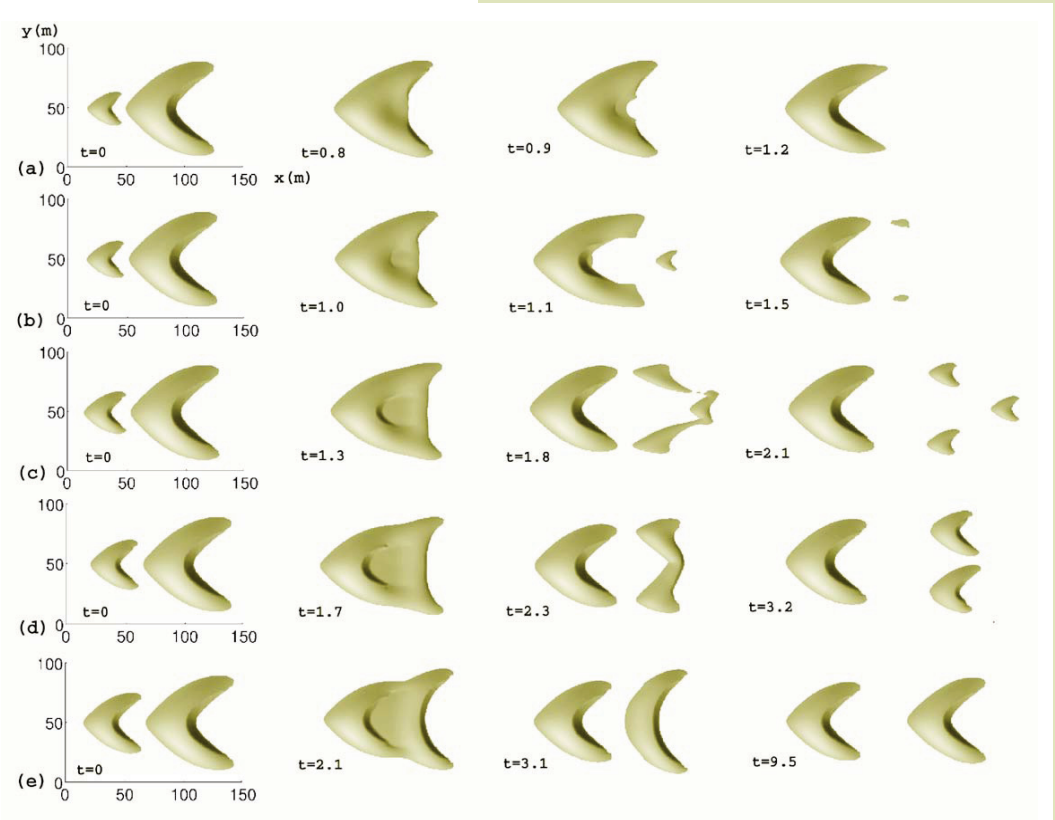
CSE

Computational Science and Engineering

Annual Report 2006/2007



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CSE

Computational Science and Engineering

Annual Report
2006 / 2007

July 2006 to July 2007

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Cover:
Different situations during the collision of two Barchan dunes using open boundary conditions. Coalescence (a), breeding (b),(c), budding (d), and solitary wave behavior (e) take place. The time (t) is in month and the x and y labels in (a) are the same for all axes. [Durán et al, Phys. Rev. E 72, 021308 (2005)]

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Introduction

This year is the 10th anniversary of the curriculum in Computational Science and Engineering, CSE, at ETH and this is already the seventh Annual CSE Report. It is the fourth report which is done electronically only. We have become adjusted to the fact that it is much more convenient to obtain information in electronic form. Two years ago we have started with the Master Program in CSE and the first students have already finished their Master thesis. We are ready to advertise the Master Program on a world wide scale. Our website http://www.cse.ethz.ch/master/ describing the Master Program contains all the information in English. For potential students it is of great interest to have this CSE report and the previous ones electronically available to get an impression on the breadth and depth and the dynamics of CSE related research in all of ETH. More and more persons are interested in research and education in CSE, not only students but also colleagues, visitors and people form other universities. They all want to know what is going on at the ETH in this exciting field. This new edition documents the changes that happened in the last year and gives a glimpse of the developments immediately ahead of us.

