthquake in Japan. This earthquake generated high frequency (HF) extreme accelerations of 3.9g and 3.5g recorded at IWTH25 station (figure below). In order to understand the generation mechanism of these HF events, we perform a dynamic fault rupture model of this earthquake and identify the source of this extreme event.

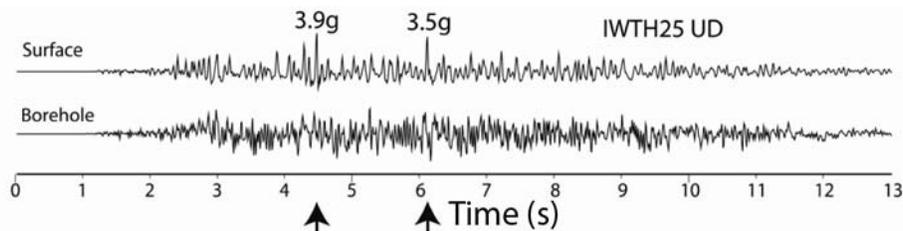


Figure. Observed UD acceleration component (surface and borehole) at IWTH25 station

References:

N. Nelson Pulido, L. A. Dalguer, and S. Aoi
Dynamic fault rupture model of the 2008 Iwate-Miyagi Nairiku earthquake, Japan; Role of rupture velocity changes on extreme ground motions
AGU Fall meeting (2009).

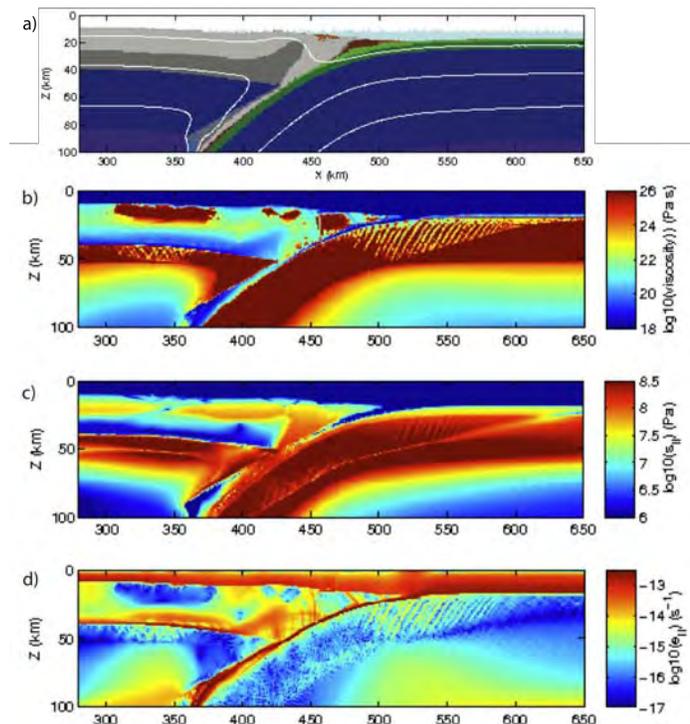
Title: Genesis of mega-thrust earthquake events at convergent plate boundaries: 3D modelling of seismic coupling combining geodynamic and earthquake-faulting models

Researchers: PhD student Ylona van Dinther (ETHZ)
Dr. Taras Gerya (ETHZ)
Dr. Luis A. Dalguer (ETHZ)
Dr. P. Martin Mai, (KAUST, Saudi Arabia)
Dr. Gabriele Morra (University of Sydney, Australia)
Dr. Francesca Funiciello (university Roma Tre, Italy)

Description:

We develop a coupled system of geodynamic and earthquake faulting dynamic models to investigate long-term earthquake cycle on a convergent margin, from large, geodynamical space-time scales to small, seismological ones. Our numerical simulations link kinematic observables and long-term deformation phenomena to earthquake dynamic occurrences. This investigation contributes to understand the physical relationship between geodynamics mechanism, seismicity and thrust-faulting dynamics. Our current geodynamic simulations show outer-rise localization features influenced by both regional and bending stresses, characterized in terms of seismic properties. This work is very computationally intensive, to cover the complete process of earthquake occurrence at small and large scale in time and space.

Figure. Geodynamic visco-elasto-plastic 1500x200 km subduction model showing a) compositional rock type (Purple: mantle, Blue: lithosphere, Grey: continental crust, Green: oceanic crust, Brown: sediments) and temperature contours (white lines, 100-500-900 degrees Celsius), b) viscosity, c) second invariant of the stress tensor, and d) second invariant of the strain rate tensor. The last three sub-figures demonstrate the trench-ward intra-plate localizations within the outer-rise area between 480 and 600 km.



References:

Y. van Dinther; T. Gerya, P. M. Mai, and L. Dalguer
Toward earthquake seismicity variability studies inferred from geodynamic numerical simulations of a subduction zone. AGU fall meeting (2009).

Title: On the development of improved Pseudo-Dynamic (PD) models for ground motion simulation

Researchers: PhD student Banu Mena Cabrera (ETHZ)
Dr. P. Martin Mai (KAUST, Saudi Arabia)
Dr. Luis A. Dalguer (ETHZ)

Description:

We are currently performing a suite of dynamic rupture simulation of different sizes with stochastic initial stress distribution to investigate correlations between dynamic source parameters. The identified correlations are used to improve the pseudo-dynamic model that will lead to a more realistic, physics based ground motion prediction. The suite of dynamic models is developed using a parallelized FDM numerical model scalable to thousand of processors, currently running on our 20 processors linux cluster.

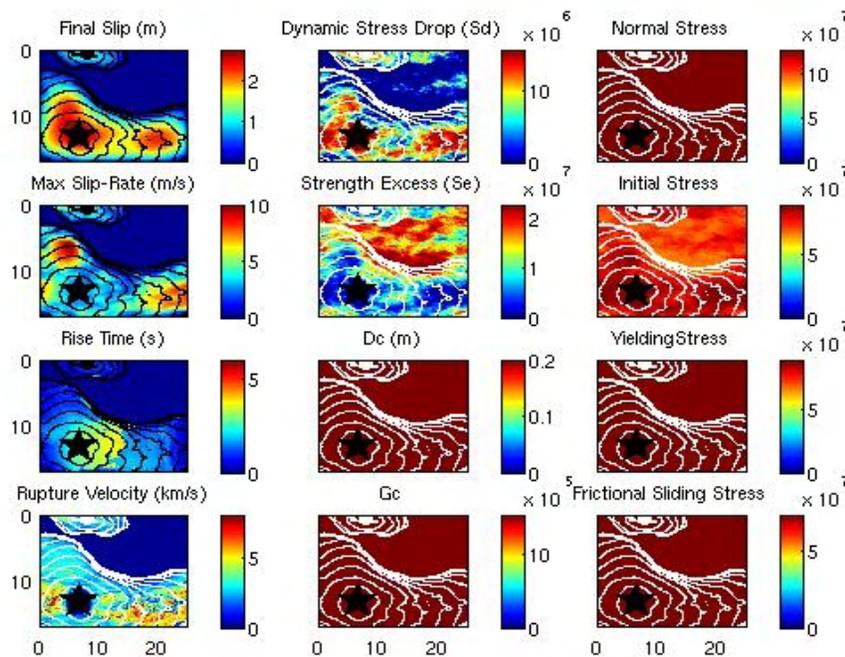


Figure. Source parameters distribution calculated from dynamic rupture simulations.

References:

B. Mena, P. M. Mai, K. B. Olsen, M. D. Purvance, and J. N. Brune, Hybrid Broadband Ground Motion Simulation Using Scattering Green's Functions: Application to Large Magnitude Events. *Bull. Seism. Soc. Am.*, in press (2009).
B. Mena and P. M. Mai, Selection and Quantification of Near-Fault Velocity Pulses due to Source Directivity. *Georisk*, in press (2009).

Title: Broad-Band Ground Motion Simulations in The Messina Straits Area (Southern Italy)

Researchers: PhD student Walter Imperatori (ETHZ)
Dr. P. Martin Mai, (KAUST, Saudi Arabia)

Summary: In this project we focus on the Messina Straits area (southern Italy) earthquake (Mw 7.1) that struck the area about one century ago (see figure below). The purpose of this study is to investigate the source and ground motion characteristics of this earthquake in order to predict variability of ground shaking levels for future events in this area of study. For that we need to perform hundreds of simulations accounting for realistic sources and available velocity models, that requires accurate and efficient numerical techniques and powerful computational resources.

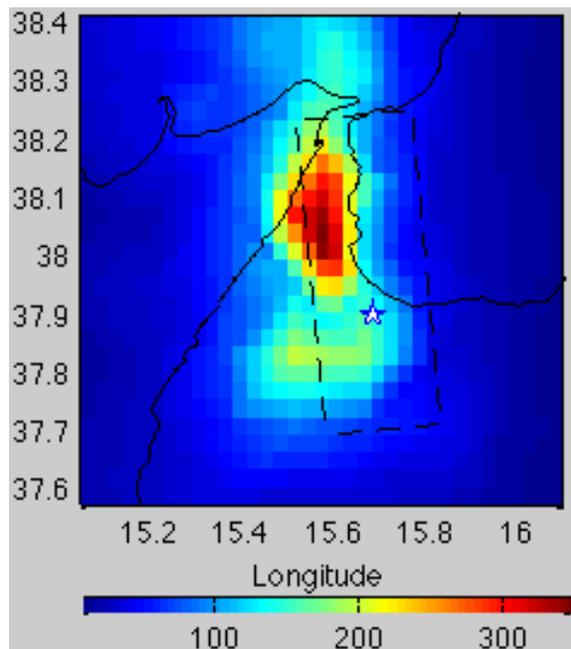


Figure: Peak Ground Acceleration values (cm/s^2) for one of our scenario models

References:

W. Imperatori and P. M. Mai
Broad-Band Ground Motion Simulations in The Messina Straits Area (Southern Italy)
in *1908-2008: Scienza e Societa' a 100 anni dal grande terremoto*, Reggio Calabria, Italy (2008).

Title: Broad-Band Ground Motions Combining Low-Frequency Deterministic Simulations and High Frequency Scatterograms: Validation Against the 1994 Northridge Earthquake

Researchers: PhD student Walter Imperatori (ETHZ)
Dr. K. Olsen (SDSD, USA)
Dr. P. Martin Mai, (KAUST, Saudi Arabia)

Description:

Broadband scenario ground motions (0-10 Hz) play an important role in seismic hazard analysis, and accurate broadband synthetics are needed for performance-based earthquake engineering analysis. Validation and verification of the broadband methods is critical to ensure realistic synthetic seismograms. In this study we present a validation of the most recent version of the ETH/SDSU broadband method against strong-motion data from the 1994 Northridge earthquake. The synthetics are compared to data using the bias of the response spectral residuals, as well as a goodness-of-fit measure recently proposed. We also test two different approaches to estimate frequency-dependent site amplification factors.

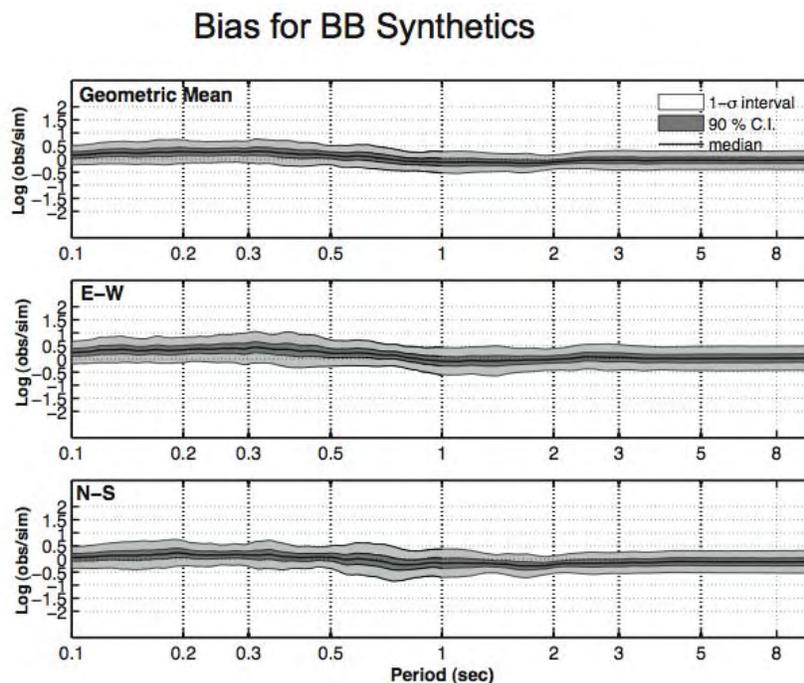


Figure. Bias of the response spectral residuals for broadband synthetics.

References:

W. Imperatori, K. Olsen and P. M. Mai
Broad-Band Ground Motions Combining Low-Frequency Deterministic Simulations and High Frequency Scatterograms: Validation Against the 1994 Northridge Earthquake
SCEC 2009 annual meeting, Palm Springs, California (2009).

Title: Development of kinematic and dynamic rupture models, in an elastic medium, equivalent to a dynamic rupture model with off-fault plastic yielding.

Researchers: PhD student Alice-Agnes Gabriel (ETHZ)
Dr. Jean-Paul Ampuero (Caltech, USA)
Dr. Luis A. Dalguer (ETHZ)
Dr. P. Martin Mai, (KAUST, Saudi Arabia)

Description:

In this project we plan to develop a set of dynamic rupture models, incorporating off-fault plastic yielding (macroscopic representation of damage) in the bulk, to investigate the effect of the non-elastic response on the dynamic rupture propagation and near source ground motion as well as the physical limits on the slip velocity function and extreme ground motion.

Emphasis is given to examine the slip velocity pulse as a measure of ground-motion excitation, since it is well known that rupture directivity associated with propagating slip pulse can generate large amplitude of near-source velocity ground motion.

In the current stage of the project, we focus our study on the conditions to generate steady-state pulse-like ruptures and how this regime operates when off-fault inelastic deformation is considered during rupture simulation. We target to characterize the conditions to generate steady-state pulse-like ruptures and compare these to analogous results in purely elastic media. This study needs an extensive application of numerical methods and codes for dynamic rupture simulations in the presence of off-fault plasticity.

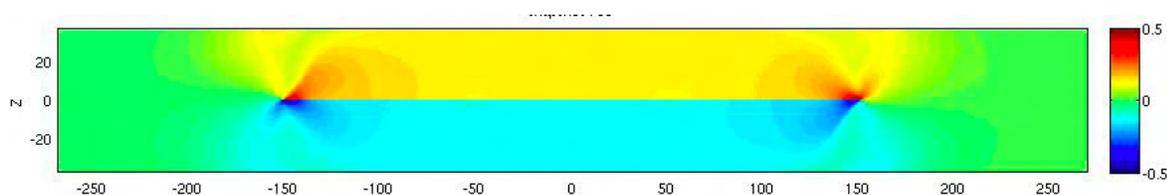


Figure. Velocity snapshot of pulse-like dynamic rupture simulated by the spectral element method (SEM)

References:

A.-A. Gabriel; J.-P. Ampuero, L.A. Dalguer and P. M. Mai
Properties of Steady State Dynamic pulse-like ruptures with off-fault plasticity
AGU fall meeting (2009).

Title: Coupled seismogenic Geohazards in Alpine Regions (COGEAR)

Researchers: Dr. D. Fäh
Dr. J. Burjanek
PhD candidate G. Stamm
PhD candidate V. Poggi
Dr. S. Alvarez-Rubio
Prof. D. Giardini

Institute/Group: Institute of Geophysics, ETH Zurich; Swiss Seismological Service

Description:

COGEAR is an interdisciplinary natural hazard project with the goal to investigate the hazard chain induced by earthquakes. It is supported by the *Competence Center for Environment and Sustainability (CCES)* of ETH Zurich. It includes the tectonic processes and the related variability of seismicity in space and time, earthquake forecasting and short-term precursors, and strong ground motion as a result of source and complex path effects. In soils and rock, we will study nonlinear wave propagation phenomena and liquefaction as well as the triggering of landslides; the potential of earthquake-induced snow avalanches is also estimated. Here the focus is on the physics of the non-linear processes in relation to topography, geological disposition and slope stability. The Valais and specifically the area of Visp, as well as the Visper and Matter valleys have been selected as study areas. The tasks include detailed field investigations, the development of 3D structural models at different scales, and the application of numerical ground motion modeling techniques, assessment of the susceptibility to seismically induced effects and installation of different monitoring systems to test and validate our models. The monitoring systems are for long-term operation and include a continuous GPS and seismic network, a test installation for the observation of earthquake precursors, and two test areas (Visp, St. Niklaus-Randa) to study site-effects and non-linear phenomena. The probability of observing a major earthquake in the next 40 years is high, and project COGEAR is the first step in preparing for such observations as well as setting up a scientific base for detailed monitoring and analysis. This project will prepare a follow-up risk-related project including the impacts on buildings, infrastructure, and society.

References:

- H. B. Havenith, D. Fäh, S. Alvarez-Rubio, and D. Roten, Response spectra for the deep sediment-filled Rhône Valley in the Swiss Alps, *Soil Dynamics and Earthquake Engineering* **29**, 17-38 doi:10.1016/j.soildyn.2008.01.016 (2008).
- D. Roten, D. Fäh, C. Cornou, and D. Giardini, 2D resonances in Alpine valleys identified from ambient vibration wavefields. *Geophys. J. Int.*, **165**, 889-905 (2006).
- D. Roten and D. Fäh, A combined inversion of Rayleigh wave dispersion and 2D resonance frequencies. *Geophysical J. Int.*, **168**, 1261–1275 (2007).
- D. Roten, D. Fäh, K. B. Olsen, and D. Giardini, A comparison of observed and simulated site response in the Rhone valley, *Geophysical J. Int.*, **173**, 3, 958-978 (2008)
- D. Roten, D., Fäh, F. Bonilla, S. Alvarez-Rubio, T. Weber, and J. Laue, Estimation of nonlinear site response in a deep Alpine valley, *Geophys. J. Int.*, **178**, 1597–1613 (2009).
- S. Steimen, D. Fäh, F. Kind, C. Schmid and D. Giardini, Identifying 2-D Resonance in Microtremor Wave Fields, *Bull. Seism. Soc. Am.*, **93**, 583-599 (2003).

Title: Deforming Meshes that Split and Merge

Researchers: Chris Wojtan¹, Nils Thuerey², Markus Gross², Greg Turk¹

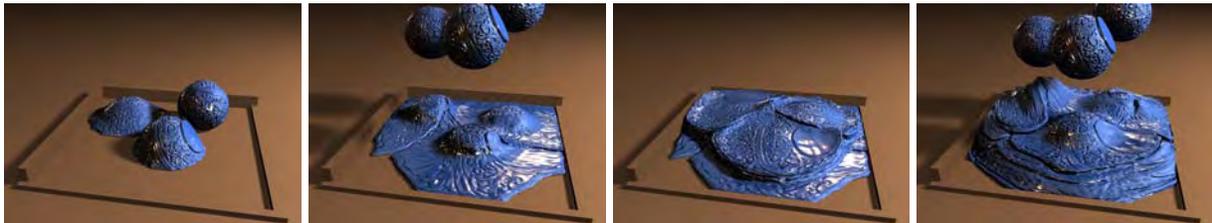
Institutes:

- 1) Computer Graphics Group, Georgia Institute of Technology
- 2) Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich

Description:

We present a method for accurately tracking the moving surface of deformable materials in a manner that gracefully handles topological changes. We employ a Lagrangian surface tracking method, and we utilize a triangle mesh for our surface representation so that fine features can be retained. We make topological changes to the mesh by first identifying merging or splitting events at a particular grid resolution, and then locally creating new pieces of the mesh in the affected cells using a standard isosurface creation method. We stitch the new, topologically simplified portion of the mesh to the rest of the mesh at the cell boundaries. Our method detects and treats topological events with an emphasis on the preservation of thin features, while simultaneously simplifying those portions of the material that are not visible.

Our surface tracker is not tied to a particular method for simulating deformable materials. In particular, we show results from two significantly different simulators: a Lagrangian FEM simulator with tetrahedral elements, and an Eulerian grid-based fluid simulator. Although our surface tracking method is generic, it is particularly well-suited for simulations that exhibit thin features and numerous topological events. Highlights of our results include a taffy-pulling animation with many fold and merge events, the creation and separation of thin strands in the simulation of viscoelastic materials, and the retention of thin sheets and surface details in a splashing fluid animation.



These images show an example simulation of several ornamental spheres being dropped on top of each other in an Eulerian visco-elastic fluid simulation. Invisible geometry is quickly deleted, while the visible surfaces retain their detailed geometry even after translating through the air and splashing on the ground.

References: C. Wojtan, N. Thuerey, M. Gross, G. Turk, Deforming Meshes that Split and Merge, Proceedings of ACM SIGGRAPH (New Orleans, USA, August 3-7, 2009), ACM Transactions on Graphics, vol. 28, no. 3

Title: Synthetic Turbulence using Artificial Boundary Layers

Researchers: Tobias Pfaff¹, Nils Thuerey¹, Andrew Selle², Markus Gross¹

Institutes:

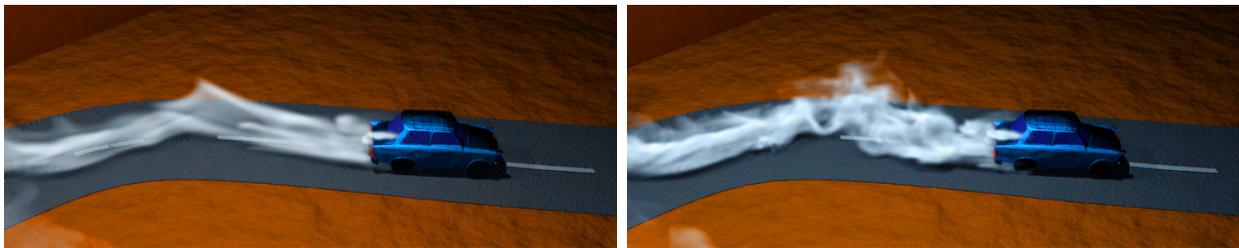
- 1) Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich
- 1) Walt Disney Animation Studios

Description:

Turbulent vortices in fluid flows are crucial for a visually interesting appearance. However, most standard fluid solvers in graphics are not able to represent highly turbulent phenomena due to numerical properties.

While there has been a significant amount of work on turbulence in graphics recently, these algorithms rely on the underlying simulation to resolve the flow around objects. We build upon work from classical fluid mechanics to design an algorithm that allows us to accurately precompute the turbulence being generated around an object immersed in a flow. This is made possible by modeling turbulence formation based on an averaged flow field, and relying on universal laws describing the flow near a wall. We precompute the confined vorticity in the boundary layer around an object, and simulate the boundary layer separation during a fluid simulation. Then, a turbulence model is used to identify areas where this separated layer will transition into actual turbulence. We sample these regions with vortex particles, and simulate the further dynamics of the vortices based on these particles.

In our paper, we show how our method complements previous work on synthetic turbulence, and yields physically plausible results. In addition, we demonstrate that our method can efficiently compute turbulent flows around a variety of objects including cars, whisks, as well as boulders in a river flow. We can even apply our model to precomputed static flow fields, yielding turbulent dynamics without a costly simulation.



The images above show a fluid simulation of a car's wake. The left image is produced using a standard fluid solver, which is not able to resolve the turbulence. The right image shows the same simulation augmented with our turbulence method.

References: T.Pfaff, N. Thuerey, A. Selle, M. Gross, Synthetic Turbulence using Artificial Boundary Layers. Proceedings of ACM SIGGRAPH Asia (Yokohama, Dec. 16-19, 2009) – to appear.

Title: Enrichment Textures for Detailed Cutting of Shells

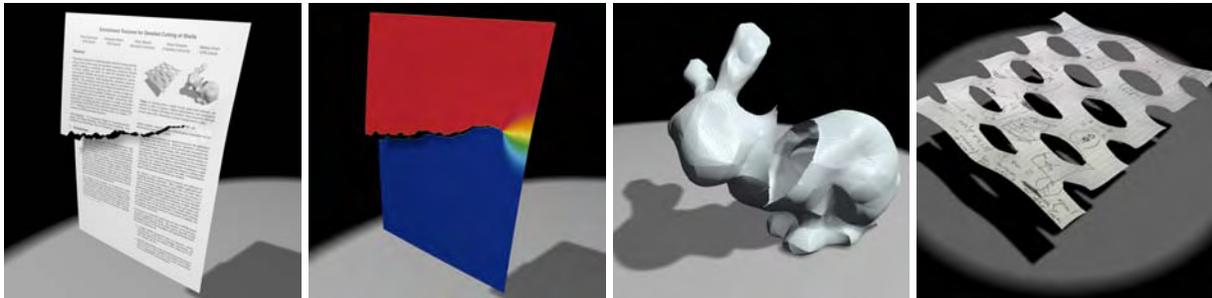
Researchers: Peter Kaufmann¹, Sebastian Martin¹, Mario Botsch², Eitan Grinspun³, Markus Gross¹

Institutes:

- 1) Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich
- 2) Bielefeld Graphics and Geometry Group, Bielefeld University
- 3) Columbia Computer Graphics Group, Columbia University

Description:

We present a method for simulating highly detailed cutting and fracturing of thin shells using low-resolution simulation meshes. Instead of refining or remeshing the underlying simulation domain to resolve complex cut paths, we adapt the extended finite element method (XFEM) and enrich our approximation by custom-designed basis functions, while keeping the simulation mesh unchanged. The enrichment functions are stored in enrichment textures, which allows for fracture and cutting discontinuities at a resolution much finer than the underlying mesh, similar to image textures for increased visual resolution. Furthermore, we propose harmonic enrichment functions to handle multiple, intersecting, arbitrarily shaped, progressive cuts per element in a simple and unified framework. Our underlying shell simulation is based on discontinuous Galerkin (DG) FEM, which relaxes the restrictive requirement of C^1 continuous basis functions and thus allows for simpler, C^0 continuous XFEM enrichment functions.



The above images show a single shell element being progressively fractured (far left) and a visualization of the underlying enrichment texture (left). Our method can also be applied to more complex meshes such as the bunny consisting of 552 triangle elements (right). A single element can be cut multiple times, resulting in one enrichment per cut (far right).

References: P. Kaufmann, S. Martin, M. Botsch, E. Grinspun, M. Gross, Enrichment Textures for Detailed Cutting of Shells. Proceedings of ACM SIGGRAPH (New Orleans, USA, August 3-7, 2009), ACM Transactions on Graphics, vol. 28, no. 3, pp. 50:1-50:10

Title: Polyhedral Finite Elements using Harmonic Basis Function

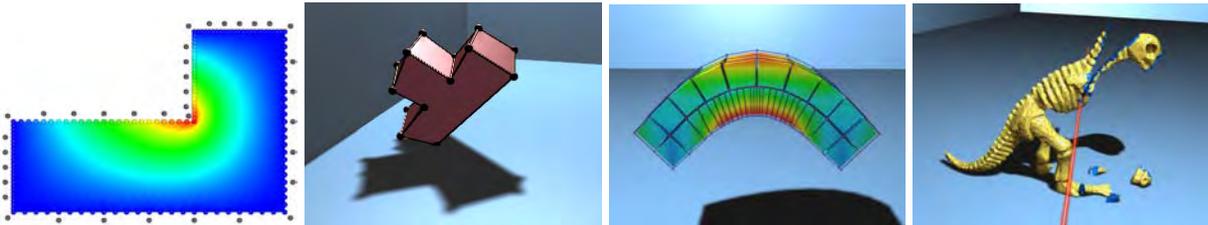
Researchers: Sebastian Martin¹, Peter Kaufmann¹, Mario Botsch², Markus Gross¹

Institutes:

- 1) Computer Graphics Laboratory, Institute of Visual Computing, ETH Zurich
- 2) Bielefeld Graphics and Geometry Group, Bielefeld University

Description:

Finite element simulations in computer graphics are typically based on tetrahedral or hexahedral elements, which enables simple and efficient implementations, but in turn requires complicated remeshing in case of topological changes or adaptive refinement. We propose a flexible finite element method for arbitrary polyhedral elements, thereby effectively avoiding the need for remeshing. Our polyhedral finite elements are based on harmonic basis functions, which satisfy all necessary conditions for FEM simulations and seamlessly generalize both linear tetrahedral and trilinear hexahedral elements. We discretize harmonic basis functions using the method of fundamental solutions, which enables their flexible computation and efficient evaluation. The versatility of our approach is demonstrated on cutting and adaptive refinement within a simulation framework for corotated linear elasticity.



The above images show an example of a harmonic basis function (far left) and its application to a single nonconvex elastically deformable element (left). Extending classical linear FEM to generalized linear basis function allows a simple handling of topological changes in the simulation mesh as shown for adaptive refinement (right) and cutting (far right).

References: S. Martin, P. Kaufmann, M. Botsch, M. Gross, Polyhedral Finite Elements using Harmonic Basis Functions. Proceedings of Eurographics Symposium on Geometry Processing (Copenhagen, Denmark, July 2-4, 2008), Computer Graphics Forum, vol. 27, no. 5, 2008, pp. 1521-1529.

Title: Onion-like Network Topology Enhances Robustness against Malicious Attacks

Researchers: Christian Schneider
Prof. Hans Hermann

Institute: Institute for Building Materials
ETH Zürich

Description:

We develop a method to generate robust networks against malicious attacks, as well as to substantially improve the robustness of a given network by swapping edges and keeping the degree distribution fixed. A novel measure for network robustness, which is based on persistence of the size of the largest cluster during attacks, is introduced. The method was applied to several types of networks with broad degree distributions including a real network, the Internet. We find that our method can improve the robustness significantly. Our extensive calculations show that robust networks have a novel "onion-like" topology consisting of a core of highly connected nodes hierarchically surrounded by rings of nodes with decreasing degree.

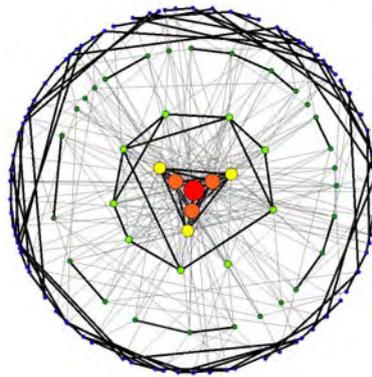


Figure 1: The onion-like topology of a robust network with $N = 124$ nodes and $M = 366$ edges. The size of the nodes is proportional to their degree k . Edges between nodes with equal degree and the fully connected core are highlighted. In onion-like networks between nearly each pair of nodes of equal k there is a path that does not contain nodes with higher degree.

References:

[1] C. M. Schneider, A. A. Moreira, J. S. Andrade Jr., S. Havlin and H. J. Herrmann *Onion-like Network Topology Enhances Robustness against Malicious Attacks*, submitted

Title: Probing the supercooled region of water by ab initio methods

Researchers: Tobias Kesselring
Prof. Dr. Hans Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

Several experimental and computational evidences for a critical point in supercooled water exist. Since Water crystallizes before entering into the assumed area of the critical point it is nearly impossible to do experiments to verify the hypothesis. For computer simulations crystallization is no problem, because their runtimes (pico- to nanoseconds) are too short for crystallization processes. Usually such simulations are done with (classical) molecular dynamics (MD) which need empirical Potentials. But no such potentials exist for supercooled water. Therefore ab initio methods are used to explore the response functions in supercooled water. Another advantage of ab initio methods in contrast to classical MD is that they are treating hydrogen bonds as covalent bonds and not as a pure electrostatic effect.

First simulations at ambient conditions will be made to compare the response functions with experiments. After this the region of the critical point comes into the focus.

Title: The Growth and Impact of the Wood Decay Fungi *Physisporinus vitreus* on Norway Spruce (*Picea abies* [L.] Kast.)

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The white-rot wood decay fungi *Physisporinus vitreus* preferentially degrade the pit membranes in wood whereby the fungi increases the wood permeability. Thus, *P. vitreus* can be used to improve the uptake of wood preservatives and environmentally-benign wood modification substances. The objective of the proposed research project is to develop a mathematical model of hyphal growth and expansion of *P. vitreus* in heartwood of Norway spruce. In addition, we wish to examine degradation patterns of the fungus, the mechanisms that are responsible for enhancing wood permeability and those related with alterations of the strength properties of the heartwood. By focussing on these fundamental processes we hope to improve our knowledge on how the complex system (fungus wood) interacts under defined conditions. The project consists in computational and laboratory experiments (Collaboration with Prof. Dr. F.W.M.R. Schwarze from EMPA).

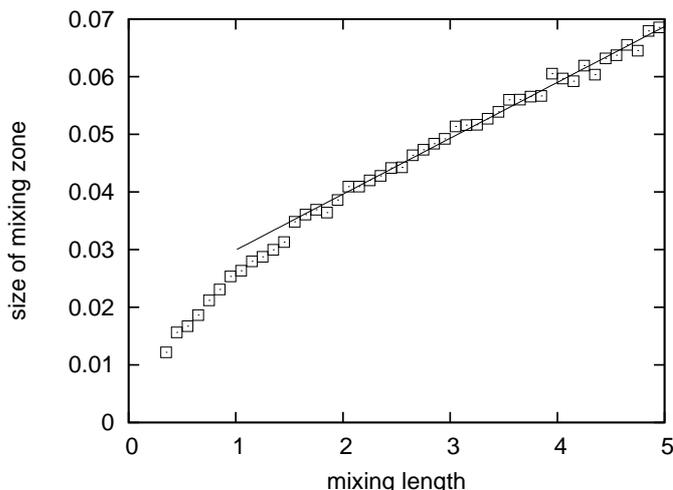
Title: Mixing Properties of Flowing Powder

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

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



The size of the mixing zone increases linearly with the mixing length.

Two dimensional simulations of a tube where two different kind of particles flow through were performed. The different types of particle were initially separated and started to mix as they flew through the system. With our current model the increase of the mixing zone was found to be linear with increasing mixing length. But our simulations also revealed, that the modeling of the forces due to the turbulent flow play an important role within such systems. More sophisticated models for turbulence that correctly reproduce the probability density functions (PDF) as well as the temporal and spatial correlations of the velocities and accelerations within the fluid are certainly needed. Models that seem to correctly reproduce the needed properties of fully developed turbulence usually consist of systems of stochastic differential equations (SDE). Finding and implementing an adequate turbulence model and incorporating the fluid-particle interactions will be the next steps of our work.

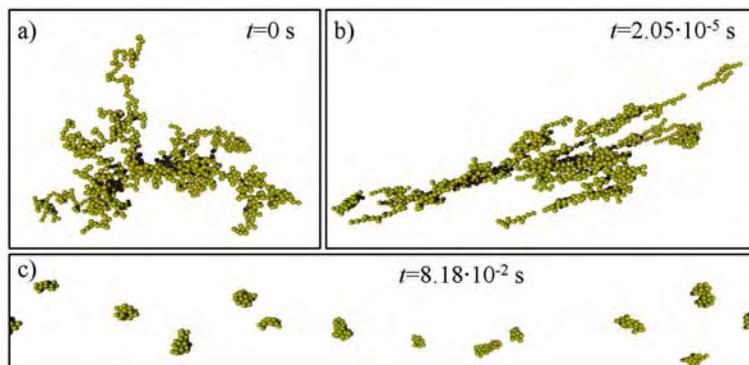
Title: Fragmentation and Restructuring of Soft-Agglomerates under Shear

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Soft-agglomerate restructuring, break-up (or fragmentation) and relaxation are studied in a simple shear flow by a discrete element method (DEM). The agglomerates, held together by van der Waals forces, are stretched and rotate in the shear flow until they fracture at their weakest point resulting in lognormally-shaped fragment size distributions asymptotically. The evolution of the average number of particles per fragment is described by generalized scaling laws between shear rate, onset (time-lag) of fragmentation, asymptotic fragment mass and size consistent with experimental and theoretical studies in the literature. Individual fragments relax in the flow towards more compact agglomerates and the initial effective fractal dimension of the agglomerates determines the final one of the fragments.



Snapshots of soft-agglomerate break-up in a linear shear profile with constant shear rate. a) The initial parent agglomerate ($t = 0$ s). b) The agglomerate rotates and is stretched in the flow field until it breaks at the weakest point ($t = 2.05 \cdot 10^{-5}$ s). c) The final fragment distribution where fragments rotate like rigid agglomerates ($t = 8.18 \cdot 10^{-2}$ s).

References:

- [1] Max L. Eggersdorfer, D. Kadau, H.J. Herrmann, Sotiris E. Pratsinis, *Fragmentation and Restructuring of Soft-Agglomerates under Shear*, Preprint.

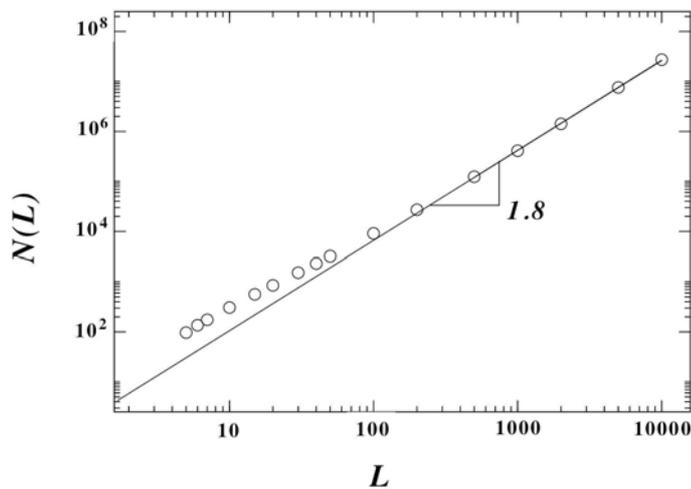
Title: Self-similarity of watershed lines

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

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

Description:

The concept of watershed arises naturally in the field of Geomorphology, where it plays a fundamental role in e.g. water management, landslide and flood prevention. Moreover, important applications can also be found in seemingly unrelated areas such as Image Processing and Medicine. Watersheds have been used since ancient times to delimit boundaries. Border disputes between countries, like for example the case of Argentina and Chile, have shown that it is important to fully understand the subtle geometrical properties of watersheds. They were studied extensively in the past and there have also been preliminary, but inconclusive, claims about fractality. Despite the far reaching consequences of scaling properties on the hydrological and political issues connected to watersheds no detailed numerical or theoretical study has yet been performed. We use an advanced algorithm for the determination of watershed lines on Digital Elevation Models (DEMs), which is based on the iterative application of Invasion Percolation (IIP). The main advantage of our method over previously proposed ones is that it has a sub-linear time-complexity. This enables us to process systems comprised of up to 10^8 sites in a few cpu seconds. Using our algorithm we are able to demonstrate, convincingly and with high accuracy, the fractal character of watershed lines. We find the fractal dimension of watersheds to be $D_f = 1.211 \pm 0.001$ for artificial landscapes, $D_f = 1.10 \pm 0.01$ for the Alpes and $D_f = 1.11 \pm 0.01$ for the Himalaya.



Log-log plot of the number $N(L)$ of sites visited by the IP-based algorithm, in order to determine the watersheds on artificial landscapes, as a function of linear dimension L (circles). Solid line shows the least squares fit to the five last data points, which gives a dimension $D = 1.8 \pm 0.01$ for large scales ($N \propto L^D$).

References:

[1] E. Fehr, J.S. Andrade Jr., S.D. da Cunha, L.R. da Silva, H.J. Herrmann, D. Kadau, C.F. Moukarzel, and E.A. Oliveira, *New efficient methods to calculate watersheds*, J. Stat. Mech. (2009) P09007

Title: Microscopic Modelling of Shear-Thickening Fluids

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

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

Description:

The interest in micro-macro-transitions is growing, especially in the field of complex fluids, where one can tune the rheology by simply changing the mixture. Up to date the microscopic parameters that describe the viscosity of non-Newtonian fluids, in particular the intrinsic shear thickening, are not well understood. Earlier, shear thickening was thought to be related to dilatancy, but recent studies prove that also materials show shear thickening behavior, which consist of attractively interacting particles and hence do not have any measurable dilatancy. As basic model we use a simple suspension, containing identical particles together with a drag force, to account for the surrounding fluid. In molecular dynamics (MD) simulations we study extensions of this basic model and their effects on the shear thickening behavior. More generally we study what properties, features or interactions on the particle scale are needed to achieve shear thickening behavior in the model. In a second step we try to control the strength of the effect and compare with experimental results. Further studies will consider irreversibilities and/or hysteresiseffects, i.e. time- and path-dependent effects like thixotropy or rheopexy.

Title: River Delta Formation

Researchers: Hansjörg Seybold
José Soares de Andrade
Peter Molnar
Hans Herrmann
Wolfgang Kinzelbach

Institute: Institut für Baustoffe
ETH Zürich

Description:

The prediction of the evolution of river beds and the understanding of erosion and sedimentation processes in the river delta region are very important for coastal management and the prevention of floods. While the water flow changes on the time scale of days and weeks, sedimentation and erosion in the river delta takes place on geological time scales. This large range of different time scales makes it impossible to apply classical hydrodynamical models to describe these phenomena.

In recent years cellular automata models have come into focus in geomorphological modelling as these models can be efficiently implemented and parallelized. While they have been successfully applied to braided river systems and other topography driven flows, they failed to reproduce the characteristic features of coastal deltas. This comes mainly from the fact, that coastal currents cannot be described by topographic flow routing rules like Manning Strickler formula.

Based on the ideas of cellular automata a new model simulating the time-series of river delta evolution is proposed in this study, providing insight into the theoretical processes of the delta formation. The model combines the simplicity of cellular models with the essential hydrodynamic features necessary to reproduce realistic river delta patterns. Simulated ocean deltas show comparable features to real deltas with respect to surface pattern and deep time evolution of major changes. Furthermore the subaqueous morphology and the formation of levees could be reproduced for the first time with a reduced complexity model.

References:

- [1] H. Seybold, P. Molnar, H.M. Singer, J. S. Andrade, H.J. Herrmann and W. Kinzelbach *Simulation of birdfoot delta formation with application to the Mississippi Delta*, **J. Geophys. Res.**, 114, F03012, (2009)
- [2] H.J. Herrmann, H. Seybold *Computational Modelling of River Delta Formation*, accepted for publication in **IJMPB** (2009)

Title: Modeling dynamics of botnet activity in spamming

Researchers: Dr. Tamara Mihaljev
Prof. Lucilla de Arcangelis
Prof. Hans Jürgen Herrmann

Institute: Institut für Baustofe
ETH Zürich

Description:

Networks of compromised computers, botnets, are nowadays the main source of malicious internet traffic. Since botnets are used for sending unsolicited commercial emails, spams, studying characteristics of temporal patterns in the receiving of such emails can be used for revealing botnet properties.

We use dynamical processes on directed complex networks to model sending of the botmaster orders inside a botnet with a complex ordering hierarchy, or sending of the spam emails through internet. Our goal is to understand the source of correlations in inter-arrival times of spam messages. This way we learn about the way spammers operate and about the structure of botnets used for spamming.

In the first approximation we model messages by random walkers, sent using different dynamical rules from the chosen source nodes. We use the first arrival times of random walkers to the chosen receiver node to calculate the inter-arrival time distribution of messages. In exhaustive numerical simulations this process is then studied for different topologies of the underlying network, different rules for sending messages, input degrees of the receiver node, different numbers of the source nodes and of the messages sent. We find that even in this simple model, when underlying networks are scale free, distribution of inter-arrival times deviates from exponential distribution, meaning that dynamical processes studied are not random. The distributions of inter-arrival times obtained in our model allow for bursts in receiving spam, which is a property of spamming process observed in the analysis of the real spam data.

Title: Instability Effects in Porous Media and Adhesive Penetration into Spruce Wood Structure

Researchers: M. Sc. Miller Mendoza Jimenez
Dr. Falk Wittel
Prof. Hans J. Herrmann

Institute: Institute for Building Materials
ETH Zürich

Description:

The goal of the present work is investigate numerically an experimentally the instability of the displacement of a miscible mixture in a porous medium and determine the causes of the formation and growth of the fingers. For this, we use a modified lattice Boltzmann model for simulating the fluid dynamics and the concentration of adhesive. In order to reproduce the hardening process we make a viscosity model based on experimental data that lets the viscosity changes with time and local concentration. Finally, we find that there is a critical point that controls the shape of the interface fluid-air and the formation of the fingers when the fluid becomes unstable.

Also with this model, we study the penetration of the adhesives into the spruce wood structure using the lattice Boltzmann model to study the maximum penetration depth and the final volumen of adhesive into the wood sample. In the simulations, we consider the wood as an anisotropic porous media with a permeability tensor field based on experimental data of the wood density.

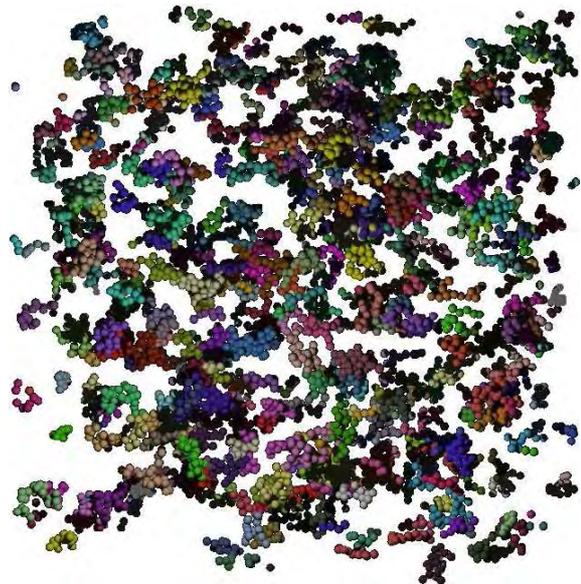
Title: Simulation of Particle Aggregation

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

Particle-Aggregation is a phenomenon encountered in various industrial processes either influencing the product result or e.g. as outgased particles which remain in the atmosphere. As the form and sizes of these aggregates is of physical and chemical relevance predicting typical aggregate properties via computer simulation is of importance. Using a simple model to represent motion in a sheared velocity field additionally with Brownian motion one can receive qualitative results regarding particle-particle, cluster-particle and cluster-cluster aggregation with varying parameters. Using an off-lattice model and simple particle and particle-interaction models, representative simulation results can be obtained for a sheared velocity field and Brownian particle-particle aggregation with relatively low computational requirement.



Snapshot of the simulated aggregation process.

References:

- [1] C. Riday, D. Kadau, H.J. Herrmann, *Simulation of Aggregation and Fragmentation under Shear*, Preprint

Title: Numerical simulations of underwater dune formation and experimental validation

Researchers: Thomas Pähtz
Prof. Hans Herrmann

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

Description:

In this project we will develop the first computationally efficient simulation for underwater dune formation including free surface effects. We expect to detect significant differences to aeolian dunes due to the influence of water depths and because the saturation length of our model, describing the spatial lag between water flow and sand motion, will have a very different behavior compared to models for aeolian land dunes according to our preliminary investigations. We will also simulate antidune formation, what has never been done before. Our computed simulation outputs will be experimentally validated by a first comprehensive study of underwater barchan topologies and dynamics. Our morphodynamic model can be extended to real situations. It will predict sand motion driven by water flow as it occurs in coastal rivers and fluvial landforms. This sand motion leads to changes of the coastal landscape, what in turn alters the water flow. All these aspects will be predicted by our model.

Title: Simulation of Ultrasound Assisted Impact Fragmentation

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

Institute: IFB - Computational Physics for Engineering Materials

Description: Impact fragmentation is a widely used principle for comminution processes of dry bulk solids. In the past researchers tried to manipulate the outcome of the fragmentation e.g. by modifying target shapes, impact angles or velocities. The available energy for fracture initiation and propagation is mainly considered as determined by the impact velocity. The resulting fragment mass distribution is described by power laws with universal exponents. In this paper we demonstrate via a 3D Discrete Element Model, starting from an impact on a rigid target, how fragmentation of impactors can be influenced by vibrating targets. In our studies the target is considered as rigid, but with the possibility of rigid body motion along the axis of impact with varying amplitude and frequency. The models consist of agglomerates of many spherical particles interconnected by beam-truss elements. In an earlier study this setup was used to study fragmentation mechanisms with meridional crack formation and propagation in particular. Our simulation results enable us to understand the fragmentation process and the differences for fracture due to impact against vibrating targets. Since the proposed ultrasound assisted impact comminution is a yet unexplored process, results are compared to classical impact fragmentation and dynamic FEM calculations.



Figure 1: Fragmented impactor for vibrating (left) stationary target (right) ($v_i=200\text{m/s}$). Intensities represent different clusters.

Title: Constrained Wire Crumpling in 3D Space

Researchers: Norbert Stoop
Surya Kusuma
Falk K. Wittel
Prof. Hans J. Herrmann

Institute: IFB - Computational Physics for Engineering Materials

Description: The process of crumpling a long piece of wire into a three dimensional container is studied. Previous studies on wire crumpling in 2D have shown the importance of friction and plastic yielding on the morphology. It was found that the potential energy and insertion force follow a power law as a function of the packing density. In this study, experiments were performed pushing nylon wires of various thickness into spherical plastic containers of varying sizes. The morphology of the crumpled structure, the maximum packing ratio, and the required wire insertion force were further investigated and confirmed with the aid of a 3D discrete element simulation. It is found from the simulation that the maximum pressure exerted by the wire on the container and the maximum potential energy of the system is dependent on the friction between wires and friction of wire with the container. Divergence of potential energy, contact energy, pressure on container and insertion forces are observed.

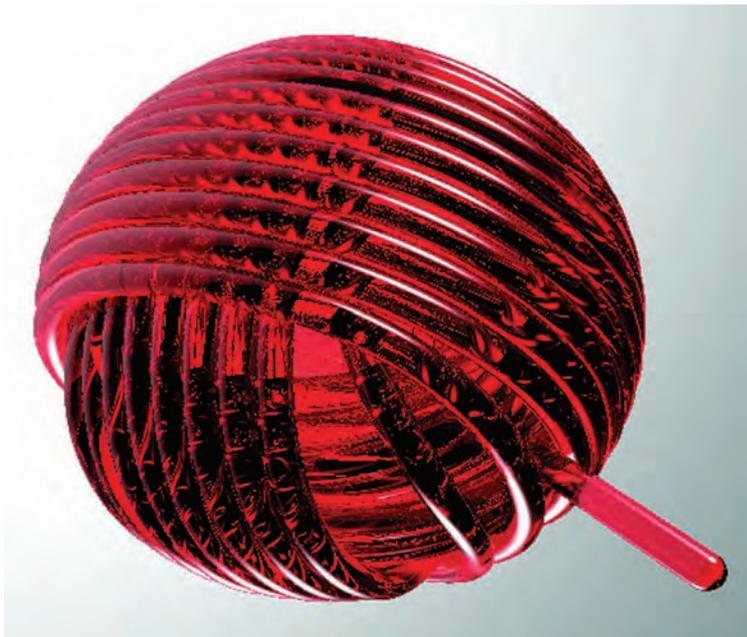


Figure 1: Rendering of simulated wire, crumpling inside the spherical cavity.

Title: Anisotropic growth of planar discs

Researchers: Norbert Stoop
Falk K. Wittel
Prof. Hans J. Herrmann

Institute: IFB - Computational Physics for Engineering Materials

Description: Shell structures are nature's reply to optimizing shape and function. In biology, a rich variety of shapes arises from different couplings of growth laws with initial geometry, if we think of shells, bladders, algae, fungi, jellyfish etc. We study the growth of initially flat discs, using an implementation of subdivision surface based finite elements (FE) and various growth laws. We find that analytical solutions of the problem lose stability when self-contact is included, leading to an energetically favored morphology, characterized by repetitive coiling and anti-symmetry. Identical behavior is found for ring like objects. Apart from discovering stable growth shapes, the system serves as a verification example for the simulation of constrained membrane growth via subdivision surface FE with self-contact and adaptive refinement (ARC).