By now the whole Bachelor and Master curricula are in full place and the first students have finished both degrees. We have currently 61 students (40 in the BSc Program and 21 in the MSc Program). This is the moment to review the program as a whole and therefore the CSE committee has already decided on further developments which are described in the outlook.

On the research side we have seen again new professors being hired who use computing as one of their important tools to do science and/or engineering. In this year our colleague Hans J. Herrmann from the Institute for Building Materials at ETH will show in the featured report 'Simulation of Dunes' progress in his field.

Last year I could announce that we expected a large turnout for the International Congress on Industrial and Applied Mathematics, ICIAM 2007, which then took place at ETH and the University of Zürich 16-20 July this year. Indeed, the attendance with about 3200 participants was tremendous. Overall 2873 talks have been given as invited or special lectures, minisymposia talks or contributed papers. In addition 120 posters have been presented. Due to this huge number of presentations we had up to 70 parallel sessions. At this point I would like to thank all people involved for their enthusiastic commitment to make the event a success. I think the University of Zürich and ETH have shown their strength and as a large portion of the lectures covered CSE it gave excellent publicity to our field. Our Study Advisor, Kaspar Nipp, organized a four hour minisymposium together with tow colleagues from Germany on *Computational science and engineering*. You find more on the whole congress at the website: http://www.iciam07.ch/.

At this point we thank the Executive Board of the ETH for supporting CSE in research and education. Moreover, we thank all those at the ETH who have contributed to this report.

Zürich, November 27, 2007
Rolf Jeltsch, Head of Student Studies CSE and member of the CSE Committee

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Education

In October 2006, 16 new students have started their CSE Bachelor studies. The students had done their first year's studies in another curriculum at ETH in the following fields: Mathematics 2 students, Computer Science 2, Mechanical Engineering 3, Electrical Engineering 2, Civil, Environmental and Geomatic Engineering 4, Biology 1; and from other Swiss universities in Computer Science 1 and from Swiss Fachhochschulen in Electrical Engineering 1.

From outside ETH 2 students entered the CSE Master curriculum, 1 from EPF Lausanne with a Master degree in Science et Génie des Matériaux, 1 from the University of Berne with a Diploma degree in Physics.

The total number of CSE students enrolled at the end of the academic year 2006/2007 was 49 (32 in the BSc program and 17 in the MSc program).

The presentation of the CSE Bachelor/Master curricula for ETH students of the second semester of May 24, 2007 was attended by around 60 students. It is hoped that a fair number of them will start with the CSE Bachelor studies this fall.

In the past academic year 19 students have successfully finished a CSE curriculum, Bachelor, Master and Diploma, respectively, and have received a CSE degree, some with very good scores. In the two and a half years Diploma curriculum in CSE existing since October 1997 and started for the last turn in October 2003 the last 4 students finished their studies. In the following list we give the name of the student, the title of the Bachelor/Master/Diploma thesis and, in parentheses, the name and the department/institute of the advisor.

Bachelor Theses

R. Andreev — Stochastic Galerkin-Wavelet Methods for Diffusion Problems
(C. Schwab, Applied Mathematics)

H. Avenhaus — Molekulardynamik in GROMOS
(A. Mark / W. van Gunsteren, Computational Chemistry)

C. Heitzmann — Gesture-based Image Selection User Interface for Large Screen Interaction Environments
(M. Gross, Computer Graphics Lab)

N. Kannookadan — Motiva-The Next Generation Configuration Device: Planning, Design and Evaluation.
(A. Kunz, Machine Tools and Manufacturing)

C. Scherrer — Valuation of American Contracts in Stochastic Volatility Models
(C. Schwab, Applied Mathematics)

Master Theses

M. Blattmann	Nonparametric Volatility Estimation with a Functional Gradient Descent Algorithm for Univariate Financial Time Series (P. Bühlmann, Statistics)
R. Carnecky	Interactive Skeleton-Based Character Deformation (M. Gross, Computer Graphics Lab)
L. Gamper	Graph Algorithms for Quantum Many Body Systems (M. Troyer, Theoretical Physics)
S. Gerster	Learning Graphs from Data: A Comparison of Different Algorithms with Application to Tissue Microarray Experiments (P. Bühlmann, Statistics)
C. Heitzmann	Computer-Supported Creativity Processes in Research and Development (A. Kunz, Machine Tools and Manufacturing)
M. Koller	Rolle von numerischen Verfahren und Parametrisierungen in atmosphärischen Simulationen mit expliziter Konvektion (C. Schär, Atmospheric and Climate Science)
M. Müller	Sedimentation von Hydrometeoren in ECHAM (U. Lohmann, Atmospheric and Climate Science)
K. Schüpbach	Numerical Investigation of Radiative Exchange in a Polydispersion of Coal Particles Undergoing Steam Gasification Using the Monte Carlo Method (A. Steinfeld, Energy Technology)
S. Villiger	Basket Option Pricing on Sparse Grids Using Fast Fourier Transform (C. Schwab, Applied Mathematics)
B. Wüthrich	Simulation and Validation of Compressible Flow in Nozzle Geometries and Validation of Open FOAM for this Application (L. Kleiser, Fluiddynamics)

Diloma Theses

L. Blaser	Boundary Analysis for Numerical Weather Prediction Models (C. Schär, Atmospheric and Climate Science)
C. Bosshard	Implementation of a Finite-Volume Code for the Solution of the Incompressible Navier-Stokes equations (P. Jenny, Fluid Dynamics)

J. Nart — Large-Scale Dynamic Models
(Jörg Stelling, Computer Science)

S. Riva — Computation of Electrostatic forces by Virtual Work Methods
(R. Hiptmair, Applied Mathematics)

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

Term Papers

M. Blattmann — Nonparametric volatility estimation for financial time series
(P. Bühlmann, Statistics)

F. Fruth — Implement the Use of Tesis veDYNA at a Chassis Development Stage by Creating a Bespoke Ad-on Tool to Facilitate Lab-car Evaluations
(T.Fussey/M. Erzsaenger, Bentley; R. Jeltsch, Applied Mathematics)

L. Gamper — FFT on Hyperbolic Sparse Grids
(W. Petersen, Applied Mathematics)

S. Gerster — Prediction of pI and Retention Time shifts due to posttranslational Modification"
(M. Müller, Molecular Biology and Biophysics: R. Jeltsch, Applied Mathematics)

C. Heitzmann — Lattice Visualization and Editor for Physics Simulations
(M. Troyer, Theoretical Physics)

N. Kannookadan — Discretization of Linear Dirac Equations in 1D
(R. Hiptmair, Applied Mathematics)

M. Koller — Numerische Aspekte vertikaler Koordinaten in atmosphärischen Modellen
(C. Schär, Atmospheric and Climate Science)

H. Piehl — Simulieren von Array-Elektroden in Femlab"
(M. Morari, Automatics)

C. Scherrer — Assessment fo the Variational Stochastic Method for the Many-Body Problem in Quantum Chemistry
(M. Reiher, Physical Chemistry)

S. Villiger — Effiziente Fouriertransformation auf dünnen Gittern
(C. Schwab, Applied Mathematics)

B. Wüthrich Numerical Simulation of the Endolymph Flow in the Vestibular Organ
(L. Kleiser, Fluiddynamics)

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 31, 2007
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 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 WS06/07