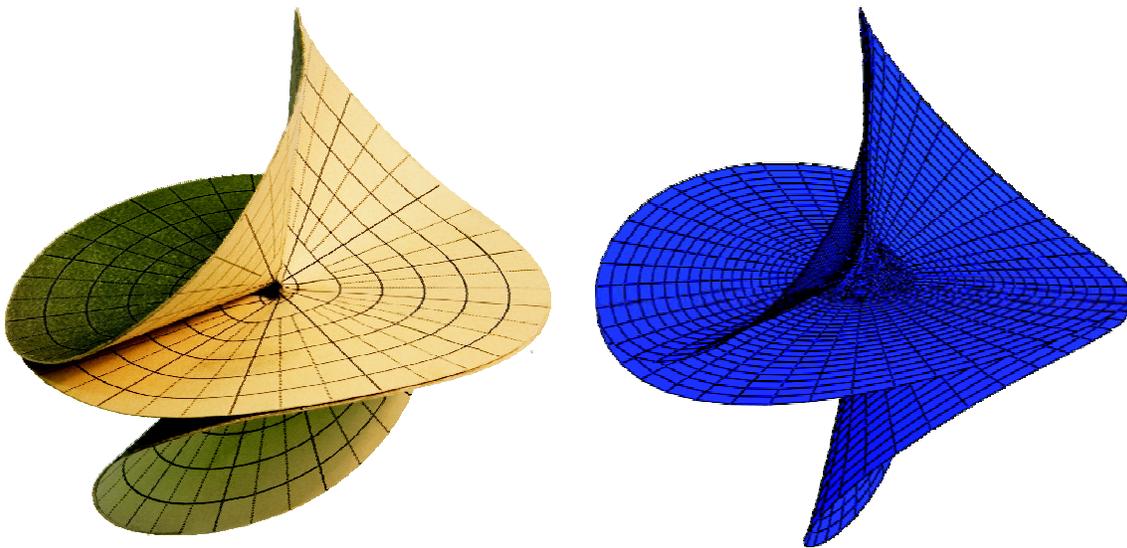


Figure 1: Toy paper model and simulation for a circumferentially growing disc in a stable growth configuration.

Title: Efficient Algorithms for Radiative Transfer

Researcher: Gisela Widmer
Prof. Ralf Hiptmair
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

When simulating a dense gas at very high temperatures, energy transport by means of radiation has to be taken into account. However, as even the stationary monochromatic radiative transfer equation is stated in five dimensions, with the intensity depending on space and direction, it is a bottleneck of such computations.

An adaptive sparse discretization [1] allows to significantly reduce the number of degrees of freedom in the discretization with essentially no loss of accuracy. This, however, does not guarantee that the computational time to solve the equation scales down at the same rate.

In this project we develop and implement efficient algorithms tailored to adaptive sparse finite elements. The C++-implementation is based on tree-structures and uses the conjugate gradient method with a multiplicative subspace preconditioner [2] in order to solve the problem at overall computational costs that are proportional to the number of degrees of freedom in the adaptive sparse discretization.

References:

- [1] G. Widmer and R. Hiptmair and Ch. Schwab. Sparse Adaptive Finite Elements for Radiative Transfer. *J. Comput. Phys.*, 227(12): 6071-6105, 2008.
- [2] G. Widmer. An Efficient Sparse Finite Element Solver for the Radiative Transfer Equation. *J. Heat Trans.*: accepted for publication, 2009.

Title: Robust Maxwell Formulation

Researcher: Florian Krämer
Prof. Ralf Hiptmair
Dr. Jörg Ostrowski

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

A novel method for the stable numerical solution of the time-harmonic Maxwell's equations for any frequency was presented in [1]. The method is based on an extended $\mathbf{a}\text{-}\varphi$ variational formulation of the full linear Maxwell's equations. This formulation avoids stability problems in the stationary limit in non-conductive parts, where the usual formulation loses control of the scalar potential.

During the last year we have focused on the development of a \mathcal{H} -Matrix preconditioner. The first step was to derive the preconditioner (1). In table 1 we see the comparison between the new real and positive definite preconditioner and the old complex, unsymmetric preconditioner. In (1) σ, μ, ϵ are material parameters and ω is $2 \cdot \pi \cdot$ frequency

$$\begin{pmatrix} \mathbf{curl}_{\mu}^{\frac{1}{2}} \mathbf{curl} + \sigma \omega & 0 & 0 \\ 0 & -\text{div}(\epsilon \mathbf{grad}) & 0 \\ 0 & 0 & -\text{div}(\epsilon \mathbf{grad})|_{\Omega_C} \end{pmatrix} \quad (1)$$

The second step was to approximate the blocks of (1) with \mathcal{H} -Matrices. The first block has posed a problem. Similar to the approach in [2] we have added an regularization term to the first block. We have chosen the regularization term to be depending on the average conductivity of the conductor.

Number of complex d.o.f.	Time old min	Memory old GB	Time new min	Memory new GB
199 000	4.2	6.0	0.6	1.4
405 000	16.8	15.3	1.4	3.3

Table 1: Total memory and time consumption of the old and new preconditioner

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

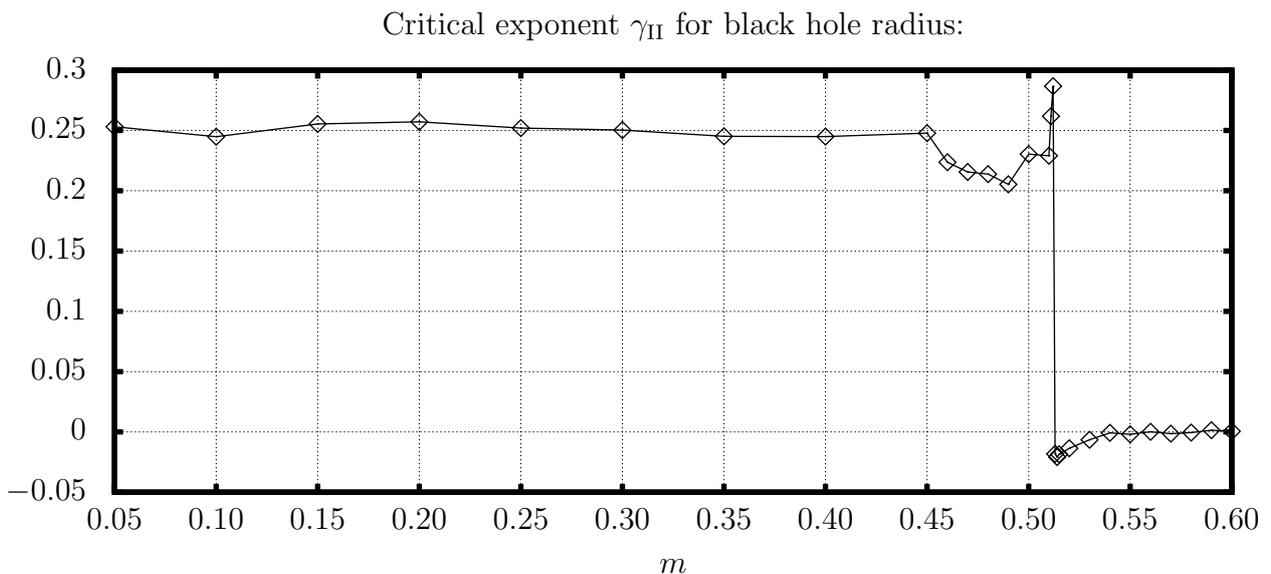
Title: The spherically symmetric EINSTEIN-DIRAC system

Researchers: BENEDIKT ZELLER
RALF HIPTMAIR

Institute: Seminar for Applied Mathematics, ETH Zürich

Description: We develop a spatial GALERKIN method, suitable for finding numerical solutions of the EINSTEIN-DIRAC equations in spherically symmetric spacetime (in polar/areal coordinates). The method features exact conservation of the total electric charge and allows for a spatial mesh adaption based on physical arclength.

- A lot of physically relevant phenomena have been observed successfully within recent simulations: black hole formation, critical collapse, propagating DIRAC waves, nontrivial zero mass solutions and structure and stability of static solutions.
- For particle masses $0.05 \leq m \leq 0.512$ we observed type II critical collapse. In particular, our data indicates that critical exponent γ_{II} does actually not depend on the particle mass m , as may be seen in the following figure.



References:

- [1] B. ZELLER and R. Hiptmair. *Conservative discretization of the Einstein-Dirac equations in spherically symmetric spacetime*, 2006, *Class. Quantum Grav.* 23 S615-S634.
- [2] Douglas W. Schaefer, Daniel A. Steck and Jason F. Ventrella. *Critical collapse of the Einstein-Dirac field*. PHY 387N Group 4 Term Project, 1998.
- [3] Felix Finster, Joel Smoller and Shing-Tung Yau. *Particle-like solutions of the Einstein-Dirac equations*. arXiv:gr-qc/9801079 v3, 1999.

Title: Simulation of cross roll straightening

Researchers: A. Mutrux
B. Berisha
P. Hora

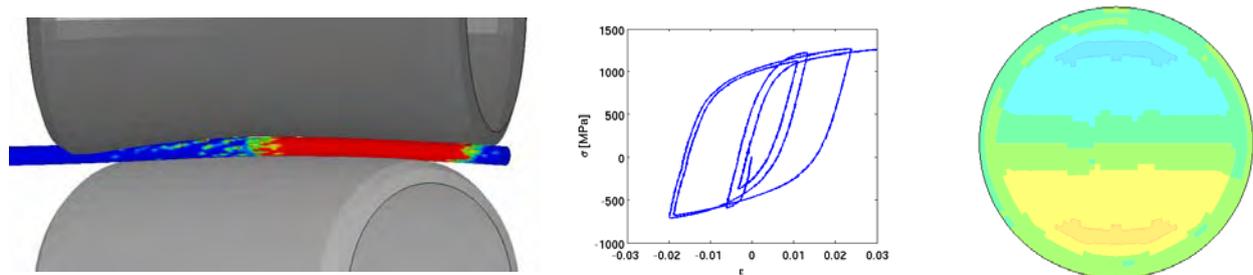
**Institute/
Group:** Institute of Virtual Manufacturing

Description:

Cross roll straightening is an operation aimed at reducing the undesirable curvature of drawn round bars. This reduction is achieved by bending the bar and simultaneously rotating it between two rolls, a convex and a concave one. For bars of large diameter, the rolls are set in a way such that a lateral stamping is also applied.

Previous work in the field is mainly based on analytical considerations. In this project, a first approach is to simulate the whole process using a finite element (FE) code [1]. Due to the large computation time required by this procedure and the only limited accuracy achieved, a second approach is taken. In this second approach, based on submodeling, the problem is reduced to the deformation of a ‘slice’ of the bar [2]. In order to incorporate stamping, which is neglected in the submodel, a third approach is used. The deformation history of a material point of the bar is build, based on similarities between straightening and bending.

The deformations involved in the straightening process being cyclical, constitutive models incorporating kinematic hardening effects have to be considered. In order to describe the strain-stress hysteresis curves observed for the tension-compression tests carried, a slightly modified version of the Chaboche model is used.



Plastification during straightening process, corresponding deformation of an element over time and final normal stress distribution.

References:

- [1] *Numerical modeling of cross rolls straightening* A. Mutrux, B. Berisha, B. Hochholdinger, P. Hora. Proc. 7th LS-Dyna Anwederforum, Bamberg, Germany 2008
- [2] *FE simulation of cross roll straightening: a submodel approach* A. Mutrux, B. Berisha, M. Weber, P. Hora. Proc. Complas X, Barcelona, Spain 2009

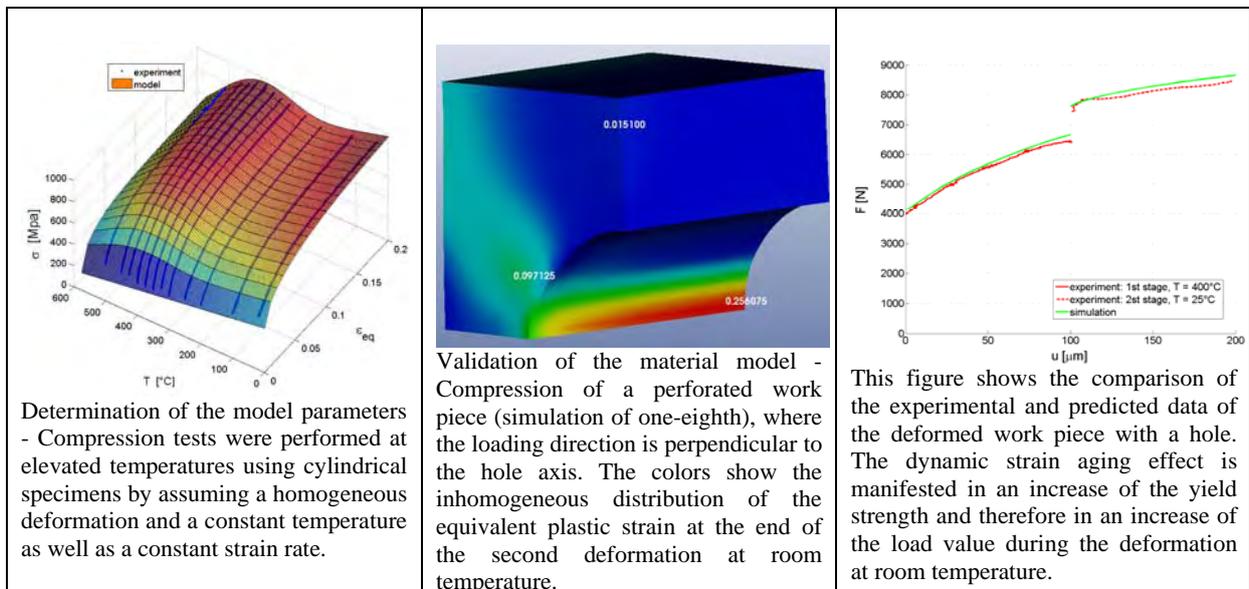
Title: An Investigation of Dynamic Strain Aging Effect on a Medium Carbon Steel with a Dislocation based Material Model

Researchers: B. Berisha
P. Hora
L. Tong

Institute/ Group: Institute of Virtual Manufacturing

Description:

A coupled isotropic-kinematic hardening material model was developed based on phenomenological observations of performed two stage experiments on a medium carbon steel – SAE 1144, where the first deformation is performed at elevated temperatures and the second deformation at room temperature. Bergström's theory of work hardening as well as the nonlinear kinematic hardening of an Armstrong-Frederick type were used as a basis for the model development. In the proposed model a relationship between material coefficients of the classical Bergström model and temperature was investigated. The developed model was implemented in an in-house Finite-Element-Code for 8-node brick elements. Due to the large computation time needed by 3D computer simulations of dislocations, in this approach, instead of concerning individual interactions of dislocations to define the stress-strain relationship, the dislocation density was computed in the middle of the element by assuming a large amount of dislocations. Representative simulation results were compared with the experimental data in order to validate the efficiency and the application range of the model.



References:

B. Berisha, P. Hora, A. Wahlen, L. Tong
A combined isotropic-kinematic hardening model for the simulation of warm forming and subsequent loading at room temperature, *International Journal of Plasticity*, 2009, doi: 10016/j.ijplas.2009.06.001

Title: 3D Fineblanking simulation

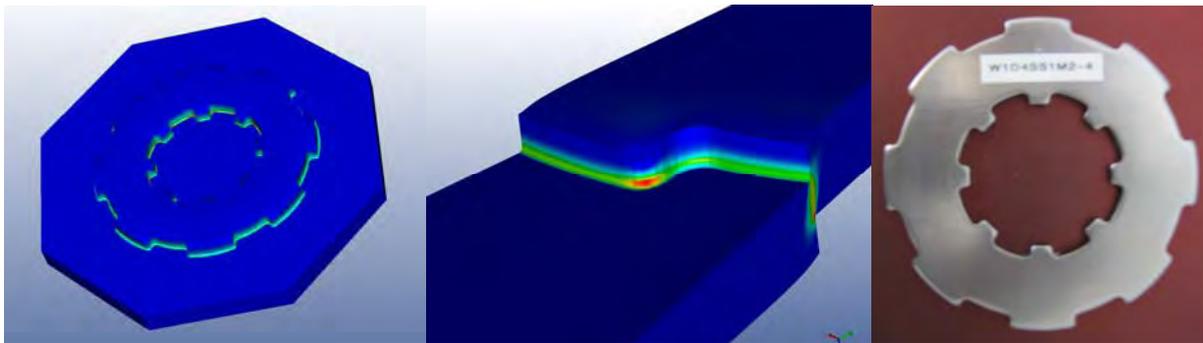
Researchers: N. Manopulo
L. Tong
P. Hora

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

Description:

Fineblanking is a manufacturing process which allows the mass production of blanked products with superior surface quality [1]. The 3D numerical simulation of this particularly precise process is however challenging. This is because quality-critical tool features such as the die clearance and the shape of the cutting edges have dimensions up to two orders of magnitude smaller than the average part dimensions. If commercial Updated Lagrange codes are used, a very high FE mesh resolution becomes a must in order to accurately represent the surface evolution along the edge, which in turn makes the computation unfeasible. The methodology presented in this paper makes use of the Arbitrary Lagrangian Eulerian FE Formulation [2] in order to keep control over the mesh region in contact with the tools. This way an optimal FE mesh can be guaranteed throughout the computation. This not only reduces the computational cost considerably, but also avoids mesh distortion along the cutting edge, allowing an accurate representation of the tool features.

Used in conjunction to the stress limit criterion delineated in [3] surface failure can also be accurately predicted. Numerical results are validated against the experiments carried out with a specially designed fineblanking tool in use at our institute.



References:

- [1] Schmidt R.-A.: Umformen und Feinschneiden. Carl Hanser Verlag München Wien, 2007
- [2] Belytschko T., Liu W. K. Moran B. : Nonlinear Finite Elements for Continua and Structures. John Wiley and Sons, Ltd., pp. 393-450, ISBN 471-98774-3, 2001
- [3] P. Hora, L. Tong and B. Berisha: Stress Limit Model with Deformation Dependent Damage for Failure Prediction in Bulk Forming Processes, NumiForm 2007, pp. 1401-1406, Porto Portugal, 2007

Title: Metamodels applied to save knowledge of planning complex fineblanking processes

Researchers: R. Hitz
N. Manopulo
P. Hora

Institute: Institute of Virtual Manufacturing

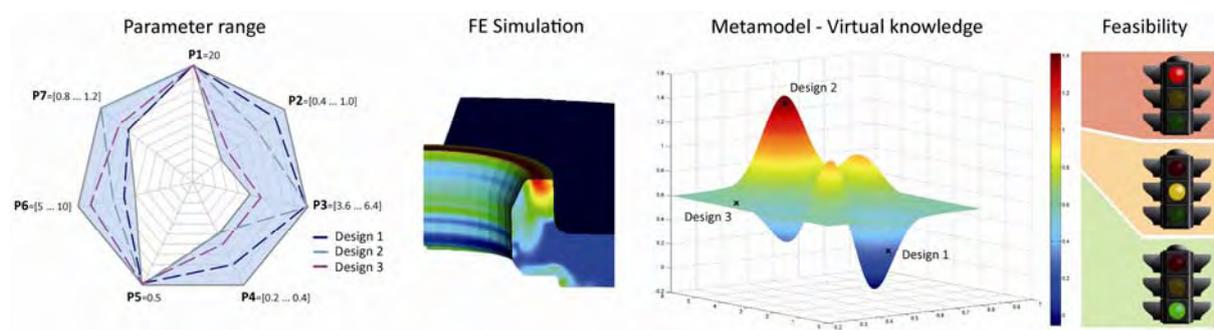
Description:

Designing an appropriate method plan for a fineblanking process with complex geometry and forming features [1] is a challenging task in regard to the systems complexity of dependencies between geometric work piece and method parameters. The designer makes a lot of decisions based on his experience.

In this work metamodels [2] are used as a repository to conserve the expert knowledge and expand it with results of FE simulations by approximating the system.

For the feasibility analysis of a certain method in conjunction with a specific geometry and method parameter values, thousands of FE simulations are needed to cover the whole parameter range. To handle this amount of load, an automated workflow (MetaDesigner) was developed based on scripts and FE tools. The results are the parameter value combinations with specific target values (formability, maximum forces, geometric deviations) forming the support points of the metamodels. The newly developed software MetaGenerator, implemented in the Institute of Virtual Manufacturing, is capable of generating miscellaneous metamodels (different regression and correlation models), including k-fold cross validation in a row, to determine the most suitable model to describe the systems behavior.

To access the knowledge stored in the metamodels a graphical user interface (MetaPlanner) is being developed. It allows the evaluation of generated metamodels concerning target values by entering values of the parameterized work piece geometry. Moreover the models can be used for fast optimization [3] given small computational cost of the function evaluation of metamodels. The designer can use this tool in an early stage of method planning to get hints regarding feasibility when no accurate numerical simulation results are yet available.



References:

- [1] Schmidt R.-A.: Umformen und Feinschneiden. Carl Hanser Verlag München Wien, 2006
- [2] K.-T. Fang, R. Li, A. Sudjianto: Design and Modeling for Computer Experiments. Tylor & Francis Group, 2006
- [3] M.H.A. Bonte: Optimisation Strategies for Metal Forming Processes. 2007

Title: Residual structure in a peptide fragment of the outer membrane protein X under denaturing conditions: A molecular dynamics study.

Researchers: Vincent Kräutler*
Sebastian Hiller**
Philippe H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group: ** Institute of Molecular Biology and Biophysics

Description :

The *Escherichia coli* outer membrane protein X (OmpX) contains two polypeptide segments that present non-random residual structure in 8 M aqueous urea, whereas the remainder of the protein is in a flexibly disordered conformation (Tafer *et al.*, Biochemistry 43:860-869 (2004)). In the present study, the results of two long-timescale (0.4 μ s) unrestrained explicit-solvent molecular dynamics (MD) simulations of a tetradecapeptide representative of one of these two segments in 8 M aqueous urea are reported and analyzed. The two simulations were initiated either from the conformation of the corresponding segment in an NMR model structure of the unfolded protein or from an entirely extended configuration. The sampled conformational ensembles agree qualitatively with the experimentally observed NOEs, but not quantitatively, suggesting that a number of relevant configurations have not been visited on the $2 \times 0.4 \mu$ s timescale. Major conformational transitions occur on the 0.1 μ s timescale and the ensembles corresponding to the two independent simulations overlap only to a limited extent. However, both simulations show in multiple events the reversible formation and disruption of α -helical secondary structure (characteristic of the urea-denatured state) and β -turn secondary structure (characteristic of the native state). Events of helix formation are correlated with the appearance of hydrogen bonds between two side chains (Asp75-Ser78) and of a persistent hydrophobic contact (Trp76-Tyr80). They also evidence a peculiar helix stabilization and N-terminal capping role for a negatively charged residue (Asp75). These features are in good qualitative agreement with the NMR model for the structured state of the corresponding segment in the urea-denatured protein. The analysis of the simulations provides a detailed picture of the structural and dynamical features of the considered peptide at atomic resolution that is of high relevance in the understanding of the OmpX folding process.

References: V. Kräutler, S. Hiller and P.H. Hünenberger
Eur. Biophys. J., submitted (2009).

Title: The Martini coarse grained force field: Extension to carbohydrates.

Researchers: Cesar A. Lopez**
Andrzej Rzepiela**
Alex H. de Vries**
Lubbert Dijkhuizen***
Philippe H. Hünenberger*
Siewert J. Marrink**

**Institute/
Group:** * Laboratory of Physical Chemistry
** Zernike Institute for Advanced Materials, University of
Groningen (The Netherlands)
*** Groningen Biomolecular Sciences and Biotechnology Institute,
University of Groningen (The Netherlands)

Description :

We present an extension of the Martini coarse grained force field to carbohydrates. The parameterization follows the same philosophy as was used previously for the parameterization of lipids and proteins, focusing on the reproduction of partitioning free energies of small compounds between polar and non polar phases. The carbohydrate building blocks considered are the monosaccharides glucose and fructose, and the disaccharides sucrose, trehalose, maltose, cellobiose, nigerose, laminarabiose, kojibiose, and sophorose. Bonded parameters for these saccharides were optimized by comparison to conformations sampled with an atomistic force field, in particular with respect to an accurate representation of the rotameric states. Application of the new coarse grained carbohydrate model to the oligosaccharides amylose and curdlan showed a preservation of the main structural properties, with three orders of magnitude more efficient sampling than the atomistic counterpart. Finally we investigated the cryoprotective effect of glucose and trehalose on a lipid bilayer, and found a strong decrease of the melting temperature, in good agreement with both experimental findings and atomistic simulation studies.

References: C.A. Lopez, A. Rzepiela, A.H. de Vries, L. Dijkhuizen, P.H. Hünenberger and S.J. Marrink
J. Chem. Theor. Comput., submitted (2009).

Title: Absolute single-molecule entropies from quasi-harmonic analysis of microsecond molecular dynamics: Correction terms and convergence properties.

Researchers: Riccardo Baron**
Philippe H. Hünenberger*
J. Andrew McCammon**

**Institute/
Group:** * Laboratory of Physical Chemistry
** Department of Chemistry and Biochemistry,
University of California San Diego, La Jolla (USA).

Description :

The convergence properties of the absolute single-molecule configurational entropy and the correction terms used to estimate it are investigated using microsecond molecular dynamics simulation of a peptide test system. The results are compared with previous applications for systems of diverse chemical nature. It is shown that: *(i)* the effect of anharmonicity is small; *(ii)* the effect of pairwise correlation is typically large; *(iii)* the latter affects to a larger extent the entropy estimate of thermodynamic states characterized by a higher motional correlation. The causes of such deviations from a quasi-harmonic behavior are explained and improved entropies calculated. Overall, this study emphasizes the need for extensive phase-space sampling in order to provide a reliable estimation of entropic contributions.

References: R. Baron, P.H. Hünenberger and J.A. McCammon
J. Chem. Theor. Comput., submitted (2009).

Title: Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling.

Researchers: Lovorka Perić-Hassler*
Halvor S. Hansen*
Riccardo Baron**
Philippe H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group: ** Department of Chemistry and Biochemistry,
University of California San Diego, La Jolla (USA).

Description :

Molecular dynamics simulations of the 11 glucose-based disaccharides in water at 1 bar and 300K are reported. The simulations were carried out using the GROMOS 45A4 force-field and the sampling along the glycosidic dihedral angles ϕ and ψ was artificially enhanced using the local elevation umbrella sampling (LEUS) method. The trajectories are analyzed in terms of free-energy maps in the space of the glycosidic dihedral angles, stable and metastable conformational states (relative free-energies and estimated transition timescales), intramolecular hydrogen-bonding (H-bonding), solute configurational entropies and agreement with experimental data. All disaccharides considered are found to be characterized either by a single stable (overwhelmingly populated) state ((1 \rightarrow n)-linked disaccharides with $n = 1, 2, 3$ or 4) or by two stable (comparably populated) states with a low interconversion barrier ((1 \rightarrow 6)-linked disaccharides). Metastable states are also identified with relative free energies in the range 8-22 kJ mol⁻¹. The 11 compounds can be classified into four families (which correlate with approximate topological symmetries) : (i) the $\alpha(1 \rightarrow 1)\alpha$ -linked disaccharide trehalose (axial-axial linkage) presents no metastable state, the lowest configurational entropy and no intramolecular H-bonds; (ii) the four $\alpha(1 \rightarrow n)$ -linked disaccharides ($n = 1, 2, 3$ or 4; axial-equatorial linkage) present one metastable state, an intermediate configurational entropy and two alternative intramolecular H-bonds; (iii) the four $\beta(1 \rightarrow n)$ -linked disaccharides ($n = 1, 2, 3$ or 4; equatorial-equatorial linkage) present two metastable states, an intermediate configurational entropy and one intramolecular H-bond; (iv) the two (1 \rightarrow 6)-linked disaccharides (additional glycosidic dihedral angle) present no (isomaltose) or a pair of (gentiobiose) metastable states, the highest configurational entropy and no intramolecular H-bonds. The results suggest that the observed conformational preferences are dictated by four main driving forces (conformational preferences of the residue rings, *exo*-anomeric effect, steric constraints, possible presence of a third glycosidic dihedral angle), leaving a secondary role to intramolecular H-bonding and specific solvation effects. In spite of the weak conformational driving force attributed to solvent-exposed H-bonds in water (highly polar protic solvent), intramolecular H-bonds may still have a significant influence on the physico-chemical properties of the disaccharide by decreasing its hydrophilicity. The calculated average values of the glycosidic torsional angles agree well with available experimental data, providing validation for the force-field and simulation methodology employed.

References: L. Perić-Hassler, H.S. Hansen, R. Baron and P.H. Hünenberger
J. Phys. Chem. B, to be submitted (2009).

Title: Interaction of alginate single-chain polyguluronate segments with mono- and divalent metal cations: A comparative molecular dynamics study.

Researchers: Lovorka Perić-Hassler*
Philippe H. Hünenberger*

Institute/ * Laboratory of Physical Chemistry
Group:

Description :

The interaction of a set of monovalent (Na^+ , K^+) and divalent (Mg^{2+} , Ca^{2+}) metal cations with single-chain homopolyguluronate segments of alginates (periodic chain based on a dodecameric repeat, 2_1 -helical conformation) is investigated using explicit-solvent molecular dynamics (MD) simulations (at 300 K and 1 bar). A total of 14 (neutralizing) combinations of the different ions are considered (single type of cation or simultaneous presence of two types of cation, either in the presence or absence of chloride anions). The main observations are that : (i) the chain conformation and intramolecular hydrogen-bonding is insensitive to the counter-ion environment; (ii) the binding of the cations is essentially non-specific for all ions considered (counter-ion atmosphere confined within a cylinder of high ionic density, but no well-defined binding sites); (iii) the density and tightness of the distributions of the different cations within the counter-ion atmosphere follow the approximate order $\text{Ca}^{2+} > \text{Mg}^{2+} > \text{K}^+ > \text{Na}^+$ (preferential affinity for divalent over monovalent cations, and for Ca^{2+} over Mg^{2+}); (iv) the solvent-separated binding of the cations to the carboxylate groups of the chain is frequent, and its occurrence follows the approximate order $\text{K}^+ > \text{Na}^+ > \text{Ca}^{2+} > \text{Mg}^{2+}$ (contact binding events as well as the binding of a cation to multiple carboxylate groups are very infrequent); (v) the counter-ion atmosphere typically leads to a complete screening of the chain charge within 1.0-1.2 nm of the chain axis, and charge to a reversal at about 1.5 nm (*i.e.* the effective chain charge becomes positive and as high in magnitude as one quarter of the bare chain charge at this distance, before slowly decreasing to zero). These findings agree well (in a qualitative sense) with available experimental data and predictions from simple analytical models, and provide further insight concerning the nature of alginate-cation interactions in aqueous solution.

References: L. Perić-Hassler and P.H. Hünenberger
Mol. Simul., to be submitted (2009).

Title: Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection.

Researchers: Daan P. Geerke*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/Group: * Laboratory of Physical Chemistry

Description :

Molecular dynamics simulation is used to investigate the interaction of the polyhydroxylated cosolutes (CSLs) methanol (MET), ethylene glycol (ETG), glycerol (GLY), glucose (GLU) and trehalose (TRH) in aqueous solution with the surface of rigid Lennard-Jones walls. The walls are designed to represent simplified models for biomolecular (membrane, protein) surfaces and include three functionalization variants: *(i)* non-polar (NP, no functionalization); *(ii)* semi-polar (SP, surface hydroxyl groups); *(iii)* highly-polar (HP, positive and negative surface charges). The simulations are performed to investigate, in a simplified context, the preferential affinity/exclusion properties of the different CSLs (compared to water), which are relevant for the phenomenon of bioprotection by polyhydroxylated compounds. The simulations are carried out at three different temperatures (300, 475 and 600 K), and a comparison to simulations involving pure water or the pure liquid CSLs MET, ETG and GLY is also undertaken. In aqueous solution, all CSLs considered evidence preferential affinity (compared to water) for the NP and SP walls. This effect increases in magnitude with increasing CSL size, and is due to the favorable driving force associated with the replacement of multiple water molecules at the wall surface by a single polyhydroxylated CSL molecule (the partial substitution occurring without significant change in the total number of wall-solution hydrogen bonds). The preferential affinity is significantly reduced for the HP wall (for MET, ETG and GLY, preferential exclusion is actually observed). This change is probably related to the higher efficiency of water (compared to the CSLs) in terms of electrostatic solvation (higher dielectric permittivity), and provides an interpretation for the observation that polyhydroxylated CSLs appear to show preferential affinity for the surface of membranes, but preferential exclusion for the surface of proteins.

References: D.P. Geerke, W.F. van Gunsteren and P.H. Hünenberger
Mol. Simul., to be submitted (2009).

Title: Convection and Magnetic Field Generation in Earth and Other Planets

Researchers:

Jon Rotvig
Martha Evonuk
Andrew Jackson
Chris Finlay
Andrey Sheyko

Institute Institut für Geophysik, Dept Erdwissenschaften
Group Earth and Planetary Magnetism Group

Description:

Convection in the liquid part of planets is a ubiquitous feature of the solar system. It is the mechanism by which heat is efficiently transported from the interior to the exterior, thus either cooling the planet through time or extracting heat generated internally, through radioactivity, gravitational contraction, chemical differentiation, or other processes. We see the signature of convection in the surface patterns of flow on the giant planets such as Jupiter and Saturn; planets that also possess strong magnetic fields. On the Earth we cannot see the convection in the liquid core *per se*, but we can detect the magnetic field with high resolution, observe its changes through time, and via paleomagnetic measurements of the magnetization of rocks attest to the fact that the magnetic field has been extant for the last 4 billion years. Thus our work is aimed at elucidating convection and magnetic field generation in the Earth and other planets. We use a mixture of spectral and finite volume codes to evolve the underlying fluid dynamical (Navier-Stokes, heat, electrodynamic) equations in time. Our recent work has concentrated on the generation of differential rotation in density-stratified giant planets, and mechanisms for reversals in the Earth.

References:

- Rotvig, J. (2009) An investigation of reversing numerical dynamos driven by either differential or volumetric heating . *Phys. Earth. Plan. Int.*, 176, 69-82.
- Glatzmaier, G.A., Evonuk, M. and Rogers, T. (2009) Differential rotation in giant planets maintained by density-stratified turbulent convection . *Geophys. Astrophys. Fluid Dyn.*, 103, 31-51.

Title: Mapping 3-D mantle conductivity from satellite data

Researchers: J. Velínský
Z. Martinec (DIAS Dublin)

Institute/ Institute of Geophysics

Group: Earth and Planetary Magnetism

Description:

The study of lateral variability in physical properties of Earth's mantle using geophysical methods is a topic of modern fundamental science. It gives insight into geodynamic processes such as mantle convection, the fate of subducting slabs and the origin of continents. Global seismic tomography provides today a variety of three-dimensional (3-D) mantle velocity models that can be interpreted in terms of cratonic roots, mantle plumes and slab graveyards. The goal of global electromagnetic (EM) induction studies is to identify complementary large-scale spatial variations (3-D structures) in the electrical conductivity of the mantle. This is an important issue since conductivity reflects the connectivity of constituents as fluids, partial melt, and volatiles (all of which may have profound effects on rheology and, ultimately, mantle convection and tectonic activity), while seismology ascertains bulk mechanical properties.

A new method of inverse global EM induction modeling has been developed, which is based on the time-domain approach. The core of the inverse method is a computationally effective evaluation of data sensitivity to changes of mantle conductivity using the solution of an adjoint problem. Nevertheless, the computational demands of the method are still high, as the diffusion equation for magnetic field has to be solved in the entire Earth's mantle many times. So far, the method has been benchmarked on synthetic data sets related to the future ESA multi-satellite mission *Swarm*. A simplified 2-D inversion was performed using data provided by the *Champ* satellite. These results suggest, that in the upper mantle, the northern hemisphere is more conducting, while at depths below 670 km, the situation is reversed.

References:

Martinec, Z., J. Velínský, The adjoint sensitivity method of global electromagnetic induction for CHAMP magnetic data. *Geophys. J. Int.*, in press.
Another manuscript in preparation

Title: The generation of seismic anisotropy in the Earth's inner core

Researchers:

Philippe Marti

Andrew Jackson

Institute Institut für Geophysik, Dept Erdwissenschaften

Group Earth and Planetary Magnetism Group

Description:

The Earth's inner core is elastically anisotropic. Seismic waves travel faster along the Earth's rotation axis than in the equatorial plane and display complex variations with depth. It has been proposed that this is caused by a preferred orientation of iron alloy crystals, for example due to Maxwell stresses, originating from magnetic forces, on the inner core. The Maxwell stresses and the resulting pattern of crystal alignment have been computed for candidate magnetic fields created by a self-consistent code simulating convection in the outer core of the Earth. As a result of motional induction associated with the convection, magnetic fields are self-excited by feedback from an existing field. For this project an existing 3D dynamo simulation code, based on a spectral expansion and finite differences, has been modified to improve its scalability and extended to use the HDF5 file format. It is used for the computation of more realistic magnetic forces acting on the inner core.

After stresses are calculated we compute the flow induced in the highly viscous inner core. Our ultimate aim is to couple the finite strains that develop with crystal slip systems (for example iron is thought to be hexagonally close-packed in the core) to predict and possibly explain the existence of observed seismic anisotropy.

Title: Simulations for High Current Plasma Arc in Three Dimensions for Circuit Breakers

Researchers: Harish Kumar
Prof. Rolf Jeltsch, Prof. Manuel Torrihon
Prof. Ralf Hiptmair, Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics, ETH Zürich

Description: The high-energy, high-current thermal plasma arc that develops between electric contacts in a gas circuit breaker during circuit interruption is an important phenomenon in the power transmission industry. The high temperature and pressure arc dissipates the tremendous amount of energy generated by the fault current, hence it protects the other parts of the circuit. In order to interrupt the current, the arc must be weakened and finally extinguished.

To simulate the complicated process containing high current plasma arc we use the equations of magnetohydrodynamics(MHD), that describe flow of plasma in presence of a magnetic field. In this project Runge-Kutta Discontinuous Galerkin (RKDG) methods for MHD are investigated and found suitable for these simulation. For the simulation of the problem containing shocks, we have implemented the various Riemann solvers and limiters in the code. We investigate the role of various Riemann solver in RKDG simulations, by examine the results of first-, second-,third-, and fourth-order simulations for both smooth and non-smooth problems. The spectral properties of RKDG schemes are also investigated by computing their approximate modified wavenumber.

To simulate the behavior of a plasma arc in 3D using RKDG methods for resistive MHD, we first generates the *numerical arc*. For this we assumes that there is an initial arc with the given current 100kA and applies boundary conditions for magnetic field depending on the incoming fault current of 100kA. This initial arc is simulated till steady state is reached. This is now considered to be the *actual arc*, that is used to study the effects of external magnetic fields on the arc. We apply an external magnetic field in the axial direction by adding it to the magnetic field of the arc and modifying boundary condition accordingly. This results in the rotation of the arc. In the Figure 1 above, the resulting velocity field is presented that is corresponding to the arc of 100kA and external magnetic field of 0.5 Tesla in axial direction. This rotation can be used to build a pressure in a adjacent chamber that can be used to extinguish the arc. This can result in significant reduction of the operating energy of the circuit breaker.

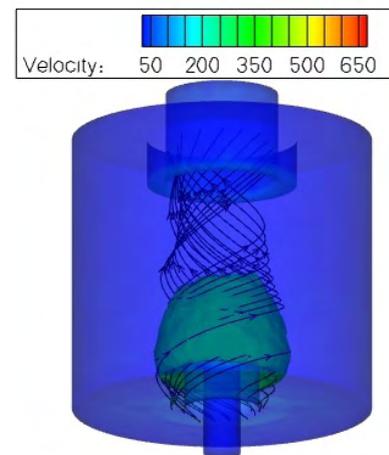


Figure 1: Rotation of the arc generated by the external magnetic field: Velocity profile in m/s .

Title: Turbulent reactive flow

Researchers: Michael Hegetschweiler
Gaurav Anand
Michael Wild
Mathias Hack
Benjamin Zoller
Patrick Jenny

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

Description:

Worldwide, more than 80% of the consumed energy is converted by burning fossil fuels. Therefore, improving emission rates and efficiency of combustion devices automatically has a significant impact on our environment and is of crucial importance. To achieve such improvements, however, the capability of accurately predicting the governing physical processes (which involve turbulence-reaction interaction) is essential. A modeling approach, which proved to be very general and powerful, is based on solving a joint probability density function (PDF) transport equation. Opposed to other approaches, such PDF methods require no model for turbulent convection and there exist no closure issues with averaging the reaction source terms.

PDF solution algorithm: Compared with Reynolds-averaged Navier-Stokes (RANS) models, PDF methods are computationally more expensive and challenging. Due to its high dimensionality, the PDF transport equation is solved by a particle method. Two algorithmic issues of great concern have been addressed. The first one deals with local particle time stepping, which allows to deal more efficiently with very slow flow regions and/or heterogeneous grids. The method greatly enhances the robustness and efficiency of PDF methods in general, but it is only applicable for statistically stationary scenarios. The second issue is related to accurate time integration of coupled systems of stochastic differential equations. Although applied here for PDF simulations, the devised scheme is more fundamental; e.g. we also employ it to solve problems related to kinetic gas theory.

Turbulent combustion modeling: In terms of modeling, we focus on five topics: multi-scalar mixing of reactive scalars, non-premixed turbulent combustion with local extinction and re-ignition, premixed turbulent combustion, spray combustion and NO_x formation. In all projects we employ a hybrid particle/finite-volume PDF framework and employ scale separation ideas to describe the statistics at the unresolved fine scales.

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M. A. Wild, B. T. Zoller, J. Allegrini, P. Jenny. Efficient NO Calculations in Turbulent Non-Premixed Flames Using PDF Methods. *Proceedings of the European Combustion Meeting*, 2009

M. L. Hack, J. Schmoker, P. Jenny. A Joint Probability Density Function (PDF) Model for Turbulent Premixed Combustion. *Proceedings of the European Combustion Meeting*, 2009

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M. Hegetschweiler, C. Handwerk, P. Jenny. Combustion Model Based on Joint Statistics of Progress Variable, Mixture Fraction and Scalar Dissipation Rate. *Combustion Science and Technology*, 2009

G. Anand, P. Jenny. A unified probability density function formulation to model turbulence modification in two-phase flow. *Phys. Fluids*, 2009

G. Anand, P. Jenny. Stochastic modeling of evaporating sprays within a consistent hybrid joint PDF framework. *Journal of Computational Physics*, 2009

G. Anand, P. Jenny. On the Influence of Droplet Parameters on Gas Turbulence. *Flow, Turbulence and Combustion*, 2009

Title: Flow and transport in porous and fractured media

Researchers: Manav Tyagi
Hadi Hajibeygi
Dimitris Karvounis
Giuseppe Bonfigli
Zarah Lakdawala
Patrick Jenny

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

Description:

Flow and transport in porous media has many applications in earth science, energy science, and many other areas. Examples in which we are interested are oil and gas recovery, CO₂ storage in geological sub-surface formations, geothermal power exploration, and automotive filters.

Multi-scale modeling: This is a collaboration with Dr. Seong Lee (Chevron). One of the major challenges in macroscopic simulations is the correct treatment of complex permeability distributions with strong variations and many length scales. To deal with this issue, various upscaling and multi-scale methods have been developed. In collaboration with the company Chevron we devised and developed a new multi-scale finite-volume (MSFV) algorithm, which has several advantageous properties compared with previous multi-scale methods. The MSFV method allows for very efficient studies of realistic multi-phase flow scenarios in heterogeneous porous media. Recently, we devised a general well model in this context and an iterative procedure, which allows to converge to the corresponding fine scale solutions, was developed. Moreover, a more rigorous treatment of compressibility effects was introduced. Currently, the MSFV method is used for a multi-physics framework, where Navier-Stokes and Darcy govern different regions of a domain. All contributions are relevant for the practical use of the MSFV method; not only for subsurface simulations, but e.g. also for computational fluid dynamics.

Hierarchical model of fractured reservoirs: This is an interdisciplinary collaboration with various earth scientists of ETH Zürich and Prof. Stephan Matthai (Mining University Leoben). In the context of geothermal power production, a modeling framework for flow and transport in fractured porous media is currently being created. It has proper interfaces which allow to interfere with rock mechanics and rock chemistry models. Moreover, everything is coupled with heat conduction in the rock. Due to the very large number of fractures, only the large ones will be resolved. The cloud of small fractures will be homogenized and treated by effective permeabilities. This project is a collaboration with various earth scientists.

Unconditionally stable non-linear solver: This is a collaboration with Prof. Hamdi Tchelepi (Stanford University) and Dr. Seong Lee (Chevron). While flow in porous media is governed by an elliptic or parabolic PDE, a hyperbolic system has to be solved to obtain the phase saturation distributions. The flux function for immiscible phase transport is S-shaped and with classical iteration schemes the time step size is severely restricted due to stability constraints.

A novel scheme was developed resulting in a much more efficient, unconditionally stable solver for phase transport.

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

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M. Tyagi, P. Jenny. Probability Density Function Modeling of Multi-Phase Flow in Porous Media. Submitted to *Journal of Computational Physics*, 2009

M. Tyagi, P. Jenny. Probability density function framework for modeling multi-phase ganglia flow in porous media. Submitted to *Journal of Fluid Mechanics*, 2009

Title: Radiation and light scattering in turbid media

Researchers: Milos Sormaz
Patrick Jenny

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

Description:

Radiation and scattering of electromagnetic waves are crucial for many research areas, including energy sciences. Two fundamentally different approaches are employed to model the governing phenomena: the first one, the analytic theory, is based on solving Maxwell's equations; the second one, the transport theory, considers transport of photons. Although less rigorous, the transport theory is the basis for most modeling efforts, which is due to major mathematical difficulties with the analytic theory.

PDF method to compute photon statistics: This is a collaboration with Tobias Stamm and Dr. Safer Mourad (EMPA). Based on the transport theory, we developed a modeled evolution equation for the photon number density and the joint PDF of photon propagation direction (and additional properties in the future). Compared with other models, which simply assume diffusion of the scattered photon concentration in the medium, the level of closure is much higher and the solutions contain more relevant statistical information. The algorithm was implemented and validated. In the course of this work, its value for color investigations related to halftone printing could be demonstrated. Recently, optical surface effects, fluorescence, polarization and spatially varying absorption characteristics were incorporated. Moreover, a second multi-scale level to deal with realistic halftone print has been developed. Depending on the scenario, this multi-scale approach can lead to speedup factors of several orders of magnitude.

References:

M. Sormaz, T. Stamm, S. Mourad, P. Jenny. Stochastic modeling of light scattering with fluorescence using a Monte Carlo based multi-scale approach. *Journal of Optical Society of America*, 2009

M. Sormaz, T. Stamm, P. Jenny. Stochastic modeling of polarized light scattering using a Monte Carlo based stencil method. Submitted to *Journal of Optical Society of America*, 2009

Title: Fluid dynamics in biological systems

Researchers: Johannes Reichold
Prof. Patrick Jenny

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

Description:

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

Modeling the cerebral blood flow: This is a collaboration with Prof. Bruno Weber (University of Zürich) and Prof. Alfred Buck (University Hospital Zürich). Cerebral blood flow (CBF) can be defined as the rate of delivery of arterial (nutritive) blood to the capillary beds of a particular mass of brain tissue. CBF assumes a fundamental role in homeostasis and neural activity as it regulates the supply of glucose and oxygen. A multi-scale approach has been developed to model CBF in a realistic vascular network. High-resolution 3D data of the cerebral angioarchitecture in animal models acquired by Prof. Weber's group are utilized. The imaged blood vessels are divided into groups of large, medium and small lumen. While large and medium vessels are fully resolved, the capillary bed is modeled as an isotropic grid. Pressure is assumed to be constant in the large vessels while it may vary for smaller sizes. Other vessel properties such as diameter and curvature are represented by a corresponding transmissibility value. Vasodilation during neural activity or partial occlusion in cerebrovascular impairment are examples of localized changes in vessel attributes. Recently, motivated by difficulties with appropriate boundary condition specifications, a stochastic framework for the generation of artificial but realistic vessel networks has been devised and implemented. Moreover, a hierarchical numerical homogenization approach to deal with the large number of capillaries was devised and tested.

Dynamics of flow with particles (erythrocytes) in capillary networks: This is a collaboration with Dr. Dominik Obrist (Institute of Fluid Dynamics, ETH), Prof. Bruno Weber (University of Zürich) and Prof. Alfred Buck (University Hospital Zürich). Although known that there is a rheological effect, if blood flows through capillary networks, this turned out to be much more dramatic than previously thought. It was first demonstrated with a discrete simulations, where simple, but well confirmed rules were applied at bifurcations to predict where along a blood cell proceeds. Then, a continuum model (average number of blood cells in a capillary segment is treated as a real number) was devised. The consequences are fascinating and have an enormous impact on our understanding of blood flow, erythrocyte transport and supply regulation e.g. in the brain cortex.

Stochastic modeling of hierarchical Salmonella infection: This is a collaboration with Prof. Wolfgang Hardt (ETH Zürich). After a Salmonella bacterium has docked to a host cell, various proteins get injected in a hierarchical order. Therefore, first a series of reactions have to take place. In order to confirm a hypothesis explaining the injection hierarchy of proteins,

stochastic particle simulations were performed. Later, it was shown how and under which conditions such a Monte Carlo modeling framework can be described by deterministic reaction mechanism, which can be solved much more efficiently.

References:

J. Reichold, M. Stampanoni, A. L. Keller, A. Buck, P. Jenny, B. Weber. Vascular graph model to simulate the cerebral blood flow in realistic vascular networks. *Journal of Cerebral Blood Flow and Metabolism*, 2009

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F. Haiss, R. Jolivet, M. T. Wyss, J. Reichold, F. Scheffold, M. P. Krafft, B. Weber. Lifting the curtain: Improved In vivo two-photon imaging after blood replacement by perfluorocarbon. Submitted to *Neuron*, 2009

Title: Development of numerical schemes and solution algorithms

Researchers: Giuseppe Bonfigli
Florian Müller
Patrick Jenny

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

Description:

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

Multi-scale finite-volume method for incompressible flows: The multi-scale finite-volume (MSFV) method, which we originally developed for multi-phase flow in porous media, was extended and modified to solve the Poisson equation for pressure arising in incompressible Navier-Stokes simulations. It was shown that especially in combination with the immersed boundary technique the performance of this new iterative linear solver, which can be interpreted as a domain decomposition or multi-grid method, is excellent.

High order immersed boundary method: A novel immersed boundary technique was developed to treat complex geometries with Cartesian grids. It was shown that 4th order spatial accuracy can be maintained at the boundary. Recently the method was extended for moving boundaries and will be generalized for fluid structure interaction problems.

Rankine Hugoniot solver: In this finite-volume approach, viscous and source terms are consistently distributed from the cell volumes to the cell surfaces. Moreover, the same idea can be employed to treat the time derivative term and flux derivatives perpendicular to the face normal direction. This results in piecewise constant states (in cells) fulfilling the Rankine Hugoniot conditions at all cell interfaces. As show earlier, this results e.g. in more accurate pressure solutions in flames. Currently, the method is revisited and further analyzed.

References:

G. Bonfigli, P. Jenny. An efficient multi-scale Poisson solver for the incompressible Navier-Stokes equations with immersed boundaries. *Journal of Computational Physics*, 2009

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P. Jenny, H. Tchelepi, S. Lee. Unconditionally convergent nonlinear solver for hyperbolic conservation laws with S-shaped flux functions. Journal of Computational Physics, 2009

G. Bonfigli, P. Jenny. Recent developments in the multi-scale-finite-volume procedure. Lecture Notes in Computer Science, LNCS, 2009

G. Bonfigli. Influence of the discretization order on the accuracy of an immersed-boundary procedure for incompressible flows. AIAA, 2009

Title: PDF modeling of non-equilibrium gas flow

Researchers: Hossein Gorji
Patrick Jenny

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

Description:

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

Stochastic particle method based Focker-Planck model: This is a collaboration with Prof. Manuel Torrilhon (ETH Zürich) and Prof. Stefan Heinz (University of Wyoming). A stochastic model and a solution algorithm to simulate the flow of gases, which are not in thermodynamic equilibrium was developed. For the interaction of a particle with others, statistical moments of the local ensemble have to be evaluated, but unlike in molecular dynamics simulations or DSMC, no collisions between computational particles are considered. In addition, a novel integration technique allows for time steps independent of the stochastic time scale. The stochastic model represents a Fokker-Planck equation in the kinetic description, which can be viewed as an approximation to the Boltzmann equation. This allows for a rigorous investigation of the relation between the new model and classical fluid and kinetic equations. The fluid dynamic equations of Navier-Stokes and Fourier are fully recovered for small relaxation times, while for larger values the new model extends into the kinetic regime. It could be demonstrated that the stochastic model is consistent with Navier-Stokes in that limit, but also that the results become significantly different, if the conditions for equilibrium are invalid. It could also be shown that the mass flow rate through a channel is correctly predicted as a function of the Knudsen number. Recently, a non-linear extension of the model do achieve consistency with respect to the Prandtl number has been devised.