02.11.06	Per Lötstedt, Scientific Computing, Uppsala University The Master Equation: Applications and Numerical Methods
09.11.06	D. Obrist, Fluiddynamik Understanding Top-Shelf Vertigo: Modeling of a Pathophysiological Process
16.11.06	H. Maurer, Geophysik Tomographische Inversion geophysikalischer Daten
23.11.06	S. Malamud, Alinpa AG, Wollerau, und Mathematik ETH Asset Pricing in Heterogeneous Economies
30.11.06	A. Gunzinger, Supercomputing Systems AG, Zürich Hardware-Optimierung versus algorithmische Optimierung
07.12.06	H. Katzgraber, Theoretische Physik Spin Glasses: Still Frustrating after all these Years
11.01.07	P. Hora, Virtuelle Produktion Module der digitalen Fabrik am Beispiel der virtuellen Karosserieplanung
18.01.07	A. Schmid, P. Stucki, Savannah Simulations AG, Herrliberg Praktische Anwendung der agentenbasierten Simulation am Beispiel der Fussgängersimulation SimWalk

Case Studies Seminar SS07

29.03.07	M. Kastenholz, Credit Suisse, Zürich Econophysics and Option Pricing
12.04.07	C. Winkelmann, Analyse et Calcul Scientifique, EPFL Finite Elements for Incompressible Two-Fluid Flow – Efficient Matrix Assembly and Reinitialization A. Burri, sd&m Schweiz AG, Zürich Ein Leben nach dem Studium: Das Berufsbild des Software-Ingenieurs
19.04.07	M. Torrilhon, Seminar für Angewandte Mathematik Modellierung in der Kontinuumsphysik
26.04.07	D. Würtz, Theoretische Physik Exponential Brownian Motion or How to Valuate Continuous Sampled Asian Options
03.05.07	P. Spichtinger, Atmosphäre and Klima Wolken in Atmosphärenmodellen - ein Multiskalenproblem
31.05.07	P. Tackley, Geophysik Numerical modelling of mantle convection, plate tectonics and the long-term evolution of Earth and other terrestrial planets
07.06.07	L. Zschiederich, ZIB (Zuse Institute Berlin) und JCMwave GmbH Computational Photonics: Modellierung, Numerik, Anwendersoftware

4

Computational Highlight

Simulation of Dunes

Hans J. Herrmann
Institute of Building Materials, DBAUG, ETH Zurich

Abstract:

Sand dunes are found in a wide variety of shapes in deserts and coasts, and also on the planet Mars. The basic mechanisms of dune formation could be incorporated into a continuum saltation model, which simulated successfully reproduced the shape of the dunes and has been also applied to calculate interaction of dunes in a field. We also present numerical simulation of the transformation of barchan dunes, under influence of vegetation, into parabolic dunes, which appear frequently on coasts. Further, we apply our model to simulate the shape of dunes observed on Mars. Our model could reproduce unusual dune shapes of the Martian north polar region, like rounded barchans and elongated linear dunes.

1 Introduction

Sand dunes develop wherever sand is exposed to an agitated medium that lifts grains from the ground and entrains them into a surface flow. Dunes are constituted of sand which comes from the sea. Once the grains are exposed to the air, they dry and some can be carried by the wind, initiating sand transport.

The morphology of sand dunes and the conditions under which each dune type appears have been studied by several authors. Quantitatively, however, the selection of dune size and shape and the mechanisms of dune stabilization are far from being understood, and are the challenges which motivated the present simulations.

The mechanism responsible for dune formation is called *saltation* (Bagnold 1941; Almeida et al. 2006). Grains are lifted from the ground by the wind, accelerated downwind, and after a certain distance ℓ they collide back onto the ground. Each grain impact may eject further grains — a mechanism called "splash" (Anderson and Haff 1988) — and thus a cascade process occurs, until the saltation flux achieves saturation, since the air transfers momentum back to the grains. Dunes appear because an exposed sand sheet is unstable, evolves into mounds, and next into dunes with a slip face. The existence of a saturation transient of the sand flux is reponsible for the existence of a minimum dune size.

2 The Dune Model

We have recently proposed a minimal dune model which provides an understanding of important features of real dunes, such as their longitudinal shape and aspect ratio, the formation of a slip face, the breaking of scale invariance, and the existence of a minimum dune size (Sauermann et al. 2001; Kroy et al. 2002). This model combines an analytical description of the turbulent wind velocity field above the dune with a continuum saltation model that allows for saturation transients in the sand flux. The fundamental idea of the dune model is to consider the bed-load as a thin fluid-like granular layer on top of an immobile sand bed. The model has been latter improved by Schwämmle and Herrmann (2005) to take into account lateral sand transport due to perturbations transverse to the main wind direction.

We studied the formation and evolution of barchans and transverse dunes. In particular we could successfully reproduce the crescent shape of dunes which develop in areas of unidirectional winds, their rate of motion, stability and interaction with each other. There are, indeed, several different sand patterns which can be observed according to wind condition, sand availability, humidity level and vegetation. A model of sand dunes which accounts for such variables yields an powerful tool in the understanding of processes and morphology in deserts and along coasts.

Sand transport takes place near the surface, in the turbulent boundary layer of the atmosphere (Pye and Tsoar 1991). In this turbulent layer, the wind velocity $u(z)$ at a height z may be written as

$$u(z) = \frac{u_*}{\kappa} \ln \frac{z}{z_0}, \tag{1}$$

where $\kappa = 0.4$ is the von Kármán constant, u_* is the wind shear velocity, which is used to define, together with the fluid density ρ_{fluid}, the shear stress $\tau = \rho_{\text{fluid}} u_*^2$, and z_0 is called aerodynamic roughness.

A dune or a smooth hill can be considered as a perturbation of the surface that causes a perturbation of the air flow onto the hill. In the model, the shear stress perturbation is calculated in the two dimensional Fourier space using the algorithm of Weng et al. (1991) for the components τ_x and τ_y, which are, respectively, the components parallel and perpendicular to wind direction. In what follows, we present the sand transport equations introduced in Sauermann et al. (2001) and refer to Schwämmle and Herrmann (2005) for a two-dimensional extension of the model.

The sand transport model uses the air shear stress in the boundary layer to calculate the sand flux. The equation for the sand flux (Sauermann et al. 2001) is a differential equation that contains the saturated flux q_{s} at the steady state, and the characteristic length ℓ_{s} that defines the transients of the flux:

$$\frac{\partial}{\partial x} q = \frac{1}{\ell_{\text{s}}} q \left(1 - \frac{q}{q_{\text{s}}} \right). \tag{2}$$

In eq. (2), the saturation length ℓ_{s} is written as

$$\ell_{\text{s}} = \frac{1}{\gamma} \left[\frac{\ell}{(u_*/u_{*\text{t}})^2 - 1} \right], \tag{3}$$

where ℓ is the average saltation length and $u_{*\mathrm{t}}$ is the threshold wind shear velocity for sustained saltation, which defines the threshold shear stress $\tau_\mathrm{t} = \rho_\mathrm{fluid} u_{*\mathrm{t}}^2$. The parameter γ models the average number n of grains dislodged out of equilibrium, and is written as

$$\gamma = \frac{\mathrm{d}n}{\mathrm{d}(\tau_\mathrm{a}/\tau_\mathrm{t})}, \tag{4}$$

where τ_a is the air born shear stress, which is distinguished from the grain born shear stress, i.e. the contribution of the saltating grains near the ground to the total shear stress τ due to their impacts onto the surface. The parameter γ, thus, gives the amount of grains launched into the saltation sheet when the wind strength deviates from the threshold by an amount $\tau_\mathrm{a}/\tau_\mathrm{t}$. The air born shear stress τ_a is lowered if the number of grains in the saltation layer increases and vice versa, which is called the "feedback" effect: At threshold, the wind has a strength $\tau_\mathrm{a} \approx \tau_\mathrm{t}$ sufficient to just maintain saltation. The parameter γ depends on microscopic quantities such as the time of a saltation trajectory or the grain-bed interaction, which are not available in the scope of the model.