References:

P. Jenny, M. Torrilhon, S. Heinz. A Solution Algorithm for the Fluid Dynamic Equations Based on a Stochastic Model for Molecular Motion. *Journal of Computational Physics*, 2009

Title: Hybrid LES/RANS modeling framework

Researchers: Heng Xiao
Patrick Jenny

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

Description:

While large eddy simulation (LES) is a very powerful approach to model turbulent flows, it is not yet widely used in industrial workflows. This is mainly due to the high computational cost, which is Reynolds number dependent, if wall turbulence is involved. Another difficulty is the choice of an appropriate computational grid. Motivated by these shortcomings, various hybrid LES/RANS methods have been proposed. A major challenge thereby is to determine the RANS and LES regions and to provide valid boundary conditions between them. Recently we started a project dealing with this topic in collaboration with Prof. Leonhard Kleiser (Institute of Fluid Dynamics).

Title: Morphing wing aerodynamics

Researchers: Vitali Dmitriev
Michael Gloor
Patrick Jenny

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

Description:

The technology of morphing wings has a high potential, since many more degrees of freedom can be employed to adapt and control a wing for different purposes in different environments. This project started recently and is a collaboration with Profs. Paolo Ermanni, Eduardo Mazza and Manfred Morari (ETH Zürich). Our role is to build predictive virtual models, which allow to design therequired structure and control algorithms.

References:

M. Gloor, D. Schafroth, P. Jenny. Efficient Algorithm for Aerodynamic Investigations of Micro Helicopters. Submitted to the Journal of the American Helicopter Society, 2009

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

Researchers: Lars Gräf, Andreas Jocksch and Leonhard Kleiser

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

Description:

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

In one project, we implemented ADM in the semi-industrial finite-volume code NSMB with full support of domain decomposition and parallel computing. We used NSMB with ADM to investigate film cooling of turbine blades, a state-of-the-art cooling technique. First, the dominant vortex structures (counter-rotating vortex pair, horseshoe vortex, hairpin vortices) of the flow were visualized. Furthermore, the flow inside and beneath the cooling holes, which is generally inaccessible to experimental measurements, has been analyzed. Second, the cooling efficiency is strongly influenced by the turbulence properties of the oncoming boundary layer. Using a recent technique for turbulent inflow generation which uses randomly distributed synthetic eddies of deterministic size, we have been able to demonstrate the effect of turbulent versus laminar boundary layer flow on this specific scenario.

In another project, we investigated the development of isolated turbulent spots in boundary layers at Mach numbers $M = 1.1$ and $M = 5$ by numerical simulations. The turbulent spots show typical properties known from the incompressible regime, e.g., the arrowhead-like shape of the spot with the downstream overhang region and streaks in the tail region. In the core region of the turbulent spots velocity profiles, skin friction and heat transfer were evaluated. For one parameter set at $M = 1.1$ turbulence statistics were analyzed by considering an ensemble of turbulent spots with slightly varying initial disturbances. Strong wall cooling leads to elongated turbulent spots. Simulations for the development of isolated turbulent spots have shown a good agreement between DNS and LES.

References: See separate list.

Title: Prediction of Jet Flows and Aeroacoustic Jet Noise using Large-Eddy Simulation

Researchers: Stefan Bühler, Felix Keiderling, Leonhard Kleiser, Tobias Luginsland, Dominik Obrist

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

Description:

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

In the work of Keiderling (Diss. ETH No. 17955, 2008) large-eddy simulations (LES) were performed using ADM as a subgrid-scale model. In order to trigger the turbulent breakdown of the jet, controlled disturbances were added to the initially laminar shear layer. These disturbances were derived from a linear stability analysis of the base flow configuration. Based on this and other numerical and experimental work it became obvious that the jet nozzle itself plays an important role in the jet noise simulations in order to bring results in closer agreement with experiments.

The present work deals with the integration of the nozzle into the existing simulation setup. The computational expense for the simulation at relevant Reynolds numbers is immense and will be further increased as the viscous sublayer of the flow within the nozzle now needs to be resolved in order to obtain reliable results with the LES approach. A massively parallel version of the existing code was developed using the Message Passing Interface (MPI) to achieve acceptable turn-around times of the jet simulations. The validation of the parallel code version including the necessary adaptations to account for the nozzle geometry in the simulation domain has been completed. The focus now lies on further optimizing the most time consuming routines so that the simulations including the nozzle can be performed more efficiently.

The perceived noise at remote observer locations can be determined most efficiently with an acoustic far-field solver which extrapolates the information of the underlying LES to the acoustic far-field. Apart from this classical application of far-field solvers, we also started to use such a solver for “listening” to different regions of the jet. With this “directional microphone” we try to understand which regions of the jet are emitting what frequencies in what directions.

References: See separate list.

Title: Simulation of Particle-Laden Flows

Researchers: Rolf Henniger, Leonhard Kleiser, Anna Kubik

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

Description:

This project is concerned with the direct and large-eddy simulation of miscible fluid flows. The motion of such flows is at least partially governed by its density differences. They can be caused either by different densities of the involved fluids or differential loadings of small suspended particles. The density differences are described either as concentration fields in an Eulerian framework or as Lagrangian particles. Accordingly, additional transport equations have to be solved.

For this purpose, a high-order accurate simulation code for the incompressible Navier-Stokes equations has been developed which is able to simulate flows with relatively high Reynolds numbers. A high order (typically fourth or sixth order) implies that high accuracy of the solution is reached at relatively little computational cost. In addition, the simulation code must be highly scalable with the problem size on massively-parallel computers. To this end, compact finite differences on staggered grids in space and a (semi-)implicit time integration scheme are employed to minimize the number of grid points and time steps at a prescribed accuracy. This approach allows an iterative solution for the pressure and an efficient 3D data decomposition. The scalability with the problem size has been demonstrated for a channel flow in a weak scaling test with up to 100 billion grid points and 400 billion unknowns. To further increase the Reynolds number, we added different sub-grid scale models to the simulation code to enable large-eddy simulations in the future.

Currently, the flow solver is applied to transitional and turbulent channel flows as well as multiphase flows such as simulations of a model estuary. There, it is the aim to study the mixing of fresh- with saltwater as well as the transport of suspended sediment particles or pollutants in the fluid.

Another sub-project aims at modeling abrasive water jet cutting. We carried out preliminary numerical studies on the particle-water interaction and air entrainment in compressible jets with high Reynolds numbers. Water jets with free surfaces were simulated with commercial and open-source CFD codes. We achieved good agreement with analytical solutions for single-phase configurations and reasonable and perspicuous results for two-phase flows.

References: See separate list.

Title: Fluid Mechanics of the Inner Ear

Researchers: Francesco Boselli, Leonhard Kleiser, Dominik Obrist, Stefan Hegemann*

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

* Dept. of Otorhinolaryngology, University Hospital Zurich

Description:

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

We study the (patho-)physiology of the semicircular canals and the cochlea with numerical simulations. While the cochlea requires a careful simulation of a highly unsteady flow with tight fluid-structure interaction, the simulation of the semicircular canals involves the simulation of particle sedimentation.

Settling particles in the semicircular canals (SCC) of the inner ear are suspected to be the most common cause for vertigo. This pathological condition is known as benign paroxysmal positional vertigo (BPPV) and affects almost 10% of all elderly people. However, only little is known about the mechanisms of BPPV.

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

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

References: See separate list.

Title: Preconditioned Methods for Large-Scale Model Reduction

Researchers: Christine Tobler
Daniel Kressner

Institute: Seminar for Applied Mathematics

Description:

A typical use of numerical simulations is the measurement and control of output quantities such as heat, noise, and stress at critical parts of the computational domain with respect to a selected set of input parameters. The fundamental idea of *mathematical model reduction* is that this input-output behaviour can often be well approximated by a much simpler model than needed for describing the entire state of the simulation.

Once model reduction has been performed, the original model can be replaced by the resulting simpler model, leading to reduced simulation times and greatly facilitating the further analysis and design of a control system. For instance, often only a low-order model allows for the use of more sophisticated robust and optimal control techniques. With the advances of modern control theory, model reduction has become an important and rapidly changing field with a large diversity of application areas, including structural and fluid dynamics, biosystems, and micro-electro-mechanical systems.

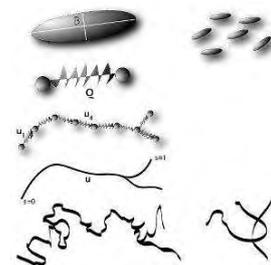
A wide variety of techniques has been developed to perform model reduction. For example, balanced truncation produces reduced models for which reliable a priori and a posteriori bounds on the approximation error are known. However, the computational demand of existing numerical algorithms currently precludes the application of balanced truncation to more complex models. The major goal of this project consists of the development and analysis of novel preconditioned and adaptive algorithms that retain the reliability of balanced truncation at a much lower computational cost. In the long run, these algorithms can be expected to significantly extend the applicability of model reduction to a wider range of models.

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D. Kressner. Memory-efficient Krylov subspace techniques for solving large-scale Lyapunov equations. In IEEE International Symposium on Computer-Aided Control Systems Design, San Antonio, pages 613-618, 2008.

Title: Theory for entangled polymeric melts and brushes, filamentous physical and chemical gels

Researchers: Prof. Martin Kröger¹
Prof. Yitzhak Rabin²
Prof. Avraham Halperin³
Prof. Manuel Laso⁴
Prof. Marc L. Mansfield⁵



Institutes: ¹ Computational Polymer Physics, D-MATL, ETH Zürich
² Tel Aviv University, Israel
³ CEA Grenoble, France
⁴ ETSII Madrid, Spain
⁵ Stevens Institute of Technology, Hoboken, U.S.A.

Description:

In order to understand the phase behavior and formation dynamics of helically wound networks we generalized the Janus chain model [1]. We investigated the structure, dimensions, and entanglement statistics of long linear polyethylene chains [2]. There is some demand to tune polymer thickness. To this end we developed a scaling theory for dendronized polymers, and compared with experiments performed in D-MATL [3]. Strong versus weak ternary protein adsorption onto brushes has been explored based on scaling theory [4]. In the area of topological analysis of polymeric melts we studied chain-length effects and developed fast-converging estimators for entanglement length [5]. A systematic time-scale-bridging molecular dynamics applied to flowing polymer melts has been developed [6], and detailed atomistic molecular-dynamics simulations of α -conotoxin AuIB in water were performed [7]. We studied the random packing of model polymers: Local structure, topological hindrance and universal scaling has been observed by us [8]. We reveal an effect of network topology on phase separation in two-dimensional Lennard-Jones networks [9]. Details available at <http://www.complexfluids.ethz.ch>

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- [5] R.S. Hoy, K. Foteinopoulou, M. Kröger, *Phys. Rev. E* **80** (2009) 031803.
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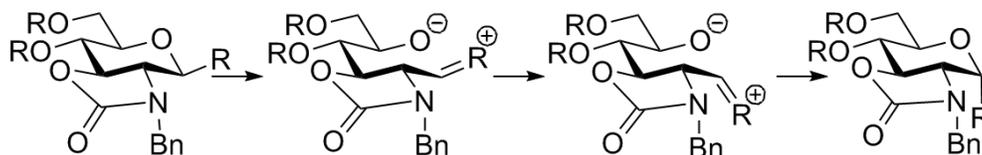
Title: *Endo*-cleavage Induced Anomerization of Pyranosides

Researchers: Hiroko Satoh^{1,2}
Shino Manabe³
Jürg Hutter⁴
Teodoro Laino⁴
Hans Peter Lüthi¹

Institute/Group: ¹Laboratory of Physical Chemistry, ETH Zurich, Switzerland
²National Institute of Informatics, Tokyo, Japan
³Advanced Science Institute, RIKEN, Saitama, Japan
⁴Institute of Physical Chemistry, University of Zürich, Switzerland

Description:

In carbohydrate chemistry, the mechanism of glycoside cleavage is a fundamental issue. Glycosides with an *N*-benzyl-2,3-*trans*-oxazolidinone group, a glycosyl donor for 1,2-*cis* stereoselective glycosylation, easily anomerize under mild acidic conditions.[1] Experimental evidence that the anomerization is caused by *endo*-cleavage rather than by *exo*-cleavage was obtained (Scheme below). *Endo*-cleavage in glycosides is rather uncommon, however.



Based on quantum chemical calculations, we found pronounced differences in the transition state energies between pyranosides with and without oxazolidinone groups attached.[2] This observation was confirmed by experiment. Based on this study, we are now exploring the reaction mechanism at greater detail performing *ab initio* molecular dynamics studies.

References:

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[2] Satoh, H.; Hutter J.; Lüthi H.P.; Manabe S.; Ishii K.; Ito Y. *Eur. J. Org. Chem.*, **2009**, 1127.

Title: Electron Delocalization and Conjugation Efficiency in Linearly π -Conjugated Compounds: A Donor-Acceptor Based Scheme

Researchers: Peter A. Limacher¹
Maurizio Bruschi²
Hans Peter Lüthi¹

Institute/Group: ¹Laboratory of Physical Chemistry, ETH Zurich, Switzerland
²Università degli Studi Milano-Bicocca, Milan, Italy

Description:

For the design of donor/acceptor functionalized π -conjugated compounds, electron delocalization is a widely used concept to make structure-property predictions. We developed a various schemes based on the Natural Bond Orbital (NBO) analysis to “measure” electron delocalization in π -conjugated compounds.[1] The method maps rather complex information obtained from quantum chemical calculations onto simple concepts used by the general chemist, and has been proven useful in a number of applications. For example, we were able to address the issues of efficiency of cross (*geminal*) versus through (*cis/trans*) conjugation.[2]

More recently, the method was extended towards the study of the conjugation efficiency, i.e. the ability of a conjugation path to support the interaction of donors and acceptors.[3] Different protocols were suggested and applied towards the study of the conjugation efficiency in various polyacetylenes. The study shows that the incorporation of triple bonds in a polyacetylene (PA) chain, to give polydiacetylene (PDA) or polytriacetylene (PTA), increases the total amount of π -delocalization, but, on the other hand, reduces the efficiency with which π -delocalization extends along the chain. This observation can be explained by means of the (donor-acceptor-)orbital-interaction patterns along the polymer chain. Whereas the interactions between like orbitals (double with double, triple with triple bonds) leads to smooth energy profiles, the interaction between unlike orbitals is usually smaller. The relatively weaker interaction between double and triple bonds results in a more limited flow of charge, i.e. a lesser degree of charge delocalization.[3]

References:

- [1] M.G. Giuffreda, M. Bruschi, and H.P. Lüthi, *Chemistry Eur. J.*, **2004**, *10*, 5671-5680.
- [2] M. Bruschi, M.G. Giuffreda, and H.P. Lüthi, *Chimia*, **2005**, *59*, 1-6.
- [3] M. Bruschi, P.A. Limacher, J. Hutter, and H.P. Lüthi, *J. Chem. Theory Comput.*, **2009**, *5*, 506–514.

Title: The COST Molecular Annotation Project (COSTMAP):
Quantum Chemical Data Archival, Retrieval and Search

Researchers: Stefano Borini¹
Peter A. Limacher¹
Martin Brändle²
Hans Peter Lüthi¹

Institute/Group: ¹Laboratory of Physical Chemistry, ETH Zurich
²Chemistry Biology Pharmacy Information Center, ETH Zurich

Description:

The availability of high-throughput computing of molecular properties is defining the need for databases of molecular structures, where each configuration can be decorated with QM-evaluated properties, data relationships, and user-generated annotations and evaluation. Sensible proof exist that this concept adds value for the user community (examples: the bioinformatics or the Cambridge Structural Database). However, the computational chemistry community is still missing a standard, public access database to share scientific knowledge and information.

The COST Molecular Annotation Project (COSTMAP) [1] is a prototype database implemented in our group, following an earlier feasibility study.[2] COSTMAP employs a graph-based data model to store, retrieve and represent molecular information. When fully operative, the database will allow search and retrieval of information both from the web and via scripting. Search criteria will be based on structural features, property values and user-produced annotations. Standard data formats, such as CML, RDF, and Q5Cost[2] will be used for maximum interoperability.

COSTMAP has been employed in discovery and active exploration of structural features of end-cap substituted polyacetylenes. Different combinations of substituents (two acceptor groups: NO₂ and CN, and two donors OH and NH₂) were applied to the polyene backbone. The geometries, optimized at the CAM-B3LYP level were then imported into COSTMAP. Thanks to the availability of visual inspection and easy access to all the computed molecules, we were able to find a systematic distortion pattern of the backbone shape, toward either Bow or S-shaped, depending on the chosen substitution (see corresponding article in this report).

References:

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- [3] S. Borini, A. Monari, E. Rossi, A. Tajti, C. Angeli, G.L. Bendazzoli, R. Cimiraglia, A. Emerson, S. Evangelisti, D. Maynau, J. Sanchez-Marin, P. G. Szalay, *J. Chem. Inf. Model.*, **2007**, *47*, 1271-1277.

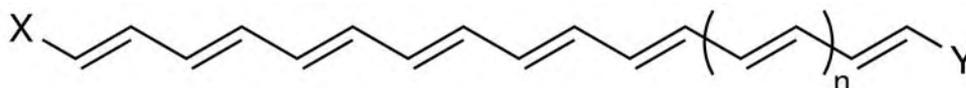
Title: Analyzing Bond Length Alternation and (Hyper)polarizability Properties of Polyacetylene Oligomer Chains using the Coulomb-Attenuating CAM-B3LYP Density Functional

Researchers: Peter A. Limacher
Hans Peter Lüthi

Institute/Group: Laboratory of Physical Chemistry, ETH Zürich

Description:

Although electron delocalization is a concept rather than a physical observable, it is used to explain a plethora of properties in π conjugated systems such as the polyacetylenes. Its presence and strength can be estimated by inspection of the carbon-carbon bond distances, especially the difference in length of a single and a double bond. Electronic properties such as the dipole polarizability and hyperpolarizabilities are also expected to depend strongly on the amount of π conjugation present in the system.[1]



However, it is known that standard density functional theory fails in predicting accurate geometries and, more importantly, severely overestimates hyperpolarizabilities for polymers of extended size due to an incorrect electric field dependence modeled by the the commonly used exchange functionals. This led to the development of long-range corrected density functionals containing range dependent contributions of DFT and HF exchange. We could show that the CAM-B3LYP functional delivers accurate geometries for polyacetylenic systems and removes the overestimation of hyperpolarizabilities to large parts.[2] Recent CCSD investigations on elongated oligomer chains show that the second hyperpolarizability might be calculated accurately even at the HF level of theory.[3]

References:

- [1] M. Bruschi, P.A. Limacher, J. Hutter, and H.P. Lüthi, *J. Chem. Theory Comput.*, **2009**, 5, 506–514.
- [2] P.A. Limacher, K.V. Mikkelsen, and H.P. Lüthi, *J. Chem. Phys.*, **2009**, 130, 194114.
- [3] P.A. Limacher, H.P. Lüthi, *in preparation*.

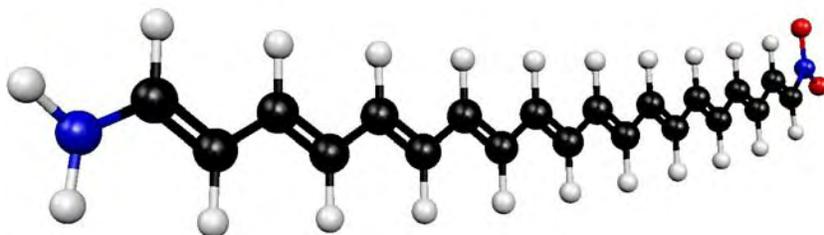
Title: A systematic analysis of the structure and (hyper-) polarizability of donor-acceptor substituted polyacetylenes using a Coulomb-attenuating density functional

Researchers: Stefano Borini
Peter A. Limacher
Hans Peter Lüthi

Institute/Group: Laboratory of Physical Chemistry, ETH Zurich

Description:

We performed a systematic investigation on all-*trans* polyacetylene chains of different lengths, end-capped with moieties of different donor or acceptor natures and different strengths, to infer useful structure/property relationship rules and behavioral patterns. The values for bond length alternation (BLA), longitudinal polarizability, and first and second hyperpolarizabilities have been computed by means of density functional theory with the Coulomb-attenuating B3LYP functional, using response theory. A comparison of the relative effect that each end-capping combination contributes to BLA, linear, and nonlinear optical coefficients has been performed. This results in useful insights and general rules to *ad hoc* tailoring the molecular response for a specific characteristic. [1]



The inspection of the optimized structures revealed that the donor-acceptor substituted polyacetylene chains are not perfectly linear, but take a slight bow- or S-shape, depending on the chosen substitution (bow shape for heteropolar- and S-shape for homopolar substitution). [2]

References:

- [1] S. Borini, P.A. Limacher and H.P. Lüthi, *J. Chem. Phys.*, **2009**, *131*, 124105.
[2] S. Borini, P.A. Limacher and H.P. Lüthi, *J. Phys. Chem. A*, *accepted*.

Title: Systematic Study of Electronic Properties of
Zintl Phases with Novel Magnetism

Researchers: Eduardo Cuervo Reyes
Reinhard Nesper

Institute/ Laboratory of Inorganic Chemistry
Group: Solid State

Description

Zintl phases are formally considered diamagnetic semiconductors. Nevertheless, it has been observed recently in some theoretical calculations, that when they contain 1-dimensional silicon substructures, they can be bad metals and show weak paramagnetism. In addition, unexpected ferromagnetic behaviour has been recently observed in some of these main group compounds (CaSi, SrSi and BaSi). We wonder about how ferromagnetism can take place in systems without d and/or f electrons. Aiming to understand this, DFT first-principles electronic structure calculations have been performed. Since the actual details of the electrons density can be an important clue for the observed behaviour and the theoretical partitioning of the charge can depend of the basis used, systematic-calculations have been carried using several basis and projection techniques. Consistently, these solids are predicted as metallic due to a small overlap of the anion-derived and cation-derived bands with a significant contribution of d states. The density of states at the fermi level is too low to satisfy the Stoner criterion. These results, together with the complementary experimental data, suggest that the ferromagnetism observed can be due to a Bloch's transition of the low density electron gas. On a slightly different line, a minimal tight-binding model was elaborated and is being solved in the time-dependent Hartree-Fock approximation at finite temperature, in order to understand the role of different interactions in the band-insulator metal transition.

References

Manuscripts in preparation

Title: Time-Dependent Visualization of Lagrangian Coherent Structures by Grid Advection

Researchers: F. Sadlo, R. Peikert

**Institute/
Group:** Institute of Visual Computing
Computer Graphics Laboratory

Description:

Lagrangian coherent structures play an important role in the analysis of unsteady vector fields because they represent the time-dependent analog to vector field topology. Nowadays, they are often obtained as ridges in the finite-time Lyapunov exponent of the vector field. However, one drawback of this quantity is its very high computational cost because a trajectory needs to be computed for every sample in the space-time domain. One of the foci of this paper are Lagrangian coherent structures that are related to predefined regions such as boundaries, i.e. related to flow attachment and flow separation phenomena. It presents an efficient method for computing the finite-time Lyapunov exponent and its height ridges only in these regions, and in particular, grid advection for the efficient computation of time series of the finite-time Lyapunov exponent, exploiting temporal coherence.

References:

in: Topology-Based Methods in Visualization III, Springer (to appear), 2009.

Title: Predictor-Corrector Schemes for Visualization of Smoothed Particle Hydrodynamics Data

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

**Institute/
Group:** Institute of Visual Computing
Computer Graphics Laboratory

Description:

In this paper we present a method for vortex core line extraction which operates directly on the smoothed particle hydrodynamics (SPH) representation and, by this, generates smoother and more (spatially and temporally) coherent results in an efficient way. The underlying predictor-corrector scheme is general enough to be applied to other line-type features and it is extendable to the extraction of surfaces such as isosurfaces or Lagrangian coherent structures. The proposed method exploits temporal coherence to speed up computation for subsequent time steps. We show how the predictor-corrector formulation can be specialized for several variants of vortex core line definitions including two recent unsteady extensions, and we contribute a theoretical and practical comparison of these. In particular, we reveal a close relation between unsteady extensions of Fuchs et al. and Weinkauff et al. and we give a proof of the Galilean invariance of the latter.

When visualizing SPH data, there is the possibility to use the same interpolation method for visualization as has been used for the simulation. This is different from the case of finite volume simulation results, where it is not possible to recover from the results the spatial interpolation that was used during the simulation. Such data are typically interpolated using the basic trilinear interpolant, and if smoothness is required, some artificial processing is added. In SPH data, however, the smoothing kernels are specified from the simulation, and they provide an exact and smooth interpolation of data or gradients at arbitrary points in the domain.

References:

IEEE Transactions on Visualization and Computer Graphics, Vol. 15, (to appear), 2009.

Title: HFN, a 128-bit High Precision Arithmetic Package for IBM CELL and Intel Multi-core processors.

Researchers: Wes Petersen†, David H. Bailey§
François Gaignat†, Mauro Calderara‡
Tobias Setz†, Aneesh Pande†

Institute: †Seminar for Applied Mathematics, ETH Zürich
‡Dept. of Physics, ETH Höggerberg
§NERSC, Lawrence Berkeley National Laboratory

Description:

Due to ill-conditioning, many applications require high precision arithmetic to supplement double or single precision available in multi-core hardware. In particular, the IBM CELL Broadband Engine used in Playstations and various blades, has strong 32-bit support, and now double (64-bit) on expensive blades. Because the CELL has powerful hardware facilities for handling 128-bit *vectors*, it seems reasonable to use this hardware for extended arithmetic. Two projects were completed: 128-bit arithmetic on the SPU (synergistic processing units) on the CELL, and likewise a similar SSE implementation on Intel multi-core. Both processors have extensive facilities for handling parallel 4-word (ea. 32-bit) data streams. One master's thesis (Gaignat), one Diplomarbeit (Calderara), and two Bachelorarbeit theses (Setz and Pande) were completed. Parallel versions over the 8 SPUs per CELL, each close to the hardware using 128-bit vectors on each SPU, were implemented by Gaignat. Calderara took the basic arithmetic operations (+, −, *, /) and implemented $\sqrt{\quad}$, log, exp, and powers x^m distributed over the SPUs.

Since the vector hardware on Intel multi-core is similar to that of the CELL, Setz and Pande ported and optimized the (+, −, *, /) operations on an Intel 4-core processor donated by Intel, Munich. The work was supervised by W. Petersen, SAM, ETHZ and D. Bailey, NERSC, Lawrence Berkeley National Laboratory, Berkeley, CA.

References:

- [1] M. Calderara, DiplomaArbeit, Sept. 8, 2009, ETHZ
- [2] F. Gaignat, Master's Thesis, 6 Aug. 2009.
- [3] T. Setz & A. Pande, Bachelor Theses, 5 Nov. 2009.

Title: Global Analysis of the High Resolution Infrared Spectrum of Methane $^{12}\text{CH}_4$ in the Region from 0 to 4800 cm^{-1}

Researchers: S. Albert *, S. Bauerecker**, V. Boudon***, L. R. Brown****, J.-P. Champion**, M. Loëte**, A. Nikitin*****, M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106 Braunschweig
*** Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9 Avenue Alain Savary, F-21078 Dijon
**** Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, California 91109, USA
***** Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 634055 Tomsk, Russia

Description:

We report the global analysis of methane ($^{12}\text{CH}_4$) lines from high resolution rovibrational spectra including accurate line positions and intensities in the region 0 – 4800 cm^{-1} . This covers four polyads: The Ground State Monad (rotational levels), the Dyad (940–1850 cm^{-1} , 2 vibrational levels, 2 sublevels), the Pentad (2150–3350 cm^{-1} , 5 vibrational levels, 9 sublevels) and the Octad (3550–4800 cm^{-1} , 8 vibrational levels, 24 sublevels) and some of the associated hot bands (Pentad–Dyad and Octad–Dyad). New Fourier transform infrared (FTIR) spectra of the Pentad and Octad regions have been recorded with a very high resolution (better than 0.001 cm^{-1} instrumental bandwidth, unapodized) at 78 K using the Bruker IFS 125 HR Zürich prototype (ZP2001) spectrometer in combination with a long optical path collisional cooling system [2]. Existing spectra previously recorded with the FTIR spectrometer at the National Solar Observatory on Kitt Peak in Arizona were remeasured selectively to provide new intensities and positions of weaker lines above 4400 cm^{-1} . These were combined with previously reported absorption data from FTIR and laser absorption, as well as high-resolution stimulated Raman and microwave spectra. The effective hamiltonian was expanded up to order 6 for the Ground State, order 6 for the Dyad, order 5 for the Pentad and order 5 for the Octad. Using extensive computations, a total of 16738 line positions were used in the least squares adjustment.

References:

1. S. Albert, S. Bauerecker, V. Boudon, L. R. Brown, J.-P. Champion, M. Loëte, A. Nikitin, and M. Quack, *Chem. Phys.* 356, 131 – 146 (2009).
2. S. Albert, S. Bauerecker, M. Quack and A. Steinlin, *Mol. Phys.*, 105, 541 – 558 (2007)

Title: Education about the Use of Quantities, Units and Symbols in Chemistry: The Earlier the Better

Researchers: J. Stohner*
M. Quack**

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

Description:

The so called IUPAC (International Union of Pure and Applied Chemistry) “Green Book” has a long history. The third, revised and enlarged edition was published recently by IUPAC and the Royal Society of Chemistry [1].

The intention of the Green Book ever since its appearance was not to present a list of recommendations as commandment, but rather, its aim was and still is to help the user in what may be called a “good practice of scientific usage”. Many well established conventions are used in science and technology, but mixing conventions can lead to misunderstandings or even cause severe errors. One of those errors caused by confusion of metric and imperial units led to the loss of the NASA Mars Climate Orbiter (MCO) in 1999. The failure cost about 200 Million USD worth of equipment and a non-quantifiable loss of scientific data and work. The “green book” contains a number of most up-to-date tables of particular use also in computational chemistry.

References:

1. J. Stohner, M. Quack, Education About the Use of Quantities, Units and Symbols in Chemistry: The Earlier the Better, in Chemistry Education in the ICT Age, Chapt. 31, pp. 339-344, (Eds.: M. Gupta-Bhowon, S. Jhaumeer-Laulloo, H. Li Kam Wah, P. Ramasami), Springer Science + Business Media B.V., 2009.
2. E. R. Cohen, T. Cvitas, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, and A. J. Thor, Quantities, Units and Symbols in Physical Chemistry, 3rd edition, second corrected printing. (IUPAC and Royal Society of Chemistry, RSC Publishing, Cambridge, 2008).
3. J. Stohner, M. Quack, A Concise Summary of Quantities, Units and Symbols in Physical Chemistry, IUPAC & Royal Society of Chemistry, Cambridge, 2009.
4. Japanese Translation of ref. 2 published in 2009
5. J. Stohner, M. Quack, Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular Spectroscopy, in “Handbook of High Resolution Spectroscopy, (Eds.: M. Quack, F. Merkt), Wiley, 2010, manuscript in preparation.

Title: Intramolecular Vibrational Energy Redistribution Measured by Femtosecond Pump-Probe Experiments in a Hollow Waveguide

Researchers: A. Kushnarenko*
V. Krylov**
E. Miloglyadov*
M. Quack*
G. Seyfang*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** State Optical Institute, St. Petersburg

Description:

In femtosecond pump-probe experiments the intramolecular vibrational energy redistribution has been investigated in the gas phase for CF_3CHF_2 , CH_2Br_2 , CH_2BrCl , C_6H_6 . To increase the measured probe signal the experiments have been performed in a hollow waveguide. The results were analyzed by means of computations in terms of intramolecular rate processes.

References:

A. Kushnarenko, V. Krylov, E. Miloglyadov, M. Quack, and G. Seyfang, in *Ultrafast Phenomena XVI*, Proceedings of the 16th International Conference on Ultrafast Phenomena, Stresa, Italia, June 2008, edited by P. Corkum, S. De Silvestri, K. A. Nelson, E. Riedle, and R. W. Schoenlein (Springer, Berlin, 2009), Vol. 92, pp. 349-351.

Title: High Resolution Near Infrared Spectroscopy and Vibrational Dynamics of Dideuteromethane (CH₂D₂)

Researchers: O. N. Ulenikov*
E. S. Bekhtereva*
S. Albert**
S. Bauerecker***
H. Hollenstein**
M. Quack**

Institute/Group: * Laboratory of Molecular Spectroscopy, Physics Department, Tomsk State University, RU-634050 Tomsk,
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
*** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106 Braunschweig

Description:

We report the infrared spectrum of CH₂D₂ measured in the range from 2800 to 6600 cm⁻¹ with the Zurich high-resolution Fourier transform interferometer Bruker IFS 125 prototype (ZP 2001, with instrumental bandwidth less than 10⁻³ cm⁻¹) at 78 K in a collisional enclosive flow cooling cell used in the static mode. Precise experimental values (with uncertainties between 0.0001 and 0.001 cm⁻¹) were obtained for the band centers by specific assignment of transitions to the $J = 0$ level of 71 vibrational levels. In combination with 22 previously known band centers, these new results were used as the initial information for the determination of the harmonic frequencies, force constant parameters F_{ij} , anharmonic coefficients, and vibrational resonance interaction parameters. A set of 47 fitted parameters for an effective Hamiltonian reproduces the vibrational level structure of the CH₂D₂ molecule up to 6600 cm⁻¹ with a root-mean-square deviation $d_{\text{rms}} = 0.67$ cm⁻¹. The results are discussed in relation to the multidimensional potential hypersurface of methane and its vibrational dynamics.

References:

O. N. Ulenikov, E. S. Bekhtereva, S. Albert, S. Bauerecker, H. Hollenstein, and M. Quack, *J. Phys. Chem. A* **113** (10), 2218-2231 (2009).

Title: Analysis of the High Resolution IR-Spectrum of $^{13}\text{CH}_4$ in the 2200 – 4700 cm^{-1} region: The Pentad and the Octad

Researchers: H. M. Niederer*
S. Albert*
S. Bauerecker**
M. Quack*
V. Boudon***
J. P. Champion***

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106 Braunschweig
*** Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9 Avenue Alain Savary, F-21078 Dijon

Description:

Besides many applications ranging from astrophysics to atmospheric pollution and combustion engines methane is also of fundamental importance for understanding molecular quantum dynamics and potential hypersurfaces [1,2,3]. In this context spectroscopic studies of methane are important. We have carried out new high resolution measurements of infrared spectra of methane and its isotopomers $^{12}\text{CH}_4$ [4], $^{13}\text{CH}_4$ [5], $^{12}\text{CH}_3\text{D}$, $^{12}\text{CH}_2\text{D}_2$, $^{12}\text{CHD}_3$ and $^{12}\text{CD}_4$. The spectra have been taken in the range 1800 – 8000 cm^{-1} at low temperature (80 K) and at room temperature (293 K) using the Zürich prototype Bruker 125 spectrometer (ZP 2001) in combination with a low temperature cooling cell. Low temperature, giving rise to reduced Doppler widths (by a factor of 1.9) and very high resolution (0.0027 cm^{-1} for spectra in the region around 3000 cm^{-1}), made it possible to determine line positions very accurately, i.e. for $^{13}\text{CH}_4$ better than 10^{-4} cm^{-1} around 3000 cm^{-1} . We have studied $^{13}\text{CH}_4$ spectra in its pentad region (2250 – 3250 cm^{-1}). Now we are analyzing the octad region (3800 – 4750 cm^{-1}), recently analyzed for the isotopomer $^{12}\text{CH}_4$ [4]. We present an initial analysis of this region counting 8 levels, discuss the observed strong interactions and compare to the work on $^{12}\text{CH}_4$ [4].

References:

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3. R. Marquardt and M. Quack, J. Phys. Chem. A., 108, 3166 (2004).
4. S. Albert, S. Bauerecker, V. Boudon, L. R. Brown, J. P. Champion, M. Loëte, A. Nikitin and M. Quack, Chem. Phys., 356, 131 (2009) and doi:10.1016/j.chemphys.2008.10.019
5. H. M. Niederer, S. Albert, S. Bauerecker, V. Boudon, J. P. Champion and M. Quack, Chimia, 62, 273 (2008).

Title: Nuclear Spin Symmetry Conservation of Methane in the Gas Phase at 16 K

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

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106 Braunschweig

Description:

The principles of approximate parity and nuclear spin symmetry conservation in molecular processes are among the most useful insights in molecular dynamics and spectroscopy [2]. However, as these are only approximate symmetries, attempts to find their violations have been suggested and undertaken in practice [3,4], including an early FTIR-study of CH₄ in supersonic jets and studies by cw-cavity ring down spectroscopy of supersonic jets [6]. We study here again methane CH₄ in the gas phase at very low temperature for the understanding of the spin conversion mechanism and energy transfer within excited quantum levels with a new experimental technique in this context. Methane was cooled down to at most liquid Helium temperature using a collisional cooling cell connected to the Zürich prototype Bruker 125 FTIR spectrometer. Spectra have been taken in the spectral region between 2800 and 3600 cm⁻¹ in which transitions to the isolated ν₃ band have been observed with an estimated absolute wavenumber accuracy better than 10⁻⁵ cm⁻¹. Due to a rapid non-equilibrium cooling process, non-thermal populations of various nuclear spin isomers have been achieved, i.e. non-equilibrium intensity ratios in infrared absorption have been observed. The spectra could be simulated with effective rotational temperatures of about 16 and 27 K under different conditions, and assuming conservation of nuclear spin symmetry upon cooling. An upper bound for the conversion rate between A, E and F nuclear spin isomers can be estimated from the residence time of the molecules in our experimental setup. We have also carried out extensive measurements of spectra of ¹²CH₄ and ¹³CH₄ under equilibrium conditions at about 80 K in the spectral range covering almost the whole infrared up to 12000 cm⁻¹ and we shall discuss the preliminary analysis of these data.

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Title: High Resolution Infrared Spectroscopy of Oxirane Carbonitrile

Researchers: K. K. Albert*
S. Albert*
M. Quack*
J. Stohner**

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

Description:

Precursor molecules of evolution like oxirane carbonitrile [2] are of interest in relation to possible astrophysical observation using spectroscopy [3, 4]. As a chiral molecule, the heterocyclic molecule CH₂OCHCN (cyanooxirane or in systematic nomenclature oxirane carbonitrile) is also of potential interest when relating biomolecular evolution and molecular parity violation [4,5]. We report here results of a high resolution infrared spectroscopic study of the ν_{13} and ν_{12} bands ($\nu_0 = 849.11 \text{ cm}^{-1}$ and $\nu_0 = 915.27 \text{ cm}^{-1}$, respectively). In general, the highly resolved infrared spectra of chiral molecules are difficult to assign because of their complex structure. Many of the high resolution infrared studies of these molecules available to date have been performed in our group [6,7], including those of the three-membered heterocyclic ring compounds d1-oxirane and fluoro-oxirane [8,9]. The work reported here expands importantly upon this foundation. The analyses use extensive computations.

References:

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Title: The Rovibrational Analysis of the CH Stretching Fundamental of CHD₂I

Researchers: C. Manca Tanner*
S. Albert*
M. Quack*

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

Description:

Intramolecular vibrational energy redistribution (IVR) is a central primary process in chemical reaction dynamics [2, 3]. The corresponding time evolution can either be obtained from high-resolution IR spectra or the IVR process can be studied in femtosecond pump-probe experiments [3,4]. Recent work in our group has shown that CH₃I and its various deuterated isotopomers have IVR-times on the order of 200 fs to 400 ps [4]. This wide range of redistribution times indicates different intramolecular coupling schemes for the initially excited vibrational levels, in agreement with a recent effective hamiltonian analysis including strong anharmonic resonances up to the CH stretching polyad $N = 4$ [5].

The present work is part of a larger effort to understand IVR in CH₃I, CH₂DI, and CHD₂I on the basis of high resolution spectra ranging from the far infrared to the near infrared and visible. We have recorded spectra with our high resolution FTIR spectrometer with a resolution reaching 0.0008 cm⁻¹. Here we present a detailed rovibrational analysis of the CH-stretching fundamental ν_1 at 3029.67918 cm⁻¹. Numerous local and global resonances have been found. We compare our new results with our recent work on the overtone spectra and dynamics [4-6]. In particular, we discuss the assignment of high J value and $K_a \geq 6$ levels and possible dark states that may perturb the rotational pattern.

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3. M. Quack, Chapter 27 in Femtosecond Chemistry, J. Manz and L. Woeste, eds. Verlag Chemie (Weinheim, 1995); M. Quack, Chimia, 55, 753 (2001) and citations therein.
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Title: Second Overtone Spectra of the NH-Stretching Vibration in C₆H₅NH₂, C₆D₅NH₂ and C₆H₅NHD Measured in a Molecular Beam by Isotope Selective Overtone Spectroscopy (ISOS)

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

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

Description:

The investigation of the vibrational structure and dynamics in aniline has a long history. The inversion motion of the NH₂ group over the plane of the phenyl ring can be described by a double well potential with a saddle point of the potential hypersurface at the planar geometry. An early determination [2] led to a barrier of about 450 cm⁻¹. The tunneling process through the barrier splits the ground state and also many vibrationally excited states into two tunneling components. The dependence of the effective inversion tunneling potential upon the excitation of some vibrational modes was approximately treated using the quasiadiabatic channel reaction path Hamiltonian (RPH) [3]. Supersonic jet ISOS spectroscopy has been used in our group to measure the tunneling splitting in the first NH-stretching overtone region of C₆H₅NH₂ and C₅H₅NHD, showing NH-stretching to be an inhibiting mode [3,4]. The main goal of the present experiments is the measurement of the vibrationally state resolved spectra of the second NH-stretching overtone of rotationally cold C₆H₅NH₂, C₆D₅NH₂ and C₅H₅NHD anilines by the ISOS method [3], in a molecular beam. Comparison of the assignment for C₆D₅NH₂ and normal aniline C₆H₅NH₂ confirmed the applicability of the normal mode model to NH₂ chromophore in aniline. The vibrational analysis on the basis of overtone data, including Fermi coupling between NH-stretching and symmetric NH₂- bending overtone, is presented as well as our most recent results of the -NHD isotopomer.

References:

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Title: Cavity-Enhanced Saturation Spectroscopy of the $\nu_1 + \nu_3$ -state of ammonia

Researchers: F. Ünlü
P. Dietiker
M. Quack
A. Schneider
G. Seyfang
A. Tehlar

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

Description:

The experimental investigation of parity violation in chiral molecules is of high importance for fundamental aspects of symmetry in physics and chemistry [2, 3]. Parity violation leads to a small energy difference $\Delta_{pv}E$ (on the order of 100 aeV) between the ground states of the enantiomers of chiral molecules. While it has been discovered in theoretical work from our group in 1995 that $\Delta_{pv}E$ is much larger (one to two orders of magnitude typically) than previously anticipated, and this has been confirmed by numerous calculations reviewed in [2,3,4], this effect has not yet been measured experimentally [3]. One of the highly promising high resolution experiments to measure the parity-violating energy difference $\Delta_{pv}E$ requires a sequence of absorption and emission processes at high resolution [3,5]. In preparation for these experiments a stimulated emission experiment is set up which is also used for saturation spectroscopy of NH_3 to test the enhancement cavity for the pump laser and the stability of the frequency lock. The pump laser is a tuneable external cavity diode laser with an output of 5 mW, which has to be increased in an enhancement cavity to achieve the necessary intensities for stimulated emission and saturation spectroscopy. Using narrow line width lasers, saturation spectroscopy allows for Doppler free spectroscopy and lines can be resolved which cannot be separately detected even in cooled samples with linear spectroscopic methods, like FTIR or diode laser absorption spectroscopy. We report Lamb-dip spectra of a number of lines of the $\nu_1 + \nu_3$ -state of NH_3 with a typical width (FWHM) in the order of 3 MHz, a resolution, which could not be achieved in general in previous experiments.

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5. M. Quack, *Chem. Phys. Lett.*, 132(2), 147-153 (1986)

Title: Intramolecular Vibrational Energy Redistribution Measured by Femtosecond Pump-Probe Experiments

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

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

Description:

Intramolecular vibrational energy redistribution (IVR) is one of the key aspects for our understanding of molecular dynamics and is essential for unimolecular reaction rate theory [2,3]. From high-resolution infrared (IR) -spectra or ab initio calculations one can derive the time evolution of the vibrational wavefunction or else the IVR process can be studied by femtosecond pump-probe experiments [3-6]. In our femtosecond pump-probe experiments a strong pump pulse in the near-IR is followed by a weak and temporally delayed probe pulse either in the UV or in the IR to measure the time evolution of the effective UV- or IR-absorption cross-section.

For methyl iodides and different partially deuterated methyl iodides three different relaxation times ranging from 200 fs to 400 ps have been found, when exciting the first overtone region of the CH-stretching vibration around 6000 cm^{-1} . For CHD_2I the IVR dynamics shows also an oscillatory behaviour. From the analysis of overtone spectra of $\text{CH}_3\text{-C}\equiv\text{CH}$, $\text{CF}_3\text{-C}\equiv\text{CH}$, and $(\text{CF}_3)_3\text{C-C}\equiv\text{CH}$ in comparison with numerous alkyl-CH compounds it was concluded that IVR for the alkyl-CH-stretching vibration is typically between one and three orders of magnitude faster than the IVR of the acetylenic CH-stretching vibration [2-8]. These conclusions could be confirmed in our femtosecond pump-probe experiments for different propargyl halides of the type $\text{CH}_2\text{X-C}\equiv\text{CH}$.

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Title: Localizing normal modes in large molecules

Researchers: Christoph R. Jacob
Markus Reiher

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

Description:

While nowadays efficient quantum chemical methods allow for the calculation of vibrational spectra of large (bio-)molecules, such calculations provide a large amount of data and the results are difficult to analyze. In particular for the vibrational spectra of polypeptides, a large number of close-lying normal modes contribute to each of the experimentally observed bands, which hampers the analysis considerably.

We have shown how vibrational spectra obtained from quantum chemical calculations can be analyzed by transforming the calculated normal modes contributing to a certain band in the vibrational spectrum to a set of localized modes. This is achieved by determining the unitary transformation that leads to modes which are maximally localized with respect to a suitably defined criterion. We have demonstrated that these localized modes are more appropriate for the analysis of calculated vibrational spectra of polypeptides and proteins than the normal modes, which are usually delocalized over the whole system. Both the frequencies at which the bands in the vibrational spectra appear and the total intensities of these bands can be interpreted in terms of the localized modes. Furthermore, coupling constants for the interaction between the localized modes, which make it possible to rationalize the observed band shapes, can be extracted from the calculations.

References: Ch. R. Jacob, M. Reiher, *J. Chem. Phys.* **2009**, *130*, 084106.

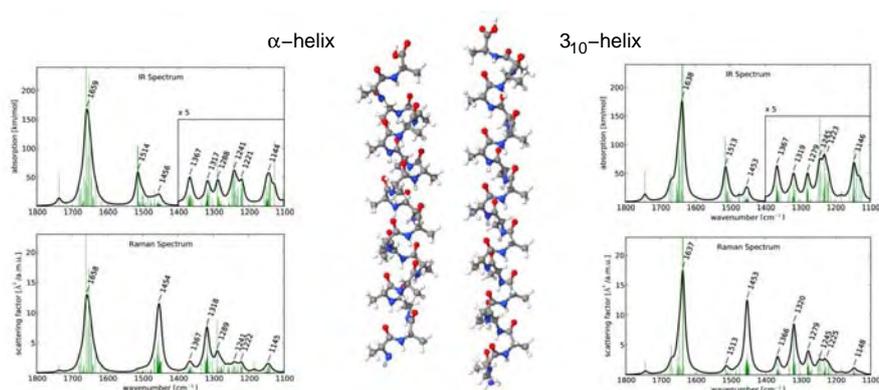
Title: Analysis of secondary structure effects on the IR and Raman spectra of polypeptides in terms of localized vibrations

Researchers: Christoph R. Jacob
Sandra Luber
Markus Reiher

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

Description:

We have demonstrated how the recently developed methodology for the analysis of calculated vibrational spectra in terms of localized modes [Ch. R. Jacob, M. Reiher, *J. Chem. Phys.* **2009**, *130*, 084106] can be applied to investigate the influence of the secondary structure on infrared and Raman spectra of polypeptides. As a model system, a polypeptide consisting of twenty (S)-alanine residues in the conformation of an α -helix and of a 3_{10} -helix was considered. Several features of the calculated spectra are analyzed in detail. Firstly, we showed for the amide II band how localized modes facilitate the decomposition of the total Raman intensities into contributions of certain groups of atoms, and how such an analysis can be used to identify the origin of differences in Raman intensity of the two helices. Secondly, we demonstrated how the shift of the position of the amide I band between the two considered structures can be rationalized and how the observed intensity distribution within the amide I band can be explained by considering the coupling constants between the localized modes. Thirdly, we showed how localized modes can be employed to analyze position of the bands found in the extended amide III region and how such an analysis makes it possible to gain a better understanding of how structural changes influence the coupling between the amide III and the C $^{\alpha}$ -H bending modes in this region.



References: Ch. R. Jacob, S. Luber, M. Reiher, *J. Phys. Chem. A* **2009**, *113*, 6558–6573.

Title: Understanding the signatures of secondary-structure elements in proteins via Raman optical activity spectroscopy

Researchers: Christoph R. Jacob
Sandra Luber
Markus Reiher

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

Description:

A prerequisite for the understanding of functional molecules like proteins is the elucidation of their structure under reaction conditions. Chiral vibrational spectroscopy is one option for this purpose, but provides only an indirect access to this structural information. By first-principles calculations, we have investigated how Raman optical activity (ROA) signals in proteins are generated and how signatures of specific secondary structure elements arise. As a first target we have focused on helical motifs and considered polypeptides consisting of twenty alanine residues to represent α -helical and of 3_{10} -helical secondary structure elements. While ROA calculations on such large molecules have not been carried out before, our main goal is the step-wise reconstruction of the ROA signals. By analyzing the calculated ROA spectra in terms of rigorously defined localized vibrations [Ch. R. Jacob, M. Reiher, *J. Chem. Phys.* **2009**, *130*, 084106], we have investigated in detail how total band intensities and band shapes emerge. We found that the total band intensities can be understood in terms of the reconstructed localized vibrations on individual amino acid residues. Two different basic mechanisms determining the total band intensities can be established and it is explained how structural changes affect the total band intensities. The band shapes can be rationalized in terms of the coupling between the localized vibrations on different residues, and we show how different band shapes arise as a consequence of different coupling patterns. As a result, it was demonstrated for the chiral variant of Raman spectroscopy how collective vibrations in proteins can be understood in terms of well-defined localized vibrations. Based on our calculations we were able to extract characteristic ROA signatures of α -helices and of 3_{10} -helices, which our analysis directly relates to differences in secondary structure.

References: Ch. R. Jacob, S. Luber, M. Reiher, *Chem. Eur. J.*, **2009**, accepted.

Title: Intensity-Driven Resonance Raman Calculations

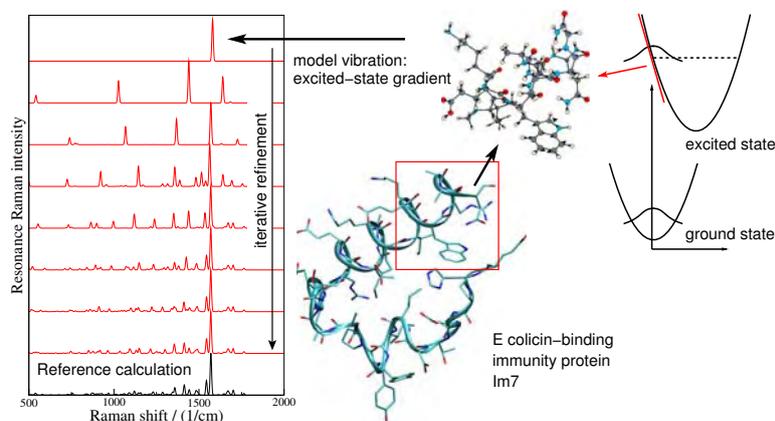
Researchers: Karin Kiewisch
Johannes Neugebauer
Markus Reiher

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

Description:

Resonance Raman (RR) spectroscopy is a powerful and versatile technique due to its highly sensitive and selective nature. Resonance enhancement allows the detection of molecules in low concentration and simplifies the interpretation of the spectra, since high intensities are observed for a few characteristic modes only.

For the study of biomolecules, the experimental selectivity of RR spectroscopy is of great advantage: The excitation wavelength can be tuned to the absorption band of a specific chromophore, e.g. an aromatic amino acid residue, resulting in an intensity increase of a local subset of modes at the chromophore. This local character of the spectra can be exploited to avoid the enormous computational effort required for the calculation of the complete harmonic force field. Intensity tracking [1] for resonance Raman allows the selective determination of the subset of intense modes. Starting from a single basis vector constructed from the gradient of the excited-state energy, the high-intensity features of a spectrum can be obtained in an iterative way. We applied the intensity-tracking algorithm to calculate RR spectra of tryptophan-containing protein models to demonstrate the efficiency of the method [1,2].



References: [1] K. Kiewisch, J. Neugebauer, and M. Reiher, *J. Chem. Phys.* **2008**, *129*, 204103.
[2] K. Kiewisch, S. Lubner, J. Neugebauer and M. Reiher, *Chimia* **2009**, *63*, 270.

Title: Haptic Quantum Chemistry

Researchers: Konrad H. Marti
Markus Reiher

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

Description:

Theoretical studies of molecular reactivity are governed by two major approaches: The static quantum chemical approach aims at the search for stationary points on the potential energy surface that can be identified as minima representing stable educts, intermediates, or products as well as transition states, while molecular dynamics extracts mechanistic and even kinetic information from the analysis of trajectories. Both of these approaches have one aspect in common and that is the fact that all implementations try to provide this information with as little guidance as possible. Of course, transition state searches in quantum chemistry benefit from educational guesses of transition structures and molecular dynamics simulations may be controlled via constraints and restraints. However, *all* of these approaches are designed to produce insight into chemical reactions with as little human interference as possible. Still, chemists would like to play with molecules in order to figure out what the reactivity might be. For this, hardly any method is available that allows the exploration of chemical reactivity with sufficient rigor, namely on the *first-principles* basis of quantum mechanics.

We presented the first implementation designed to *physically experience* quantum mechanical forces between reactants in chemical reactions. This allows one to screen the profile of potential energy surfaces for the study of reaction mechanisms. For this, we have developed an interface between the user and a virtual laboratory by means of a force-feedback haptic device. Potential energy surfaces of chemical reactions can be explored efficiently by rendering in the haptic device the gradients calculated with *first-principles* methods. The underlying potential energy surface is accurately fitted on the fly by the interpolating moving least-squares (IMLS) scheme to a grid of quantum chemical electronic energies (and geometric gradients) [G. G. Maisuradze, D. L. Thompson, *J. Phys. Chem. A* **2003**, *107*, 7118–7124]. In addition, we introduced a new IMLS-based method to locate minimum-energy paths between two points on a potential energy surface.

References: K. H. Marti, M. Reiher, *J. Comput. Chem.* **2009**, *30*, 2010–2020

Title: Quantum Chemical Study of a Stable Inverse Sandwich Complex with Unprecedented Ca(I)

Researchers: Lian Yu[†]
S. Krieck[‡]
M. Westerhausen[‡]
Markus Reiher[†]

Institute/Group: [†] Laboratorium für Physikalische Chemie, ETH Zürich, Zürich
[‡] Institut für Anorganische Chemie, Universität Jena, Jena

Description:

The reaction of bromo-2,4,6-triphenylbenzene with activated magnesium in THF yields the Grignard reagent [(thf)₂Mg(Br)-C₆H₂-2,4,6-Ph₃] with a Mg-C bond length of 214.8(3) pm. A similar reaction of bromo-2,4,6-triphenylbenzene with activated calcium led to an inverse sandwich complex [(thf)₃Ca-C₆H₃-1,3,5-Ph₃Ca(thf)₃] with the calcium atoms on opposite sides of the central arene ring showing small Ca-Ca and Ca-C distances of 427.9(3) and 259.2(3) pm. This extremely air- and moisture-sensitive complex exhibits thermochromic and solvatochromic behavior. It is paramagnetic with spin of S = 1 (triplet) with an ESR resonance at g = 2.0023. Quantum chemical calculations shed light on the bonding situation in this very unusual dinuclear Ca(I) compound.

References: S. Krieck, H. Görls, L. Yu, M. Reiher, M. Westerhausen, *J. Am. Chem. Soc.*, **2009**, *131*, 2977-2985.

Title: Organofluorosilanes as model compounds for ^{18}F -labeled silicon-based PET tracers and their hydrolytic stability — experimental data and theoretical calculations

Researchers: L. Yu[†]
A. Höhne[‡]
L. Mu[‡]
U. Voigtmann⁺
U. Klar⁺
K. Graham⁺
P. A. Schubiger[‡]
A. M. Ametamey[‡]
M. Reiher[†]

Institute/Group: [†] Laboratorium für Physikalische Chemie, ETH Zürich, Zürich
[‡] Center for Radiopharmaceutical Science of ETH, PSI and USZ, ETH Zurich, Zurich
⁺ Bayer Schering Pharma AG, Global Drug Discovery, Berlin

Description:

Radiochemists have recently discovered silicon chemistry as a tool for the introduction of ^{18}F into biomolecules for positron emission tomography (PET) imaging. ^{18}F -labeled PET tracers must be stable towards defluorination under physiological conditions. We performed an extensive investigation on the hydrolytic stability of various synthesized organofluorosilane model compounds and developed a theoretical model of organofluorosilane hydrolysis that correlates with the experimentally determined hydrolytic half-lives and allows estimation of the stability of newly designed compounds. The calculation of the difference of Si–F bond lengths between the optimized structures of the starting material and an important intermediate structure allows the estimation of the hydrolytic stability of newly designed compounds. This model permits the facilitated development of improved building blocks for the synthesis of novel ^{18}F -silyl-modified biomolecules for PET imaging.

References: A. Höhne, L. Yu, L. Mu, M. Reiher, U. Voigtmann, U. Klar, K. Graham, P. A. Schubiger, A. M. Ametamey, *Chem.—Eur. J.* **2009**, *15*, 3736-3743

Title: Restrained Optimization of Broken-Symmetry Determinants

Researchers: Maren Podewitz
Carmen Herrmann
Markus Reiher

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

Description:

One goal of this work was to provide an overview on how Lagrange multipliers can be used in self-consistent-field algorithms for convergence control. In particular, a scheme has been proposed with the purpose to guide any set of initial guess molecular orbitals to those of a Slater determinant which (1) has certain expectation values (i.e., molecular properties) within a predefined range and which (2) corresponds to a true (local) energy minimum, if such a minimum exists within the property range chosen. The most important practical application of such an algorithm is the calculation of minimum-energy broken-symmetry determinants which are often used in Kohn–Sham density functional calculations to model antiferromagnetically coupled states. This is achieved by (a) combining a constrained optimization [Q. Wu, T. Van Voorhis, *Phys. Rev. A* **2005**, *72* 024502] with a subsequent optimization where the constraints are released, i.e., the Lagrange multipliers are set to zero. Alternatively, (b) a modified scheme may be employed, where the constraints are released as soon as the energy starts to rise in the SCF algorithm. Both alternatives are combined with intermediate and final automatic control of whether the properties of interest are within the desired range. A parameter study using scheme (a) has been carried out for a set of small test systems. Applications to a synthetically available trinuclear copper complex and to the Crabtree and Brudvig’s water-oxidizing complex [R. H. Crabtree, G. W. Brudvig *et al.*, *J. Am. Chem. Soc.* **2001**, *123*, 423.] highlight the benefits and limitations of restrained optimization.

References: C. Herrmann, M. Podewitz, M. Reiher, *Int. J. Quantum Chem.* **2009**, *109*, 2430.

Title: Theoretical study of dioxygen induced inhibition of [FeFe]-hydrogenase

Researchers: Martin T. Stiebritz
Markus Reiher

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

Description:

A thorough quantum chemical investigation of O₂ addition to the H-cluster of [FeFe]-hydrogenase revealed detailed insight into possible decomposition pathways of this active site.

Hydrogenases comprise a variety of enzymes that catalyze the reversible oxidation of molecular hydrogen. Out of this group [FeFe]-hydrogenase shows the highest activity for hydrogen production which is therefore of great interest in the field of renewable energies. Unfortunately, this comes with the flaw of a generally very high sensitivity against molecular oxygen that irreversibly inhibits this enzyme. While many studies have already addressed the mechanism of hydrogen formation by [FeFe]-hydrogenase little is known about the molecular and mechanistic details leading to enzyme inactivation by O₂. In order to elucidate this process we performed density functional theory calculations on several possible O₂-adducts of the catalytic center — the so called H-cluster — and show that the direct interaction of the [2Fe]_H subsite with dioxygen is an exothermic and specific reaction in which O₂ most favorably binds in an end-on manner to the distal Fe_d. Based on the results we proposed a protonation mechanism that can explain the irreversibility of dioxygen-induced enzyme inactivation by water release and degradation of the ligand environment of the H-cluster.

References: M. T. Stiebritz, M. Reiher, *Inorg. Chem.* (2009), **48**, 7127–7140

Title: The Douglas–Kroll–Hess Electron Density at an Atomic Nucleus

Researchers: Remigius Mastalerz¹
Roland Lindh²
Markus Reiher¹

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich
²Department of Chemical Physics, Lund University P.O.B. 124,
221 00 Lund, Sweden

Description:

The electron density at a specific nucleus (the contact density) is a quantity which is of special interest to Mössbauer spectroscopy, since the chemical isomer shift, which is a characteristic parameter in compounds containing Mössbauer active isotopes, depends on the electron density at the position of the Mössbauer nucleus.

In general, the electron density at the position of an atomic nucleus is strongly affected by relativity. The scalar-relativistic variant of the Douglas–Kroll–Hess (DKH) unitary transformation technique provides a suitable framework to treat relativistic effects and has been extended to the analytical calculation of molecular properties avoiding the so-called picture change error [1], which results from calculating the desired property from non-DKH-transformed (i.e. non-relativistic) property integrals. An analytical approach to the picture-change transformation of DKH electron densities at atomic nuclei has been presented and applied to the hydrogen halides series [2]. For a truly accurate prediction of the absolute electronic charge density at heavier nuclei (accuracy better than 10^{-3} a.u.⁻³) DKH transformations beyond the 10th order in orbitals and property operator are necessary. The numerical examples have shown that the picture-change-affected density is vastly overestimated compared to the picture-change-corrected results. Moreover, the picture-change error on the contact density is strongly increasing with nuclear charge number but is generally high even in case of lighter elements. Regarding different finite nuclear charge distribution models the effect on the contact density is small compared to the effect of the DKH order of the property-operator transformation. The results presented in Ref. [2] have demonstrated that a proper high-order picture-change-corrected approach is necessary to recover the correct electronic densities at atomic nuclei. However, for the prediction of contact density *differences* — as required for the Mössbauer isomer shift — already low-order DKH transformations are likely to provide sufficiently accurate results for elements up to the third row of the periodic table.

References: [1] M. Reiher, A. Wolf, *Relativistic Quantum Chemistry. The Fundamental Theory of Molecular Science* **2009**, Wiley VCH, Weinheim
[2] R. Mastalerz, R. Lindh, M. Reiher, *Chem. Phys. Lett.* **2008**, *465*, 157

Title: Calculated Raman optical activity spectra
of 1,6-Anhydro- β -*D*-glucopyranose

Researchers: Sandra Luber
Markus Reiher

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

Description:

Raman and Raman optical activity spectra calculations of the carbohydrate molecule 1,6-anhydro- β -*D*-glucopyranose have been carried out. It has been shown that a change from the chair to the boat conformation has a strong influence on the Raman optical activity intensities. Similar results have been found for different rotamers of this molecule. In order to investigate solvent effects, we performed calculations with and without the continuum model COSMO. In addition, explicit solvation with water molecules has been investigated and shown to significantly affect the Raman optical activity spectrum. The final spectra have been constructed by overlapping of spectra of single conformers leading to a good agreement with the experimental spectra.

References: S. Luber, M. Reiher, *J. Phys. Chem. A* **2009**, *113*, 8268-8277.

Title: Intensity-Carrying Modes in Raman and Raman optical activity spectroscopy

Researchers: Sandra Luber
Markus Reiher

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

Description:

A quantum-chemical approach for the determination of modes with maximum Raman and Raman optical activity (ROA) intensity via eigenvalue equations has been described. The intensity-carrying modes are in general hypothetical molecular distortions and do not directly correspond to a particular normal mode in the spectrum. However, they provide information about those molecular distortions leading to intense bands in the spectrum. Modes with maximum Raman intensity have been presented for propane-1,3-dione, propane-1,3-dionate, and Λ -tris(propane-1,3-dionato)cobalt(III). Moreover, the mode with highest ROA intensity was examined for this chiral cobalt complex and also for the (chiral) amino acid *L*-tryptophan. The Raman and ROA high-intensity modes are an optimal starting guess for intensity-tracking calculations, in which selectively normal modes with high Raman or ROA intensity are converged. The first Raman and ROA intensity-tracking calculations have been presented. These reveal a high potential for large molecules, for which the selective calculation of normal modes with high intensity is desirable in view of the large computational effort required for the calculation of Raman and ROA property tensors.

References: S. Luber, M. Reiher, *ChemPhysChem* **2009**, *10*, 2049-2057.

Title: Intensity-Tracking for Theoretical
Infrared Spectroscopy of Large Molecules

Researchers: Sandra Luber
Johannes Neugebauer
Markus Reiher

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

Description:

An approach for the direct calculation of vibrational normal modes with high infrared intensities has been developed [1], which is based on a mode-tracking-like algorithm [*J. Chem. Phys.*, **2003**, *118*, 1634] but with distinct features: no collective guess vibration is utilized but high-intensity distortions are constructed. Only the modes of interest with the highest infrared intensities are then targeted irrespective of a pre-definition of the underlying collective normal coordinates. This leads to a fast access to the most important features in infrared spectra. Different implementations of the mode selection procedure have been validated for a set of small organic molecules as well as for the metal complex $\Delta(\delta\delta\delta)$ -tris(ethylenediaminato)cobalt(III) and the peptide all-(*S*)-decaalanine. As a critical test case, approximate infrared spectra of Schrock's dinitrogen molybdenum complex have been calculated via intensity-tracking.

References: S. Luber, J. Neugebauer, M. Reiher, *J. Chem. Phys.* **2009**, *130*, 064105.

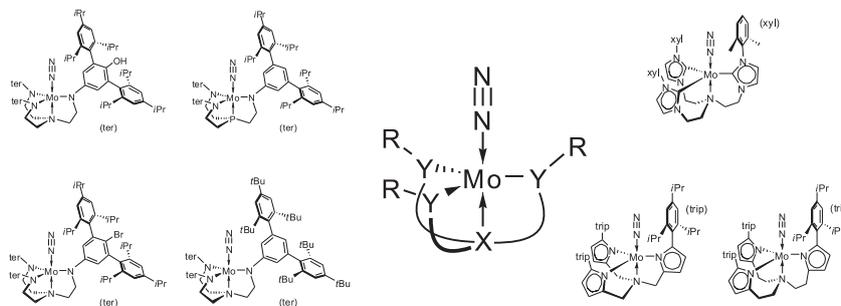
Title: Ligands for Dinitrogen Fixation at Schrock-type Catalysts

Researchers: Stephan Schenk
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich

Description:

Catalytic dinitrogen reduction with the Schrock complex is still hampered by low turnover numbers that are likely to result from a degradation of the chelate ligand [1,2]. In this work, we investigated modifications of the original HIPTN₃N ligand applied by Schrock and co-workers in catalytic reduction of dinitrogen with density functional methods [3]. We focused on ligands that are substituted in *para* position of the central phenyl ring of the terphenyl moieties and on a ligand where the bridging nitrogen is exchanged by phosphorus. In addition, results for tris(pyrrolyl- α -methyl)amine, tris(pyrrolyl- α -ethyl)amine and tris[2-(3-xylyl-imidazol-2-ylidene)ethyl]amine were reported. For this study, we took into account the full ligands without approximating them by model systems. Reaction energies for the various derivatives of HIPTN₃N were found to be similar to those of the unchanged parent system. However, the most promising results for catalysis were obtained for the [$\{$ tris[2-(3-xylyl-imidazol-2-ylidene)ethyl]amine $\}Mo$](N₂) complex. Feasibility of the exchange of NH₃ by N₂ was found to be the pivotal issue whether a complex can become a potential catalyst or not. A structure–reactivity relationship was derived which allows for the convenient estimation of the reaction energy for the NH₃/N₂ exchange reaction solely from the wavenumber of the N \equiv N stretching vibration. This relationship may guide experiments as soon as a dinitrogen Mo complex is formed.



- References:**
- [1] D. M. Yandulov, R. R. Schrock, *Science*, **2003**, *301*, 76–78.
 - [2] S. Schenk, B. Le Guennic, B. Kirchner, M. Reiher, *Inorg. Chem.*, **2008**, *47*, 3634–3650.
 - [3] S. Schenk, M. Reiher, *Inorg. Chem.*, **2009**, *48*, 1638–1648.

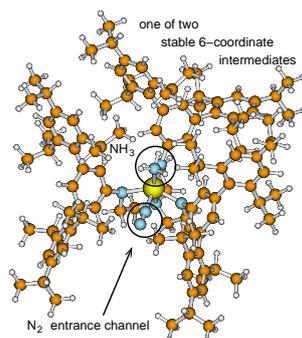
Title: A Stable Six-Coordinate Intermediate in Ammonia–Dinitrogen Exchange at Schrock’s Molybdenum Catalyst

Researchers: Stephan Schenk*
Markus Reiher*
Barbara Kirchner**

Institute/Group: * Laboratorium für Physikalische Chemie, ETH Zürich
**Universität Leipzig, Lehrstuhl für Theoretische Chemie,
Linnestr. 2, D-04103 Leipzig

Description:

In this work [1], we investigated the mechanism of the ammonia–dinitrogen exchange reaction which is the decisive step [2] to close the catalytic cycle of Schrock’s dinitrogen reduction sequence under ambient conditions [3]. We identified several viable pathways for the approach of dinitrogen to the five-coordinate molybdenum center of the ammonia complex by means of *first-principles* molecular dynamics simulations. These exploratory simulations were then complemented by rigorous quantum chemical structure optimizations. Our calculations have been performed for the full Schrock catalyst without simplifying the large chelate ligand, and are hence not affected by model assumptions. We have shown that the reaction obeys an addition–elimination mechanism via a *stable* six-coordinate intermediate. This intermediate has been fully characterized by stationary quantum chemical methods. The predicted infrared spectrum of this species features an N≡N stretching vibration which is well separated in frequency from all other N≡N stretching vibrations of N₂-binding complexes involved in the Schrock cycle. Depending on the life time of this intermediate in the reaction liquor, the production of this intermediate might even be monitored by the absorption of the N≡N stretching vibration.



- References:**
- [1] S. Schenk, B. Kirchner, M. Reiher, *Chem.–Eur. J.* **2009**, *15*, 5073–5082.
 - [2] S. Schenk, B. Le Guennic, B. Kirchner, M. Reiher, *Inorg. Chem.*, **2008**, *47*, 3634–3650.
 - [3] D. M. Yandulov, R. R. Schrock, *Science*, **2003**, *301*, 76–78.

Title: A Vibrational Raman Optical Activity study of 1,1'-Binaphthyl Derivatives

Researchers: Vincent Liégeois
Markus Reiher

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

Description:

Vibrational Raman Optical Activity (VROA) spectroscopy is a powerful tool to unravel the configurations as well as the conformations of molecules [J. Haesler, I. Schindelholz, E. Riguet, C. G. Bochet, W. Hug, *Nature* **2007**, *446*, 526] and macromolecules [L. D. Barron, F. Zhu, L. Hecht, *Vib. Spectrosc.* **2006**, *42*, 15]. The $3N - 6$ vibrational degrees of freedom leads to substantial information about the structures, which need theoretical tools for their detailed interpretation. We have therefore elaborated a quantum chemistry procedure [V. Liégeois, K. Ruud, B. Champagne, *J. Chem. Phys.* **2007**, *127*, 204105] for the analytical evaluation of the optical molecular responses [electric dipole-electric dipole polarizability (α), electric dipole-electric quadrupole polarizability (A), and the optical activity tensor (G')] as well as of their geometry derivatives entering into the expressions of the VROA intensities.

Our methodology was then applied to the simulation of the Raman polarized and VROA backward spectra of a series of 2,2'-substituted 1,1'-binaphthyl compounds presenting a variety of torsion angle between the two naphthalene rings. Contrary to the Raman spectra, which are very similar to each other, the VROA spectra present some signatures that are changing as a function of the torsion angle. Indeed, the signatures of the cisoid conformation for the compounds with substituents R=H, F and OH are very different from those of their transoid counterparts.

This study has thus revealed VROA signatures associated to the atropisomerism. They are dominated by the $\beta_{G_p}^2$ invariant while the $\beta_{A_p}^2$ invariant is smaller but has generally the same sign as the $\beta_{G_p}^2$ one.

References: V. Liégeois, *ChemPhysChem* **2009**, *10*, 2017

Title: State-averaged Density Matrix Renormalization Group
Calculations for Unsaturated Organic Molecules

Researchers: Vincent Liégeois
Konrad H. Marti
Markus Reiher

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

Description:

Since its development by White in 1992 [S. R. White, *Phys. Rev. Lett.* **1992**, *69*, 2863], the Density Matrix Renormalization Group (DMRG) algorithm has been used in *ab initio* quantum chemistry calculations where a large active space was required [G. Moritz and M. Reiher, *J. Chem. Phys.* **2007**, *126*, 244109; D. Ghosh, J. Hachmann, T. Yanai, and G. K.-L. Chan **2008**, *J. Chem. Phys.*, *128*, 144117]. Indeed, this method enables one to treat a large number of active orbitals which is not feasible with CASSCF due to the factorial scaling. The DMRG approach is therefore interesting to study highly delocalized systems like β -carotene [D. Ghosh, J. Hachmann, T. Yanai, and G. K.-L. Chan **2008**, *J. Chem. Phys.*, *128*, 144117] or chlorophyll.

Here, we have elaborated on a sound strategy for the efficient and accurate calculation of excited states, *i.e.* accurate excitation energies. In order to prevent root flipping or losing states due to the numerical Davidson subspace iteration technique, the state-averaged (averaged reduced density matrix) approach proposed by Garnet G.-L. Chan and coworkers [J. J. Dorando, J. Hachmann, and G. K.-L. Chan **2007**, *J. Chem. Phys.*, *127*, 084109] was implemented in our DMRG code. Our program is then applied on polyene systems for which accurate reference data are available [D. Ghosh, J. Hachmann, T. Yanai, and G. K.-L. Chan **2008**, *J. Chem. Phys.*, *128*, 144117]. Different effects on the relative energies such as the number of DMRG states, the number of roots in the state-averaged approach, different weighting of the reduced density matrix of the excited states, levelshift, noise, ... are tested for five polyenes of increasing size (ranging from C₈H₁₀ to C₂₄H₂₆). While for the small systems, reference CASSCF calculations can be conducted, the largest systems benefit from the polynomial scaling of the DMRG algorithm. Moreover, we have compared our results to TDDFT and CC2 calculations on the bases of the energy and the spatial symmetry ordering of the states.

References: V. Liégeois, K. H. Marti, M. Reiher, *in preparation*

Title: Investigation of the vibrational Raman optical activity signatures associated to $(TG)_N$ and $(GG)_N$ conformations of 20-unit polypropylene chain by mean of localized mode

Researchers: Vincent Liégeois¹
Christoph R. Jacob¹
Markus Reiher¹
Benoît Champagne²

Institute/Group: ¹Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
²Unité de Chimie Physique Théorique et Structurale, FUNDP, Rue de Bruxelles 61, B-5000 Namur, Belgium

Description:

The control of polymer conformations and structures is crucial for applications as widespread as self-assembled monolayers, biological membranes, biosensors, and polymeric bulk materials. Indeed, the properties of the materials build from polymers are strongly dependent of the tacticity, the ramifications, the defects, ... of the chains. In order to control them, techniques such as NMR or Raman spectroscopies are used to characterize the polymer chains and their surrounding. Vibrational Raman optical activity (VROA) spectroscopy, which measures the tiny difference of interaction between a right-handed and a left-handed circularly polarized incident light, appears to be an ideal tool for probing polymer structures that exhibit chirality. It has been applied, during the last decades, to a broad range of systems including fragrances, sugars, polypeptides, ... [L. D. Barron, F. Zhu, L. Hecht, *Vib. Spectrosc.* **2006**, *42*, 15].

In this project, using *ab initio* approaches, we address the potential of VROA for detecting and interpreting polymeric helical structures. One of the major challenge is to analyse the normal modes which are most of the time delocalized over the whole molecule. The localized mode methodology [Ch. R. Jacob, M. Reiher, *J. Chem. Phys.* **2009**, *130*, 084106] enables us to analyse how the total band intensities and band shapes emerge. This scheme is therefore used on a 20-unit isotactic polypropylene chain. The signature of two different conformers, namely the $(TG)_{19}$ and $(GG)_{19}$, are investigated, especially the couplet at around 1100 cm^{-1} that was already point out as a signature of the $(TG)_N$ conformation [E. Lamparska, V. Liégeois, O. Quinet, B. Champagne, *ChemPhysChem* **2006**, *7*, 2366].

References: V. Liégeois, Ch. R. Jacob, B. Champagne, M. Reiher, *in preparation*

Title: Systematic quantitative analysis and modeling of the endocytic membrane system in mammalian cells

Researchers: Jo A. Helmuth¹⁾
Mirko Birbaumer²⁾
Christoph J. Burckhardt³⁾
Lucas Pelkmans²⁾
Urs F. Greber³⁾
Ivo F. Sbalzarini¹⁾

**Institute/
Group:** ¹⁾MOSAIC Group
²⁾Institute of Molecular Systems Biology, ETH Zurich
³⁾Institute of Zoology, University of Zurich

Description:

The endocytic membrane system consists of a variety of entry routes and organelles, mechanisms of vesicle formation and cargo sorting, and a wide range of trafficking kinetics. Endocytosis is the prime cellular system used by many pathogens, including toxins, viruses, and intracellular bacteria. To understand the complex endocytic system in mammalian cells, realistic computer simulations are needed. To reach this goal, we will perform systematic perturbation studies of the endocytic membrane system with high-resolution light microscopy. New image processing and object detection algorithms, combined with novel machine learning methods, will be applied to identify quantitative parameters for classification, and to extract the physical properties of endocytic organelles and trafficking dynamics. The obtained large sets of characteristic parameters, describing endocytic phenotypes and their dynamic behavior, will be used to formulate and numerically simulate integrative spatio-temporal models of the membrane trafficking network, enabling predictions of the collective behavior of the endocytic membrane system.

References:

J. A. Helmuth, C. J. Burckhardt, U. F. Greber, and I. F. Sbalzarini. Shape reconstruction of subcellular structures from live cell fluorescence microscopy images. *Journal of Structural Biology*, 167:1–10, 2009.

J. A. Helmuth, C. J. Burckhardt, P. Koumoutsakos, U. F. Greber, and I. F. Sbalzarini. A novel supervised trajectory segmentation algorithm identifies distinct types of human adenovirus motion in host cells. *J. Struct. Biol.*, 159(3):347–358, 2007.

Presented at the International Symposium on Visual Computing (ISVC), Las Vegas, USA, 2009; International Conference on Information Processing in Cells and Tissues (IPCAT), Lugano, Switzerland, 2009; BioImage Informatics Conference, Janelia Farm, Howard Hughes Medical Institute, Ashburn (VA), USA, 2009; Swiss Institute of Bioinformatics Scientific Meeting, Fribourg, Switzerland, 2009.

Title: Predictive physical models and large-scale computer simulations to study the role of electrostatics and couplings in the nonequilibrium dynamics of biological membranes in relation to lipid rafts and endocytosis

Researchers: Nérido González-Segredo¹⁾
Ivo F. Sbalzarini¹⁾

**Institute/
Group:** ¹⁾MOSAIC Group

Description:

Membranes in live cells are complex, organized mixtures of different lipids and proteins. They contain several functional sub-domains (“rafts”) that are believed to be ordered microphases, resulting from lipid phase segregation. The existence of lipid rafts is, however, still not unanimously accepted. Nevertheless, rafts are suspected to have many important biological functions, e.g., in signal transduction, protein transport and sorting, diffusive transport, endocytosis, and membrane budding, fusion, fission, and tether formation (“BFFT”). Membrane sub-domains are currently intensively studied using both theoretical and experimental methods. To the best of our knowledge, however, no simulation studies have been carried out so far and the physical mechanisms and dynamics of raft formation and evolution are largely unknown. Currently available membrane models and simulations neglect the dynamic feedback loops between lipids and proteins. Moreover, they neglect electrostatics and hydrodynamics. Most membrane-binding proteins, as well as the membranes themselves, are however electrically charged. We propose a novel physical model that will fully account for the feedback-loops, electrostatic, and hydrodynamic effects in biomembranes. We will develop a multi-phenomenon hybrid particle-continuum computer model to bridge the gap between the scales of individual (electrically or mechanically active) proteins, lipid rafts, and vesicle budding and fission.

References:

R. Ramaswamy, N. González-Segredo, and I. F. Sbalzarini. A new class of highly efficient exact stochastic simulation algorithms for chemical reaction networks. *J. Chem. Phys.*, 130(24):244104, 2009.

F. Mallamace, C. Corsaro, M. Broccio, C. Branca, N. González-Segredo, J. Spooren, S.-H. Chen, and H. E. Stanley. NMR evidence of a sharp change in a measure of local order in deeply supercooled confined water. *Proc. Natl. Acad. Sci. USA*, 105(35):12725–12729, 2008.

Presented at the CECAM workshop on Computational Systems Biology, Lausanne, Switzerland, 2009; Swiss Institute of Bioinformatics Scientific Meeting, Fribourg, Switzerland, 2009; All SystemsX.ch day, Basel, Switzerland, 2008; CCP5 Annual Meeting, Surfaces and Interfaces, London, UK, 2008; Water and Aqueous Solutions Gordon Research Conference, New Hampshire, USA, 2008.

Title: Image analysis based on physical models and non-linear optimal state observers

Researchers: Grégory Paul¹⁾
Janick Cardinale¹⁾
Ivo F. Sbalzarini¹⁾

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

Description:

Many biological experiments are based on light microscopy to observe dynamic processes in living cells. Manual analysis and intuitive interpretation of image data are hereby more and more replaced by automated analysis. The use of large data sets and high degrees of automation results in improved significance and results that are less biased by prior expectations, i.e. that have better reproducibility.

We are developing image analysis algorithms for many different biological applications. A large class of these algorithms shares the property that a physical model of the object of interest is used to process the image data. The algorithms for image enhancement, filtering, model implementation, and estimation hereby remain unchanged. We focus at implementing new algorithms in a standardized framework that will enable fast software development and reduce the amount of redundant code.

In a first step, we will apply this framework to the problem of object detection. The dynamics of the observed objects and the transfer function of the imaging equipment are given by state-space system models. Image processing is based on the optimal reconstruction of the system states using methods of Sequential Monte Carlo, Kalman Filtering, or Particle Filtering. A method for the segmentation of images under conditions of structured backgrounds and temporary occlusion will be implemented. The method is flexible enough to accommodate arbitrary dynamical systems, including the possibility of switching behavior between different state space models.

References:

Presented at the American Society for Cell Biology Annual Meeting (ASCB), San Diego, USA, 2009; IEEE International Symposium on Biomedical Imaging (ISBI), Boston, USA, 2009; Swiss Institute of Bioinformatics Scientific Meeting, Fribourg, Switzerland, 2009.

Title: Modeling and simulation of lipid membrane bilayers and microdomains

Researchers: Birte Schrader¹⁾
Rajesh Ramaswamy¹⁾
Nélido González-Segredo¹⁾
Sylvain Reboux¹⁾
Ivo F. Sbalzarini¹⁾

**Institute/
Group:** ¹⁾MOSAIC Group
(part of the SystemsX.ch RTD project *LipidX*)

Description:

We will integrate experimental and theoretical results into a spatiotemporal biophysical model of lipid membranes at three scales: the microscopic atomistic scale, the mesoscopic scale of membrane domain organization, and the macroscopic scale of continuum mechanics and electrostatics. Once the lipids are synthesized and inserted into the membranes, they undergo complex self-organization, giving rise to a variety of membrane behaviors, sub-domains, and functions. We will study the dynamics of self-organization and the resulting membrane structures using spatiotemporal biophysical models. These models will link for the first time the atomistic scale (biochemical composition and structural conformation of lipid molecules in bilayers) with the continuum scale (membrane sub-domains, endocytosis). The main goal of the project is the modeling and simulation of cell membrane structure in order to study lateral association in micro-domains in lipid mixtures, and their interactions with proteins including molecular sorting. Ultimately, the present project will link regulatory events in the genetic and metabolic systems to concrete phenotypic effects such as virus endocytosis. This link will help us predict how changes at the activities of metabolism alter the lipid composition and how these changes in composition alter membrane properties.

References:

R. Ramaswamy, N. González-Segredo, and I. F. Sbalzarini. A new class of highly efficient exact stochastic simulation algorithms for chemical reaction networks. *J. Chem. Phys.*, 130(24):244104, 2009.

I. F. Sbalzarini. Abstractions and Middleware for Petascale Computing and Beyond. *International Journal of Distributed Systems and Technologies*, in press, 2009.

M. Bergdorf, I. F. Sbalzarini, and P. Koumoutsakos. A Lagrangian particle method for reaction-diffusion systems on deforming surfaces. *J. Math. Biol.*, submitted, 2009.

B. Schrader, S. Reboux, and I. F. Sbalzarini. Discretization Correction of General Integral PSE Operators in Particle Methods. *J. Comput. Phys.*, submitted, 2009.

Presented at the Swiss Institute of Bioinformatics Scientific Meeting. Fribourg, Switzerland, 2009; Scottish-Swiss Forum for Bioinformatics, Edinburgh, UK, 2008.

Title: Parallel evolutionary algorithms for molecular structure and conformation prediction and analysis

Researchers: Christian L. Müller¹⁾
Grégory Paul¹⁾
Ivo F. Sbalzarini¹⁾
Bojan Zagrovic²⁾
Phillippe Hünenberger³⁾
Wilfred van Gunsteren³⁾

Institute/ ¹⁾MOSAIC Group
Group: ²⁾Mediterranean Institute for Life Sciences, Split, Croatia
³⁾Laboratory of Physical Chemistry, ETHZ

Description:

Optimization and systems identification in high dimensions is a recurring topic in many areas of computational science. In addition, information about global parameter sensitivities is often desired for model reduction, experimental design, or uncertainty analysis. The systems considered in computational biophysics are frequently non-linear, highly multimodal, and modeled by computer simulations where no gradient information is available. Evolutionary optimizers are, therefore, the method of choice. The project aims at developing a parallel version of a coupled, adaptive swarm-evolution strategy that provides on-line estimates of the global parameter sensitivities during an optimization run. The global sensitivity estimator uses the same samples that are generated by the optimization strategy, thus having a high computational efficiency. It is based on a novel sensitivity measure that can be statistically estimated on arbitrary, scattered sampling points in parameter space.

References:

C. L. Müller, I. F. Sbalzarini, W. F. van Gunsteren, B. Žagrović, and P. H. Hünenberger. In the eye of the beholder: Inhomogeneous distribution of high-resolution shapes within the random-walk ensemble. *J. Chem. Phys.*, 130(21):214904, 2009.

Presented at the third Workshop on Theory of Randomized Search Heuristics (TRSH), Birmingham, UK, 2009; International Conference on Evolutionary Computation (ICEC), Funchal, Madeira (Portugal), 2009; CCP5 Conference on Structure Prediction, London, UK, 2009; ACM Genetic and Evolutionary Computing Conference (GECCO), Montréal, Canada, 2009; IEEE Congress on Evolutionary Computation (CEC), Trondheim, Norway, 2009; Swiss Institute of Bioinformatics Scientific Meeting, Fribourg, Switzerland, 2009.

Title: Middleware and Abstractions for Transparent Parallel Computing

Researchers: Omar Awile¹⁾
Ivo F. Sbalzarini¹⁾
Jens H. Walther²⁾

Institute/ ¹⁾MOSAIC Group
Group: ²⁾Technical University of Denmark, Copenhagen, Denmark

Description:

The increasing complexity of the models studied in computational science, together with the proliferation of parallel computing platforms at all levels (e.g. multi-core processors), has made parallel programming a key challenge. Present programming models for parallel computers are processor-centric, but memory-transparent. This means that every processor (and hence the communication between them) needs to be programmed explicitly and separately, while it is transparent to the programmer whether data are in memory, cache, or registers. In order to exploit multi-core architectures, reduce code development times, and increase parallel scalability, a new programming paradigm is required. This new paradigm should be processor-transparent and data-explicit. Programs should be independent of the number of processors they will later run on, but the programmer needs to be in control of data locality in order to exploit the benefits of shared memories and shared caches. We are developing and applying a set of parallel data and operation abstractions that provide such functionality for scientific numerical simulations. Their implementation is based on a middleware library on which the application codes can be implemented.

References:

J. H. Walther and I. F. Sbalzarini. Large-scale parallel discrete element simulations of granular flow. *Engineering Computations*, 26(6):688–697, 2009.

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

I. F. Sbalzarini. Abstractions and Middleware for Petascale Computing and Beyond. *International Journal of Distributed Systems and Technologies*, in press, 2009.

Presented at the 5th international congress of Nano-Bio & Clean Tech, San Francisco, USA, 2008; 21st Nordic Seminar on Computational Mechanics, Trondheim, Norway, 2008.

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

Researchers: Adeline Bichet, Thomas Bosshard, Peter Brockhaus, Marc Chiacchio, Tracy Ewen, Erich Fischer, Doris Folini, Cathy Hohenegger, Sven Kotlarski, Wolfgang Langhans, Daniel Lüthi, Knut Makowski, Pardeep Pall, Christoph Schär, Linda Schlemmer, Jürg Schmidli, Martin Wild, Elias Zubler.

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

Description:

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

The high-resolution modeling uses the COSMO-CLM limited-area atmospheric model. The main thrust of this work is dedicated to the understanding and simulation of the European summer climate. Comprehensive European-scale climate-change scenario simulations are conducted at a horizontal resolution of 25 km covering the period 1950-2100. Current work is addressing potential changes in heatwave and heavy precipitation events. In parallel, we are developing a high-resolution climate simulation capability with a horizontal resolution of 2 km. Both idealized and real-case simulations are conducted. The main motivation behind this work is the desire to explicitly simulate convective clouds (as opposed to using convective cloud parameterization schemes in lower-resolution models).

The global scale simulations are carried out with the climate model ECHAM5-HAM, developed at the Max Planck Institute in Hamburg, Germany. This work is led by Dr. Martin Wild, and it also exploits collaborations with the group of Prof. Ulrike Lohmann. The model contains sophisticated aerosol and cloud microphysics schemes. These are essential for realistic simulations of radiation and precipitation processes in the atmosphere. This model is used to study the link between anthropogenic and natural perturbations of the radiation balance and the intensity of the hydrological cycle. The time period under consideration covers 1870-2100. The global model simulations provide also boundary conditions to drive the regional model.

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

Title: Wavelet finite element method for option pricing in high-dimensional diffusion models

Researchers: Norbert Hilber
Sohrab Kehtari
Christoph Schwab
Christoph Winter

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The numerical solution of high-dimensional partial differential equations arising when pricing of financial derivatives is considered in this project. In order to reduce the otherwise exponentially growing complexity in the number of degrees of freedom, sparse tensor product spaces are applied for the discretization. This technique enables the pricing of multi-asset options with up to eight underlying assets – leading to 10^8 active degrees of freedom – for the Black-Scholes framework and eight additional dimensions for the stochastic volatility models.

Dimensionality reduction by principal component analysis is investigated in order to price options on indices by considering the whole vector process of all of their constituents.

References:

- [1] N. Hilber, A.-M. Matache, and C. Schwab, Sparse wavelet methods for option pricing under stochastic volatility, *The Journal of Computational Finance*, 8(4):1-42, 2005.
- [2] N. Hilber, C. Schwab, and C. Winter, Variational sensitivity analysis of parametric Markovian market models, in L Stettner, editor, *Advances in Mathematics of Finance*, volume 83, pages 85–106, Banach Center Publ., 2008.
- [3] C.C.W Leentvaar and C.W Oosterlee, On coordinate transformation and grid stretching for sparse grid pricing of basket options, *J. Comput. Appl. Math.*, 222(1):193–209, 2008.
- [4] C. Reisinger and G. Wittum, Efficient hierarchical approximation of high-dimensional option pricing problems, *SIAM J. Sci. Comput.*, 29(1), 2007.
- [5] T. von Petersdorff and C. Schwab, Numerical solution of parabolic equations in high dimensions, *M2AN Math. Model. Numer. Anal.*, 38(1):93–127, 2004.

Title: Sparse techniques for elliptic sPDEs

Researchers: Roman Andreev
Marcel Bieri
Claude Gittelsohn
Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The project encompasses the analysis and implementation of algorithms for the deterministic numerical solution of elliptic and parabolic boundary value problems with stochastic coefficients in a d -dimensional physical domain. We also consider the corresponding stochastic eigenvalue problems.

A separation of deterministic and stochastic parts of the input data is achieved for example by a Karhunen-Loève expansion. This reduces the original stochastic problem to a high-dimensional parametric deterministic problem.

The main goal of the project is to overcome this high complexity by using

- sparse techniques for approximating the solution's random behavior,
- a priori and a posteriori adaptivity to represent the solution's randomness by as few terms as possible,
- and computer parallelism to efficiently overcome potential bottlenecks in our proposed algorithms.

We apply sparse approximation techniques and adaptivity in the context of two methods, namely *stochastic Galerkin FEM* (sGFEM) and *stochastic collocation FEM* (sCFEM), see also [1, 2, 3] and references therein. Both methods allow for parallelization to enhance their performance in terms of run-time behavior.

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

References

- [1] M. Bieri, R. Andreev and C. Schwab. Sparse tensor discretization of elliptic sPDEs. *SIAM Journal on Scientific Computing*, to appear.
- [2] M. Bieri. A sparse composite collocation finite element method for elliptic sPDEs. Submitted.
- [3] C.J. Gittelsohn. Stochastic Galerkin discretization of the lognormal isotropic diffusion problem. *Mathematical Models and Methods in Applied Sciences*, to appear.

Title: Computational Performance of a Parallelized Three-Dimensional High-Order Spectral Element Toolbox

Researchers: Michel Deville¹
Sohrab Kehtari²
et al. (see remark)

Institute: ¹ Laboratory of Computational Engineering
École Polytechnique Fédérale de Lausanne
² Seminar for Applied Mathematics
ETH Zürich
³ Vortical Flow Research Laboratory
Massachusetts Institute of Technology

Description:

A comprehensive performance review of an MPI-based high-order three-dimensional spectral element method C++ toolbox is presented with focus on the parallel efficiency. The performance evaluation is analyzed with help of a time prediction model based on a parametrization of the application and the hardware resources. A tailor-made CFD computation benchmark case is introduced and carried out, stressing the particular interest for clusters with up to 8192 cores. Some problems in the parallel implementation have been detected and corrected. The theoretical complexities with respect to the number of elements, to the polynomial degree, and to communication needs are correctly reproduced. It is concluded that this type of code has a nearly perfect speedup on machines with thousands of cores, and is ready to take the step to next-generation petaflop machines.

Remark: This is a collaborative work with Christoph Bosshard¹, Christian Cléménçon¹, Roland Bouffanais³, Nicolas Fiétier¹, Ralf Gruber¹, Vincent Keller¹, and Jonas Latt¹.

References:

- [1] Bosshard, et al., Computational Performance of a Parallelized Three-Dimensional High-Order Spectral Element Toolbox, *APPT 2009*, LNCS 5737, pp. 323–329, 2009.

Title: Self-Consistent Generation of Plate Tectonics in Spherical Mantle Convection

Researchers: H. van Heck
P. J. Tackley

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

Description:

In convection with strongly temperature-dependent viscosity appropriate to rocks, the cold upper thermal boundary layer becomes so stiff that it forms a stagnant lid around the planet. This is similar to Venus or Mars, but on Earth the lid is broken into several plates that move around, with deformation taking place at narrow plate boundaries. Various simulations have shown that introducing plastic yielding to model brittle or semi-brittle failure of the rock, breaks the stagnant lid and leads to plate tectonic-like behaviour. In this project we investigate self-consistent plate tectonics using simulations in a 3-D spherical shell using the code StagYY by P. Tackley. In an initial study (listed below) we found two new modes of convection in this geometry, including "great circle" subduction with weak spreading centers at low yield stress, and a two-plate solution at higher yield stress. We are now systematically investigating the behaviour as a function of heating mode (internal, basal or a combination), Rayleigh number and yield stress. This leads to scaling laws that can then be applied to understand the evolution of Earth and other terrestrial planets, including "super-Earths".

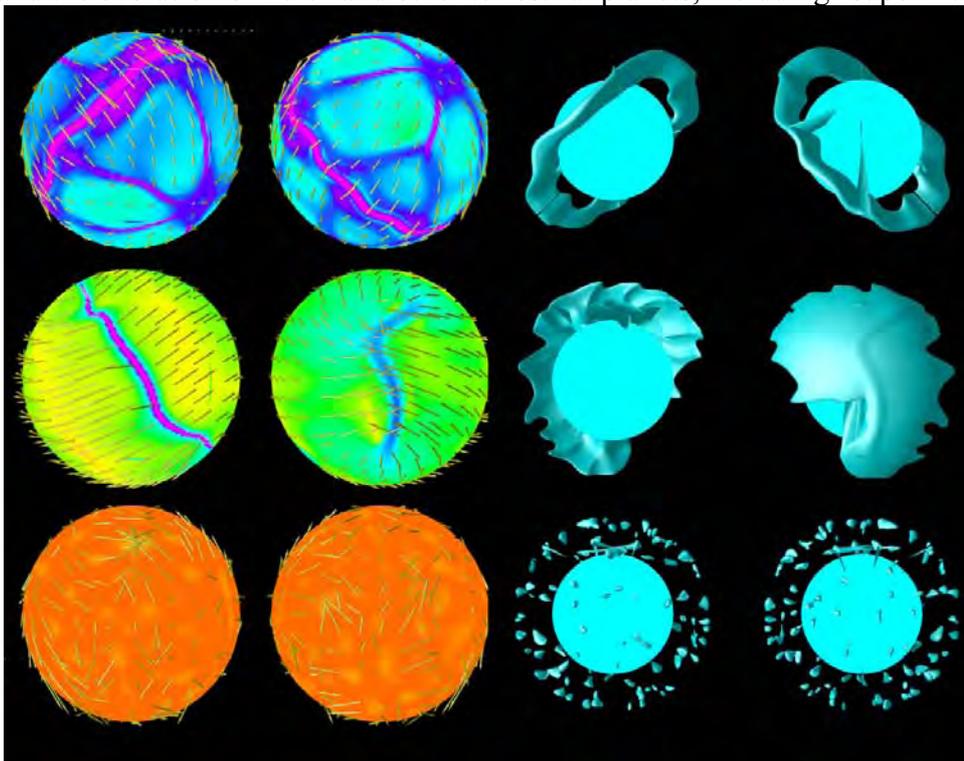


Figure. Surface viscosity (left 2 columns) and cold temperatures (right 2 columns) showing 'great circle subduction' mode (top), two-plate solution (middle) and stagnant lid (bottom).

References: van Heck, H. and P. J. Tackley, Planforms of self-consistently generated plate tectonics in 3-D spherical geometry, *Geophys. Res. Lett.* 35, L19312, doi:10.1029/2008GL035190.

Title: Scaling Laws for Thermal Convection in Spherical Geometry

Researchers: F. Deschamps
P.J. Tackley

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

Description:

Reconstruction of the thermal history of planetary mantles requires a good description of the heat flux that can be transported through planetary mantles. A convenient way to quantify heat flux, internal temperature and other important observables is to build appropriate scaling relationships, which relate these observables to controlling parameters. Scaling relationships strongly depend on the system physical (geometry, boundary conditions, mode of heating) and rheological properties. A key ingredient is a realistic, spherical geometry. The curvature, measured by the ratio f of the core radius to the total radius, has a strong influence on the flow pattern and on the heat transfer. Using STAGYY, we performed two series (one for bottom heating, e.g. Figure 1, the other for mixed heating) of numerical experiments of thermal convection for an isoviscous fluid in spherical geometry. We then invert our results for appropriate heat flux and temperature scaling relationships as a function of the curvature, the Rayleigh number, and the internal heating. Additional complexities of planetary mantles include temperature dependent viscosity and the presence of chemical heterogeneities. A more realistic description of the thermal history of planetary mantles thus requires scaling relationships that account for these parameters, which we will consider in future steps.

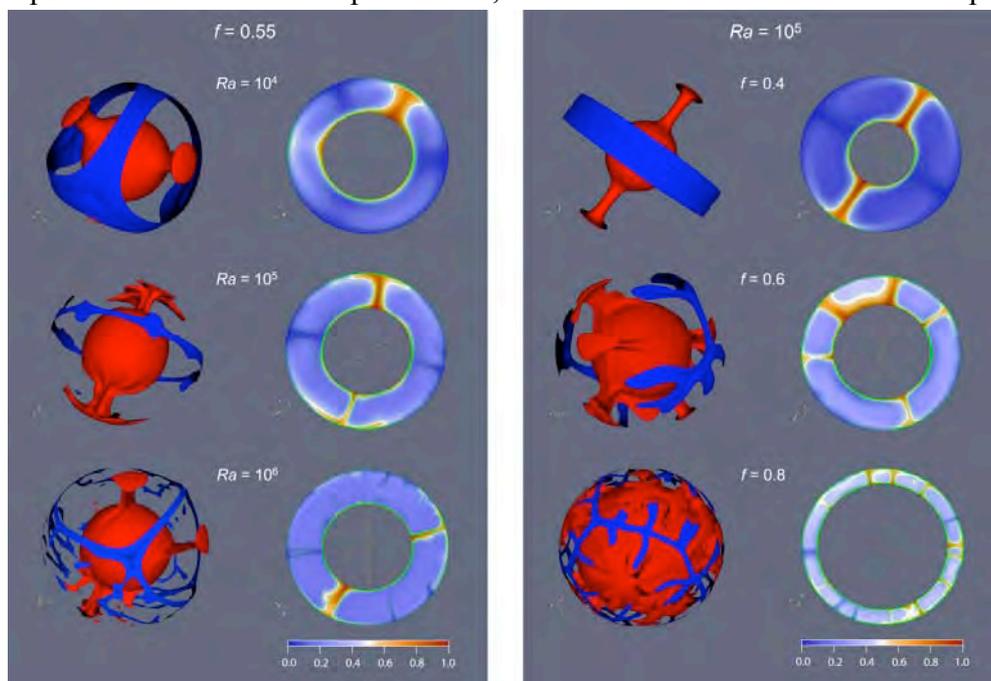


Figure 1. Thermal convection simulations. Left: fixed curvature ($f = 0.55$) and 3 Rayleigh numbers. Right: fixed Rayleigh number (10^5) and 3 curvatures. Left columns contain temperature isosurfaces, right columns show temperature slices.