The steady state is assumed to be reached instantaneously, since it corresponds to a time scale several orders of magnitude smaller than the time scale of the surface evolution. Thus, time dependent terms are neglected.

The time evolution of the topography $h(x,t)$ is given by the mass conservation equation

$$\frac{\partial h}{\partial t} = -\frac{1}{\rho_\mathrm{sand}} \frac{\partial q}{\partial x}, \tag{5}$$

where $\rho_\mathrm{sand} = 0.62 \rho_\mathrm{grain}$ is the mean density of the immobile dune sand (Sauermann et al. 2001), while ρ_grain is the grain density. If sand deposition leads to slopes that locally exceed the angle of repose $\theta_\mathrm{r} \approx 34^\circ$ of the sand, the unstable surface relaxes through avalanches in the direction of the steepest descent. Avalanches are assumed to be instantaneous since their time scale is negligible in comparison with the time scale of the dunes.

For a dune with slip face, flow separation occurs at the brink, which represents a discontinuity of the surface. The flow is divided into two parts by streamlines connecting the brink with the ground. These streamlines define the separation bubble, inside which eddies occur and the flow is re-circulating (Kroy et al. 2002). In the model, the dune is divided into several slices parallel to wind direction, and for each slice, one separation streamline is defined at the lee side of the dune. Each streamline is fitted by a third order polynomial connecting the brink with the ground, at the reattachment point. The distance between the brink and the reattachment point, and thus the length of the separation bubble is determined by the constraint of a maximum slope of 14° for the streamlines (Kroy et al. 2002). Inside the separation bubble, the wind shear stress and sand flux are set to zero.

Simulation steps may be summarized as follows: (i) the shear stress over the surface is calculated using the algorithm of Weng et al. (1991); (ii) from the shear stress, the sand flux is calculated with eq. (2); (iii) the change in the surface height is computed from mass conservation (eq. (5)) using the calculated sand flux; and (iv) if the inclination of the surface gets larger than θ_r, avalanches occur and a slip face is developed. Steps (i) – (iv) are iteratively computed until the steady state is reached.

3 Barchan dunes and barchan fields

In spite of its apparent complexity, the procedure presented above is so far the simplest method calculate the evolution of sand dunes. In particular for barchan dunes the dune model has been extensively tested and its results have been found to be quantitatively in good agreement with field measurements (Sauermann et al. 2003). Moreover, the model has been applied to calculate interaction of barchan dunes in a field, and revealed that dunes may interact in different ways, depending on their sizes. Since smaller dunes have higher velocities, they may easily "collide" with larger, slower larger ones during their downwind motion in a field. Our simulations show that very small dunes in this case may be "swallowed up" by larger dunes downwind. But if the size difference between the interacting dunes is not too large, then the smaller dune upwind gains sand from the larger one, which then becomes smaller and may wander away (fig. 1). Effectively, it is like if the smaller dune were crossing over the larger one (Schwämmle and Herrmann 2003), as proposed before by Besler (1997). A systematic study of dune interaction has been presented in Durán et al. (2005).