Title: Thermo-Chemical Convection and the Survival of Reservoirs of Dense Material

Researchers: F. Deschamps
P.J. Tackley

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

Description:

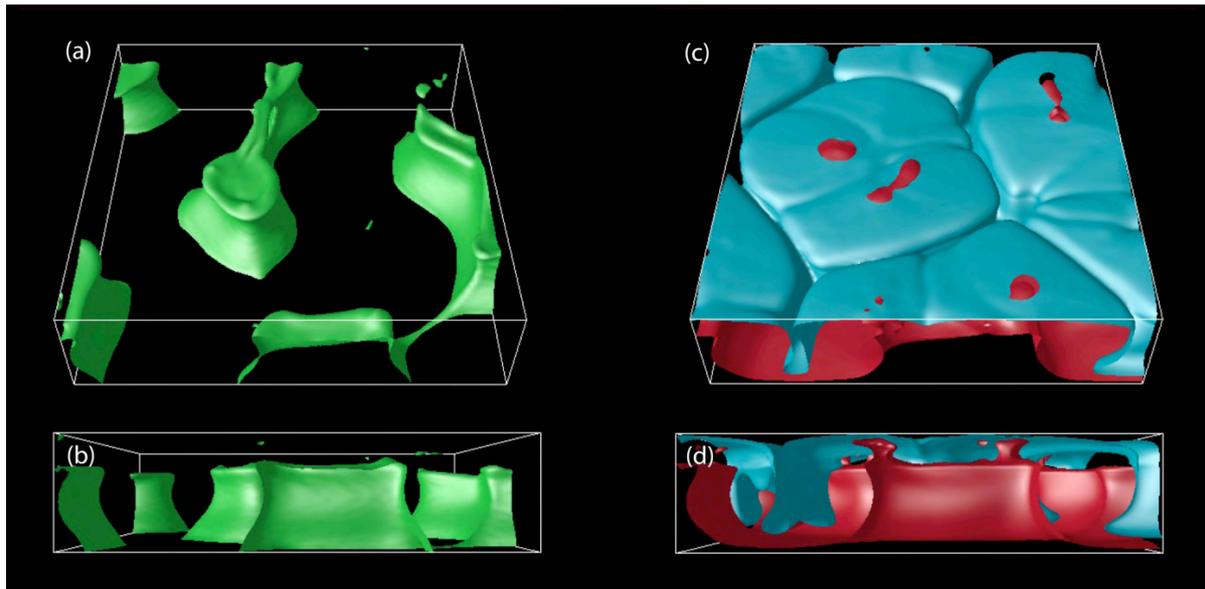


Figure 1. A thermo-chemical model of convection combining a moderate buoyancy ratio ($B = 0.2$), a moderate compositional viscosity contrast ($R\mu_c = 18$), a large thermal viscosity contrast ($R\mu_T = 10^6$), a 660-km viscosity jump of 30, and a Clapeyron slope of the phase transition at 660 km equal to -2.3 MPa/K. Plots (a) and (b) display isosurface ($C = 0.5$) of the chemical field, and plots (c) and (d) display isosurfaces of the residual temperature (red is hot, blue is cold). For these parameter values, large pools of dense material are generated at the bottom of the system, and survive convection for at least 4.5 Gyr. The thermo-chemical structures predicted by such model fit those observed by probabilistic tomography very well.

A growing body of seismological observations indicate that strong density anomalies, likely due to compositional anomalies, are present in the Earth's deep mantle. We aim to identify models of thermo-chemical convection that can generate strong thermo-chemical density anomalies in the lower mantle – particularly at its base, and maintain them for a long period of time. For this, we explored the model space of thermo-chemical convection using STAG3D. Five main conclusions can be drawn from this search. (i) Large (≥ 100 kg/m³) chemical density contrasts induce stable layering. For smaller contrasts, with no other ingredient added, dense material is rapidly entrained. (ii) For strong ($\geq 10^4$) thermal viscosity contrasts, large pools of dense material are generated at the bottom of the system and survive convection. (iii) Small chemical viscosity contrasts allow rapid mixing, whereas large chemical viscosity contrasts give stable layering. This influence is however of 2nd order compared to those of the buoyancy ratio and of thermal viscosity contrast. (iv) A 660-km viscosity contrast of 30 or more reduce the vertical mass transfer around this depth. (v) An

endothermic phase transition at 660-km with a Clapeyron slope around -3.0 to -1.5 MPa/K strongly inhibits the rise of dense material above 660 km but still allows the penetration of downwellings in the lower mantle. Thus, models that include both a large thermal viscosity contrast and an endothermic 660-km phase transition (Figure 1) are able to create and maintain large pools of dense material at the bottom of the system.

References: Phys. Earth Planet Int. (2008) doi:10.1016/j.pepi.2008.04.016
Phys. Earth Planet Int. (2009) doi:10.1016/j.pepi.2009.03.012

Title: Coupled Models of Mantle Geochemical Evolution, Plate Tectonics, Magmatism and Core Evolution Incorporating Self-consistently Calculated Mineralogy

Researchers: T. Nakagawa, P. J. Tackley, F. Deschamps, J.A.D. Connolly

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

Description:

In the mantle, many different mineral phases exist as a function of pressure, temperature and composition, and these have a first-order influence on properties such as density, which has a large effect on the dynamics. Numerical models of thermo-chemical mantle convection have typically used a simple approximation to treat these complex variations in material properties, such as the extended Boussinesq approximation. In order to get closer to a realistic mineralogy, we here calculate composition-dependent mineral assemblages and their physical properties using the code *Perple_X* by J. Connolly, which minimizes free energy for a given combination of oxides as a function of temperature and pressure, and use this in a numerical model of thermo-chemical mantle convection in a three-dimensional spherical shell, to calculate three-dimensionally-varying physical properties. The numerical models treat the evolution of a planet over billions of years, including self-consistent plate tectonics arising from plastic yielding, melting-induced differentiation, and a parameterised model of core evolution based on heat extracted by mantle convection.

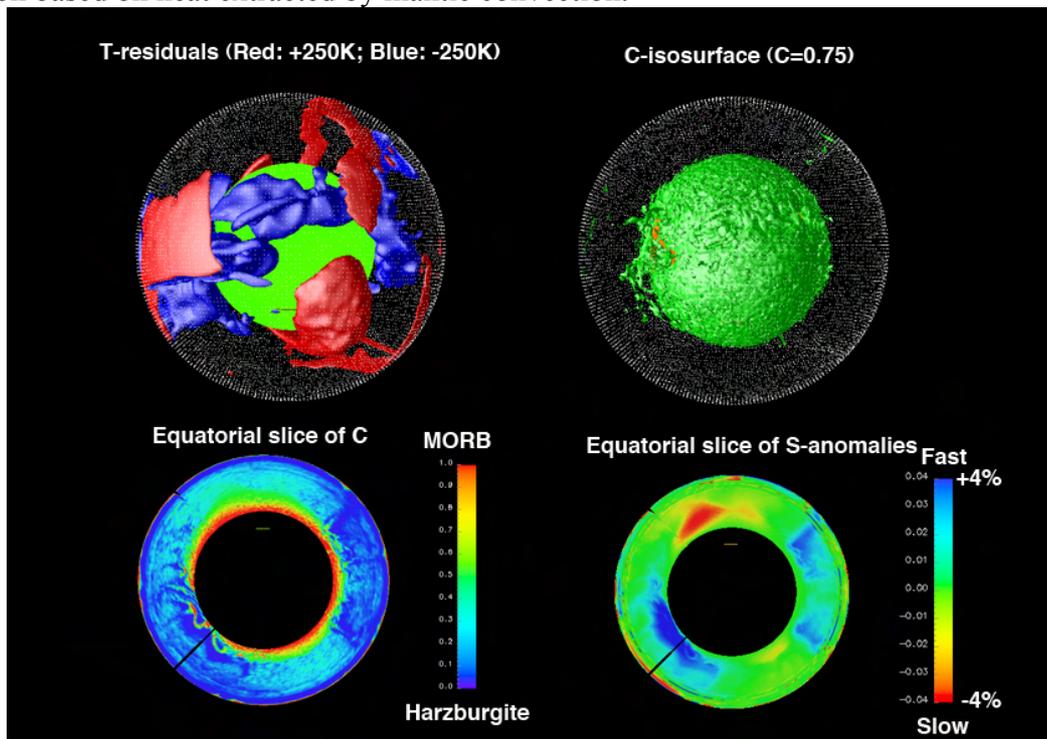


Figure 1. Example simulation with PERPLEX-calculated mineralogy and physical properties.

References: Nakagawa, T., P. J. Tackley, F. Deschamps and J. A. D. Connolly (2009) Incorporating self-consistently calculate mineral physics into thermo-chemical mantle convection simulations in a 3D spherical shell and its influence on seismic anomalies in Earth's mantle, *Geochem. Geophys. Geosys.*, 10, Q03004, doi:10.1029/2008GC002280.

Title: Robust Preconditioning in CitcomS via PETSc

Researchers: Dave May

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

Description:

The use of numerical simulations to study convection in the mantle has a long history in geodynamics. The Citcom family of mantle convection codes are in widespread use through out the geodynamics community. Since the inception of the original Cartesian version written by Louis Moresi in the early 1990's, many variants have been developed. Two important contributions were made by Shijie Zhong in the form of the parallel 3D Cartesian version and the parallel, full spherical version.

The Computational Infrastructure for Geodynamics (CIG) have been providing maintenance and support for CitcomS over the last 5 years. The CIG effort to provide a community mantle convection code has resulted in several developments to CitcomS. These include the addition of new physics (rheology, compressibility), coupling with other software, the inclusion of additional geologically relevant input/outputs and improved portability. Such improvements have seen a further increase in the development and usage of this particular version of Citcom. Today, CitcomS is routinely used to solve mantle convection and subduction models with approximately one hundred million unknowns on large distributed memory clusters.

In simulations of convection and slab subduction, one of the major challenges preconditioned iterative methods face, is to be able to effectively handle a wide range of viscosity contrasts and viscosity structures. Viscosity contrasts may vary by up to $O(10^8)$ and viscosity structures may be either smooth and continuous functions, or discontinuous. Many advances have been made in both numerical linear algebra and the software encapsulating these mathematical concepts since the development of the original Citcom. However, the solver used by all Citcom software has remained largely unchanged from the original version. Incorporating modern techniques into CitcomS has the potential to greatly improve the flexibility and robustness of the iterative method used to solve the underlying saddle point problem. Here we describe how PETSc (<http://www.mcs.anl.gov/petsc>), a flexible linear algebra package, has been integrated into CitcomS in a non-invasive fashion which i) preserves all the pre-existing functionality and ii) enables a rich infrastructure of preconditioned Krylov methods to be used to solve the discrete Stokes flow problem.

We demonstrate the advantages of including PETSc in CitcomS by comparing the convergence rate and solution time of the new Stokes solver with the original CitcomS approach. As a preconditioner for the Schur complement, we utilise a scaled BFBt preconditioner which is constructed via the assumption of the existence of an approximate commutator. The BFBt preconditioner is composed of smaller sub-problems for which efficient, robust and scalable algebraic multigrid (AMG) methods exist. Specifically, we utilise PETSc's interfaces to the Hypre (BoomerAMG) and ML algebraic multigrid libraries to rapidly prototype our preconditioner. We demonstrate that the scaled BFBt we utilise is robust and yields convergence rates largely independent of the element resolution and the viscosity contrast. Using this preconditioner, we can accommodate higher viscosity contrasts than were possible with the original CitcomS solver. The test problems

used for these comparisons include simulations of variable viscosity mantle convection (regional, full spherical) and slab subduction (regional).

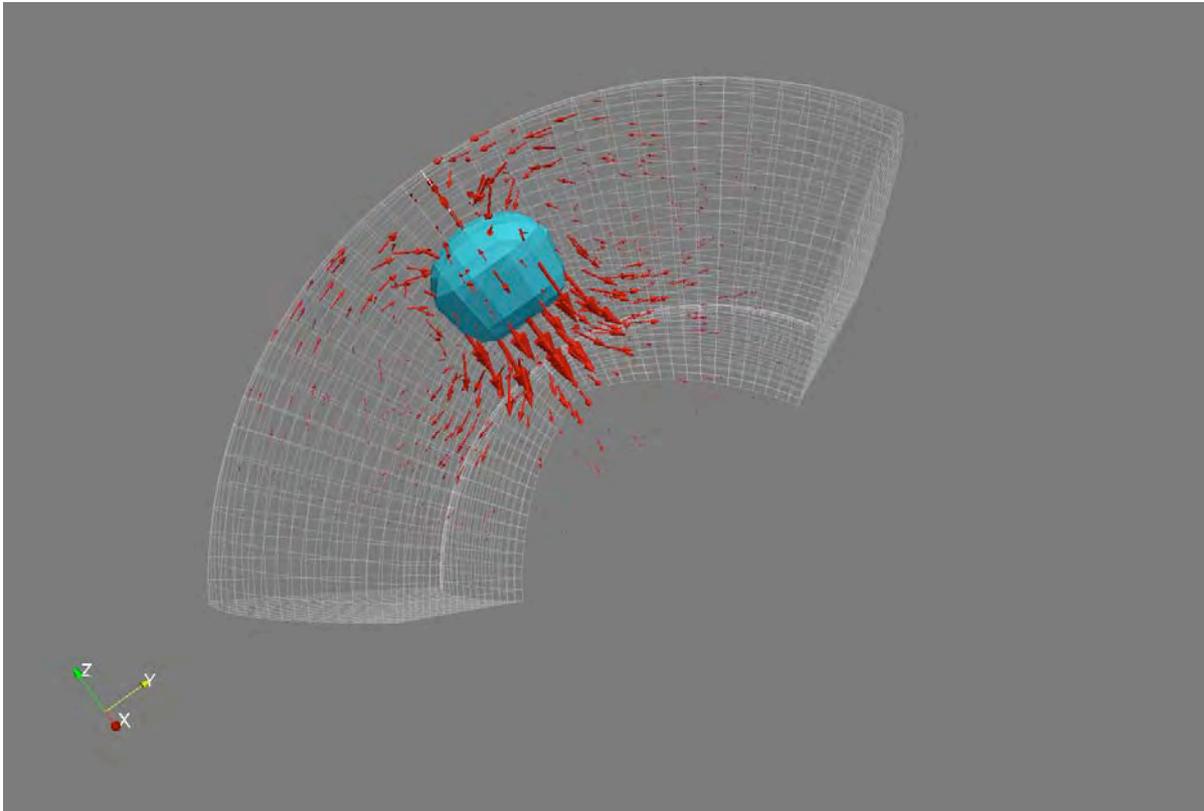


Figure: Illustration of an idealised geodynamic model referred to as the "viscous sinker" problem. Here, a cube with viscosity 10^6 Pa.s sinks into the surrounding mantle which possesses a viscosity of 10 Pa.s. Despite the simple geometric setup, the discontinuity in the viscosity field and the magnitude of the viscosity contrast between the mantle and cube make this problem challenging for preconditioned iterative methods. The resulting flow field is shown.

References:

May, D.A. & Moresi, L., (2008), Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, *Physics of Earth and Planetary Interior*, 171, pp. 33-47.

An additional publication is in preparation to be submitted to "Geochemistry, Geophysics, Geosystems".

Title: Comparing Thin-Sheet Models with Three-Dimensional Numerical Models for India-Asia collision

Researchers: S. M. Lechmann¹
S. M. Schmalholz¹
B. J. P. Kaus²

Institute/Group: ¹ Geological Institute/ Structural Geology and Tectonics, D-ERDW
² Institute of Geophysics/ Geophysical Fluid Dynamics, D-ERDW

Description:

Knowledge about the tectonic evolution of the Tibetan Plateau is still incomplete and many open questions remain concerning the deformation style of the crustal thickening, causing the abnormally high elevation of the Tibetan Plateau. Different models have been suggested explaining the crustal thickening by (1) homogeneous, continuous deformation using thin-sheet models, (2) discrete movement along thrusts developing crustal wedges and (3) lateral crustal flow due to pressure gradients resulting from topography. Most existing numerical models are not fully three-dimensional (3D) (e.g. thin-sheet models) and assume a certain deformation style a priori, which makes it difficult to judge the applicability of such constrained models to the formation of the Tibetan Plateau.

We performed a comparison of deformation styles during continent indentation resulting from a fully 3D numerical model and a thin-sheet model. The rheology for both models is linear viscous. The 3D model consists of four layers representing a simplified lithosphere: strong upper crust, weak lower crust, strong upper mantle and weak lower mantle. From the effective viscosity distribution of the 3D model a vertically averaged effective viscosity is calculated and used for the thin-sheet model to make direct comparisons between the two models.

Simulating indentation is achieved by assigning a tripartite velocity profile at one lateral boundary (fig. 1): A constant horizontal velocity is applied at one section. The velocity then gradually decreases towards zero, applying a cosine-function. The last section of the indenting boundary is fixed. The other three lateral boundaries show free slip. The 3D model additionally exhibits a free surface and a bottom boundary allowing free slip.

The 3D code employs the finite element method with a mixed velocity-pressure formulation to simulate incompressible flow. A Lagrangian mesh with 27-node brick elements and 27 integration points is employed. The thin-sheet model is also based on the finite element method using 7-node triangles.

We quantified the differences in the horizontal velocity field resulting from the two models. Special attention was paid on two scenarios: First, active indentation is taking place, while in a second phase indentation velocity is set to zero and only gravity is acting. We focused on the area around the indentation corner (the so-called syntaxis), as there the differences in both models are largest.

During indentation the overall velocities of the thin-sheet model and the full 3D model are of the same order of magnitude and differences are marginal. However, when indentation velocity is set to zero and gravitational collapse is equilibrating the differences in topographic elevation, the two models are not in agreement anymore (fig. 2).

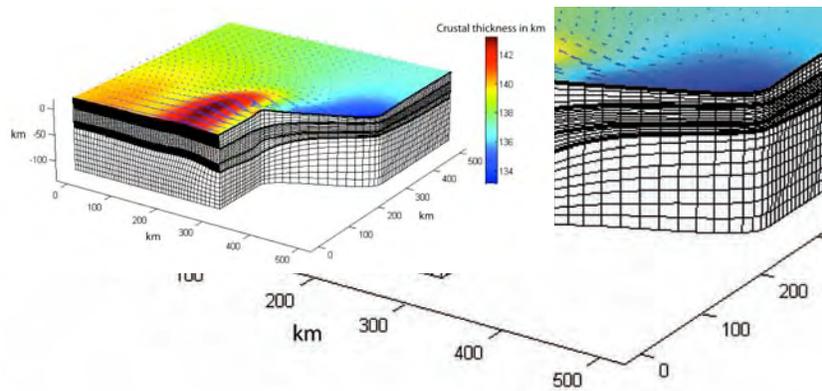


Figure 1: Indentation in 3D model. Kinematic boundary conditions account for the indentation of India into Asia. Colours indicate crustal thickness in km and blue arrows indicate velocity field at the surface.

In the 3D model we can observe strong gradients in magnitude and direction of velocities with depth in the area of the syntaxis.

The employed 3D model, including a viscosity profile with two strong layers, is still quite basic but already includes large strain indentation, multilayer buckling, lower crustal flow and differential thickening. The thin-sheet model, on the other hand, ignores deformation styles like buckling and lower crustal flow.

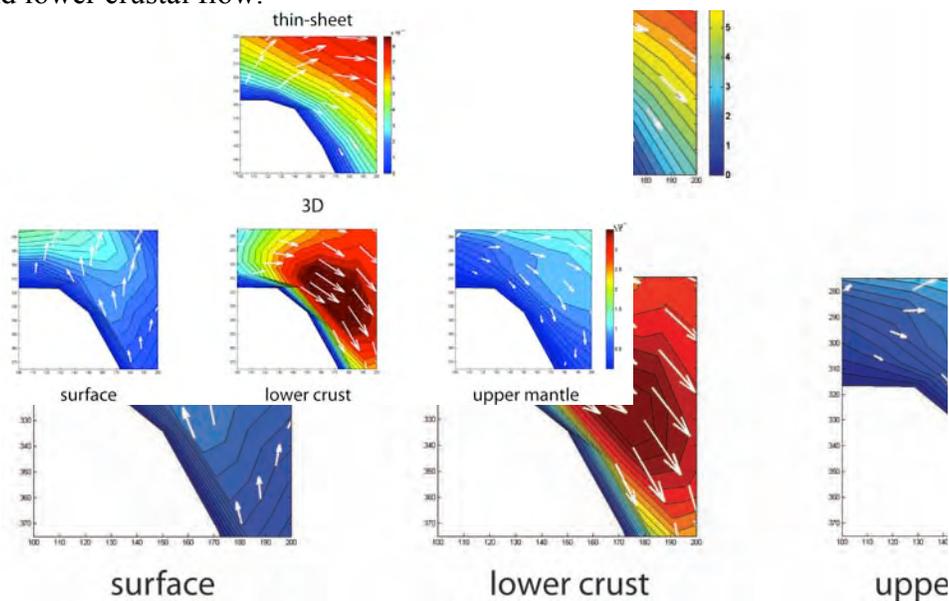


Figure 2: Zoom of situation at the syntaxis during gravitational collapse. White arrows indicate the horizontal flow field and colours the magnitude of the horizontal velocity ($v = \sqrt{v_x^2 + v_y^2}$). Largest velocity in the thin-sheet model is $9 \cdot 10^{-12} \text{ m/s} \approx 0.3 \text{ mm/yr}$. Largest velocity in the 3D model is $3.5 \cdot 10^{-11} \text{ m/s} \approx 1 \text{ mm/yr}$.

Title: Understanding the Dynamics of Subduction by Combining Semi-Analytical and Numerical Models

Researchers: B.J.P. Kaus¹
T.W. Becker²

Institute/Group: ¹ Institute of Geophysics/ Geophysical Fluid Dynamics, D-ERDW
² Dep. of Earth Sciences, University of Southern California, USA.

Description:

Subduction zone dynamics has been extensively studied with laboratory models in which a dense, high viscosity slab sinks into a less dense and less viscous mantle. Recently, it was found that these laboratory results could be reproduced with numerical models if the upper boundary condition is a true free surface, or if a weak ‘sticky-air’ layer is employed [Schmeling et al, PEPI, 2008]. Yet, our insight in the dynamics of subduction remains somewhat limited and no scaling law exists that *predicts* slab velocity (or slab behavior) as a function of slab thickness, slab/mantle viscosity ratio and slab/mantle density difference. Existing scaling laws rely on knowing the radius of curvature of subducting slabs, which is a parameter that is typically known only *after* an experiment has been performed. For this reason, we here perform additional 2D numerical simulations in which we address the effects of numerics (resolution, time step), initial geometry (slab tip length and angle), and rheology on subduction dynamics in the presence of a free surface.

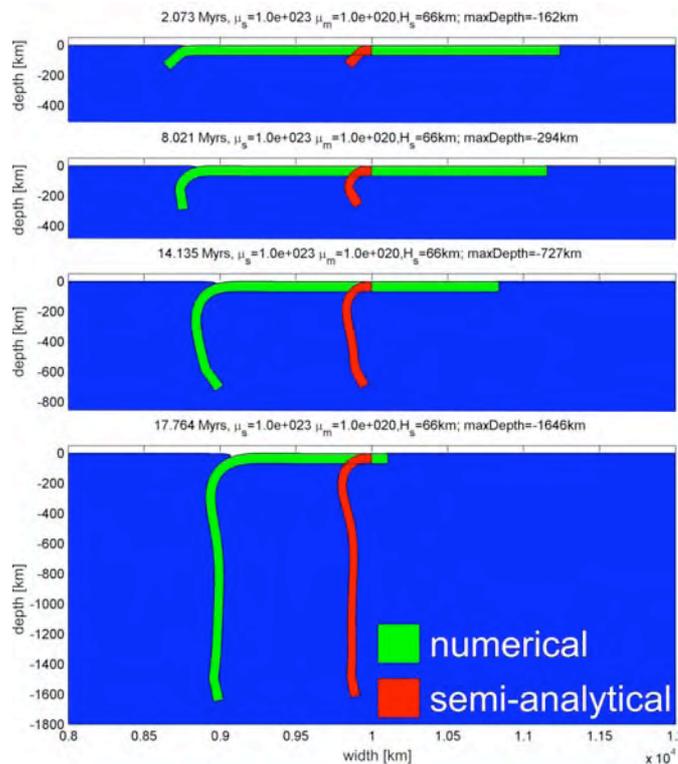


Figure: Comparison between numerical simulations (green) and the semi-analytical model (red). The semi-analytical model is shifted in the horizontal direction for visualization purposes.

Results confirm earlier findings that slab dynamics is to a large extent controlled by the effective viscosity contrast between slab and mantle. Two main deformation modes exist as a function of viscosity contrast: the ‘drip’ or ‘Rayleigh-Taylor’ mode occurs for viscosity contrasts smaller than about 100, and is dominated by slab-stretching and non-constant horizontal plate velocities. The ‘plate’ mode, on the other hand, occurs for viscosity contrasts larger than 500 and is characterized by slabs that do not change their initial length during subduction. Horizontal plate velocities are homogeneous along the slab top and bending occurs in the trench area, with a bending radius that depends on viscosity contrast and slab thickness. In the plate mode, the initial slab tip length and angle have a significant effect on the initial subduction rate. After the slab tip reached a depth of several hundreds of km, however, subduction velocities are largely independent on the initial geometry and are described by a modified Stokes law. We developed a semi-analytical subduction model by combining this velocity parameterization with thin viscous sheet equations. Good agreement exists between numerical and analytical models, both in terms of geometry and in terms of temporal evolution, and we are currently exploring the dynamics of subduction with the help of this semi-analytical model.

Title: Factors That Control the Angles of Shear Bands in Geodynamic Numerical Models of Brittle Deformation

Researchers: B.J.P. Kaus

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

Description:

Numerical models of brittle deformation on geological timescales typically use a pressure-dependent (Mohr-Coulomb or Drucker-Prager) plastic flow law to simulate plastic failure. Despite its widespread usage in geodynamic models of lithospheric deformation, however, certain aspects of such plasticity models remain poorly understood. One of the most prominent questions in this respect is: what are the factors that control the angle of the resulting shear bands? Recent theoretical work suggest that both Roscoe (45°), Coulomb angles ($45^\circ \pm \phi/2$, where ϕ is the angle of internal friction) and Arthur angles ($45^\circ \pm (\phi + \Psi)/4$ where Ψ is the dilation angle), as well as all intermediate angles are possible. Published numerical models, however, show a large range of shear band angles with some codes favoring Arthur angles, whereas others yield Coulomb angles.

In order to understand what causes differences between the various numerical models, I here perform systematic numerical simulations of shear localization around an inclusion of given length-scale. Both numerical (element-type), geometrical and rheological (viscoplastic versus viscoelastoplastic) effects are studied. Results indicate that the main factor, controlling shear band angle, is the non-dimensional ratio between the length scale of the heterogeneity d and the size of the numerical mesh Δx . Coulomb angles are observed only in cases where $d/\Delta x > 5-10$, and in which the inclusion is located sufficiently far from the boundary of the box. In most other cases, either the Arthur orientation or the Roscoe orientation is observed. Whereas differences in element-types and rheology do have consequences for the maximum obtainable strain rates inside the shear bands, they only have a minor effect on shear band angles. Shear bands, initiated from random noise or from interactions of shear bands with model boundaries or other shear bands, result in stress heterogeneities with dimensionless length scales $d/\Delta x \sim 1-2$. Such shear bands are thus expected to form Roscoe or Arthur orientations, consistent with the findings in previous numerical models.

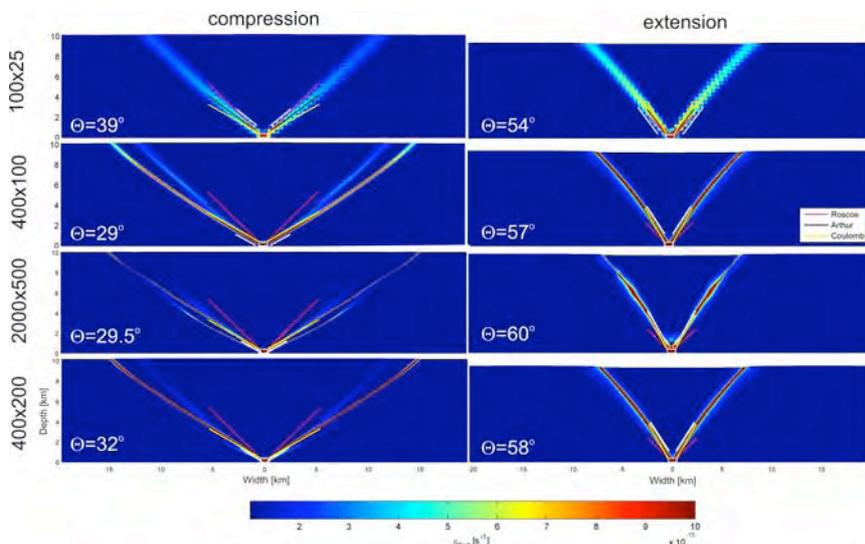


Figure 1: Examples of shearband angles under compression and extension, for various numerical resolutions. Numbers indicate the resulting shear-band angle. Coulomb angles form at sufficiently large resolutions.

Title: MILAMIN_VEP: A Fast MATLAB-based Finite Element Code to Model Large-Strain Geodynamic Processes

Researchers: B.J.P. Kaus

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

Description:

Numerical modelling of geodynamic processes is challenging since it involves a number of complexities, both physical (rocks in a brittle manner if cold or subjected to large differential stresses, but in a viscous manner if they are hot), and numerical (dealing with extremely large strains in the presence of a free surface). Moreover, material properties are a function of pressure, temperature and composition, and might change once partial melting occurs.

To deal with these complexities I have developed a general 2D MATLAB-based finite element code called MILAMIN_VEP. The solver of the code is based on the high-performance viscous Stokes solver MILAMIN (a MILlion degrees of freedom a MINute), developed by Dabrowski et al. (2008, G-cubed; see also www.milamin.org). In addition, I have added elasticity, plasticity, and powerlaw rheologies. Moreover, the mechanical solver is coupled with an energy solver, to allow modelling of processes such a shear-heating induced localization. Tracers in combination with a remeshing algorithm are employed to deal with large deformations and which also allows for a relatively straightforward implementation of phase transitions. The use of a direct solver ensures that a solution can be obtained even in the presence of large variations in effective viscosity contrast, as they typically arise during such simulations. A simple surface processes algorithm is included to allow to study the effects of a free surface, erosion and sedimentation on tectonics. Moreover, both quadrilateral and triangular elements are implemented which allows using the code with both structured and unstructured meshes.

MILAMIN_VEP has been verified against a range of available analytical solutions. Moreover, the code participated in a two recent benchmark studies (on subduction dynamics and brittle deformation. Currently MILAMIN_VEP is used in a routinely manner by a number of researchers to address problems that range from a grain-size (“what is the effective rheology of a partially molten rock?”), to crustal and lithospheric scale (e.g. crustal scale-buckling in the Zagros mountains, or initiation of lithospheric shear localization), or planetary scale (e.g. to study subduction dynamics, interaction between mantle convection and lithospheric deformation or to study coronae formation on Venus).

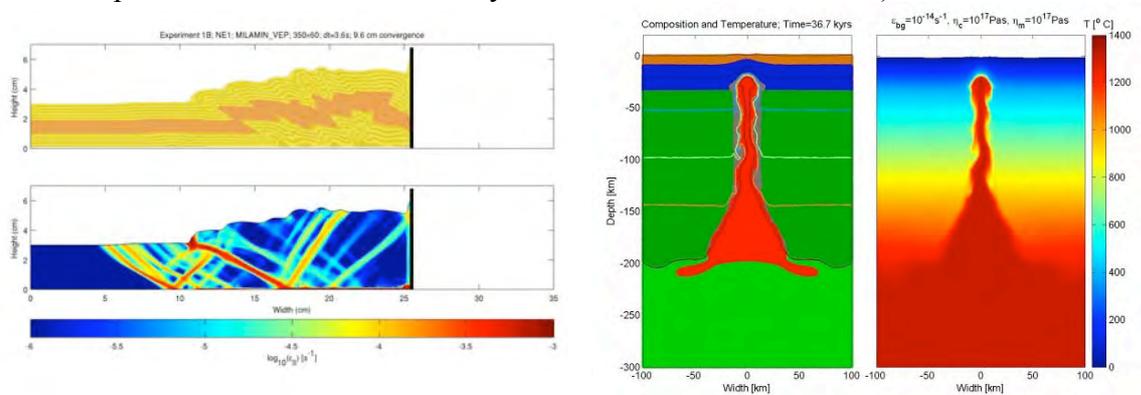


Figure. Simulations performed by MILAMIN_VEP. Left: part of a benchmark study on crustal-scale brittle deformation. Right: melt migration through the lithosphere.

Title: Development of a 3D Lithosphere and Mantle Evolution Model (LaMEM)

Researchers: B.J.P. Kaus
D. May

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

Description:

Mantle convection modelling is well established in the field of geodynamics. Over the last 25 years, numerous mantle convection codes have been developed for distributed memory computer architectures to enable high resolution, three-dimensional simulations to be performed. Together with parallelism, such codes also incorporate some form of multigrid implementation (typically geometric multigrid) to provide a scalable solution. Effectively treating problems with large viscosity contrasts is a continually active area of research in the mantle convection community.

By comparison, numerical models of lithospheric dynamics are far less mature. This is especially true if we consider codes capable of three-dimensional simulations. Part of the reason for the development in lithospheric dynamics lagging behind mantle convection may be due to the fact that finite elements have typically been the favoured discretisation method for these models. Compared to the finite volume discretisation advocated in mantle convection models, finite elements typically possess much larger memory requirements, and as such, three-dimensional simulations were beyond the computational resources of many research groups. Several additional computational challenges face numerical models of lithospheric deformation i) the inclusion of complex non-linear, visco-elasto-plastic rheologies and ii) the need to track distinct compositional and rheologically different materials. Both of these attributes complicate the development of scalable three-dimensional models, particularly with respect to the choice of preconditioned iterative method, which is suitable to solve the discrete set of equations.

The "Lithosphere and Mantle Evolution Model" (LaMEM) is a three-dimensional, arbitrary Lagrangian-Eulerian (ALE) visco-plastic finite element code which is being developed to study high resolution models of lithospheric deformation. Important to the success of this code is its ability to scale well up to hundreds of CPU's. At the core of LaMEM is the discretisation of a variable viscosity Stokes flow problem. The implicit solution of the system of equations is the most computational demanding component of each time step. In addition, LaMEM has a tracer-based advection scheme to deal with large deformation. We have currently implemented both linear (Q_1P_0) and quadratic elements (Q_2P_1) and the code can be employed in either a fully Lagrangian, a fully Eulerian or in an arbitrary Lagrangian-Eulerian mode.

The software library PETSc is used to provide basic support for managing a distributed grid and parallel linear algebra operations required by preconditioned Krylov subspace methods. Through PETSc, we have access to the scalable algebraic multigrid libraries BoomerAMG (included with Hypre) and ML (included with Trilinos).

The current LaMEM development is split into several inter-related focus areas.

- i) the development and inclusion of visco-plastic and visco-elastic rheologies, as well as the inclusion of typical experimentally derived rock creep laws.
- ii) the development of scalable, robust preconditioners for highly variable viscosity Stokes flow.

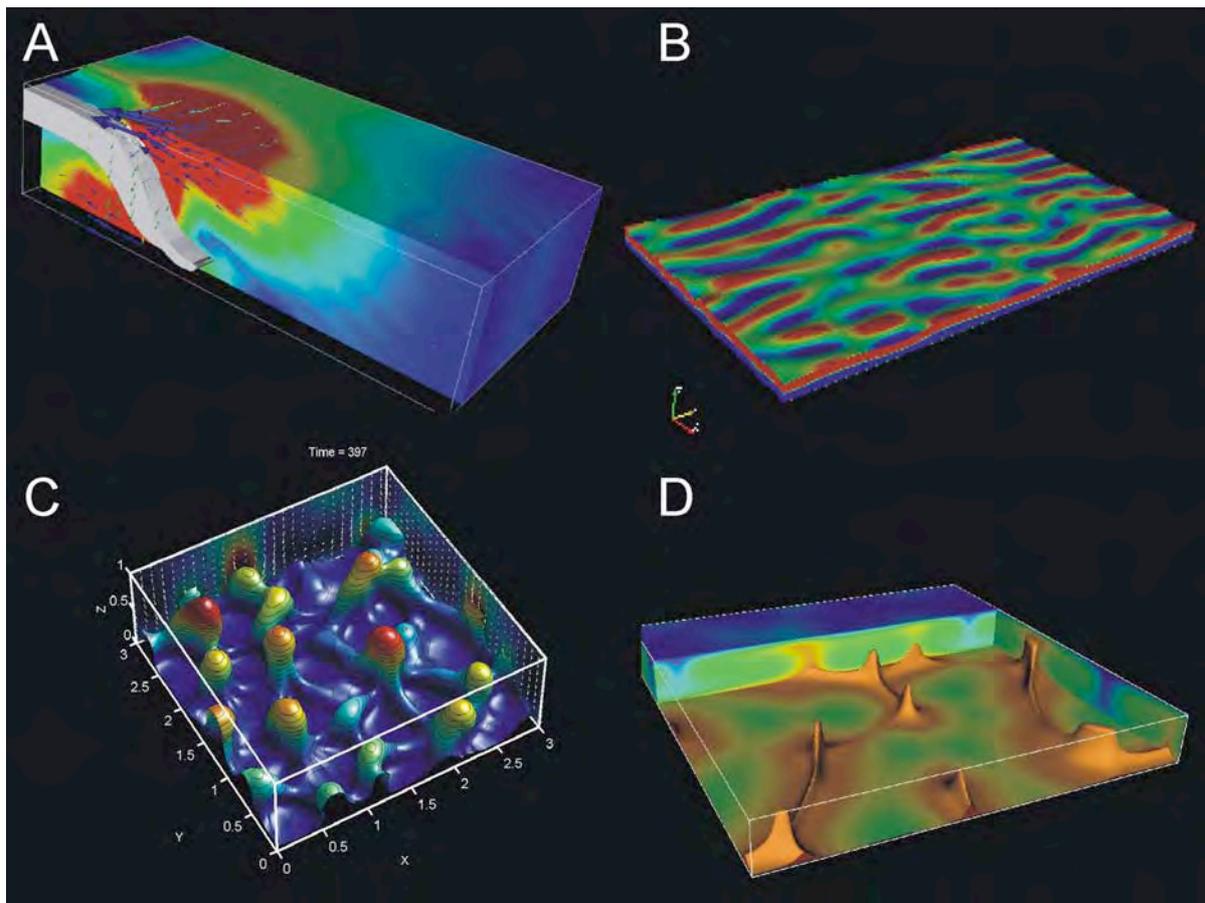


Figure 1. Geodynamic examples: A) subduction in the presence of a free surface, B) detachment folding of a high viscosity layer on top of a layer with small viscosity, C) Viscous Rayleigh-Taylor instability, D) thermal convection.

Title: Is Mars' Crustal Dichotomy a Consequence of Core Formation?

Researchers: G. Golabek¹
T. Keller¹
T. Gerya¹
J.A.D. Connolly²

Institute/Group: ¹ Institute of Geophysics/ Geophysical Fluid Dynamics, D-ERDW
² Institute of Mineralogy and Petrology, D-ERDW

Description:

One of the most striking surface features on Mars is the crustal dichotomy, a large difference in elevation and crustal thickness between the southern highlands and the northern lowlands. The dichotomy is among the oldest geological features on Mars and was formed more than 4.1 billion years ago owing to either exogenic or endogenic processes (e.g. Keller and Tackley, 2009). In order to find an internal origin of the crustal dichotomy, occurring within a maximum of 400 Ma of planetary differentiation, the thermal state of the planet resulting from core formation needs to be considered. Based on the geochemical analysis of SNC meteorites it was suggested that a primordial crust with up to 45 km thickness can be formed already during the Martian core formation. Therefore we suggest that the sinking of iron diapirs delivered by pre-differentiated impactors induced shear heating-related temperature anomalies in the mantle, which fostered the formation of early Martian crust. In this study, we examine parameter sets that will likely cause an onset of hemispherical low-degree mantle convection directly after, and coupled to, an already hemispherically asymmetrical core formation. To test this hypothesis we use a numerical model, where we self-consistently couple the formation of the Martian iron core to the onset of mantle convection. Peridotite melting is enabled to track melting and crust formation caused by heat released from core formation and radioactive heating.

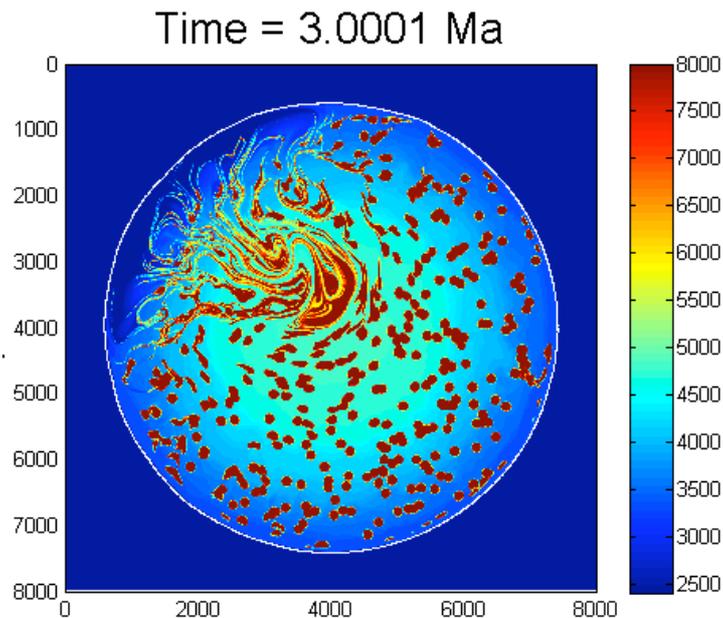


Fig. 1: Density plot showing a giant impactor triggering a fast iron silicate separation on one hemisphere of a Mars-sized body.

We perform 2D simulations using the code I2ELVIS, which combines finite differences on a fully staggered rectangular Eulerian grid with Lagrangian marker-in-cell technique to solve momentum, continuity and temperature equations as well as the Poisson equation for gravity potential in a self-gravitating planetary body. In our model setup, the planet is surrounded by a low viscosity, massless fluid to simulate a free surface. We apply a temperature- and stress-dependent viscoplastic rheology inside a Mars-sized planet. Radioactive and shear-heating as well as consumption of latent heat by silicate melting are taken into account. The depth of neutral buoyancy of silicate melt with respect to solid silicates is determined by the difference in compressibility of the liquid and solid phase. To self-consistently simulate the silicate phase changes expected inside a Mars-sized body, we employ the thermodynamical `Perple_X` database. As initial condition, we apply randomly distributed iron diapirs with 75 km radius inside the planet, representing the cores of stochastically distributed impactors characteristic for the late accretion stage of terrestrial planets. Additionally, we explore the effect of one giant impactor core on the planetary evolution.

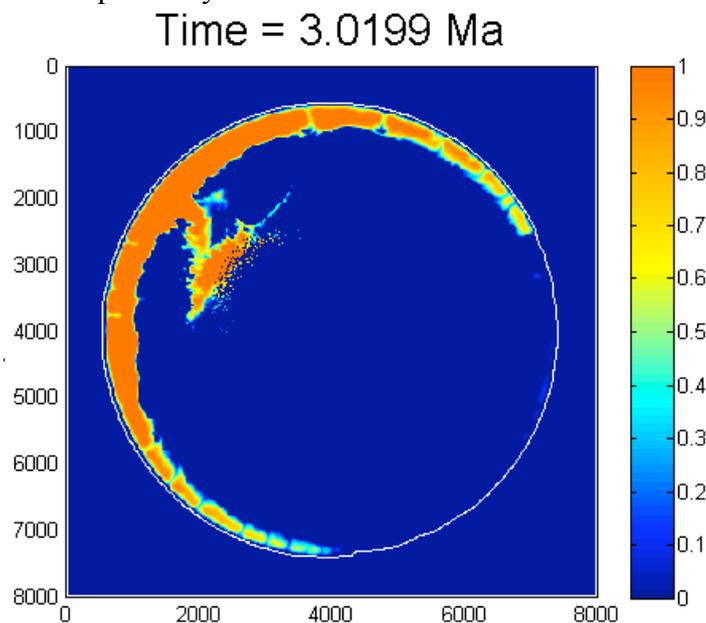


Fig. 2: Melt fraction plot showing silicate melt covering one hemisphere fostering a dichotomous structure.

Results indicate that the presence of a large impactor core induces hemispherically asymmetrical core formation. Furthermore, the amplitude of shear heating anomalies generally well exceeds the solidus of primitive mantle material. The formation of a considerable amount of silicate melt is observed. Some of the generated melt segregates to the surface to form primordial crust, whereas negatively buoyant melt from deeper sources sinks to the CMB. The hemispherical asymmetry in temperature induced by a giant impactor works in favour of an onset of low-degree mantle convection after core formation. Such a hemispherical convection geometry might subsequently be sustained by phase-dependent viscosity, and thus harbour an early development of a dichotomous crustal thickness distribution.

Title: Influence of Rheology on Terrestrial Planet Core Formation

Researchers: Gregor Golabek
Taras V. Gerya
Boris J.P. Kaus
Paul Tackley

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

Description:

Knowledge about the terrestrial core formation mechanism is still very limited. Several core formation modes have been proposed, including a fracturing mode in which a central unmelted region is displaced by a degree one mode from the center of the accreting body and is fragmented due to the large stresses created by an overlying asymmetric iron layer, and in contrast, core formation via iron diapirs, which can be formed by giant impacts. We investigate which core formation mode is active under certain conditions by performing 2D simulations using the code I2ELVIS, which combines finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations as well as the Poisson equation for gravity potential in a self-gravitating planetary body. In the model, the planetary body is surrounded by a low viscosity massless fluid to simulate a free surface. We apply a temperature- and stress-dependent viscoplastic rheology inside Mars- to Earth-sized bodies and include heat release due to radioactive decay, shear and adiabatic heating. As initial condition we use stochastically distributed iron diapirs with random sizes in the range of 50 to 100 km radius, representing the iron delivered by pre-differentiated impactors.

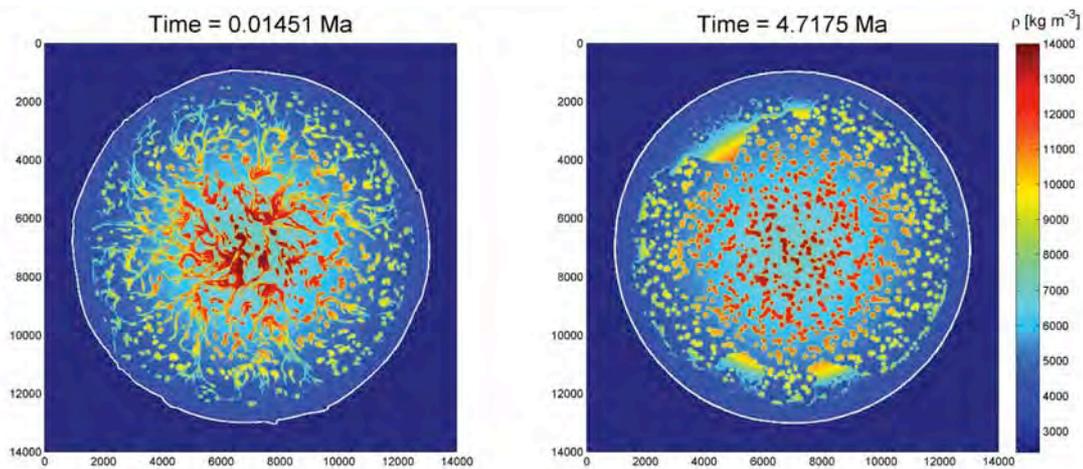


Fig. 1: Different core formation modes with different timescales can be observed for wet and dry silicate rheology.

A systematic investigation of the influence of silicate rheology, temperature and diapir radii on different-sized protoplanets is being performed. We show that depending on the silicate rheology, which is strongly dependent on the water content of olivine and the initial temperature profile, plastic yielding and shear localization take place and different regimes of core formation appear: For weak planetary interiors iron diapirs sink in collective groups. For

highly viscous planets an asymmetric iron layer forms, which surrounds the central part of the planet or a mixture of diapirism and fracturing mechanism develops. We derive scaling laws, which predict the onset of plastic yielding and shear localization in the silicates and the associated core formation modes. The final temperature profiles of the different core formation modes show dependent on the differentiation mode significant differences, which will have an influence on the onset of mantle convection.

Title: Introductory Textbook on Numerical Geodynamic Modelling

Researchers: T. Gerya

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

Description:

Numerical modelling of geodynamic processes was predominantly the domain of high-level mathematicians experienced in numerical and computational techniques. Now, for the first time, students and new researchers in the Earth Sciences can learn the basic theory and applications from a single, accessible reference text. Assuming only minimal prerequisite mathematical training (simple linear algebra and derivatives) the author provides a solid grounding in basic mathematical theory and techniques, including continuum mechanics and partial differential equations, before introducing key numerical and modelling methods. 8 well-documented, state-of-the-art visco-elasto-plastic, 2-D models are then presented, which allow robust modelling of key dynamic processes such as subduction, lithospheric extension, collision, slab break-off, intrusion emplacement, mantle convection and planetary core formation. Incorporating 47 practical exercises and 67 MATLAB examples (for which codes are available online at www.cambridge.org/gerya), this textbook provides a user-friendly introduction for graduate courses or self-study, encouraging readers to experiment with geodynamic models. <http://cambridge.org/uk/catalogue/catalogue.asp?isbn=9780521887540>

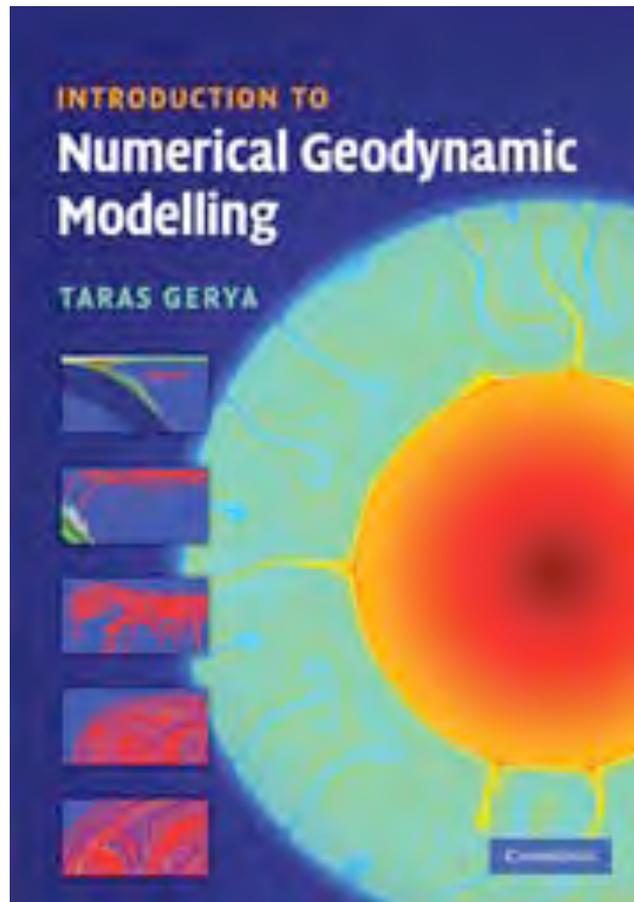


Fig.3. Cover page of the textbook.

Title: Numerical Modelling of Subduction Zones

Researchers: M. Faccenda, K. Nikolaeva, Y. Mishin, E. Sizova, G. Zhu, G. Golabek, T. Gerya, B. Kaus

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

Description:

Various aspects of subduction zone dynamics are modelled in 2D and 3D with the use of the original codes I2ELVIS and I3ELVIS combining finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations. The principal scientific directions are:

- Downward water suction (Fig. 1) due to sub-hydrostatic pressure gradients forming along normal faults in the slab bending area (Faccenda et al., 2009)
- Subduction initiation at passive margins (Nikolaeva et al., in press)
- Magmatic consequences and 3D dynamics (Fig. 2) of hydrous plumes in subduction zones (Zhu et al., 2009; Castro et al., 2009)
- Transition to plate tectonics in the early Earth (Sizova et al., 2009)

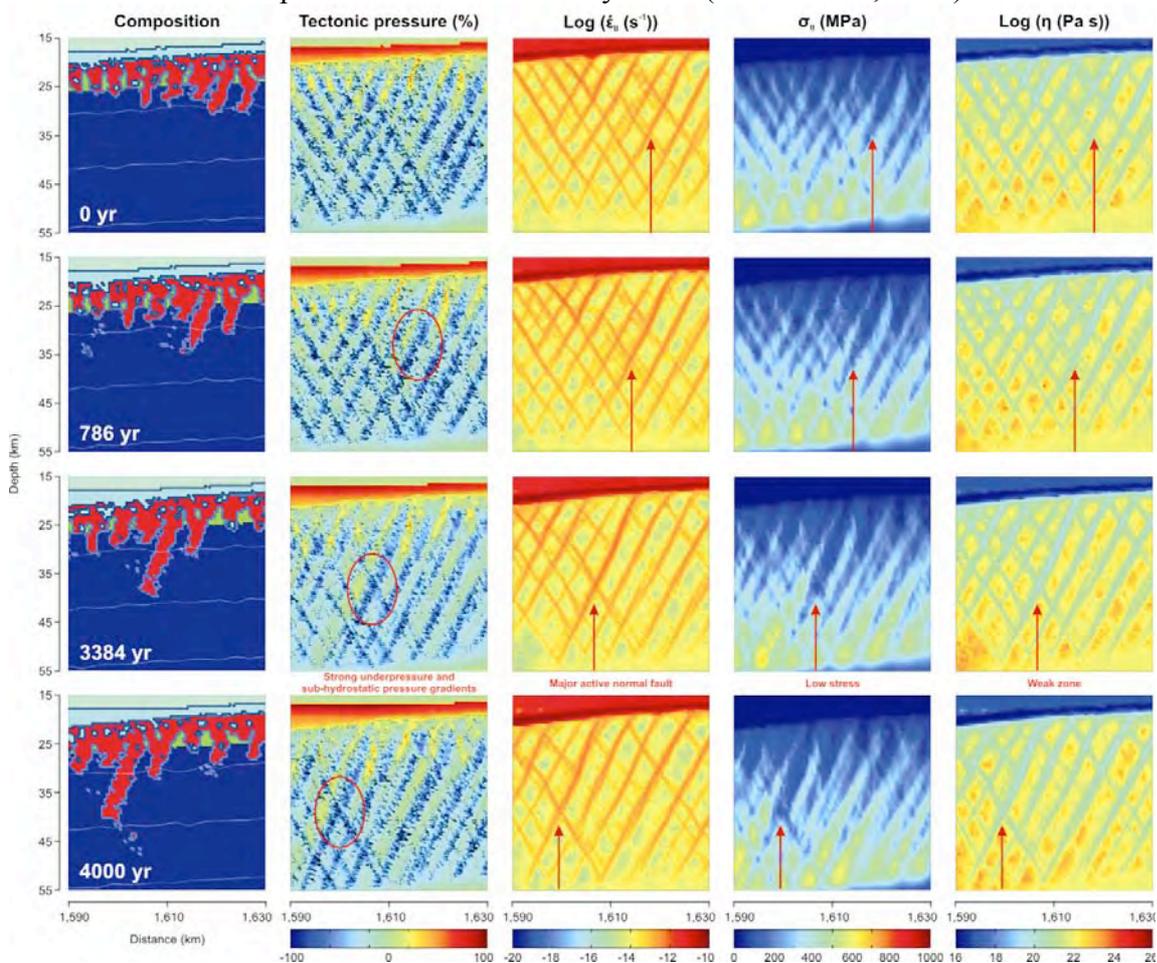


Fig. 1. Evolution of a serpentinizing normal fault. From left to right column: map of composition (color scale as in Fig. 1 and 2a)), tectonic pressure (defined as $(P - P_{\text{lith}})/P_{\text{lith}} * 100$ (%), where P is dynamic pressure and P_{lith} is lithostatic pressure), second invariant of strain

rate, second invariant of stress, effective viscosity. The black arrows in the tectonic pressure maps are the inverted (i.e. sub-hydrostatic) pressure gradients. The red circles enclose areas with strong tectonic underpressure and sub-hydrostatic gradients that tend to focus at the bottom of the serpentinizing fault. Red arrows indicate approximately the bottom tip of the serpentinizing normal fault characterized by high strain rates, low stresses and weak rheology.

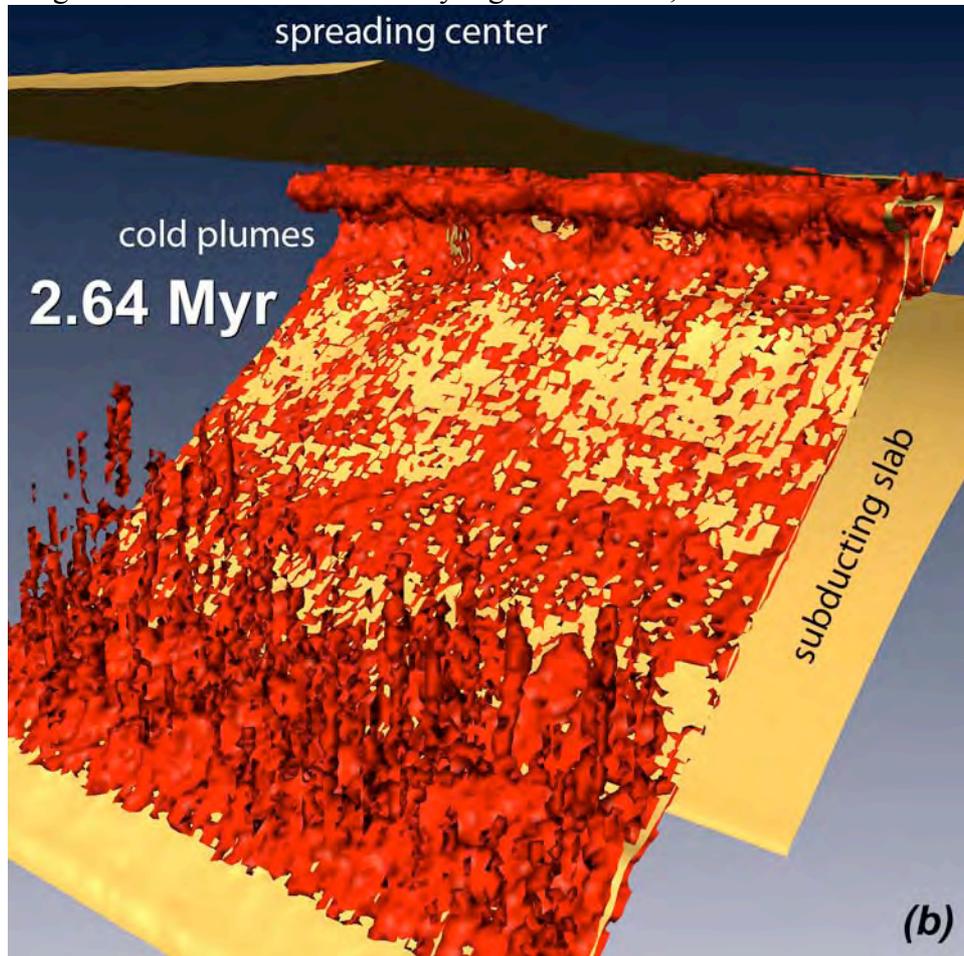


Fig. 2. 3D numerical model of partially molten hydrous plumes forming atop the slab in an intraoceanic subduction zone (Zhu et al., 2009)

References:

1. Faccenda, Gerya, T.V., M., Burlini, L. (2009) Fault-induced seismic anisotropy by hydration in subducting oceanic plates. *Nature Geosciences*, (in press).
2. Castro, A., García-Casco, A., Fernández, C., Corretgé, L.G., Moreno-Ventas, I., Gerya, T., Löw, I. (2009) Ordovician ferrosilicic magmas: Experimental evidence for ultrahigh temperatures affecting ametagreywacke source, Gondwana Research, doi:10.1016/j.gr.2008.12.011
3. Zhu, G., Gerya, T.V., Yuen, D.A., Honda, S., Yoshida, T., Connolly, J.A.D. 3-D Dynamics of hydrous thermal-chemical plumes in oceanic subduction zones. *Geochemistry, Geophysics, Geosystems*, (in press)
4. Nikolaeva, K., Gerya, T.V., Marques, F.O. (2009) Subduction initiation at passive margins: numerical modeling. *Journal of Geophysical Research*, (in press)
5. Sizova, E., Gerya, T., Brown, M., Perchuk, L.L. (2009) Subduction styles in the Precambrian: insight from numerical experiments. *Lithos*, (in press).

Title: Numerical Modelling of Continental Collision Zones

Researchers: M. Faccenda, Z. Li, T. Gerya

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

Description:

Various aspects of continental collision zones and related ultrahigh-pressure metamorphism are modelled in 2D with the use of the original code I2ELVIS combining finite differences on a fully staggered rectangular Eulerian grid and Lagrangian marker-in-cell technique for solving momentum, continuity and temperature equations. The principal directions are:

- Slab breakoff processes during continental collision (Baumann and Gerya, 2009)
- Formation and exhumation of ultrahigh-pressure rocks during continental collision with application to Sulu terrain, China (Fig. 1) (Li et al., 2009)
- Dynamics of retreating decoupled continental collision with application to Northern Apennines, Italy (Faccenda et al., 2009)

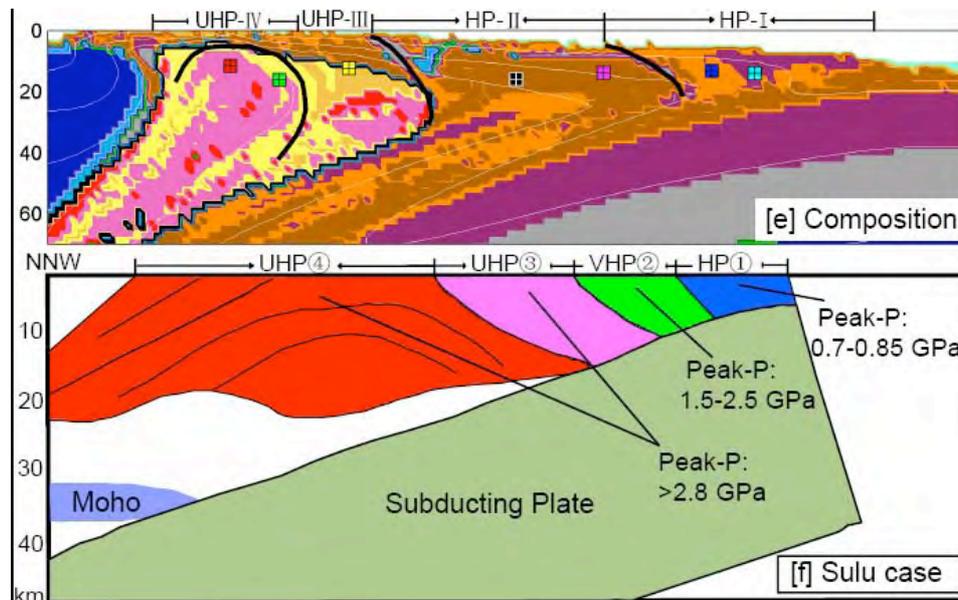


Fig. 1. Comparison of the numerical model (upper diagram) with the geological structure (lower diagram) of Sulu terrain, China (Li and Gerya, 2009).

References:

1. Baumann, C., Gerya, T., Connolly, J.A.D. (2009) Numerical modelling of spontaneous slab breakoff dynamics during continental collision. In: Advances in interpretation of geological processes: refinement of multi-scale data and integration in numerical modelling. Geological Society of London, Special Volume, (in press).
2. Faccenda, M., Minelli, G., Gerya, T.V. (2009) Coupled and decoupled regimes of continental collision: Numerical modeling. Earth and Planetary Science Letters, 278, 337–349.
3. Li, Z., Gerya, T.V. (2009) Polyphase formation and exhumation of HP-UHP rocks in continental subduction zone: Numerical modeling and application to the Sulu UHP terrane in eastern China. Journal of Geophysical Research, doi:10.1029/2008JB005935

Title: Dynamic Models of Slab Breakoff

Researchers: Thibault J.M. Duretz
Taras V. Gerya

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

Description:

We carried out a set of numerical experiments to study the effect of slab breakoff on a subduction-collision system. In order to study this case, we use a modified version of the visco-plastic numerical code I2VIS that allows the activation of the Peierls mechanism. A two-dimensional systematic study was performed by varying the oceanic slab age and initial plate convergence rate. In this parameter space, four different end-members were observed where breakoff depth can range from 40 to 400 km. Different combinations of rheological mechanisms lead to different breakoff modes. Activation of Peierls mechanism generally allows slabs to break faster and shallower.

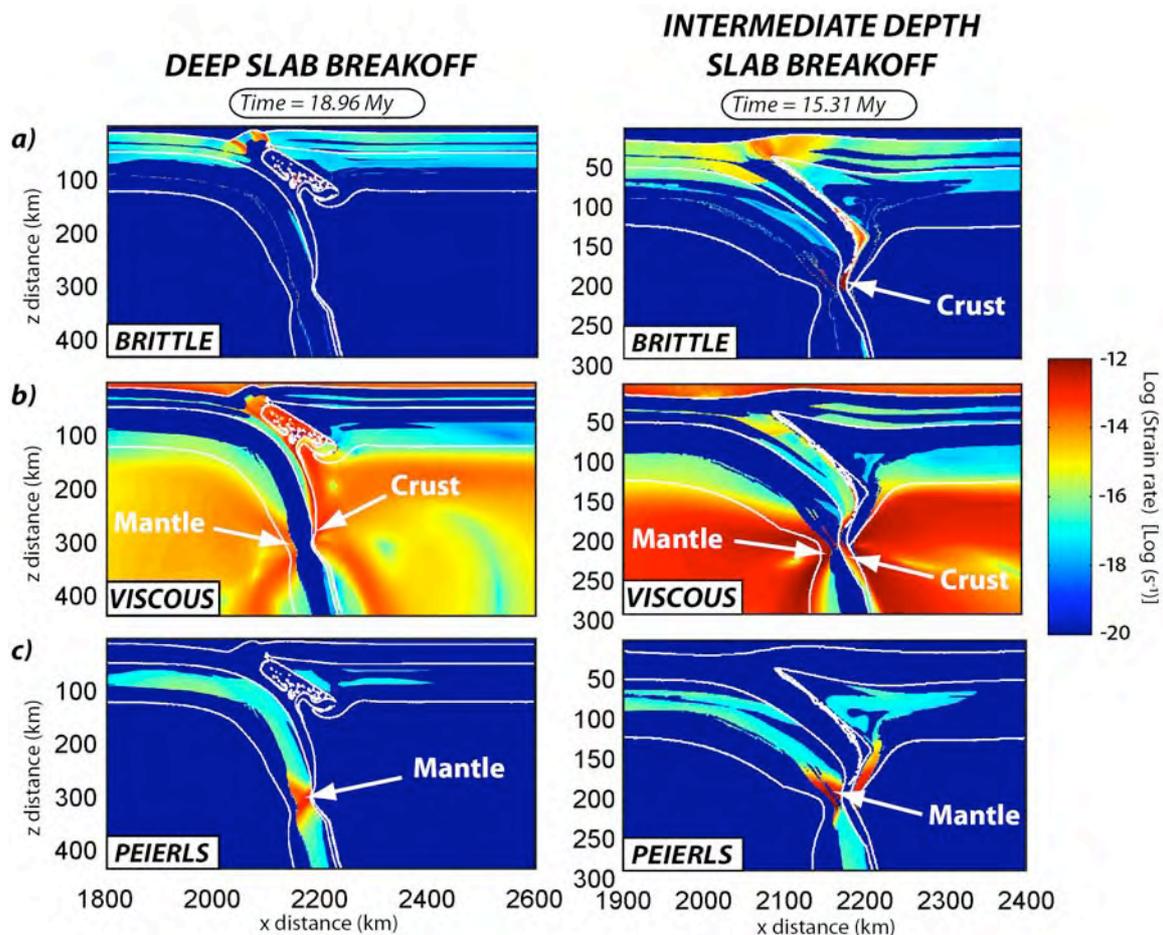


Figure : Example of two different slab breakoff end-members observed during the study (Deep and intermediate depth). Strain rate field for each rheological mechanism activated during the simulation. Dark blue color means that the rheological mechanism is not activated at the given pressure, temperature, composition condition.

Each breakoff end-member has its own topographic signal evolution and always display a sharp breakoff signal. Averaged post-breakoff uplift rates ranges between 0,8 km/My for shallow detachment and 0,2 km/My for deep detachment in foreland and hinterland basins. Initiation of continental crust subduction was observed when using an oceanic lithosphere older than 30 My. Different exhumation processes such as slab retreat and eduction were observed. Large post-breakoff rebound associated with plate decoupling occurs if the subducted oceanic slab is old enough.

Title: Exhumation of high grade rocks in Eastern Bohemian Massif and indentation mechanism: Insight from analogue and numerical modelling.

Researchers: T.J.M. Duretz¹
K. Schulmann²
B.J.P. Kaus¹
D. Gapais³

Institute/Group: ¹ Institute of Geophysics/ Geophysical Fluid Dynamics, D-ERDW
² Ctr Geochim Surf., UMR 7516, Univ Strasbourg 1, CNRS, Strasbourg.
³ Geosciences Rennes, UMR 6118, Univ Rennes 1, CNRS, Rennes.

Description:

Recent petrological, structural and geochronological studies of the eastern margin of the Bohemian Massif (Czech Republic) suggest a new conceptual geodynamical model to explain exhumation of high grade (20 kbar, 800°C) rocks. This conceptual model involves indentation of a weak orogenic lower crust by adjacent rigid mantle lithosphere, resulting in crustal scale buckling of the weak orogenic lower/middle crust interface followed by extrusion of hot ductile nappes over the rigid promontory. In order to test the hypothesis, we performed both analogue and numerical models. Analogue experiments using a 3-layer sand-silicon setup were carried out in Rennes laboratory (France). Results show that the most important features of the conceptual model can be reproduced providing a sufficient viscosity contrast between the silicones is considered. This involves: periodical buckling of silicones interface, extrusion of lowermost silicon over the indenter and flow of horizontal viscous channel underneath rigid lid above the actively progressing promontory. In addition to the laboratory experiments, we currently perform numerical simulations using the recently developed code MILAMIN_VEP. The set of numerical experiments is designed to mimic laboratory conditions and enables us to easily perform systematic studies. The experiments highlight the relative importance of viscosity and density ratio between a partially molten lower and a middle orogenic crust. Scaling relationships between vertical extrusion rate and indenter thickness and viscosity have been derived from the numerical models.

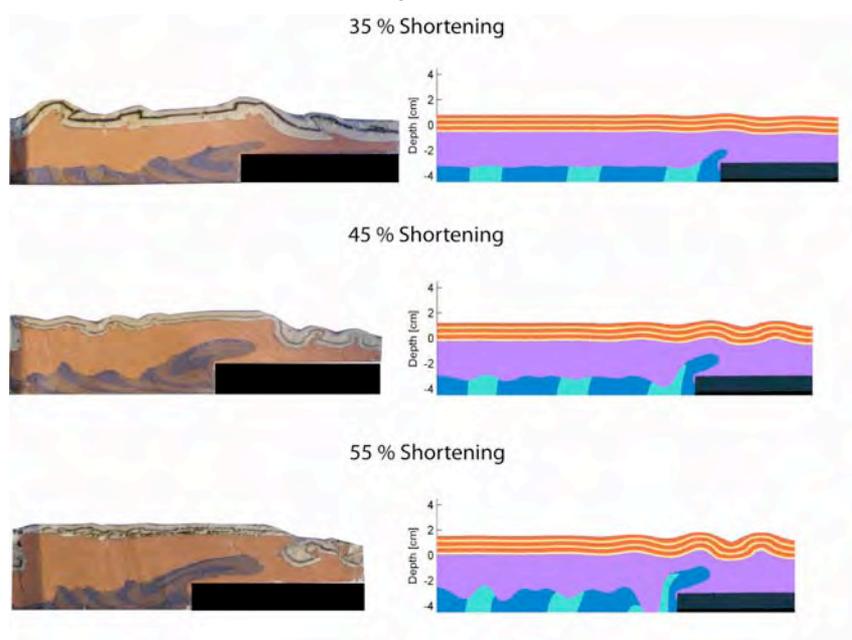


Figure : Analogue (left) and numerical model (right) evolution, for 35 %, 45 %, and 55% shortening. Viscosity ratio between the two silicones is 100 and density ratio is 1.02.

Title: The Effective Rheology of Partially Molten Rocks:
Numerical and Experimental Data

Researchers: Yolanda Deubelbeiss ^{1,2}
Boris J.P. Kaus ²
James Connolly ¹

**Institute/
Group:** ¹ Institute for Mineralogy and Petrology
² Institute of Geophysics/Geophysical Fluid Dynamics

Description:

The rheology of partially molten rocks has recently been studied experimentally. Yet, the experiments turned out to be difficult to interpret, partly because the parameters only give a picture of the system as a whole. The underlying physics are difficult to understand since different processes may compete and overlap due to coupling of different mechanical behavior. For this reason, we perform numerical experiments on an idealized system, in which we can directly monitor stress, strain and strain rate distributions inside the system and apply different rheologies for each phase separately and analyze their effect.

Experimental studies (Fig. 1) indicate that melt-solid systems behave non-linearly for moderate to high strain rates. However, the experiments are controversial. In theory, 0D visco-elastic models can be used to extract the effective rheology from laboratory experiments. However, the effects of shear-heating and non-linear rheology of the assemblage may affect the results in a non-intuitive manner. For this reason, we compare a series of 2D finite strain grain-scale numerical simulations (Fig.2) with a 0D rheology model. The 2D simulations employ an overall visco-elastic rheology, and the rheology of each phase is controlled independently. Rheologies can be either Newtonian or non-Newtonian, either constant temperature or temperature dependent viscosity according to Hess and Dingwell (1996) for the fluid phase - or - constant or power-law quartz-controlled rheology according to Ranalli (2002) for the solid phase. The simulations also account for shear heating.



Fig. 1. Back scattered electron (BSE) images of recovered, deformed sample. Simple shear experiment with sinistral shear sense of crystal bearing melt at a strain of $\gamma = 0.24$.

A 0D inversion model is developed that extracts effective material parameters from either synthetic or laboratory-derived stress-strain curves. A comparison with 2D numerical simulations (Fig. 3) indicates that non-Newtonian behaviour is important while the rheology of the solid phase has less influence on the system, a result that is in agreement with earlier findings. We are currently considering the relative importance of shear heating, non-Newtonian rheologies, elasticity and finite strain on the effective rheology of the assemblage, to better understand how rheological information can be extracted from 0D models. The results are applied to laboratory experiments on the effective rheology of partially molten rocks and have implications for volcanic eruptions and batholith emplacement.

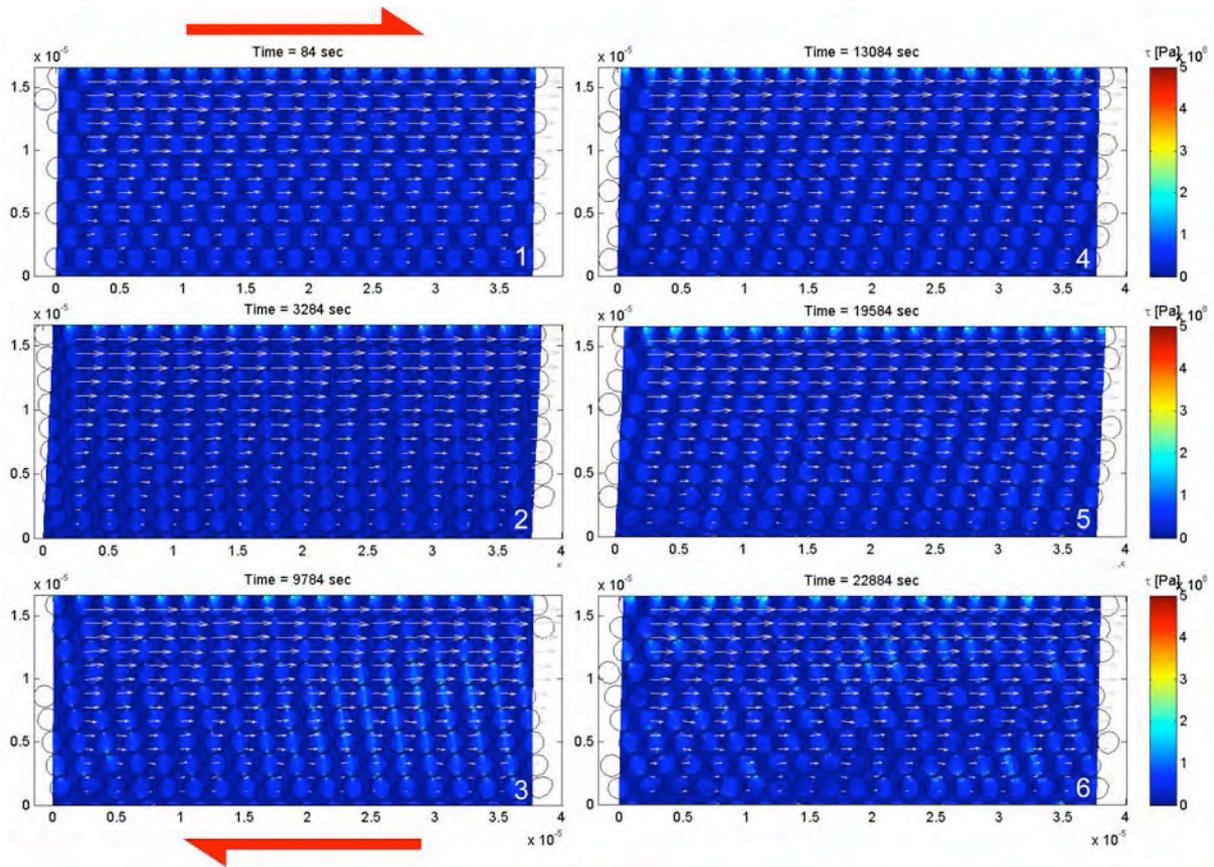


Fig. 2. A sequence of snapshots from a finite strain 2D numerical simulation of a crystal bearing melt with a that is deformed under simple shear. Sequence-figure 6 shows a strain of $\gamma = 2.5$. Periodic boundary conditions are employed.

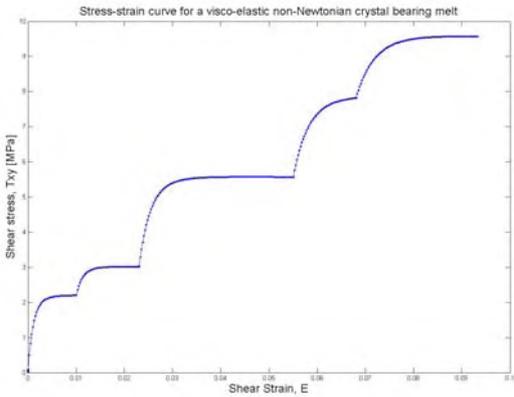


Fig. 3. Stress-strain curve representing a 2D numerical finite strain simulation with a step-wise increase of the strain rate. (similar to what is done in laboratory experiments) Here, a visco-elastic non-Newtonian temperature dependent rheology is employed. With these kinds of simulations and comparison to the laboratory experiments, the relative importance of shear heating power law rheology or finite strain can be analyzed.

Challenges and method

Modeling on these scales in Earth Sciences is insofar challenging as we have to resolve every single grain in a “rock”, which represents only a small portion of the Earth. On the other hand, models have to be large enough so that they still represent the macroscopic physical behaviour of Earth material. For these simulations we use a 2D MATLAB-based finite element code MILAMIN_VEP, with an unstructured mesh with 7-node isoparametric triangular elements.

Title: Parameters That Control the Formation of Lithospheric-Scale Shear Zones

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

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

Description:

Shear-heating induced localization might be an important process for subduction initiation. Kaus & Podladchikov (2006) showed with the help of numerical simulations that for some parameters, localization occurs and for other parameter choices, localization does not take place. Thereby, either homogeneous thickening or buckling compensates the deformation. Thermally activated thrusting in contrast to these two mechanisms is preferred for a relatively cold lithosphere. In addition to the thermal structure of the lithosphere, the deformation mode is also determined by the initial rheological structure and by the shortening rates [Burg and Schmalholz, 2008].

Here, numerous 2-D simulations (>100 #) are performed to distinguish these regions by changing the parameters that influence the shear heating process. The 2-D simulations are performed using a MATLAB-based finite element code. The standard simulations used for this work model a lithosphere consisting of an upper crust, a lower crust plus an upper mantle part. First, only temperature and strain rate are changed during systematic simulations, followed by changes in the rheology.

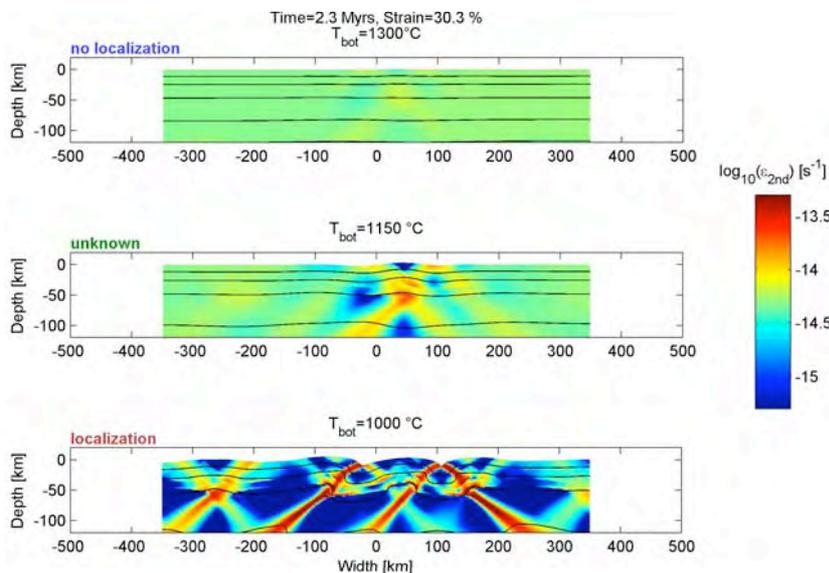


Fig. 1. Shear localization determination for simulations with a strain rate of $\epsilon_{bg} = 5 \cdot 10^{-15} s^{-1}$ and with bottom temperatures of $T_{bot} = 1300^\circ C$ (top), $T_{bot} = 1150^\circ C$ (middle) and $T_{bot} = 1000^\circ C$ (bottom) showing the second strain invariant on snapshots after $\sim 30\%$ of total strain and 2.3 Myrs, which are indicating no localization (top), no clearly determinable localization (middle) and clear localization (bottom).

In addition, a fast 1-D finite difference code was developed, that exactly reproduces the results of the 2-D code for laterally homogeneous cases. For the same input parameters, it computes information of temporal changes of both the temperature and strength profile of the Earth's upper part due to shear-heating. Even more important, it further supplies information for the occurrence of localization after comparing and validating its results with the 2-D simulations. As a powerful tool, this 1-D code can finally be used to predict the occurrence of shear localization for given input parameters. This thus yields new insights in the occurrence of shear localization in a compressed lithosphere.

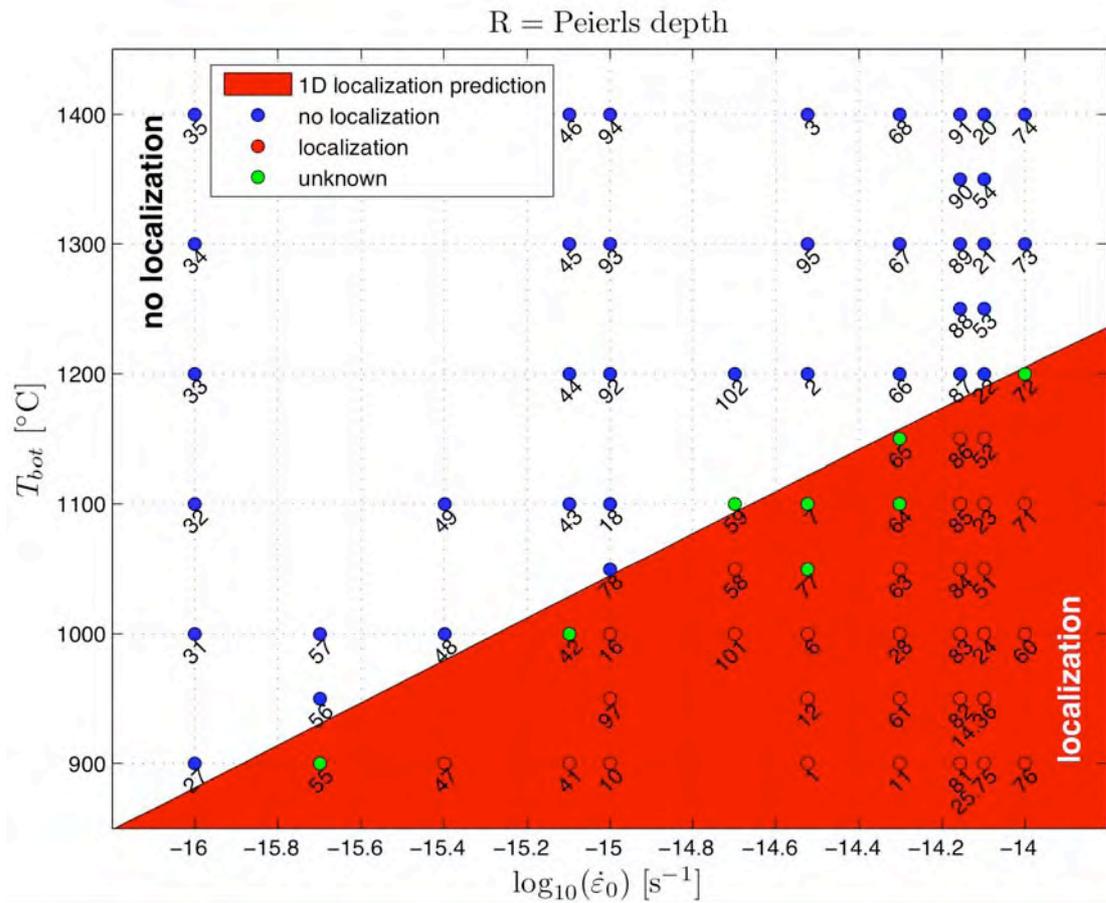


Fig. 2. Localization prediction of 1-D code (red area) are compared to 2-D simulation results shown as points and indicating no localization (blue), localization (red) and unknown (green).

References: Burg, J. P., and S. M. Schmalholz (2008), Viscous heating allows thrusting to overcome crustal-scale buckling: Numerical investigation with application to the Himalayan syntaxes, *Earth and Planetary Science Letters*, 274(1-2), 189-203.

Kaus, B. J. P., and Y. Y. Podladchikov (2006), Initiation of localized shear zones in viscoelastoplastic rocks, *Journal of Geophysical Research-Solid Earth*, 111(B4).

Title: Spherical Modelling of the Thermo-Chemical Evolution of Venus' Mantle
 π

Researchers: M. Armann
P. J. Tackley

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

Description:

Venus, although similar in size and composition to Earth, is quite different to Earth in its surface appearance, and hence also in the dynamics of its mantle, lithosphere and crust. We are performing integrated thermo-chemical convection modelling of Venus' evolution over 4.5 billion years in 3-D spherical geometry as well as 2-D spherical annulus geometry. These models include realistic ("laboratory") rheological parameters for viscous creep, which are also composition-dependent, and plastic yielding, which might cause changes in tectonic regime (e.g., episodic plate tectonics). Crustal formation and the resulting differentiation of the crust and mantle are modelled using a self-consistent melting criterion. Solid-solid phase transitions are included. Heat-producing elements decay with time, and cooling of the core is tracked. The gravitational field and surface topography are calculated using a self-gravitating formulation. Simulations are performed using StagYY by P. Tackley, which uses a finite volume multigrid solver on the Yin-Yang spherical grid. Simulations in which the lithosphere remains stagnant over the entire history indicate that over time the crust becomes as thick as the mechanical lithosphere, with delamination occurring from its base and magmatism being the dominant heat transport mechanism. A thick crust is a robust feature of these calculations. Higher mantle viscosity results in larger topographic variations, thicker crust and lithosphere and higher admittance ratios: to match those of Venus, the upper mantle reference viscosity is about 10^{20} Pa s and internal convection is quite vigorous. Several large plumes persist throughout the model history, as the core does not cool as much as in Earth. The most successful results in matching observations are those in which the evolution is episodic, being in stagnant lid mode for most of the evolution but with 2-3 bursts of activity caused by lithospheric overturn. In ongoing work we are examining the effect of crustal rheology and a more accurate melting treatment.

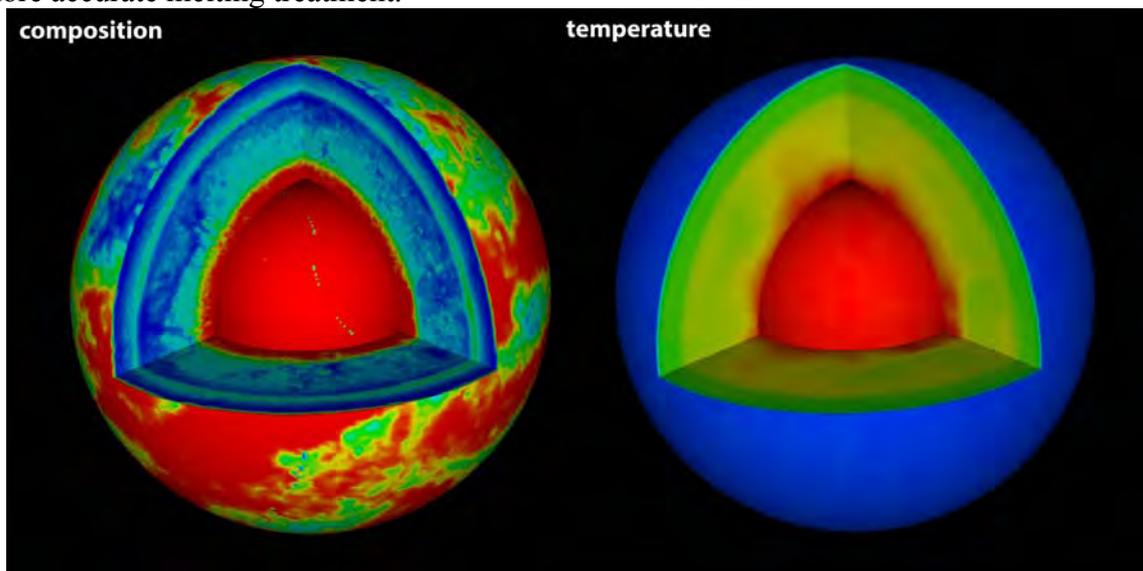


Figure. Composition (left) and temperature (right) for an episodic evolution simulation.

Title: External Gas Micro-Flows based Non-Equilibrium Gas Flow Models

Researchers: Kaspar Müller, Prof. Manuel Torrilhon

Institutes: Seminar for Applied Mathematics, ETH Zürich

Description: The description of nonequilibrium, e.g., small-scale processes in gases require mathematical modeling based on kinetic theory of gases. Due to large Knudsen numbers, classical relations of Navier-Stokes and Fourier for stress and heat-flux have to be replaced by a more accurate model. This project investigates a new mathematical model and the derivation of suitable numerical methods. The new equations, called regu-

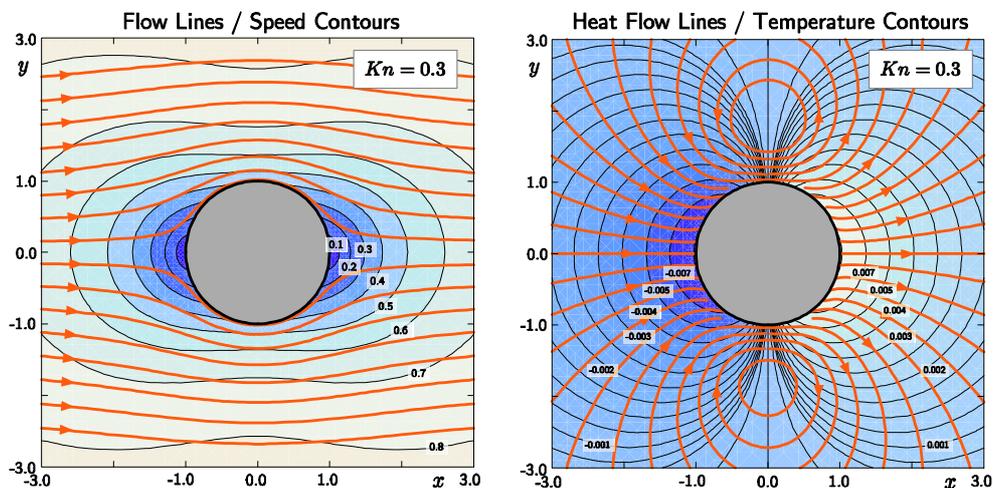


Figure 1: Slow gas flow around a micro-sphere based on extended fluid dynamics. The micro-scales induces a temperature polarization and non-trivial heat flow.

larized 13-moment system (R13), are formed by relaxational partial differential equations of hyperbolic-parabolic type. They contain first order equations for the fluiddynamic quantities, density, velocity and temperature as well as second order equations for directional temperatures, shear stress and heat flux in the form of balance laws. Recently, boundary conditions for the R13 system have been formulated. This makes it possible to consider various standard boundary value problems from fluid dynamics which now will exhibit special effects when considered with the new equations. One example is the flow around a sphere as shown in the figure. For general shapes the equations will be implemented in 2 dimensions using the finite-element framework FEnics.

References:

- [1] M. Torrilhon and H. Struchtrup, *Boundary Conditions for Regularized 13-Moment-Equations for Micro-Channel-Flows*, J. Comput. Phys. **227**(3), (2008), p.1982-2011
- [2] FEnics Software Project, www.fenics.org

Title: Scale Induced Closure for Kinetic Equations

Researcher: Prof. Manuel Torrilhon
Peter Kauf

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Ubiquitous multiparticle systems with a given interparticle potential K - e.g. gas dynamics, avalanches, traffic jams - are described by kinetic equations. We consider a linear K , scaled by the Knudsen number ε , which is the ratio of mean free path and typical length scale of a system,

$$\partial_t f + c_k \partial_k f + \frac{1}{\varepsilon} K f = 0, \quad f : \mathbb{R}^3 \times \mathbb{R}_+ \ni (\mathbf{x}, t) \mapsto f_{\mathbf{x},t}(\cdot) \in V_{\mathbf{c}}.$$

$V_{\mathbf{c}}$ is an appropriate Hilbert space containing the particle speed distribution functions $f_{\mathbf{x},t}(\cdot)$. The aim of this project is to find accurate and stable low dimensional approximations to the kinetic equation for the transition regime (ε smaller than 1.0). This is the regime of gas micro-flows or reentry problems.

Typically, such approximations exhibit a closure problem, i.e. there are more variables than equations. Classical approaches to overcome this use an expansion of f in terms of ε (Chapman-Enskog), or a reconstruction in terms of moments of f (Grad). Both of these methods expand f around the equilibrium distribution ($\varepsilon = 0$). However, Chapman-Enskog type equations become unstable for high orders, whereas Grad produces equations of unclear accuracy. We are combining both methods by introducing a scaling with ε in the moment space. This leads to a collision term induced order-of-magnitude foliation of $V_{\mathbf{c}}$ into an equilibrium subspace, a higher moments subspace and a non-equilibrium subspace. The resulting equations are stable and accurate to 2nd order in ε . Whereas mathematical theory has so far been worked out for linear K , applications of the scale-induced approach to non-linear interactions have been carried out and proven successful as well.

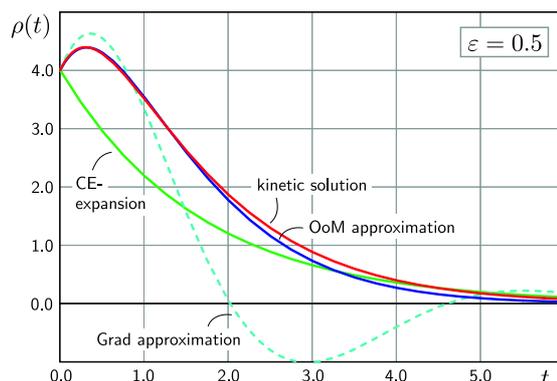


Figure 1: Approximations of the mass density $\rho = \int f d\mathbf{c}$: kinetic equation (exact result), Grad, Chapman-Enskog and Order of Magnitude.

References:

[1] M. Torrilhon, P. Kauf, C.D. Levermore, and M. Junk, *Scale-Induced Closure for Approximations of Kinetic Equations*, Proceed. 26th Intl. Symp. Rarefied Gas Dynamics, Kyoto, Japan (2008)

Title: Hybrid Numerical Methods for Kinetic Equations

Researcher: Peter Kauf
Prof. Manuel Torrilhon

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Ubiquitous multiparticle systems with a given interparticle potential - e.g. gas dynamics, avalanches, traffic jams - are described by the Boltzmann equation

$$\partial_t f + c_k \partial_k f = \mathcal{S}(f), \quad f : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \ni (\mathbf{x}, \mathbf{c}, t) \mapsto f(\mathbf{x}, \mathbf{c}, t) \in \mathbb{R}_+$$

The solution function f associates to every space-time point $(\mathbf{x}, t) \in \mathbb{R}^3 \times \mathbb{R}_+$ a 3-dimensional distribution of particle speeds $\mathbf{c} \in \mathbb{R}^3$. The operator $\mathcal{S}(f)$ is a problem dependent, usually highly non-linear integral operator.

Standard numerical discretizations of the Boltzmann equation are difficult because of the high dimensionality (3 space + 3 velocity + 1 time dimensions). Interestingly, physical equations like Euler equations, Navier-Stokes-Fourier system, or extended fluid dynamics (moment methods) can be viewed as approximations to Boltzmann's equation. In these descriptions the velocity space is replaced by a finite number of variables (e.g. density, velocity, temperature). Even though the number of parameters is comparably low, the approximation of the distribution function given by these models as solution to the Boltzmann equation is quite good. This is due to scale separation and the built-in physical asymptotics. However in many applications (e.g. micro devices for gases), scale-separation is not available and a full kinetic approach is necessary to model the behaviour of the system accurately.

Our aim is a combination of methods which are physically substantiated with state of the art numerical approaches to high dimensional problems. These include rescaling of the distribution function to obtain Galilei invariance, as well as efficient discretizations through highly adapted basis functions.

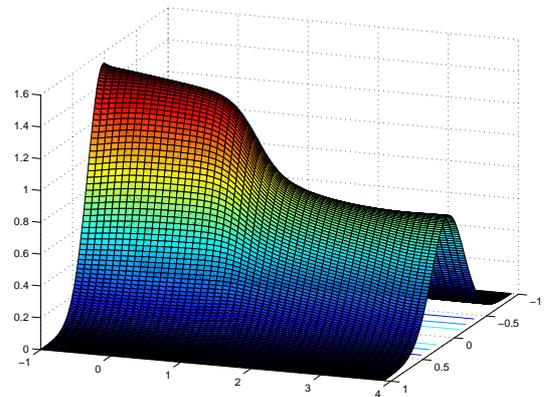


Figure 1: Velocity distribution in a Riemann-Problem: Projection to one velocity and one space dimension.

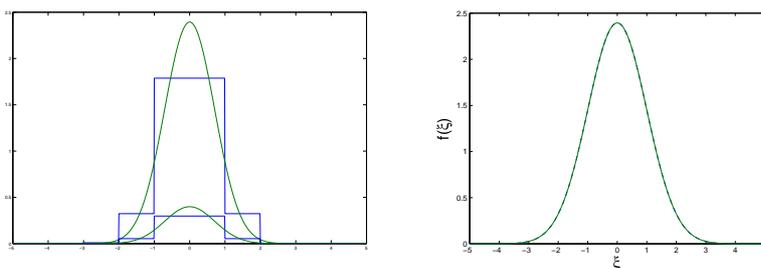


Figure 2: Approximation of equilibrium distributions by 5 piecewise constants (left) and by one Gaussian Basis function (right).

Title: Multilevel Monte Carlo methods for partial differential equations with stochastic coefficients

Researcher: Dr. Oliver Nowak
Prof. Manuel Torrilhon

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

This project is to investigate the suitability of multilevel Monte Carlo methods [1] for the computation of expected outputs from an elliptic PDE with stochastic coefficients. The motivating application is oil reservoir modelling in which it is increasingly common to model the risk porosity as a log-normal Gaussian field, with the output of interest being the oil flow in response to an applied pressure drop.

Assuming that this certain elliptic PDE with stochastic coefficients is discretised by a numerical method (for instance Finite Elements) which depends on a parameter h_l that is related to a mesh-size, let denote $g_{h_0}, g_{h_1}, \dots, g_{h_L}$ the corresponding outputs, where $h_l = N^{-l}h_0$ for $0 \leq l \leq L$. By linearity of the ‘expected value operator’ we have

$$\mathbb{E}g_{h_L} = \mathbb{E}g_{h_0} + \sum_{l=1}^L \mathbb{E}(g_{h_l} - g_{h_{l-1}}), \quad (1)$$

where $\mathbb{E}g_{h_L}$ denotes the expected output with respect to the approximate solution on the finest grid. The multilevel Monte Carlo method estimates each expected value on the right hand side of (1) such that the overall variance (which is directly related to the Monte Carlo error) is minimised under fixed computational costs.

References:

- [1] M. B. Giles: *Multilevel Monte Carlo Path Simulation*. Operations Research, **56**, pp. 607-617, 2008.

Title: Dynamical Low-Rank Approximation for Nonlinear Wave Equations

Researchers: Dr. Julia Schweitzer
Prof. Dr. Marlis Hochbruck

Institutes: Seminar for Applied Mathematics, ETH Zürich
Mathematisches Institut, Heinrich-Heine-Universität Düsseldorf
SFB TR 18 “Relativistic Laser-Plasma Dynamics”

Description:

In former projects we developed fast and efficient numerical solvers for problems arising in laser-plasma dynamics [1,2]. These are typically described by nonlinear wave equations. Even though the methods studied previously resulted in a considerable speed up and the physicist are now able to study new experimental setups, the idea arose to develop low order approximation models to reduce the storage requirements, which are still enormous in realistic two- and three-dimensional problems.

We use the localized structure of the laser pulses studied by the physicist, to reduce the discretized problem to a problem involving only low-rank matrices, which can be stored efficiently. For first order problems this has been done already by Lubich, Koch and Nonnenmacher, [3,4].

We extend their ideas to the second order case of nonlinear wave equations. Namely we derive a new system of differential equations directly advancing the low-rank decomposition in time and avoiding the storage inefficient complete system. In addition we discuss a stable time integration of the new system by using an adaptive rank control mechanism.

References:

- [1] C. Karle, J. Schweitzer, M. Hochbruck, E.W. Laedke and K.-H. Spatschek
Numerical solution of nonlinear wave equations in stratified dispersive media
J. Comp. Phys. 216 (2006) 138-152
- [2] C. Karle, J. Schweitzer, M. Hochbruck and K.-H. Spatschek
A parallel implementation of a two-dimensional fluid laser-plasma integrator for stratified plasma-vacuum systems
J. Comp. Phys. 227 (2008) 7701-7719
- [3] O. Koch and C. Lubich
Dynamical low rank approximation
SIAM J. Matrix Anal. Appl. 29 (2007), 434-454
- [4] A. Nonnenmacher and C. Lubich
Dynamical low-rank approximation: applications and numerical experiments
Math. Comput. Simulation 79 (2008), 1346-1357

Title: Computational Plasma Modeling for Electric Arcs

Researcher: Daniel Wright
Prof. Manuel Torrilhon

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The flow of plasma in interaction with a magnetic field is described by the equations of magnetohydrodynamics (MHD). Traditionally, many applications for magnetohydrodynamics can be found in the field of astrophysics. However, in recent technological applications, extreme settings or sophisticated devices lead to the creation of plasmas which have to be modeled by magnetohydrodynamics. A major role is played by electric arcs and discharges. Examples are circuit breakers, micro-drilling devices, nuclear fusion and advanced flow control.

In many cases electric arcs can be considered as a multi-physics research field since not only gas dynamics and electrodynamics are combined but also other many other phenomena such as turbulence, chemical reactions or radiation have to be taken into account. The correct combination of different phenomena has to be investigated and their interaction with numerical methods has to be clarified. Furthermore, the analysis of the mathematical structure of the MHD system is still ongoing.

In this project we investigate the evolution and extinction of generic electric arcs in a high pressure environment. Extinction is linked to the mathematical stability of solutions, which can be studied using reduced models. Due to the interaction of the electric arc with the external network, boundary conditions and driving forces need special dynamic real-time modeling. The results deepen our physical understanding of the underlying processes and influence the construction of suitable numerical methods. In order to incorporate special effects like Hall-currents, electron pressure and ionization in a mathematically transparent way, we investigate plasma flow based on a three-fluid description where electrons, ions and neutrons are considered separately. This extends the MHD equations to a multi-phase model with interesting hyperbolic properties. In particular, two different momentum equations change the type of the equations because one of Maxwell equations turns into a global constraint. This requires a special numerical treatment and leads to interesting deviations of the results from standard models.

Title: A classical picture of the role of vacancies and interstitials in Helium-4

Researchers: L. Pollet, M. Troyer*
P.N. Ma, F.-C. Zhang **

Institute/Group: * Theoretische Physik, ETH Zürich
** University of Hong Kong

Description:

Motivated by experimental hints for supersolidity in Helium-4, we perform Monte Carlo simulations of vacancies and interstitials in a classical two- and three-dimensional Lennard-Jones solid. We confirm a strong binding energy for vacancies, of the order of the Lennard-Jones attraction, which is reminiscent of what was found for vacancies in Helium-4. We also find, in two-dimensional simulations, a strong attraction and large binding energy of interstitials since by clustering interstitials the elastic deformation energy is minimized thanks to the formation of dislocations. We interpret the results in light of the properties of Helium-4.