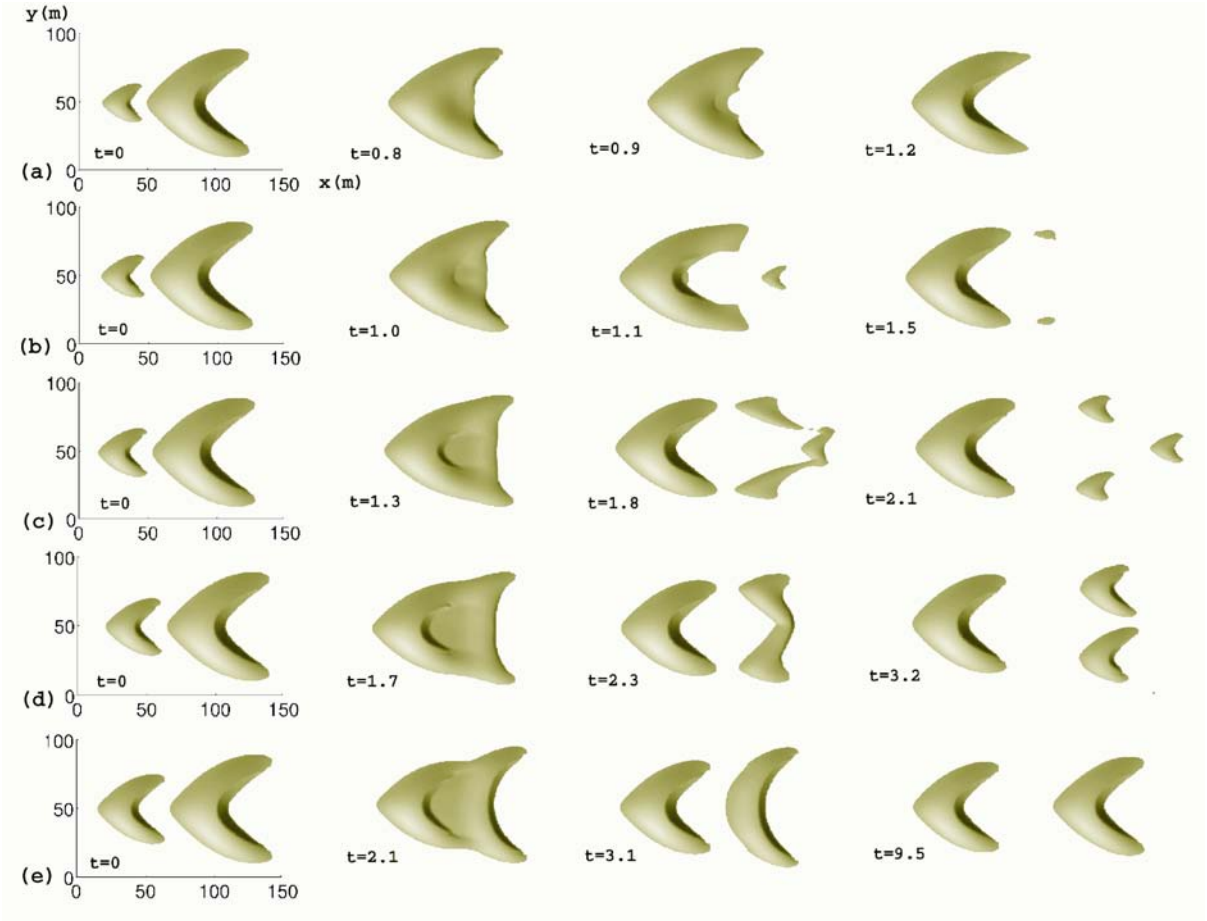

Figure 1: Four simulation snapshots of barchan dune interaction. Cases (a) — (e) correspond to different initial heights for the upwind, smaller barchan (Durán et al. 2005).

4 Sand mobility competing with vegetation

Dunes wandering onto the continent often compete with vegetation, which grows close to the sea where it finds favorable, humid conditions. We all know that plants fix the sand on the ground, but we also expect that the efficiency to stop sand transport should depend for instance on vegetation amount. We investigated with our dune model what happens with a barchan dune when it encounters a vegetated area. A recent investigation of aerial photographs covering a time span of 50 years (Tsoar and Blumberg 2002) found that barchans can invert their shape to form parabolic dunes and vice versa when the amount of vegetation changes. Parabolic dunes are U-shaped dunes the arms of which point toward the direction of the prevailing wind. We propose a model for vegetation growth taking into account sand erosion and deposition and use the saltation model (Sauermann et al. 2001) for simulating the sand transport which determines the evolution of the dunes.