References:

J. Low Temp. Phys 152, 156 (2008)

Title: Supersolidity in ^4He

Researchers: M. Boninsegni^{*}
B. Svistunov^{**}, ^{***}
N. Prokof'ev^{**}, ^{***}
A. Kuklov^{****}
P. Corboz, L. Pollet, M. Troyer^{*****}

Institute/Group: Department of Physics, University of Alberta^{*}
Department of Physics, University of Massachusetts^{**}
Kurchatov Institute, Moscow^{***}
Department of Physics, CUNY, Staten Island^{****}
Theoretische Physik, ETH Zürich^{*****}

Description:

More than half a century ago Penrose asked: are the superfluid and solid state of matter mutually exclusive or do there exist "supersolid" materials where the atoms form a regular lattice and simultaneously flow without friction? Recent experiments provide evidence that supersolid behavior indeed exists in Helium-4 -- the most quantum material known in Nature. In this paper we show that large local strain in the vicinity of crystalline defects is the origin of supersolidity in Helium-4. Although ideal crystals of Helium-4 are not supersolid, the gap for vacancy creation closes when applying a moderate stress. While a homogeneous system simply becomes unstable at this point, the stressed core of crystalline defects (dislocations and grain boundaries) undergoes a radical transformation and can become superfluid.

Using first-principle simulations for the probability density of finding a ^3He atom in the vicinity of the screw dislocation in solid ^4He , we determine the binding energy to the dislocation nucleus $E_B = 0.8 \pm 0.1$ K and the density of localized states at larger distances. The specific heat due to ^3He features a peak similar to the one observed in recent experiments, and our model can also account for the observed increase in shear modulus at low temperature. We further discuss the role of ^3He in the picture of superfluid defects.

We present results of a theoretical study of ^4He films adsorbed on graphite, based on the continuous space worm algorithm. In the first layer, we find a domain-wall phase and a $(7/16)$ registered structure between the commensurate $(1/3)$ and the incommensurate solid phases. For the second layer, we find only superfluid and incommensurate solid phases. The commensurate phase found in previous simulation work is only observed if first layer particles are kept fixed; it disappears upon explicitly simulating them.

References:

Phys. Rev. Lett., 101, 097202 (2008)
Phys. Rev. Lett. 101, 155302 (2008)
Phys. Rev. B 78, 245414 (2008)

Title: Local interactions and non-Abelian quantum loop gases

Researchers: S. Trebst, C. Nayak *
M. Troyer **
K. Shtengel ***

Institute/Group: * Station Q, Microsoft
** Theoretische Physik, ETH Zürich
*** University of California, Riverside

Description:

Two-dimensional quantum loop gases are elementary examples of topological ground states with Abelian or non-Abelian anyonic excitations. While Abelian loop gases appear as ground states of local, gapped Hamiltonians such as the toric code, we show that gapped non-Abelian loop gases require non-local interactions (or non-trivial inner products). Perturbing a local, gapless Hamiltonian with an anticipated "non-Abelian" ground-state wavefunction immediately drives the system into the Abelian phase, as can be seen by measuring the Hausdorff dimension of loops. Local quantum critical behavior is found in a loop gas in which all equal-time correlations of local operators decay exponentially.

References:

Phys. Rev. Lett. 101, 230401 (2008)

Title: Engineering exotic phases for topologically-protected quantum computing by emulating quantum dimer models

Researchers: A.F. Albuquerque, H. G. Katzgraber, M. Troyer, and G. Blatter

Institute/Group: Theoretische Physik, ETH Zürich

Description:

Topological quantum liquids with degenerate ground states protected by topological properties and an excitation gap to thermal excitations form the basis of topological quantum bits. We use a nonperturbative generalized Contractor Renormalization (CORE) to investigate the mapping of realistic microscopic models proposed to exhibit such topological phases to effective low-energy Hamiltonians for which the existence of a topological phase is established: the quantum dimer model on the triangular lattice. By tuning the couplings of the device, topological protection is achieved if the ratio between effective two-dimer interactions and flip amplitudes lies in the liquid phase of the phase diagram of the quantum dimer model. For a proposal based on a quantum Josephson junction array [L. B. Ioffe et al., *Nature* 415, 503 (2002)], our results show that the highest operational temperature is below 1 mK, and can only be obtained if extra interactions and dimer flips not present in the quantum dimer model and involving three or four dimers are included. The effects of these terms to the liquid phase are presently unknown. Removing these multi-dimer terms would require nK-scales for the device's operation. An alternative implementation based on cold atomic or molecular gases loaded into optical lattices is also discussed, and it is shown that also there small energy scales, implying long operational times, make such a device impractical. Given the many orders of magnitude between bare couplings in the devices, and the topological gap, the realization of topological phases in quantum devices requires careful attention to engineering limits and large bare interaction scales of the order of few eV.

References:

Phys. Rev. B 78, 014503 (2008)

Title: ENCORE: An Extended Contractor Renormalization algorithm

Researchers: A.F. Albuquerque, H. G. Katzgraber, M. Troyer,

Institute/Group: Theoretische Physik, ETH Zürich

Description:

Contractor Renormalization (CORE) is a real-space renormalization group method to derive effective Hamiltonians from microscopic models. The original CORE method is based on a real-space decomposition of the lattice into small blocks and the effective degrees of freedom on the lattice are tensor products of those on the small blocks. We present an extension of the CORE method (ENCORE) that overcomes this restriction. Our generalization allows the application of CORE to derive arbitrary effective models whose Hilbert space is not just a tensor product of local degrees of freedom, such as quantum dimer models, loop gases or string nets. The method is especially suitable in the the search for microscopic models to emulate low-energy exotic models and can guide the design of quantum devices.

References:

Phys. Rev. E 79, 046712 (2009)

Title: Spin Freezing Transition and Non-Fermi-Liquid Self-Energy in a 3-Orbital Model

Researchers: E. Gull, M. Troyer*
P. Werner, A.J. Millis**

Institute/Group: * Theoretische Physik, ETH Zürich
** Columbia University, New York

Description:

A single-site dynamical mean-field study of a three band model with the rotationally invariant interactions appropriate to the t_{2g} levels of a transition metal oxide reveals a quantum phase transition between a paramagnetic metallic phase and an incoherent metallic phase with frozen moments. The Mott transitions occurring at electron densities $n=2, 3$ per site take place inside the frozen moment phase. The critical line separating the two phases is characterized by a self-energy with an inverse square root frequency dependence and a broad quantum critical regime. The findings are discussed in the context of the power law observed in the optical conductivity of SrRuO_3 .

References:

Phys. Rev. Lett. 101, 166405 (2008)

Title: Binding of a ^3He impurity to a screw dislocation in solid ^4He

Researchers: P. Corboz,¹ L. Pollet,¹ N. V. Prokof'ev,^{2, 3, 1} and M. Troyer¹

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
³Russian Research Center "Kurchatov Institute", 123182 Moscow, Russia

Description:

Using first-principle simulations for the probability density of finding a ^3He atom in the vicinity of the screw dislocation in solid ^4He , we determine the binding energy to the dislocation nucleus $E_B = 0.8 \pm 0.1$ K and the density of localized states at larger distances. The specific heat due to ^3He features a peak similar to the one observed in recent experiments, and our model can also account for the observed increase in shear modulus at low temperature. We further discuss the role of ^3He in the picture of superfluid defects.

References: Phys. Rev. Lett. 101, 155302 (2008)

Title: Collective states of interacting Fibonacci anyons

Researchers: Simon Trebst,¹ Eddy Ardonne,^{2, 3} Adrian Feiguin,¹ David A. Huse,⁴ Andreas W. W. Ludwig,⁵ and Matthias Troyer⁶

Institute/Group: ¹Microsoft Research, Station Q, University of California, Santa Barbara, California 93106
²California Institute of Technology, Pasadena, California 91125
³Nordita, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden
⁴Department of Physics, Princeton University, Princeton, New Jersey 08544
⁵Physics Department, University of California, Santa Barbara, California 93106
⁶Theoretische Physik, Eidgenössische Technische Hochschule Zürich, 8093 Zürich, Switzerland

Description:

We show that chains of interacting Fibonacci anyons can support a wide variety of collective ground states ranging from extended critical, gapless phases to gapped phases with ground-state degeneracy and quasiparticle excitations. In particular, we generalize the Majumdar-Ghosh Hamiltonian to anyonic degrees of freedom by extending recently studied pairwise anyonic interactions to three-anyon exchanges. The energetic competition between two- and three-anyon interactions leads to a rich phase diagram that harbors multiple critical and gapped phases. For the critical phases and their higher symmetry endpoints we numerically establish descriptions in terms of two-dimensional conformal field theories. A topological symmetry protects the critical phases and determines the nature of gapped phases.

References: Phys. Rev. Lett., 101, 050401 (2008)

Title: Search for Deconfined Criticality: $SU(2)$ D´ej`a Vu

Researchers: A.B. Kuklov,¹ M. Matsumoto,^{2, 3} N.V. Prokof’ev,^{2, 4, 5} B.V. Svistunov,^{4, 5} and M. Troyer²

Institute/Group: 1Department of Engineering Science and Physics, CUNY , Staten Island, NY 10314
2Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
3Department of Physics, University of California, Davis, CA 95616
4Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
5Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia

Description:

Monte Carlo simulations of the $SU(2)$ -symmetric deconfined critical point action reveal strong violations of scale invariance for the deconfinement transition. We find compelling evidence that the generic runaway renormalization flow of the gauge coupling is to a weak first order transition, similar to the case of $U(1)\times U(1)$ symmetry. Our results imply that recent numeric studies of the $N\{e\}$ el antiferromagnet to valence bond solid quantum phase transition in $SU(2)$ -symmetric models were not accurate enough in determining the nature of the transition.

References: Phys. Rev. Lett. 101, 050405 (2008)

Title: Influence of the trap shape on the detection of the superfluid-Mott transition

Researchers: Ping Nang Ma,¹ Kai Yu Yang,² Lode Pollet,² J. V. Porto,³ Matthias Troyer,² and Fu Chun Zhang^{4, 5}

Institute/Group: ¹Center of Theoretical and Computational Physics and Department of Physics,
The University of Hong Kong, Hong Kong, China
²Institut Theoretische Physik, ETH Z^urich, 8093 Z^urich, Switzerland
³JQI, National Institute of Standards and Technology, Gaithersburg, MD 20899-8424
⁴Center of Theoretical and Computational Physics, The University of Hong Kong, China
⁵Department of Physics, The University of Hong Kong, China

Description:

The coexistence of superfluid and Mott insulator, due to the quadratic confinement potential in current optical lattice experiments, makes the accurate detection of the superfluid-Mott transition difficult. Studying alternative trapping potentials which are experimentally realizable and have a flatter center, we find that the transition can be better resolved, but at the cost of a more difficult tuning of the particle filling. When mapping out the phase diagram using local probes and the local density approximation we find that the smoother gradient of the parabolic trap is advantageous.

References: Phys. Rev. A 78, 023605 (2008)

Title: Critical Temperature Curve in the BEC-BCS Crossover

Researchers: Evgeni Burovski,¹ Evgeny Kozik,^{2, 3} Nikolay Prokof'ev,^{2, 3, 4} Boris Svistunov,^{2, 4} and Matthias Troyer³

Institute/Group: ¹Laboratoire de Physique Théorique et Modèles Statistiques, Université Paris-Sud, 91405 Orsay Cedex, France
²Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
³Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
⁴Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia

Description:

The strongly-correlated regime of the BCS-BEC crossover can be realized by diluting a system of two-component fermions with a short-range attractive interaction. We investigate this system via a novel continuous-space-time diagrammatic determinant Monte Carlo method and determine the universal curve T_c/ϵ_F for the transition temperature between the normal and the superfluid states as a function of the scattering length with the maximum on the BEC side. At unitarity, we confirm that $T_c/\epsilon_F = 0.152(7)$.

References: Phys. Rev. Lett. 101, 090402 (2008)

Title: Local stress and superfluid properties of solid ^4He

Researchers: L. Pollet,¹ M. Boninsegni,² A.B. Kuklov,³ N.V. Prokof'ev,^{1, 4, 5} B.V. Svistunov,^{4, 5} and M. Troyer¹

Institute/Group: 1Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland
2Department of Physics, University of Alberta, Edmonton, Alberta T6G 2J1, Canada
3Department of Engineering Science and Physics, CUNY, Staten Island, NY 10314, USA
4Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
5Russian Research Center "Kurchatov Institute", 123182 Moscow, Russia

Description:

More than half a century ago Penrose asked: are the superfluid and solid state of matter mutually exclusive or do there exist "supersolid" materials where the atoms form a regular lattice and simultaneously flow without friction? Recent experiments provide evidence that supersolid behavior indeed exists in Helium-4 -- the most quantum material known in Nature. In this paper we show that large local strain in the vicinity of crystalline defects is the origin of supersolidity in Helium-4. Although ideal crystals of Helium-4 are not supersolid, the gap for vacancy creation closes when applying a moderate stress. While a homogeneous system simply becomes unstable at this point, the stressed core of crystalline defects (dislocations and grain boundaries) undergoes a radical transformation and can become superfluid.

References: Statistical Mechanics (cond-mat.stat-mech)

Title: Expansion of a quantum gas released from an optical lattice

Researchers: F. Gerbier,¹ S. Trotzky,² S. Fölling,³ U. Schnorrberger,² J. D. Thompson,² A. Widera,⁴ I. Bloch,² L. Pollet,⁵ M. Troyer,⁵ B. Capogrosso-Sansone,⁶ N. V. Prokof'ev,^{5, 6, 7} and B. V. Svistunov^{6, 7}

Institute/Group: ¹Laboratoire Kastler Brossel, ENS, UPMC, CNRS ; 24 rue Lhomond, 75005 Paris, France
²Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany.
³Department of Physics, Harvard University, Cambridge, MA 02138, USA.
⁴Institut für Angewandte Physik, 53115 Bonn, Germany
⁵Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
⁶Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
⁷Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia

Description:

We analyze the interference pattern produced by ultracold atoms released from an optical lattice. Such interference patterns are commonly interpreted as the momentum distributions of the trapped quantum gas. We show that for finite time-of-flights the resulting density distribution can, however, be significantly altered, similar to a near-field diffraction regime in optics. We illustrate our findings with a simple model and realistic quantum Monte Carlo simulations for bosonic atoms, and compare the latter to experiments.

References: Phys. Rev. Lett. 101, 155303 (2008)

Title: Quantum Phase Transition in a Heisenberg Antiferromagnet on a Square Lattice with Strong Plaquette Interactions

Researchers: A. Fabricio Albuquerque,¹ Matthias Troyer,² and Jaan Oitmaa¹

Institute/Group: ¹School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
²Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

We present numerical results for an $S=1/2$ Heisenberg antiferromagnet on an inhomogeneous square lattice with tunable interaction between spins belonging to different plaquettes. Employing Quantum Monte Carlo, we significantly improve on previous results for the critical point separating singlet-disordered and Néel-ordered phases, and obtain an estimate for the critical exponent ν consistent with the three-dimensional classical Heisenberg universality class. Additionally, we show that a fairly accurate result for the critical point can be obtained from a Contractor Renormalization (CORE) expansion by applying a surprisingly simple analysis to the effective Hamiltonian.

References: Rev. B 78, 132402 (2008)

Title: Mechanisms for Spin-Supersolidity in $S = 1/2$ Spin-Dimer Antiferromagnets

Researchers: J.-D. Picon,^{1, 2} A. F. Albuquerque,^{1, 3} K. P. Schmidt,⁴ N. Laflorencie,⁵ M. Troyer,¹ and F. Mila²

Institute/Group: 1Theoretische Physik, ETH Zürich, 8093 Zürich, Switzerland
2Institute of Theoretical Physics, École polytechnique fédérale de Lausanne, Switzerland
3School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
4Lehrstuhl für theoretische Physik I, Otto-Hahn-Straße 4, TU Dortmund, D-44221 Dortmund, Germany
5Laboratoire de Physique des Solides, Université Paris-Sud, UMR-8502 CNRS, 91405 Orsay, France

Description:

Using perturbative expansions and the contractor renormalization (CORE) algorithm, we obtain effective hard-core bosonic Hamiltonians describing the low-energy physics of $S=1/2$ spin-dimer antiferromagnets known to display supersolid phases under an applied magnetic field. The resulting effective models are investigated by means of mean-field analysis and quantum Monte Carlo simulations. A "leapfrog mechanism", through means of which extra singlets delocalize in a checkerboard-solid environment via correlated hoppings, is unveiled that accounts for the supersolid behavior.

References: Phys. Rev. B 78, 184418 (2008)

Title: Phase diagram of 4He adsorbed on graphite

Researchers: Philippe Corboz,¹ Massimo Boninsegni,² Lode Pollet,¹ and Matthias Troyer¹

Institute/Group: ¹Institut für theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland
²Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2J1

Description:

We present results of a theoretical study of 4He films adsorbed on graphite, based on the continuous space worm algorithm. In the first layer, we find a domain-wall phase and a $(7/16)$ registered structure between the commensurate $(1/3)$ and the incommensurate solid phases. For the second layer, we find only superfluid and incommensurate solid phases. The commensurate phase found in previous simulation work is only observed if first layer particles are kept fixed; it disappears upon explicitly including their zero-point fluctuations. No evidence of any "supersolid" phase is found.

References: Phys. Rev. B78, 245414 (2008)

Title: Discerning Incompressible and Compressible Phases of Cold Atoms in Optical Lattices

Researchers: V.W. Scarola^{1,2}, L. Pollet², J. Oitmaa³, M. Troyer²

Institute/Group: 1Department of Chemistry and Pitzer Center for Theoretical Chemistry, University of California, Berkeley, California 94720, USA
2Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
3School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia

Description:

Experiments with cold atoms trapped in optical lattices offer the potential to realize a variety of novel phases but suffer from severe spatial inhomogeneity that can obscure signatures of new phases of matter and phase boundaries. We use a high temperature series expansion to show that compressibility in the core of a trapped Fermi-Hubbard system is related to measurements of changes in double occupancy. This core compressibility filters out edge effects, offering a direct probe of compressibility independent of inhomogeneity. A comparison with experiments is made.

References: Phys. Rev. Lett. 102, 135302 (2009)

Title: Thermal Canting of Spin-Bond Order

Researchers: V.W. Scarola^{1,2}, K.B. Whaley¹ and M. Troyer²

Institute/Group: 1Department of Chemistry and Pitzer Center for Theoretical Chemistry,
University of California, Berkeley, California 94720, USA
2Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

Magnetism arising from coupled spin and spatial degrees of freedom underlies the properties of a broad array of physical systems. We study here the interplay between correlations in spin and space for the quantum compass model in a finite external field, using quantum Monte Carlo methods. We find that finite temperatures cant the spin and space (bond) correlations, with increasing temperature even reorienting spin correlations between orthogonal spatial directions. We develop a coupled mean field theory to understand this effect in terms of the underlying quantum critical properties of crossed Ising chains in transverse fields and an effective field that weakens upon increasing temperature. Thermal canting offers an experimental signature of spin-bond anisotropy.

References: Rev. B 79, 085113 (2009)

Title: Collective States of Interacting Anyons, Edge States, and the Nucleation of Topological Liquids

Researchers: Charlotte Gils,¹ Eddy Ardonne,² Simon Trebst,³ Andreas W. W. Ludwig,⁴ Matthias Troyer,¹ and Zhenghan Wang³

Institute/Group: ¹Theoretische Physik, Eidgenössische Technische Hochschule Zürich, 8093 Zürich, Switzerland
²Nordita, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden
³Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106
⁴Physics Department, University of California, Santa Barbara, CA 93106

Description:

Quantum mechanical systems, whose degrees of freedom are so-called $su(2)_k$ anyons, form a bridge between ordinary $SU(2)$ spin systems and systems of interacting non-Abelian anyons. Such a connection can be made for arbitrary spin- S systems, and we explicitly discuss spin- $1/2$ and spin- 1 systems. Anyonic spin- $1/2$ chains exhibit a topological protection mechanism that stabilizes their gapless ground states and which vanishes only in the limit (k to infinity) of the ordinary spin- $1/2$ Heisenberg chain. For anyonic spin- 1 chains we find their phase diagrams to closely mirror the one of the biquadratic $SU(2)$ spin- 1 chain. Our results describe at the same time nucleation of different 2D topological quantum fluids within a 'parent' non-Abelian quantum Hall state, arising from a macroscopic occupation of localized, interacting anyons. The edge states between the 'nucleated' and the 'parent' liquids are neutral, and correspond precisely to the gapless modes of the anyonic chains.

References: Rev. Lett. 103, 070401 (2009).

Title: Absence of a Direct Superfluid to Mott Insulator Transition in Disordered Bose Systems

Researchers: L. Pollet,¹ N.V. Prokof'ev,^{1, 2} B.V. Svistunov,^{1, 2} and M. Troyer³

Institute/Group: ¹Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
²Russian Research Center "Kurchatov Institute", 123182 Moscow, Russia
³Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

We prove the absence of a direct quantum phase transition between a superfluid and a Mott insulator in a bosonic system with generic, bounded disorder. We also prove compressibility of the system on the superfluid-insulator critical line and in its neighborhood. These conclusions follow from a general *theorem of inclusions* which states that for any transition in a disordered system one can always find rare regions of the competing phase on either side of the transition line. Quantum Monte Carlo simulations for the disordered Bose-Hubbard model show an even stronger result, important for the nature of the Mott insulator to Bose glass phase transition: The critical disorder bound, Δ_c , corresponding to the onset of disorder-induced superfluidity, satisfies the relation $\Delta_c > E_{\text{g}/2}$, with $E_{\text{g}/2}$ the half-width of the Mott gap in the pure system.

References: Phys. Rev. Lett. 103, 140402 (2009)

Title: Assessing the accuracy of projected entangled-pair states on in_nite lattices

Researchers: B. Bauer¹, G. Vidal², M. Troyer¹

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²School of Physical Sciences, The University of Queensland, QLD 4072, Australia

Description:

Generalizations of the density-matrix renormalization group method have long been sought after. In this paper, we assess the accuracy of projected entangled-pair states on in_nite lattices by comparing with Quantum Monte Carlo results for several non-frustrated spin-1/2 systems. Furthermore, we apply the method to a frustrated quantum system.

References: J. Stat. Mech. (2009) P09006

Title: Topology driven quantum phase transitions in time-reversal invariant anyonic quantum liquids

Researchers: Charlotte Gils,¹ Simon Trebst,² Alexei Kitaev,³ Andreas W. W. Ludwig,⁴ Matthias Troyer,¹ and Zhenghan Wang²

Institute/Group: 1Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
2Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106
3Institute for Quantum Information, California Institute of Technology, Pasadena, CA 91125
4Physics Department, University of California, Santa Barbara, CA 93106

Description:

Indistinguishable particles in two dimensions can be characterized by anyonic quantum statistics more general than those of bosons or fermions. Such anyons emerge as quasiparticles in fractional quantum Hall states and certain frustrated quantum magnets. Quantum liquids of anyons exhibit degenerate ground states where the degeneracy depends on the topology of the underlying surface. Here we present a novel type of continuous quantum phase transition in such anyonic quantum liquids that is driven by quantum fluctuations of topology. The critical state connecting two anyonic liquids on surfaces with different topologies is reminiscent of the notion of a 'quantum foam' with fluctuations on all length scales. This exotic quantum phase transition arises in a microscopic model of interacting anyons for which we present an exact solution in a linear geometry. We introduce an intuitive physical picture of this model that unifies string nets and loop gases, and provide a simple description of topological quantum phases and their phase transitions.

References: Nature Physics

Title: Estimating errors reliably in Monte Carlo simulations of the Ehrenfest model

Researchers: Vinay Ambegaokar*, Matthias Troyer**

Institute/Group: Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853, USA*
Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland**

Description:

Using the Ehrenfest urn model we illustrate the subtleties of error estimation in Monte Carlo simulations. We discuss how the smooth results of correlated sampling in Markov chains can fool one's perception of the accuracy of the data, and show (via numerical and analytical methods) how to obtain reliable error estimates from correlated samples.

References: Am. J. Phys.

Title: Distinguishing Phases with Ansatz Wavefunctions

Researchers: B. Bauer¹, V.W. Scarola^{1,2}, M. Troyer¹ and K.B. Whaley²

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²Department of Chemistry and Pitzer Center for Theoretical Chemistry,
University of California, Berkeley, California 94720, USA

Description:

We propose an indistinguishability measure for assessment of ansatz wavefunctions with numerically determined wavefunctions. The measure efficiently compares all correlation functions of two states and can therefore be used to distinguish phases by defining correlator classes for ansatz wavefunctions. It also allows identification of quantum critical points. We demonstrate the approach for the transverse Ising model, using the matrix product state formalism with the time evolving block decimation algorithm.

References: Preprint, submitted to Nature Physics

Title: Suppression of the critical temperature for superfluidity near the Mott transition: validating a quantum simulator

Researchers: S. Trotzky^{1,†}, L. Pollet^{2,3,†}, F. Gerbier⁴, U. Schnorrberger¹, I. Bloch^{1,5}, N.V. Prokof'ev^{2,6}, B. Svistunov^{2,6}, and M. Troyer³

Institute/Group: 1 Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany
2 Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
3 Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
4 Laboratoire Kastler Brossel, ENS, UPMC, CNRS, 24 rue Lhomond, 75005 Paris, France
5 Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany
6 Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia
† These authors contributed equally to this work

Description:

Ultracold atomic gases in optical lattices have proven to be a controllable, tunable and clean implementation of strongly interacting quantum many-body systems. An essential prospect for such quantum simulators is their ability to map out the phase diagram of fundamental many-body model Hamiltonians. However, the results need to be validated first for representative benchmark problems via state-of-the-art numerical methods of quantum many-body theory. Here we present the first ab-initio comparison between experiments and quantum Monte Carlo simulations for strongly interacting Bose gases on a lattice for large systems (up to $N = 3e5$ particles). The comparison has enabled us to perform thermometry for the interacting quantum gas and to experimentally determine the finite temperature phase diagram for bosonic superfluids in an optical lattice. Our results reveal a downshift of the critical temperature as the transition to the Mott insulator is approached.

References: Preprint, submitted to Phys. Rev. Lett.

Title: Supersolid phase with cold polar molecules on a triangular lattice

Researchers: L. Pollet,^{1, 2, 3} J. D. Picon,^{3, 4} H.P. Büchler,⁵ and M. Troyer³

Institute/Group: ¹Physics Department, Harvard University, Cambridge-MA, 02138, USA
²Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
³Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
⁴Institute of Theoretical Physics, École polytechnique fédérale de Lausanne, Switzerland
⁵Institute of Theoretical Physics III, Universität Stuttgart, 70550 Stuttgart, Germany

Description:

We study a system of heteronuclear molecules on a triangular lattice and analyze the potential of this system for the experimental realization of a supersolid phase. The ground state phase diagram contains superfluid, solid and supersolid phases. At finite temperatures and strong interactions there is an additional emulsion region, in contrast to similar models with short-range interactions. We derive the maximal critical temperature T_c and the corresponding entropy $S/N = 0.04(1)$ for supersolidity and find feasible experimental conditions for its realization.

References: Preprint, submitted to Phys. Rev. Lett.

Title: Diagrammatic Monte Carlo for the Hubbard Model

Researchers: E. Kozik,¹ K. Van Houcke,^{2,3} * E. Gull,⁴ L. Pollet,^{2, 5} N. Prokof'ev,^{2,6} B. Svistunov,^{2,6} and M. Troyer¹

Institute/Group: ¹Theoretische Physik, ETH Zürich, 8093 Zürich, Switzerland
²Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
³Universiteit Gent - UGent, Vakgroep Subatomaire en Stralingsfysica Proeftuinstraat 86, B-9000 Gent, Belgium
⁴Department of Physics, Columbia University, New York, NY 10027, USA
⁵Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA
⁶Russian Research Center Kurchatov Institute, 123182 Moscow, Russia

Description:

We show that Monte Carlo sampling of the Feynman diagrammatic series (DiagMC) can be used for tackling hard fermionic quantum many-body problems in the thermodynamic limit by presenting accurate results for the repulsive Hubbard model in the correlated Fermi liquid regime. Using perturbative Feynman diagrams (rather than skeleton, or "bold-line", graphs) for the single-particle self-energy we can study moderate values of the on-site repulsion ($U/t \sim 4$) and temperatures down to $T/t=1/40$. We compare our results with high temperature series expansion and with single-site and cluster dynamical mean-field theory. We find that going from single site to large clusters is essential for obtaining the same level of accuracy as provided by DiagMC.

References: Preprint, submitted to Phys. Rev. Lett.

Title: Phase diagram of the disordered Bose-Hubbard model

Researchers: V. Gurarie,¹ L. Pollet,² N.V. Prokof'ev,^{3, 4} B.V. Svistunov,^{3, 4} and M. Troyer⁵

Institute/Group: 1Department of Physics, University of Colorado, Boulder CO 80309, USA
2Physics Department, Harvard University, Cambridge MA 02138, USA
3Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
4Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia
5Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

We establish the phase diagram of the disordered three-dimensional Bose-Hubbard model at unity filling, which has been controversial for many years. The theorem of inclusions, proven in Ref. [1], states that the Bose glass phase always intervenes between the Mott insulating and superfluid phases. Here, we note that assumptions on which the theorem is based exclude phase transitions between gapped (Mott insulator) and gapless phases (Bose glass). The apparent paradox is resolved through a unique mechanism: such transitions have to be of the Griffiths type when the vanishing of the gap at the critical point is due to a zero concentration of rare regions where extreme fluctuations of disorder mimic a *not regular* gapless system. An exactly solvable random transverse field Ising model in one dimension is used to illustrate the point. A highly non-trivial overall shape of the phase diagram is revealed with the worm algorithm. The phase diagram features a long superfluid finger at strong disorder and on-site interaction. Moreover, bosonic superfluidity is extremely robust against disorder in a broad range of interaction parameters; it persists in random potentials nearly 50 (!) times larger than the particle half-bandwidth. Finally, we comment on the feasibility of obtaining this phase diagram in cold-atom experiments, which work with trapped systems at finite temperature.

References: Preprint, submitted to Phys. Rev. B.

Title: Numerical studies of a one-dimensional 3-spin spin-glass model with long-range interactions

Researchers: Derek Larson,¹ Helmut G. Katzgraber,^{2, 3} M. A. Moore,⁴ and A. P. Young¹

Institute/Group: ¹Department of Physics, University of California, Santa Cruz, California 95064, USA
²Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
³Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA
⁴School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, U. K.

Description:

We study a p-spin spin-glass model to understand if the finite-temperature glass transition found in the mean-field regime of p-spin models, and used to model the behavior of structural glasses, persists in the non-mean-field regime. By using a 3-spin spin-glass model with long-range power-law diluted interactions we are able to continuously tune the (effective) space dimension via the exponent of the interactions. Monte Carlo simulations of the spin-glass susceptibility and the two-point finite-size correlation length show that deep in the non-mean-field regime the finite-temperature transition is lost, whereas this is not the case in the mean-field regime, in agreement with the prediction of Moore and Drossel [Phys. Rev. Lett. 89, 217202 (2002)] that 3-spin models are in the same universality class as an Ising spin glass in a magnetic field. However, slightly in the non-mean-field region, we find an apparent transition in the 3-spin model, in contrast to results for the Ising spin glass in a field. This may indicate that even larger sizes are needed to probe the asymptotic behavior in this region.

References: Phys. Rev. B, submitted (arXiv:cond-mat/0908.2224)

Title: Error Threshold for Color Codes and Random 3-Body Ising Models

Researchers: Helmut G. Katzgraber,^{1, 2} H. Bombin,³ and M. A. Martin-Delgado⁴

Institute/Group: ¹Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
²Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA
³Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
⁴Departamento de Física Teórica I, Universidad Complutense, 28040 Madrid, Spain

Description:

We study the error threshold of color codes, a class of topological quantum codes that allow a direct implementation of quantum Clifford gates suitable for entanglement distillation, teleportation and fault-tolerant quantum computation. We map the error-correction process onto a statistical mechanical random 3-body Ising model and study its phase diagram via Monte Carlo simulations. The obtained error threshold of $p_c = 0.109(2)$ is very close to that of Kitaev's toric code, showing that enhanced computational capabilities does not necessarily imply lower resistance to noise.

References: Phys. Rev. Lett. 103, 090501 (2009)

Title: Ground-state statistics from annealing algorithms:
Quantum vs classical approaches

Researchers: Yoshiki Matsuda*, Hidetoshi Nishimori**, Helmut G. Katzgraber***

Institute/Group: Department of Physics, Tokyo Institute of Technology, Oh-okayama,
Meguro-ku, Tokyo 152-8551, Japan*
Department of Physics, Tokyo Institute of Technology, Oh-okayama,
Meguro-ku, Tokyo 152-8551, Japan**
Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
Department of Physics, Texas A&M University, College Station, Texas
77843-4242, USA***

Description:

We study the performance of quantum annealing for systems with ground-state degeneracy by directly solving the Schrödinger equation for small systems and quantum Monte Carlo simulations for larger systems. The results indicate that naive quantum annealing using a transverse field may not be well suited to identify all degenerate ground-state configurations, although the value of the ground-state energy is often efficiently estimated. An introduction of quantum transitions to all states with equal weights is shown to greatly improve the situation but with a sacrifice in the annealing time. We also clarify the relation between the spin configurations in the degenerate ground states and the probabilities that those states are obtained by quantum annealing. The strengths and weaknesses of quantum annealing for problems with degenerate ground states are discussed in comparison with classical simulated annealing.

References: New J. Phys. 11 (2009) 073021

Title: Analysis of Evolutionary Algorithms on the One-Dimensional Spin Glass with Power-Law Interactions

Researchers: Martin Pelikan* and Helmut G. Katzgraber**

Institute/Group: Missouri Estimation of Distribution Algorithms Laboratory (MEDAL)
Dept. of Mathematics and Computer Science
Univ. of Missouri in St. Louis*

Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland;
Dept. of Physics, Texas A&M University, College Station, TX 77843-4242**

Description:

This paper provides an in-depth empirical analysis of several evolutionary algorithms on the one-dimensional spin glass model with power-law interactions. The considered spin glass model provides a mechanism for tuning the effective range of interactions, what makes the problem interesting as an algorithm benchmark. As algorithms, the paper considers the genetic algorithm (GA) with twopoint and uniform crossover, and the hierarchical Bayesian optimization algorithm (hBOA). hBOA is shown to outperform both variants of GA, whereas GA with uniform crossover is shown to perform worst. The differences between the compared algorithms become more significant as the problem size grows and as the range of interactions decreases. Unlike for GA with uniform crossover, for hBOA and GA with twopoint crossover, instances with short-range interactions are shown to be easier. The paper also points out interesting avenues for future research.

References: Genetic and Evolutionary Computation Conference (GECCO-2009), ACM Press, 843-850, (arXiv:cond-mat/0901.4146)

Title: Study of the de Almeida-Thouless line using power-law diluted one-dimensional Ising spin glasses

Researchers: Helmut G. Katzgraber,^{1, 2} Derek Larson,³ and A. P. Young³

Institute/Group: 1Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
2Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA
3Department of Physics, University of California, Santa Cruz, California 95064, USA

Description:

We test for the existence of a spin-glass phase transition, the de Almeida-Thouless line, in an externally-applied (random) magnetic field by performing Monte Carlo simulations on a power-law diluted one-dimensional Ising spin glass for very large system sizes. We find that an Almeida-Thouless line only occurs in the mean field regime, which corresponds, for a short-range spin glass, to dimension d larger than 6.

References: Phys. Rev. Lett. 102, 177205 (2009)

Title: Extended scaling for ferromagnetic Ising models with zero-temperature transitions

Researchers: Helmut G. Katzgraber,¹ I. A. Campbell,² and A. K. Hartmann³

Institute/Group: ¹Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
²Laboratoire des Colloïdes, Verres et Nanomatériaux,
Université Montpellier II, 34095 Montpellier, France
³Institut für Physik, Carl-von-Ossietzky-Universität, D-26111
Oldenburg, Germany

Description:

We study the second-moment correlation length and the reduced susceptibility of two ferromagnetic Ising models with zero-temperature ordering. By introducing a scaling variable motivated by high-temperature series expansions, we are able to scale data for the one-dimensional Ising ferromagnet rigorously over the entire temperature range. Analogous scaling expressions are then applied to the two-dimensional fully frustrated Villain model where excellent finite-size scaling over the entire temperature range is achieved. Thus we broaden the applicability of the extended scaling method to Ising systems having a zero-temperature critical point.

References: Phys. Rev. B 78, 184409 (2008)

Title: Ultrametricity and clustering of states in spin glasses: A one-dimensional view

Researchers: Helmut G. Katzgraber^{1,2} and Alexander K. Hartmann³

Institute/Group: 1Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
2Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA
3Institut für Physik, Universität Oldenburg, D-26111 Oldenburg, Germany

Description:

We present results from Monte Carlo simulations to test for ultrametricity and clustering properties in spin-glass models. By using a one-dimensional Ising spin glass with random power-law interactions where the universality class of the model can be tuned by changing the power-law exponent, we find signatures of ultrametric behavior both in the mean-field and non-mean-field universality classes for large linear system sizes. Furthermore, we confirm the existence of nontrivial connected components in phase space via a clustering analysis of configurations.

References: Phys. Rev. Lett. 102, 037207 (2009)

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

Researchers: Brigitte Surer,¹ Helmut G. Katzgraber,^{1, 2} Gergely T. Zimanyi,³
Brandon A. Allgood,⁴ and Gianni Blatter¹

Institute/Group: ¹Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland
²Department of Physics, Texas A&M University, College Station, Texas
77843-4242, USA
³Department of Physics, University of California, Davis, California
95616, USA
⁴Numerate Inc., 1150 Bayhill Drive, San Bruno, CA 94066, USA

Description:

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

References: Phys. Rev. Lett. 102, 067205 (2009)

Title: ENCORE: An Extended Contractor Renormalization algorithm

Researchers: A. Fabricio Albuquerque,^{1,2} Helmut G. Katzgraber,^{1, 3} and Matthias Troyer¹

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
³Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA

Description:

Contractor renormalization (CORE) is a real-space renormalization-group method to derive effective Hamiltonians for microscopic models. The original CORE method is based on a real-space decomposition of the lattice into small blocks and the effective degrees of freedom on the lattice are tensor products of those on the small blocks. We present an extension of the CORE method that overcomes this restriction. Our generalization allows the application of CORE to derive arbitrary effective models whose Hilbert space is not just a tensor product of local degrees of freedom. The method is especially well suited to search for microscopic models to emulate low-energy exotic models and can guide the design of quantum devices.

References: Phys. Rev. E 79, 046712 (2009)

Title: Evidence for universal scaling in the spin-glass phase

Researchers: Thomas Jörg¹ and Helmut G. Katzgraber²

Institute/Group: ¹LPTMS, Université Paris-Sud, CNRS UMR 8626, 91405 Orsay Cedex, France
²Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland

Description:

We perform Monte Carlo simulations of Ising spin-glass models in three and four dimensions, as well as of Migdal-Kadanoff spin glasses on a hierarchical lattice. Our results show strong evidence for universal scaling in the spin-glass phase in all three models. Not only does this allow for a clean way to compare results obtained from different coupling distributions, it also suggests that a so far elusive renormalization group approach within the spin-glass phase may actually be feasible.

References: Phys. Rev. Lett. 101, 197205 (2008)

Title: On the momentum-sector-selective transition in the 8 site dynamical mean field approximation to the two dimensional Hubbard model

Researchers: Emanuel Gull,¹ Olivier Parcollet,² Philipp Werner,³ and Andrew J. Millis¹

Institute/Group: 1Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027, USA
2Institut de Physique Th´eorique, CEA, IPhT, CNRS, URA 2306, F-91191 Gif-sur-Yvette, France
3Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

We explore the momentum-sector-selective metal insulator transitions recently found in the 8 - site dynamical cluster approximation to the two dimensional Hubbard model. The phase diagram in the space of interaction and second neighbor hopping is established. The initial transitions from Fermi liquid-like to sector-selective phases are found to be of second order, caused by the continuous opening of an energy gap whereas the other transitions are found to be first order. In the sector-selective phase the Fermi surface regions which are not gapped are found to have a non-Fermi-liquid self energy. We demonstrate that the phenomenon is not caused by the van Hove divergence in the density of states. The sector selective and insulating phases are characterized by a cluster spin correlation function that is strongly peaked at the commensurate antiferromagnetic wavevector (π, π) , but the model has no nematic instability. Comparison to dynamical mean field studies on smaller clusters is made.

References: arXiv:0909.1795v1, submitted to PRB

Title: Magnetism and orbital-ordering in an interacting three band model: a dynamical mean field study

Researchers: Ching-Kit Chan,¹ Philipp Werner,² and Andrew J. Millis¹

Institute/Group: ¹Columbia University, 538 West, 120th Street, New York, NY 10027, USA
²Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

Single-site dynamical mean field theory is used to determine the magnetic and orbital-ordering phase diagram for a model of electrons moving on a lattice with three orbital states per site and with the fully rotationally invariant Slater-Kanamori on-site interactions. The model captures important aspects of the physics of transition metal oxides with partially filled t_{2g} shells, and of electron-doped C_{60} . We introduce an unbiased, computationally simple and inexpensive method for estimating the presence of two sublattice order, determine the regimes in which spatially uniform and two-sublattice spin and orbital orderings are present and give physical arguments for the origins of the different phases. Guidelines are determined for optimizing the presence of ferromagnetism, which may be desirable in applications

References: arXiv:0909.1499v1, submitted to PRB

Title: Krylov-implementation of the hybridization expansion impurity solver and application to 5-orbital models

Researchers: Andreas M. Läuchli¹ and Philipp Werner²

Institute/Group: ¹Max Planck Institut für Physik komplexer Systeme, Nöthnitzerstrasse 38, D-01187 Dresden, Germany
²Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland

Description:

We present an implementation of the hybridization expansion impurity solver which employs sparse matrix exact-diagonalization techniques to compute the time evolution of the local Hamiltonian. This method avoids computationally expensive matrix-matrix multiplications and becomes advantageous over the conventional implementation for models with 5 or more orbitals. In particular, this method will allow the systematic investigation of 7-orbital systems (lanthanide and actinide compounds) within single-site dynamical mean field theory. We illustrate the power and usefulness of our approach with dynamical mean field results for a 5-orbital model which captures some aspects of the physics of the iron based superconductors.

References: arXiv:0908.0681v1, submitted to PRB

Title: Correlations in a band insulator

Researchers: Michael Sentef^{1,2}, Jan Kuneš¹, Philipp Werner², and Arno P. Kampf¹

Institute/Group: ¹Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany
²Theoretical Physics, ETH Zurich, CH-8093 Zurich, Switzerland

Description:

We study a model of a covalent band insulator with on-site Coulomb repulsion at half-filling using dynamical mean-field theory. Upon increasing the interaction strength the system undergoes a discontinuous transition from a correlated band insulator to a Mott insulator with hysteretic behavior at low temperatures. Increasing the temperature in the band insulator close to the insulator-insulator transition we find a crossover to a Mott insulator at elevated temperatures. Remarkably, correlations decrease the energy gap in the correlated band insulator. The gap renormalization can be traced to the low-frequency behavior of the self-energy, analogously to the quasiparticle renormalization in a Fermi liquid. While the uncorrelated band insulator is characterized by a single gap for both charge and spin excitations, the spin gap is smaller than the charge gap in the correlated system.

References: Phys. Rev. B 80, 155116 (2009)

Title: Interaction quench in the Hubbard model: Relaxation of the spectral function and the optical conductivity

Researchers: Martin Eckstein,¹ Marcus Kollar,² and Philipp Werner¹

Institute/Group: ¹Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
²Theoretical Physics III, Center for Electronic Correlations and Magnetism,
Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

Description:

We use non-equilibrium dynamical mean-field theory in combination with a recently developed Quantum Monte Carlo impurity solver to study the real-time dynamics of a Hubbard model which is driven out of equilibrium by a sudden increase in the on-site repulsion U . We discuss the implementation of the self-consistency procedure and some important technical improvements of the QMC method. The exact numerical solution is compared to iterated perturbation theory, which is found to produce accurate results only for weak interaction or short times. Furthermore we calculate the spectral functions and the optical conductivity from a Fourier transform on the finite Keldysh contour, for which the numerically accessible timescales allow to resolve the formation of Hubbard bands and a gap in the strongly interacting regime. The spectral function, and all one-particle quantities that can be calculated from it, thermalize rapidly at the transition between qualitatively different weak- and strong-coupling relaxation regimes.

References: Phys. Rev. Lett. 103, 056403 (2009)

Title: Metal-Insulator phase diagram and orbital selectivity in 3-orbital models with rotationally invariant Hund coupling

Researchers: Philipp Werner,¹ Emanuel Gull,¹ and Andrew J. Millis²

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²Columbia University, 538 West, 120th Street, New York, NY 10027, USA

Description:

A three band model containing the essential physics of transition metal oxides with partially filled t_{2g} shells is solved in the single-site dynamical mean field approximation, using the full rotationally invariant Slater-Kanamori interactions. We compute the metal-Mott insulator phase diagram in the space of chemical potential and interaction strength, determine the response of the different phases to perturbations which break the orbital symmetry, and establish the regimes in which an orbital selective Mott phase occurs. The results are compared to data on titanates, ruthenates, vanadates and C_{60} .

References: Phys. Rev. B 79, 115119 (2009)

Title: Two-stage metal-insulator transition in the 2D Hubbard model: momentum selectivity in the 8-site dynamical cluster approximation

Researchers: Philipp Werner,¹ Emanuel Gull,² Olivier Parcollet,³ and Andrew J. Millis²

Institute/Group: 1Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
2Department of Physics, Columbia University, 538 West, 120th Street, New York, NY 10027, USA
3Institut de Physique Théorique, CEA, IPhT, CNRS, URA 2306, F-91191 Gif-sur-Yvette, France

Description:

Metal-insulator transitions in the paramagnetic phase of the two dimensional square lattice Hubbard model are studied using the dynamical cluster approximation with eight momentum cells. We show that both the interaction-driven and the doping-driven transition are multi-stage and momentum-sector specific, with Fermi liquid metal and fully gapped insulator phases separated by an intermediate phase in which some regions of the Brillouin zone are gapped while others sustain gapless quasiparticles. We argue that this is the coarse-grained version of a gradually shrinking arc or pocket. A pronounced particle-hole asymmetry is found.

References: Phys. Rev. B 80, 045120 (2009)

Title: Pressure-Driven Metal-Insulator Transition in Hematite from Dynamical Mean-Field Theory

Researchers: J. Kuneš¹, Dm. M. Korotin,² M. A. Korotin,² V. I. Anisimov,² and P. Werner³

Institute/Group: ¹Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg 86135, Germany
²Institute of Metal Physics, Russian Academy of Sciences, 620041 Yekaterinburg GSP-170, Russia
³Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Description:

The Local Density Approximation combined with Dynamical Mean-Field Theory (LDA+DMFT method) is applied to the study of the paramagnetic and magnetically ordered phases of hematite Fe_2O_3 as a function of volume. As the volume is decreased, a simultaneous 1st order insulator-metal and high-spin to low-spin transition occurs close to the experimental value of the critical volume. The high-spin insulating phase is destroyed by a progressive reduction of the charge gap with increasing pressure, upon closing of which the high spin phase becomes unstable. We conclude that the transition in Fe_2O_3 at ≈ 50 GPa can be described as an electronically driven volume collapse.

References: Phys. Rev. Lett. 102, 146402 (2009)

Title: Diagrammatic Monte Carlo simulation of non-equilibrium systems

Researchers: Philipp Werner,¹ Takashi Oka,² and Andrew J. Millis³

Institute/Group: ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
²Department of Physics, Tokyo University, Hongo, Tokyo 113-0033, Japan
³Department of Physics, Columbia University, 538 West, 120th Street, New York, NY 10027, USA

Description:

We generalize the recently developed diagrammatic Monte Carlo techniques for quantum impurity models from an imaginary time to a Keldysh formalism suitable for real-time and nonequilibrium calculations. Both weak-coupling and strong-coupling based methods are introduced, analysed and applied to the study of transport and relaxation dynamics in interacting quantum dots.

References: Phys. Rev. B 79, 035320 (2009)

Title: Transient dynamics of the Anderson impurity model out of equilibrium

Researchers: T. L. Schmidt,¹ P. Werner,^{2, 3} L. Mühlbacher,⁴ and A. Komnik⁵

Institute/Group: 1Departement Physik, Universität at Basel, Klingelbergstr. 82, 4056 Basel, Switzerland
2Columbia University, 538 West 120th Street, New York, NY 10027, USA
3Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
4Physikalisches Institut, Universität at Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany
5Institut für Theoretische Physik, Universität at Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Description:

We discuss the transient effects in the Anderson impurity model that occur when two fermionic continua with finite bandwidths are instantaneously coupled to a central level. We present results for the analytically solvable noninteracting resonant level system first and then consistently extend them to the interacting case using the conventional perturbation theory and recently developed nonequilibrium Monte Carlo simulation schemes. The main goal is to gain an understanding of the full time-dependent nonlinear current-voltage characteristics and the population probability of the central level. We find that, contrary to the steady state, the transient dynamics of the system depends sensitively on the bandwidth of the electrode material.

References: Phys. Rev. B 78, 235110 (2008)

Title: Simulation of Optical and Plasmonic Nano Structures

Researchers: Christian Hafner
Christian Engström
Patrick Leidenberger
Ludmila Raguin
Matthew Mishrikey
Aytac Alparslan
Mengyu Wang
Thomas Kaufmann
Rüdiger Vahldieck

**Institute/
Group:** Laboratory for Electromagnetic Fields and Microwave Electronics
Computational Optics, Electromagnetic Field Theory

Description:

We develop various numerical methods and software packages for the simulation of optical nano structures including lossy and dispersive material with or without electromagnetic band gaps. The applications include plasmonic waveguides, optical antennas, photonic crystals, optical bio sensors, etc. Field solvers based on boundary discretization methods - the Multiple Multipole Program (MMP), the Method of Auxiliary Sources (MAS), Boundary Element Methods (BEM), Boundary Integral Equations (BIEM) –, Method of Moments (MoM), as well as domain discretization methods in frequency and time domain, namely Finite Elements Methods (FEM), Discontinuous Galerkin (DG), and Finite Difference Time Domain (FDTD) are developed and applied. The semi-analytic MMP and MAS methods provide high accuracy, robustness, and numerical efficiency for 2D applications and exhibit no problems with material dispersion and loss. For 3D simulations, FEM and FDTD are favorable as long as moderate accuracy of the results is sufficient.

The platform MaX-1, which contains our MMP and FDTD codes, has been converted into an OpenSource project OpenMaX that should include other field solvers in the future.

In order to speed up the frequency domain solvers and nonlinear eigenvalue solvers, we take advantage of Model Based Parameter Estimation (MBPE) techniques.

The field solvers mentioned above were applied to various cases, including metallic and metallo-dielectric photonic crystals, photonic crystals with anomalous dispersion, ultra-thin plasmonic waveguides with Surface Plasmon Polariton (SPP), Wedge Plasmon Polariton (WPP), and Channel Plasmon Polariton (CPP) effects, optical antennas, and biological sensor structures.

References:

In 2008 and 2009, ten papers in reviewed journals were published based on our field solvers.

Title: Simulation and Optimization of Metamaterials and Photonic Crystals

Researchers: Christian Hafner
Christian Engstöm
Matthew Mishrikey
Arya Fallahi
Rüdiger Vahldieck

Institute/ Laboratory for Electromagnetic Fields and Microwave Electronics
Group: Computational Optics, Electromagnetic Field Theory

Description:

We have developed software packages for both the simulation and optimization of metamaterials for low frequencies up to optical frequencies, including electromagnetic bandgap materials and photonic crystals. Field solvers based on the Multiple Multipole Program (MMP), the Method of Auxiliary Sources (MAS), the Method of Moments (MoM), Rigorous Coupled Wave Analysis (RCWA), Finite Element Method (FEM), and Finite Difference Time Domain (FDTD) were implemented, tested, applied, and combined with various numerical optimizers for parameter optimization (gradient methods, downhill simplex, evolutionary strategies, genetic algorithms, particle swarm optimization, and genetic programming algorithms) as well as for binary optimization (special table-based algorithms that may be considered as improved genetic algorithms, micro genetic algorithms, binary evolutionary strategies, etc.).

The software packages mentioned were applied to various cases, frequency reflective surfaces, anti-reflective coatings, radar absorbing and shielding metamaterials, electrosmog protection, high temperature metamaterial shields, negative index metamaterials, photonic crystal structures, etc.

The platform MaX-1, which contains our MMP and FDTD codes, has been converted into an OpenSource project OpenMaX that should include other field solvers in the future.

References:

In 2008 and 2009, eight papers in reviewed journals were published.

Title: Antenna analysis and design

Researchers: Christian Hafner
Christian Engström
Thomas Kaufmann
Georgios Almpanis
Mengyu Wang
Aytac Alparslan
Rüdiger Vahldieck

**Institute/
Group:** Laboratory for Electromagnetic Fields and Microwave Electronics
Electromagnetic Field Theory, Computational Optics

Description:

We develop various numerical methods and software packages for the simulation of antennas covering a frequency range from radio frequencies to microwaves and optical frequencies.

We consider time domain solvers such as Finite Volume Time Domain (FVTD), Finite Elements Methods (FEM), Finite Integral Techniques (FIT), and mesh-free techniques as well as frequency domain solvers such as FEM, Multiple Multipole Program (MMP), the Method of Auxiliary Sources (MAS), the Method of Moments (MoM), etc. In addition to in-house codes, we apply various commercial field solvers, including COMSOL, HFSS, MicrowaveStudio, etc.

The platform MaX-1, which contains our MMP and FDTD codes, has been converted into an OpenSource project OpenMaX that should include other field solvers in the future.

In the radio frequency and microwave range, we study geometrically highly complex antenna structures, dielectric resonator antennas, antennas embedded in electromagnetic bandgap materials, etc. whereas plasmonic antennas mounted on dielectric substrates are considered at optical frequencies.

References:

In 2008 and 2009, four papers in reviewed journals were published based on our field solvers.

Title: Computational modeling and design of RF arrays for human high-field MRI

Researchers: Jürg Fröhlich (IFH)
Jan Paska (IFH)
Rüdiger Vahldieck (IFH)
David Brunner (IBT)
Klaas Prüssmann (IBT)

**Institute/
Group:** Laboratory for Electromagnetic Fields and Microwave Electronics/
Electromagnetics in Medicine and Biology Group and Institute for Biomedical
Engineering / MR Technology Group

Description:

Among the large variety of present-day biomedical imaging modalities, MRI stands out by its full 3D capability, high-spatial resolution, and enormous contrast versatility. However, many advanced MRI applications, such as functional and metabolic brain studies, are seriously hampered by the limited sensitivity of the technique. The most comprehensive response to the sensitivity issue is the transition to higher baseline magnetic fields. One pivotal challenge in implementing ultra-high-field MRI is controlling the electromagnetic radiofrequency (RF) fields through which the instrument interacts with the imaging target. These fields are key determinants of the performance and safety of MRI procedures. Upon the transition to 7 Tesla, the RF electrodynamics undergoes a fundamental regime transition, which is characterized by the fact that the RF wavelength becomes significantly smaller than typical imaging targets, such as the human head. As a consequence, 7-Tesla MRI faces a dramatic increase in complexity of the RF behaviour, entailing major challenges in terms of imaging methodology and safety, yet also great opportunities with respect to sensitivity and imaging speed.

A promising approach for addressing these challenges and opportunities is the recently proposed use of large coil arrays for highly parallel RF transmission and reception. The performance of such arrays is closely linked with their electromagnetic transmission and reception characteristics. The analysis and the design of coils and coil arrays at higher baseline magnetic fields therefore requires the electromagnetic full wave analysis of the complex structure of head coil arrays together with the resulting thermodynamic response in heterogeneous anatomical models.

References:

In 2009, one paper in a reviewed journal was published.

Title: Exploring the conserved water sites and hydration of a coiled-coil trimerization motif: a MD simulation study

Researchers: J. Dolenc
R. Baron
J.H. Missimer
M.O. Steinmetz
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

The solvent structure and dynamics around ccb-p, a 17-residue peptide that forms a parallel three-stranded alpha-helical coiled coil in solution, was analysed through 10 ns explicit solvent molecular dynamics (MD) simulations at 278 and 330 K. Comparison with two corresponding simulations of the monomeric form of ccb-p was used to investigate the changes of hydration upon coiled coil formation. Pronounced peaks in the solvent density distribution between residues Arg8 and Glu13 of neighbouring helices show the presence of water bridges between the helices of the ccb-p trimer; this is in agreement with the water sites observed in X-ray crystallography experiments. Interestingly, this water site is structurally conserved in many three-stranded coiled coils and, together with the Arg and Glu residues, forms part of a motif that determines three-stranded coiled-coil formation. Our findings show that little direct correlation exists between the solvent density distribution and the temporal ordering of water around the trimeric coiled coil. The MD-calculated effective residence times of up to 40 ps show rapid exchange of surface water molecules with the bulk phase, and indicate that the solvent distribution around biomolecules requires interpretation in terms of continuous density distributions rather than in terms of discrete molecules of water. Together, our study contributes to understanding the principles of three-stranded coiled-coil formation.

References: ChemBioChem. **9** (2008) 1749-1756, DOI: 10.1002/cbic.200800096

Title: Simple, efficient, and reliable computation of multiple free energy differences from a single simulation: a reference Hamiltonian parameter update scheme for enveloping distribution sampling (EDS)

Researchers: C.D. Christ
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

We present an automatic adaptive scheme which allows fast optimization of the reference Hamiltonian parameters in enveloping distribution sampling (EDS). Six different variants of the update scheme have been tested on a condensed phase test system which included the recurrent deletion and creation of complete water molecules in water. All six schemes gave accurate free energy estimates with absolute errors of up to 1 kJ/mol for the worst scheme and up to 0.1 kJ/mol for the best scheme. Configurational sampling is focused on the regions where the end state energy difference distributions intersect, explaining the high accuracy and precision of the free energy estimates. The new update scheme makes the application of EDS to other systems, e.g. in ligand binding studies, easy as no reference state Hamiltonian parameters have to be chosen by the user. The only necessary input are the Hamiltonians of the various end states involved.

References: J Chem. Theory Comput. **5** (2009) 276–286, DOI: 10.1021/ct800424v

Title: On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models

Researchers: M. Winger
D. Trzesniak
R. Baron
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

The use of a coarse-grained (CG) model that is widely used in molecular dynamics simulations of biomolecular systems is investigated with respect to the dependence of a variety of quantities upon the size of the used integration time step and cutoff radius. The results suggest that when using a non-bonded interaction-cutoff radius of 1.4 nm a time step of maximally 10 fs should be used, in order not to produce energy sinks or wells. Using a too-large time step, e.g. 50 fs with a cutoff of 1.2 nm, as is done in the coarse-grained model of Marrink et al. (*J. Phys. Chem. B*, 2004, 108, 250 and 2007, 111, 7812), induces errors due to the linear approximation of the integrators that are commonly used to integrate the equations of motion. As a spin-off of the investigation of the mentioned CG models, we found that the parameters of the CG water model place it at physiological temperatures well into the solid phase of the phase diagram.

References: *Phys.Chem.Chem.Phys.* **11** (2009) 1934-1941, DOI: 10.1039/b818713d

Title: Interpreting experimental data by using molecular simulation instead of model building

Researchers: Z. Gattin
J. Schwartz
R.I. Mathad
B. Jaun
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

One of the most used spectroscopic techniques for resolving the structure of a biomolecule, such as a protein or peptide, is NMR spectroscopy. Because only NMR signal intensities and frequencies are measured in the experiment, a conformational interpretation of the primary data, that is, measured data, is not straightforward, especially for flexible molecules. It is hampered by the occurrence of conformational and/or time-averaging, by insufficient number of experimental data and by insufficient accuracy of experimental data. All three problematic aspects of structure refinement based on NMR nuclear Overhauser effect (NOE) intensities and $3J$ coupling data are illustrated by using two b-heptapeptides in methanol as an example. We have performed 16 molecular dynamics (MD) simulations between 20 to 100 ns in length of unrestrained and NOE distance-restrained cases (instantaneous and time-averaged) of two bheptapeptides with a central beta-HAla amino acid in methanol at two different temperatures using two different GROMOS force-field parameter sets, 45A3 and 53A6. The created conformational ensembles were used to interpret the primary NMR data on these molecules. They also were compared to a set of NMR model structures derived by single-structure refinement in vacuo by using standard techniques. It is shown that the conformational interpretation of measured experimental data can be significantly improved by using unrestrained, instantaneous and time-averaged restrained MD simulations of the peptides by using a thermodynamically calibrated force field and by explicitly including solvent degrees of freedom.

References: Chem.Eur.J.**15** (2009) 6389–6398, DOI:10.1002/chem.200802523, incl.suppl.mat.

Title: Influence of backbone fluorine substitution upon the folding equilibrium of a beta-heptapeptide

Researchers: Z. Gattin
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Explicit solvent molecular dynamics (MD) simulations of three beta-heptapeptides with a central beta- HAla(R-F) amino acid (Figure 1) in methanol are reported. They aim at an analysis of the conformational consequences of CR carbon atom bound fluoro atoms, and the particular configuration of the central fluoro-beta-amino acid: peptide **3** with an *S* configuration of the CR bound fluor atom, peptide **4** with an *R* configuration of the CR bound fluor atom, and peptide **5** with a difluoro substitution at the CR atom of residue 4. The NMR and CD spectra of these three beta-peptides were earlier (Mathad et al. *Helv. Chim. Acta* **2005**, 88, 266-280) interpreted to indicate a decrease in propensity of 3_{14} -helical structure from peptide **4** to peptide **5** to peptide **3**. This result was at odds with previous experimental data for beta-heptapeptides with a central beta-HAla(R-Me) amino acid which showed that the beta-heptapeptide with the *S, S* configuration of the central beta-HAla(R-Me) was the most 3_{14} -helical, whereas the *S,R* configuration did not lead to any detected helicity. The reported MD simulations resolve this paradox. The MD trajectories of all three peptides do agree with the primary, measured data: NMR nuclear Overhauser effect (NOE) atom-atom distance bounds and $3J$ -coupling constants. A conformational analysis of the MD trajectory conformations shows, however, a decrease in 3_{14} -helical character from peptide **3** to peptide **5** to peptide **4**, which is in line with the results for the nonfluorinated peptides. It is shown that interpretation of NMR NOE data using single-structure refinement in vacuo based on local (along the sequence) and limited atom-atom distance data as in ref 1 (Mathad et al. *Helv. Chim. Acta* **2005**, 88, 266-280) may lead to molecular structures that are not representative for the ensemble of molecular conformations.

References: J.Phys.Chem. B **113** (2009) 8695–8703, DOI: 10.1021/jp811106e

Title: On the conformational properties of amylose and cellulose oligomers in solution

Researchers: M. Winger
M. Christen
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Molecular dynamics (MD) simulations were used to monitor the stability and conformation of double-stranded and singlestranded amyloses and single-stranded cellulose oligomers containing 9 sugar moieties in solution as a function of solvent composition, ionic strength, temperature, and methylation state. This study along with other previous studies suggests that hydrogen bonds are crucial for guaranteeing the stability of the amylose double helix. Single-stranded amylose forms a helical structure as well, and cellulose stays highly elongated throughout the simulation time, a behavior that was also observed experimentally. In terms of coordination of solute hydroxyl groups with ions, amylose shows entropy-driven coordination of calcium and sulfate ions, whereas cellulose-ion coordination seems to be enthalpy-dominated. This indicates that entropy considerations cannot be neglected when explaining the structural differences between amyloses and celluloses.

References: Int.J.Carbohydr.Chem. (2009) 1-8, DOI:10.1155/2009/307695

Title: Folding and unfolding of two mixed alpha/beta peptides

Researchers: D. Wang
B. Jaun
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

We present a molecular dynamics simulation study of two peptides containing α - and β -amino acid residues. According to experiment, the two peptides differ in the dominant fold when solvated in methanol: one shows a helical fold, the other a beta hairpin. The simulations at 300 and 340 K were done by starting from a NMR spectroscopic model structure and from an extended (denatured) structure. The typical structural features of the two peptides are reproduced and a folding/unfolding equilibrium is observed on the nanosecond timescale at 300 K. Analysis of proton–proton NOE distance bounds and backbone 3J coupling constants gives results consistent with the experimental data. We conclude that our simulations are complementary to the experiments by providing detailed information on the conformational distributions.

References: ChemBioChem. (2009) on-line, DOI: 10.1002/cbic.200900125

Title: Development of a non-linear classical polarisation model for liquid water and aqueous solutions: COS/D

Researchers: A.P. Kunz
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

A new charge-on-spring (COS) model for water is introduced (COS/D). It includes a sublinear dependence of the induced dipole on the electric field for large field strength to include the effect of hyperpolarizability by damping the polarizability. Only two new parameters were introduced to define the damping of the polarizability. In the parametrization procedure, these two damping parameters, the two Lennard-Jones parameters, the charge on the oxygen, and the distance between the virtual site and the oxygen atom were varied to reproduce the density, the heat of vaporization, the dielectric permittivity, and the position of the first peak in the radial distribution function of liquid water at room temperature and pressure. In this way, a model was obtained that correctly describes a variety of thermodynamic, dynamic, and dielectric properties of water while still preserving the simplicity of the COS model, which allows a straightforward introduction of explicit polarization into (bio)molecular force fields.

References: JPC (2009) on-line, DOI:10.1021/jp903164s

Title: Comparison of three enveloping distribution sampling Hamiltonians for the estimation of multiple free energy differences from a single simulation

Researchers: C.D. Christ
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

We test the performance of three different reference state Hamiltonians for enveloping distribution sampling (EDS). EDS is an implementation of umbrella sampling which allows estimation of various free energy differences "on the fly" from a single simulation. This is achieved by construction of a reference state, which envelopes the regions of configuration space important to the various end states of interest. The proposed Hamiltonians differ in the way energy barriers separating these regions of configuration space are reduced. The test system consisted of 17 disubstituted benzenes in water and in complex with alpha-cyclodextrin. The calculated free energy differences correlate with thermodynamic integration results ($R(2) > 0.99$ for the ligands in water and $R(2) > 0.98$ for the ligands in complex with alpha-cyclodextrin). One of the reference state Hamiltonians outperformed the others in sampling the configuration space important to the various end states. In this reference state not all barriers between all pairs of states are reduced. Instead a minimum spanning tree of states is calculated, which connects states that are "closest" in configuration space.

References: J.Comput.Chem. **30** (2009) 1664-1679

Title: A method to explore protein side chain conformational variability using experimental data

Researchers: J.R. Allison
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Experimentally measured values of molecular properties or observables of biomolecules such as proteins are generally averages over time and space, which do not contain sufficient information to determine the underlying conformational distribution of the molecules in solution. The relationship between experimentally-measured NMR 3J -couplings and the corresponding dihedral angle values is a particularly complicated case due to its non-linear, multiple-valued nature. Molecular dynamics (MD) simulations at constant temperature can generate Boltzmann ensembles of molecular structures that are free from a priori assumptions about the nature of the underlying conformational distribution. They suffer, however, from limited sampling with respect to time and conformational space. Moreover, the quality of the obtained structures is dependent on the choice of force field and solvation model. A recently proposed method that uses time-averaging with local-elevation (LE) biasing of the conformational search provides an elegant means of overcoming these three problems. Using a set of side chain 3J -couplings for the protein FKBP, we first investigate the uncertainty in the angle values predicted theoretically. We then propose a simple MD-based technique to detect inconsistencies within an experimental data set and identify degrees of freedom for which conformational averaging takes place or for which force field parameters may be deficient. Finally, we show that LE MD is the best method for producing ensembles of structures that, on average, fit the experimental data.

References: The manuscript has been accepted by *ChemPhysChem*.

Title: Temperature and urea induced denaturation of the TRP-cage mini protein TC5b: A simulation study consistent with experimental observations

Researchers: Z. Gattin*
S. Riniker*
P. J. Hore**
K. H. Mok***
W. F. van Gunsteren*

Institute/ Laboratory of Physical Chemistry, ETH Zurich, Switzerland*
Group: Physical and Theoretical Chemistry Laboratory, Department of Chemistry,
University of Oxford, United Kingdom**
School of Biochemistry and Immunology, Trinity College, University of
Dublin, Ireland***

Description:

Simulations of the TRP-cage mini protein TC5b were performed at three different temperatures in water (278, 360, and 400 K) and in 6M urea solution (278, 298, 360 K) to study the denaturation of the α -helix in the protein. A denaturation temperature well below 360 K was observed, which is 40 - 60 K lower than the denaturation temperatures found in simulation with other force fields. In addition, the MD trajectories were compared to the experimental NOE- and proton cross-polarization distances.

References: The manuscript has been submitted to *Protein Science*

Title: Comparing geometric and kinetic cluster algorithms for molecular simulation data

Researchers: B. Keller
X. Daura
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

The identification of metastable states of a molecule plays an important role in the interpretation of molecular simulation data because the free-energy surface, the relative populations in this landscape and ultimately also the dynamics of the molecule under study can be described in terms of these states. We compare the results of three different geometric cluster algorithms (neighbor algorithm, K-medoids algorithm, common-nearest-neighbor algorithm) among each other and to the results of a kinetic cluster algorithm. Firstly, we demonstrate the characteristics of each of the geometric cluster algorithms using five two-dimensional data sets. Secondly, we analyze molecular dynamics data of a beta-heptapeptide in methanol - a molecule which exhibits a distinct folded state, a structurally diverse unfolded state and a fast folding/unfolding equilibrium - using both geometric and kinetic cluster algorithms. We find that geometric clustering strongly depends on the algorithm used and that the density based common-nearest-neighbor algorithm, is the most robust of the three geometric cluster algorithms with respect to variations of the input parameters and the distance metric. When comparing the geometric cluster results to the metastable states of the beta-heptapeptide as identified by kinetic clustering, we find that in most cases the folded state is identified correctly but the overlap of geometric clusters with further metastable states is often at best approximate.

References: The manuscript has been accepted by *J.Chem.Phys.*

Title: Structure determination of flexible cyclic peptides based on NMR 3J -coupling constant data

Researchers: Z. Gattin
J. Zaugg
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Molecular dynamics (MD) simulations in which experimental values such as NOE's, dipolar couplings, 3J -coupling constants or crystallographic structure factors are used to bias the values of specific molecular properties towards experimental ones, is an often used approach in structure refinement of peptides and proteins.

Here we apply the method of adaptively enforced restraining using a local-elevation (LE) biasing potential energy function in which a memory function penalizes conformations in case both the average $\langle ^3J \rangle$ and the current 3J -value deviate from the experimental target value. Then the molecule is forced to sample other parts of the conformational space, thereby being able to cross high energy barriers and to bring the simulated average $\langle ^3J \rangle$ close to the measured $\langle ^3J \rangle$.

In the present study we show the applicability of this method in structure refinement of a cyclo- β -tetrapeptide by enforcing the 3J -value restraining with LE on twelve backbone angles. The resulting structural ensemble satisfies the experimental 3J -coupling data better than the NMR model structure derived using conventional single-structure refinement based on these data. Thus, application of local-elevation search MD simulation in combination with biasing towards 3J -coupling makes it possible to use 3J -couplings quantitatively in structure determination of peptides.

References: The manuscript has been submitted to *ChemPhysChem*.

Title: The propensity of aminoisobutyric acid (Aib) to induce helical secondary structure in an alpha-heptapeptide: a computational study

Researchers: D. Wang*
M. Friedmann*
Z. Gattin*
B. Jaun**
W.F. van Gunsteren*

Institute/ *Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry
**Laboratory of Organic Chemistry, ETH Hönggerberg, Zürich, Switzerland

Description:

We present a molecular dynamics simulation study of an alpha-heptapeptide containing an Aib residue, Val1-Ala2-Leu3-Aib4-Ile5-Met6-Phe7, and a quantum mechanical (QM) study of simplified models to investigate the propensity of the Aib residue to induce 3_{10} -helical conformation. For comparison, we have also performed simulations of three analogues of the peptide with the Aib residue being replaced by L-Ala, D-Ala and Gly respectively, which provide information on the substitution effect at C (two methyl groups for Aib, one for L-Ala and D-Ala, and zero for Gly). Our simulations suggest that in methanol the heptapeptide hardly folds into canonical helical conformations, but appears to populate multiple conformations, i.e. C_7 and 3_{10} -helical ones, which is in agreement with results from the QM calculations and NMR experiments. The populations of these conformations depend on the polarity of the solvent. Our study confirms that a short peptide, though with the presence of an Aib residue in the middle of the chain, does not have to fold to an alpha-helical secondary structure. To generate a helical conformation for a linear peptide, several Aib residues should be fused in the peptide, either sequentially or alternatively, to enhance the propensity of Aib containing peptides towards the helical conformation. A correction of a few of the published NMR data is reported.

References: The manuscript has been submitted to *J.Phys.Chem.*

Title: Investigation of disulfide bond shuffling by molecular dynamics simulation

Researchers: J. Allison*
G.-P. Moll*
W.F. van Gunsteren*

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Proteins comprising each of the two plant non-specific lipid transfer protein (LTP) families, LTP1s and LTP2s, share similar folds and biological functions and are stabilised by four native disulfide bonds. Disulfide-scrambling experiments have suggested that their biophysical properties such as stability and folding pathway are quite different, however. Here we use a computational disulfide-scrambling technique to investigate the proposed disulfide bond shuffling of rice LTP1. The application of this technique to LTP2 was precluded by the finding that the NMR model structure of LTP2 does not reflect the true structural propensities of LTP2 in solution.

References: The manuscript has been submitted to *Proteins*

Title: A GPU Solvent-Solvent Interaction Calculation Accelerator for Biomolecular Simulations using the GROMOS Software

Researchers: N. Schmid
M. Bötschi
W. F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

During the past few years, Graphics Processing Units (GPUs) have become extremely popular in the high performance computing community. In this work we present an implementation of an acceleration engine for the solvent-solvent interaction evaluation of molecular dynamics simulations. By careful optimization of the algorithm speed-ups up to a factor of 30 (single-precision GPU vs. double-precision CPU) could be achieved. The accuracy of the single-precision GPU implementation is carefully investigated and does not influence structural, thermodynamic and dynamic quantities. Therefore, the implementation enables users of the GROMOS software for biomolecular simulation to run the solvent-solvent interaction evaluation on a GPU and thus to speed-up their simulations by a factor 5 to 7.

References: *Journal of Computational Chemistry* (in press)

Title: A cyclic β -helical / β -hairpin D, L- α -peptide: study of its folding properties and structure refinement using molecular dynamics

Researchers: K. Meier
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

We present a molecular dynamics simulation study of an alpha-heptapeptide containing an Aib residue, Val1-Ala2-Leu3-Aib4-Ile5-Met6-Phe7, and a quantum-mechanical (QM) study of simplified models to investigate the propensity of the Aib residue to induce 3_{10} /alpha-helical conformation. For comparison, we have also performed simulations of three analogues of the peptide with the Aib residue being replaced by L-Ala, D-Ala and Gly respectively, which provide information on the substitution effect at C^{alpha} (two methyl groups for Aib, one for L-Ala and D-Ala, and zero for Gly). Our simulations suggest that in methanol the heptapeptide hardly folds into canonical helical conformations, but appears to populate multiple conformations, i.e. C₇ and 3_{10} -helical ones, which is in agreement with results from the QM calculations and NMR experiments. The populations of these conformations depend on the polarity of the solvent. Our study confirms that a short peptide, though with the presence of an Aib residue in the middle of the chain, does not have to fold to an alpha-helical secondary structure. To generate a helical conformation for a linear peptide, several Aib residues should be fused in the peptide, either sequentially or alternatively, to enhance the propensity of Aib containing peptides towards the helical conformation. A correction of a few of the published NMR data is reported.

References: The manuscript has been submitted to *J.Phys.Chem.A*

Title: Molecular dynamics simulation of ester-linked hen egg white lysozyme reveals the effect of missing backbone hydrogen-bond donors on the protein structure

Researchers: A.P. Eichenberger
Z. Gattin
G. Yalak
W.F. van Gunsteren

**Institute/
Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group for computer aided chemistry

Description:

The three-dimensional structure of a protein is stabilised by a number of different atomic interactions. One of these is hydrogen bonding. Its influence on the spatial structure of the hen egg white lysozyme is investigated by replacing peptide bonds (except those of the two proline residues) by ester bonds. Molecular dynamics simulations of native and ester-linked lysozyme are compared with the native crystal structure. The ester-linked protein shows a slight compaction while losing its native structure. However, it does not unfold completely. The structure remains compact due to its hydrophobic core and a changed network of hydrogen bonds involving side chains.

References: The manuscript has been submitted to *PROTEINS: Structure, Function, and Bioinformatics*

Title: The thermal isomerization of the GFP chromophore: a computational study

Researchers: D. Wang
T. Merz
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

We present a density functional theory study of the isomerization of the green fluorescent protein (GFP) chromophore in the ground state promoted by a nucleophile. Three solvents with different polarity, DMSO, methanol, and benzene, have been used to characterize the nucleophile assisted mechanism. The former two solvents have been used as nucleophile to participate in the reaction, while in benzene, we use n-propylamine as the nucleophile. The calculations predict a one-step reaction for the isomerization in DMSO, with a high energy barrier of 35.8 kcal/mol, in accord with the slow reaction observed experimentally. When methanol and n-propylamine are used as nucleophile, the isomerization is characterized as a three-step process and the addition of the nucleophile is the rate-determining step. A proton transfer from the nucleophile to the oxygen of imidazolinone (O^1) is observed during the addition step, which stabilizes the negative charge on O^1 due to the reduction of the $C^1=C^2$ double bond. The reaction assisted by n-propylamine is faster than the one assisted by methanol, which is consistent with the experimental data.

References: The manuscript has been submitted to *Phys.Chem.Chem.Phys.*

Title: Molecular dynamics simulations reveal the enthalpic and entropic driving forces that govern the sequence specific recognition between netropsin and DNA

Researchers: J. Dolenc
S. Gerster
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

With the aim to gain a better understanding of the driving forces that govern sequence specific DNA minor groove binding we performed a thermodynamic analysis of netropsin binding to an AT- and to a set of 6 mixed AT/GC-containing binding sequences in the DNA minor groove. The relative binding free energies obtained using molecular dynamics simulations and free energy calculations show significant variations with the binding sequence. While the introduction of a GC base pair in the middle or close to the middle of the binding site is unfavourable for netropsin binding, a GC base pair at the end of the binding site appears to have no negative influence on the binding. The results of the structural and energetic analyses of the netropsin-DNA complexes reveal that the differences in the calculated binding affinities cannot be explained solely in terms of netropsin-DNA hydrogen bonding or interaction energies. In addition, solvation effects and entropic contributions to the relative binding free energy provide a more complete picture of the various factors determining binding. Analysis of the relative binding entropy indicates that its magnitude is highly sequence-dependent, with the ratio $|\Delta\Delta S|/|\Delta\Delta H|$ ranging from 0.07 for the AAAGA to 1.7 for the AAGAG binding sequence, respectively.

References: The manuscript has been submitted to *Nucleic Acids Research*

Title: What stabilizes the 3_{14} -helix in β^3 -peptides? A conformational analysis using molecular simulation

Researchers: B. Keller
Z. Gattin
W.F. van Gunsteren

Institute/ Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
Group: Group for computer aided chemistry

Description:

Beta-peptides are analogs of natural alpha-peptides and form a variety of remarkably stable structures. Having an additional carbon atom in the backbone of each residue, their folded conformation is not only influenced by the side-chain sequence but also and foremost by their substitution pattern. The precise mechanism by which the side chains interact with the backbone is, however, hitherto not completely known. In order to unravel the various effects by which the side chains influence the backbone conformation, we quantify to which extent the dihedral angles of a beta³-substituted peptide with an additional methyl group on the central C_{alpha}-atom can be regarded as independent degrees of freedom and analyze the distributions of these dihedral angles. We also selectively capture the steric effect of substituents on the C_{alpha}- and C_{beta}-atoms of the central residue by alchemically changing them into dummy atoms, which have no non-bonded interactions. We find that the folded state of the beta³-peptide is primarily stabilized by a steric exclusion of large parts of the unfolded state (entropic effect) and only subsequently by mutual dependence of the psi-dihedral angles (enthalpic effect). The folded state of beta-peptides is stabilized by a different mechanism than that of alpha-peptides.

References: The manuscript has been submitted to *Proteins*

High-performance Hardware

6.1 The C⁴ Computing Facilities

C⁴ currently has one compute cluster (Obelix) operated by the System Gruppe of the ETH Informatikdienste. Furthermore, in the past year, C⁴ became a Brutus shareholder.

Obelix is an IBM Cluster e1350, Type 1410/42X, running RedHat Linux. It consists of 32 e326m clients, each with two dual core AMD Opteron CPUs with either 8 or 16 GB of memory, one e326m login node, and an x346 Storage Node DS4100 with about 1.3 TB of cluster-wide disk space

Obelix is now in his fourth year of operation. The hardware proved to be very stable. At the end of September, the file server, for example, had an uptime of over 1'160 days! The accounting shows that the cluster is being used very consistently at 80% of its peak. The number of jobs submitted for four processors, running for the maximum allowed time of 30 days and requesting 8 GB of memory or more, increased dramatically during the last year, causing many of these jobs to be in the queue. It is a common usage pattern that 50% of the CPU time of a given month is consumed by two or maximally three users. There are currently seventy users active.

In 2009, the ETH Zürich Department of Chemistry, through C⁴, became a shareholder of the Brutus Cluster, giving its computational chemists guaranteed access to this resource for special projects. About two thirds of the 408 nodes are standard Brutus nodes, whereas the remaining third consists of fat nodes for very resource-demanding applications.

Eric Müller (System Supervisor) and Hans P. Lüthi (Leiter C4),
September 2009

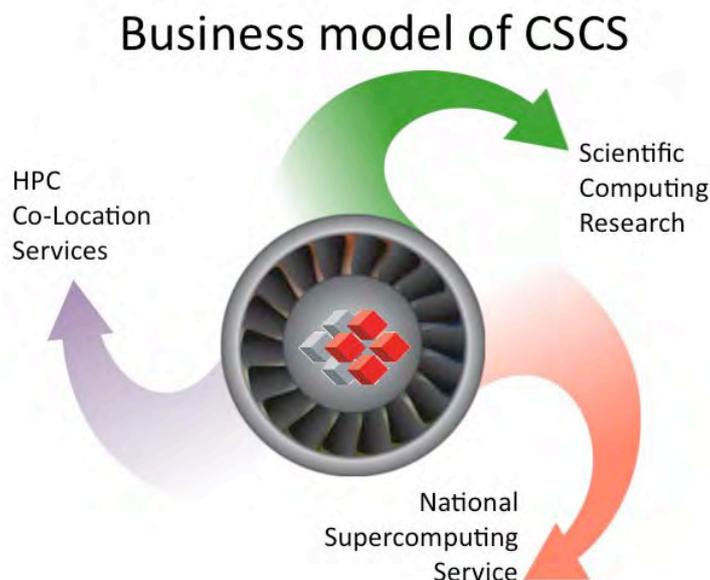
6.2 CSCS – Swiss National Supercomputing Centre

Dominik Ulmer

CSCS - Swiss National Supercomputing Centre
Galleria 2, Via Cantonale
6928 Manno, Switzerland, Tel: +41 91 610 82 11 Fax: +41 91 610 82 09
info@cscs.ch

A new CSCS business model

CSCS, the Swiss National Supercomputing Centre, develops and promotes technical and scientific services for the Swiss research community in the fields of high-performance computing. It enables world-class scientific research by pioneering, operating and supporting leading-edge supercomputing technologies. Since October 2008, CSCS is led by its new director Prof. Thomas Schulthess. Under Prof. Schulthess, research and advanced development activities will be built up at the centre. The centre has consequently developed a new business model, which reflects the different mandates of CSCS.



The business model distinguishes three business areas representing different organizational units:

- Scientific Computing Research: This unit carries out advanced development work in high-performance computing. It is run in a project-oriented manner and investigates future HPC technologies and applications.
- National Supercomputing Service: This service operates the national HPC facility and supports academic users all over Switzerland. Resources for the service are allocated to users according to scientific merit of project proposals.
- HPC Co-Location Services: This unit operates systems for contractual partners like MeteoSwiss or the Swiss Particle Physics Institute and acts as a technology transfer service.

CSCS' computing infrastructure

The compute resources of the National Supercomputing Service went through a massive upgrade during 2009. Until May 2009, CSCS operated a Cray XT3 massively parallel processing (MPP) computer system, which offered 3328 2.6GHz AMD Opteron processors on dual-core nodes as well as a further 32 processors for service activities such as providing login access and supporting the parallel file system. The system was able to deliver a peak performance of 17TFlop/s and a total of 3.3 Terabytes of memory. In May 2009, CSCS upgraded this machine to Cray XT5 technology. The new system offers 29 TB of main memory and initially consisted of 14'768 2.4 GHz AMD Opteron cores, which delivered a total of 141 TFlop/s. In early October 2009, the system was further upgraded to 22'128 2.4 GHz AMD Opteron cores with a total peak performance of 212 TFlop/s.

The processors of both systems, the XT3 and the XT5, are connected by the Cray SeaStar high-bandwidth, low-latency interconnect that uses a 3D torus typology. The parallel filesystem of the Cray XT3 provided 23 Terabytes of temporary scratch storage with a peak data transfer rate of 4.5 GB/s. This was upgraded on the Cray XT5 to 288 TB capacity and a peak data transfer rate of 20 GB/s.

In addition, CSCS operates an IBM parallel constellation cluster consisting of 48 p5-575 SMP nodes with a total of 786 Power 5 CPUs and 1.5 TB of main memory. This system offers a theoretical peak performance of 4.5 TFlop/s. A dual-link 4X SDR Infiniband interconnect links the nodes and provides a high speed network for the login nodes and the file system. A peak data transfer rate of approximately 5 GB/s is available on the GPFS parallel file system where 17 TB of storage are provided.

In the HPC C-Location Services unit, CSCS offers cluster computing capacity to the Swiss particle physics research community CHIPP by means of the Tier-2 computing cluster it hosts for the Large Hadron Collider Computing Grid. Furthermore, CSCS operates a cluster for pre- and post-processing consisting of 25 nodes, with two dual-AMD Opteron processors at 2.6 GHz. This cluster is interconnected with a 4X DDR Infiniband network. A 4X SDR Infiniband interconnect is used on the visualization cluster, which consists of 16 compute nodes, of which 6 have a special synchronization card for graphics cards.

Data management facilities

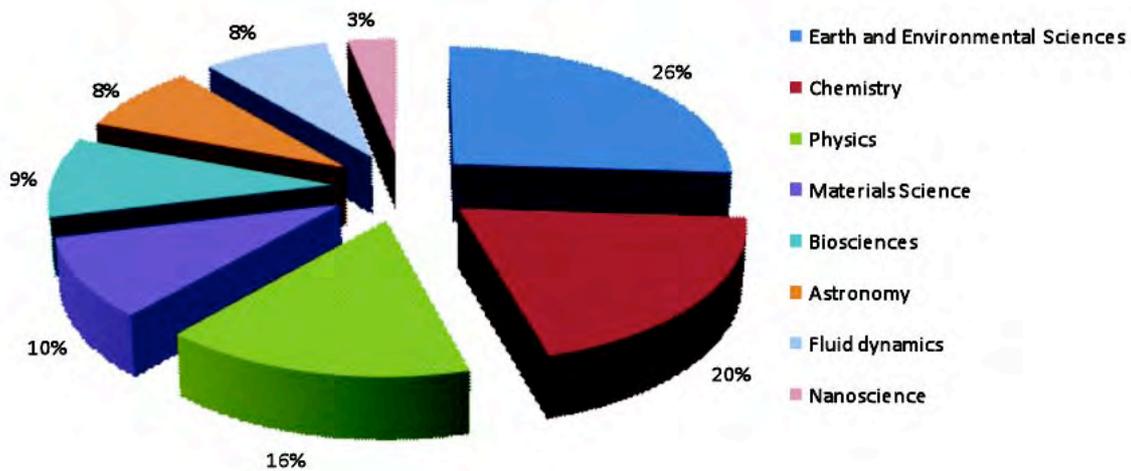
CSCS' data archive facility is based on the SAM-FS Hierarchical Storage Management (HSM) software running on a SUN Fire X4600, which controls data movement between the fast Engenio 6998 and a SUN SL8500 tape silo with Fibrechannel tape drive technology; redundant Brocade switches ensure a fully-switched FiberChannel archive environment. The archive capacity currently exceeds 2 Petabytes of total storage.

The new main storage level is a central parallel file system based on IBM GPFS technology. A high-bandwidth network based on QDR Infiniband technology connects this fast parallel file system to all major computer systems of CSCS and provides the central data management space for all research projects. Currently, this file system offers a total raw capacity of 512 Terabytes. It is expected that the file system will grow to the Petabytes level during 2010.

Users of the CSCS compute infrastructure

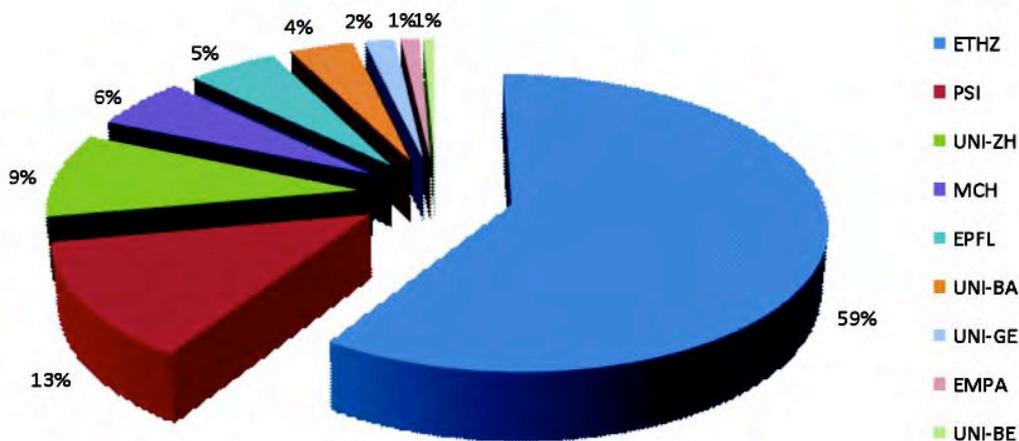
The CSCS customer base consists of researchers from the fields of chemistry, physics, material sciences, earth and planetary sciences and biosciences. Currently the vast majority of CSCS resources are used by the fields of chemistry, physics and earth and environmental sciences.

Usage of CSCS HPC resources by discipline



Of the produced CPU hours ETH Zurich consumes the largest part, followed by the Paul Scherrer Institute and the University of Zurich.

Usage of CSCS HPC resources by institution



The Production Projects and the ALPS high-impact projects that were granted during 2008, are listed in the table below.

ALPS Projects 2008

Jackson	Andrew	ETH Zurich	Investigating the origin of magnetic fields of the earth and other planets
Vogel	Viola	ETH Zurich	At the molecular level, how does cell function change under mechanical force
Parrinello	Michele	ETH Zurich	Investigate the role of protein interactions of interest for diseases such as Alzheimer and HIV
Schär	Christoph	ETH Zurich	Investigate climate change on European and Alpine scales and possible future extreme weather events

Large Projects 2008

Arbenz	Peter	ETH Zurich	Multi-level micro-finite element analysis for human bone structures
Baiker	Alfons	ETH Zurich	Surface chemistry of transition metals and catalysis for CO ₂ fixation
Bakowies	Dirk	ETH Zurich	Atomization energies from ab initio calculations without empirical corrections
Baldereschi	Alfonso	EPF Lausanne	Solid surfaces and interfaces
Boley	Aaron	University of Zurich	The accretion mechanism of T Tauri Stars
Bürgi	Thomas	University of Neuchâtel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Carollo	Marcella	ETH Zurich	Galaxy formation in the cosmic web (and its impact on measurements of the EoS of dark energy)
Carollo	Marcella	ETH Zurich	The role of environment in the formation and evolution of galaxies
Cooper	W. Anthony	EPF Lausanne	Computation of stellarator coils, equilibrium, stability and transport
Cucinotta	Clotilde	ETH Zurich	Ab initio study of LiAl alloy: a prototype for superionic conduction and hydrogen storage
Deubel	Dirk	ETH Zurich	Quantum chemical studies of transition metal anticancer drugs
Fichtner	Wolfgang	ETH Zurich	Computational science and engineering in nanoelectronics
Folini	Doris	EMPA	Inverse modelling to monitor source regions of air
Fouchet	Laure	ETH Zurich	Dust in protoplanetary disks
Gervasio	Francesco	ETH Zurich	New computational approaches to study large-scale protein conformational transitions
Gervasio	Francesco	ETH Zurich	Folding mechanism of HIV1 protease in explicit solvent

Goedecker	Stefan	University of Basel	Atomistic simulations and electronic structure
Hauser	Andreas	University of Geneva	Photophysics and photochemistry of transition metal compounds: theoretical approaches
Hutter	Jürg	University of Zurich	Development and applications of ab initio molecular dynamics methods
Iannuzzi	Marcella	PSI	Transport properties and microstructural changes in uranium dioxide
Jackson	Andrew	ETH Zurich	Models of convection and magnetic field generation in earth
Jackson	Andrew	ETH Zurich	Thermal convection in giant planets: the effect of an oblate spheroidal geometry
Joos	Fortunat	University of Bern	Modelling CARBOn cycle CLIMate Feedbacks (CARBOCLIM)
Khaliullin	Rustam	ETH Zurich	A molecular dynamics study of the phase diagram of carbon employing a neural network potential
Kleiser	Leonhard	ETH Zurich	Numerical simulation of transitional, turbulent and multiphase flows
Koumoutsakos	Petros	ETH Zurich	Aircraft wake evolutionary optimization
Koumoutsakos	Petros	ETH Zurich	Multiphysics simulations using multiscale particle methods
Kröger	Martin	ETH Zurich	Computer-aided design of nanostructured interfaces for biological sensors
Lake	George	University of Zurich	Galaxy formation (even dwarfs) in full cosmological context
Läuchli	Andreas	EPF Lausanne	Simulating quantum states of matter
Leyland	Pénélope	EPF Lausanne	Study of flight characteristics of a generic reentry launcher vehicle
Liebendörfer	Matthias	University of Basel	Three-dimensional modelling of core-collapse supernovae
Lodziana	Zbigniew	EMPA	Computational investigation of complex hydrides for hydrogen storage
Maddocks	John	EPF Lausanne	Atomistic molecular dynamics simulations of DNA minicircles
Man	Hau-Kit	ETH Zurich	Investigation of 3D size effects in numerical concrete containing realistic aggregate shapes
Mapelli	Michela	University of Zurich	Formation of massive stars in the galactic centre
Mareda	Jiri	University of Geneva	Molecular modelling of artificial multifunctional pores and their catalytic properties
Mayer	Lucio	University of Zurich	The formation of disk galaxies in a cold dark matter universe
Meher	Ayalasomayajula	ETH Zurich	Metadynamics study of large-scale pH-induced conformational changes in dengue virus envelope protein

Meuwly	Markus	University of Basel	Influence of dimerization on allostery of multidomain proteins
Meuwly	Markus	University of Basel	Electronic structure calculations for chemical reactions involving transition metals
Miniati	Francesco	ETH Zurich	Turbulence in clusters of galaxies: code testing
Oganov	Artem	ETH Zurich	Computational crystallography: crystal structure prediction and simulation of planetary materials
Parrinello	Michele	ETH Zurich	Advanced computational methods
Parrinello	Michele	ETH Zurich	Ab-initio study of GeSbTe phase change alloys
Pasquarello	Alfredo	EPF Lausanne	Atomic-scale modelling at semiconductor-oxide interfaces (2)
Passerone	Daniele	EMPA	Atomistic simulation of surface-supported molecular nanostructures and of quasicrystal surfaces
Pfaendtner	Jim	ETH Zurich	Metadynamics investigation of the dynamics of the actin cytoskeleton
Porciani	Cristiano	ETH Zurich	The physics of baryons, dark matter and dark energy
Poulikakos	Dimos	ETH Zurich	Biothermofluidics for cerebrospinal fluid diagnostics
Raible	Christoph	University of Bern	Modelling and reconstruction of north atlantic climate system variability (MONALISA II)
Röthlisberger	Ursula	EPF Lausanne	Mixed quantum mechanical/molecular mechanical (QM/MM) studies of systems of biological interest
Sbalzarini	Ivo	ETH Zurich	Simulations of biological systems and development of a parallelization framework
Schär	Christoph	ETH Zurich	Modelling weather and climate on European and Alpine scales
Seneviratne	Sonia	ETH Zurich	Land-climate interactions: modelling and analysis
Van Lenthe	Harry	ETH Zurich	What genetic loci are involved in the regulation of bone strength?
Van Swygenhoven	Helena	PSI	The atomistic modelling of size effect in plastic
Walder	Rolf	ETH Zurich	Stellar cosmic engines in galaxies
Wesolowski	Tomasz	University of Geneva	Multi-level computer simulations of electronic structure in condensed matter
Zoppi Baldrige	Laura Kim	University of Zurich	Corannulene-copper systems by a multilevel theoretical approach

6.3 Information Technology Services

The following resources are available:

- Hewlett Packard Superdome Cluster consisting of
 - 1 HP Superdome (Stardust): 128-way, 64 Dual Core Itanium2 Montecito CPUs (1600 MHz), 256 GB Memory, HP/UX Operating System
 - 1 HP Superdome (Pegasus): 64-way, 32 Dual Core Itanium2 Montecito CPUs (1600 MHz), 128 GB Memory, HP/UX Operating System

The cluster is used for parallel code taking advantage of the shared memory programming model offered by the cc-numa architecture of these systems. Many standard applications (finite element modeling, mathematics, simulations, etc.) are in this category.

The systems major usage is in the fields of thermodynamics, fluid dynamics, virtual production (FEM) and theoretical physics.

The following software is available on the Superdome cluster:

HP Fortran: Compiler and associated products

HP Fortran 90: Compiler and associated products

HP C/ansi: C Developer's Bundle for HP-UX 11.00

HP C++: Compiler

KAI Guide C++: Open MP

Abaqus 5.8: General-purpose finite element analysis

ACSL: Advanced continuous simulation language

Ampl 9.5.13: Modeling language for Mathematical Programming

ANSYS 5.5: Finite element analysis

AVS: Advanced visual system

CPLEX 65: Linear optimization solver

CFX Tascflow: CFD analysis and design tool

Diana 7.2: Finite element analysis

Gaussian 98: semi empirical and ab initio molecular orbital (MO) calculations.

MARC/MENTAT K7.3: Nonlinear finite element program

Matlab 11.1: Language for technical computing

Molcas 5: Quantum chemistry software

NAG F95: Fortran library

IMSL: Fortran Numerical Libraries

Para Phoenix 32: CFD

Patran 9.0: Finite element (Modeling, Analysis, Results evaluation)

Tecplot 8.0: Tool for visualizing a wide range of technical data

PV-Wave: Signal Processing Toolkit

Note:

These systems are becoming obsolete due to the fact, that Linux clusters based on standard hardware are today able to provide the SMP scalability necessary for most of the computations running on the Superdomes.

The phaseout of the Superdomes will start in 2010 by operating them without maintenance contract from the vendor. If a major system failure occurs, operation of the sys-

tems will be discontinued on short notice. It is not advisable to begin new projects on the superdomes any more.

- The Information Technology Services operate a Linux Cluster co-owned with the Departments Biology, Environmental Sciences, Earth Sciences, Physics, Mathematics, Material Sciences, Mechanical and Process Engineering and Computer Science. This cluster consists of the following node types:
 - 8 eight processor dual core AMD Opteron 8220 and 64-128 GB memory
 - 306 two processor AMD Opteron 250 systems with 8 GB memory
 - 272 two processor dual core AMD Opteron 2220 systems with 16 GB memory and Ethernet network
 - 420 four processor quad core AMD Opteron 8380 systems with 32 GB memory

All nodes are connected to the cluster's internal Gigabit Ethernet backbone. 256 nodes are connected to a high speed /low latency Quadrics QsNetII network. 410 nodes are connected to a high speed/low latency InfiniBand QDR network.

The peak performance of the cluster is approximately 75 teraflops.

Parts of the cluster are operated as a central resource, which can be used on a fair share base by the ETH community without being co-owner of the cluster.

The cluster nodes connected through the Quadrics QSnet II and the InfiniBand network are intended for parallel code (typically MPI based) needing high bandwidth and low latency communications, but not a globally shared memory. The Ethernet connected part of the cluster is intended for single node throughput computing and not communication intensive parallel jobs. The eight processor dual core nodes as well as the four processor quad core nodes are suited well for up to 16-way symmetric multi-processing jobs and thus are the main target for users migrating away from the Superdome systems.

7

Outlook

A few months ago a Call for proposals was published as part of the HP2C (High Performance and High Productivity Computing) initiative of the Swiss University Conference and the ETH Domain. It is meant to promote supercomputing in Switzerland, both at the CSCS in Manno and Swiss universities. Unfortunately, researchers from ETH Zürich are not eligible as principal investigators in the HP2C framework. Nevertheless, the initiative demonstrates growing awareness of the role of high performance computing for competitive science.

Indirectly, CSE research at ETH Zürich will certainly benefit from HP2C. It remains to be seen whether HP2C will be complemented and continued by other funding schemes, in which ETH Zürich will again be included.

Zürich, November 16, 2009
Ralf Hiptmair

8

Publications* in 2008/2009

*only CSE-related articles
in refereed journals

Group of P. Arbenz

A.J. Wirth, Th.L. Mueller, W. Vereecken, C. Flaig, P. Arbenz, R. Müller, G.H. van Lenthe:

Mechanical competence of bone-implant systems can accurately be determined by image-based micro-finite element analyses.

Arch. Appl. Mech., online 29.10.2009, doi:10.1007/s00419-009-0387-x.

P. Arbenz, J. Bryner, Ch. Tobler:

Parallelized transient elastic wave propagation in orthotropic structures. Proceedings of the 8th Conference on Parallel Processing and Applied Mathematics (PPAM). Wroclaw, Poland, Sept 13-16, 2009.

A. Adelman, P. Arbenz, and Y. Ineichen:

A Fast Parallel Poisson Solver on Irregular Domains Applied to Beam Dynamic Simulations, July 2009. e-Print Archive: arXiv:0907.4863v1[physics.comp-ph].

P. Arbenz, O. Chinellato:

On solving complex-symmetric eigenvalue problems arising in the design of axisymmetric VCSEL devices.

Appl. Numer. Math. 58 (4): 381-394, 2008, doi:10.1016/j.apnum.2007.01.019

P. Arbenz and C. Flaig:

On smoothing surfaces in voxel based finite element analysis of trabecular bone.

In: I. Lirkov, S. Margenov, and J. Waśniewski, editors, Large Scale Scientific Computing (LSSC 2007), pages 69–77, Berlin, 2008. Springer. (Lecture Notes in Computer Science, 4818).

P. Arbenz and R. Müller:

Microstructural Finite Element Analysis of Human Bone Structures.

ERCIM News 74, pp. 31–32, July 2008.

P. Arbenz, G. H. van Lenthe, U. Mennel, R. Müller, and M. Sala:

Multi-level μ -Finite Element Analysis for Human Bone Structures.

In: Applied Parallel Computing: State of the Art in Scientific Computing. B. Kågström, E. Elmroth, J. Dongarra, and J. Wasniewski (eds.). Lecture Notes in Computer Science 4699, pp. 240–250. Springer, Berlin, 2007, doi:10.1007/978-3-540-75755-9_30.

P. Arbenz, G. H. van Lenthe, U. Mennel, R. Müller, and M. Sala:

A Scalable Multi-level Preconditioner for Matrix-Free μ -Finite Element Analysis of Human Bone Structures.

Internat. J. Numer. Methods Engrg. 73(7):927–947, 2008, doi:10.1002/nme.2101.

P. Arbenz, S. D. Margenov, and Y. Vutov:

Parallel MIC(0) Preconditioning of 3D Elliptic Problems Discretized by Rannacher–Turek

Finite Elements.

Comput. Math. Appl. 55 (10): 2197–2211, 2008, doi:10.1016/j.camwa.2007.11.013

J. Demmel, O. Marques, B. N. Parlett, Ch. Vömel:
Performance and Accuracy of LAPACK's Symmetric Tridiagonal Eigensolvers.
SIAM J. Scientific Computing 30(3) 1508–1526, (2008)

O. Marques, Ch. Vömel, J. Demmel, B. N. Parlett:
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