Figure 2: Evolution of an initial barchan dune to a fixed parabolic shape and vice versa. Top: Transformation of barchan into parabolic dune (from the left to the right) with a characteristic time $t_g = 7$ days. Bottom: After vegetation is removed, the opposite process occurs (from the left to the right) and a barchan shape is achieved.

The continuous model for the rate of vegetation growth, follows the idea of Nishimori and Tanaka (2001). Vegetation is characterized by its local height h_v. We suppose that vegetation can grow until it reaches a maximum height H_v, and that the growth process has a characteristic time t_g, which may be enhanced or inhibited depending on the climatic conditions.

Moreover, the vegetation growth rate should be a function of the time rate of sand surface change ($\partial h/\partial t$). After any temporal change of the sand surface h, vegetation needs time to adapt to the new conditions. We introduce this phenomenological effect as a delay in the vegetation growth. In this way, the following equation holds:

$$\frac{dh_v}{dt} = \frac{H_v - h_v}{t_g} - \left|\frac{\partial h}{\partial t}\right|. \tag{6}$$

If the second term on the right-hand side of eq. (6) is larger than the first one, i.e. if the erosion rate is sufficiently high, then dh_v/dt becomes negative, which means that vegetation dies since its roots become exposed (Tsoar and Blumberg 2002).

The shear stress partitioning is the main dynamical effect of the vegetation on the flow field and, hence, on the sand transport. The vegetation acts as roughness that absorbs part of the momentum transfered to the soil by the wind. Thus, the total surface shear

stress is divided into two components, one acting on the vegetation and the other on the sand grains. The fraction of the total shear stress acting on the sand grains can be described by the expression (Buckley 1987)

$$\tau_{\mathrm{s}} = \tau \left(1 - \frac{\rho_{\mathrm{v}}}{\rho_{\mathrm{c}}}\right)^2, \tag{7}$$

where τ is the total surface shear stress, τ_{s} is the shear stress acting on the non-vegetated ground, ρ_{v} is the vegetation density, defined as $(h_{\mathrm{v}}/H_{\mathrm{v}})^2$, and ρ_{c} is a critical vegetation density that depends mainly on the geometric properties of the vegetation (Pye and Tsoar 1991).

Equation (7) represents a reduction of the shear stress acting on the sand grains, which also yields a reduction of the sand flux. Both equations (6) and (7) contain the interaction between the vegetation and the sand surface. One implication of eq. (6) is that at those places where sand erosion or deposition is small enough vegetation grows. Afterwards, the consequent decrease of the shear stress (eq. (7)), and also of the sand flux, yields sand deposition, which in turn slows down the growth of vegetation.

We performed simulations placing a 4.2 m high barchan dune on a rock bed and then allowing the vegetation to grow. A zero influx and a 0.5 m/s upwind shear velocity are set. We also fixed $\rho_{\mathrm{c}} = 0.5$, a typical value for spreading herbaceous dune plants (Pye and Tsoar 1991) and $H_{\mathrm{v}} = 1.0$ m. The dune model parameters are as in Sauermann et al. (2001).

The upper part of Figure 2 shows snapshots of the evolution of a barchan dune under the influence of vegetation with a characteristic growth time of 7 days. Calculations were performed with open boundaries and a zero influx, which means vegetation is high enough to inhibit sand transport on the flat ground. The bottom of figure 2 shows the inverse process.

We have reproduced the observed effect of the transition between barchans and parabolic dunes. After a parabolic dune is formed, it is completely covered by vegetation and rendered inactive. We studied the influence of the vegetation characteristic growth time t_{g}, which contains the information of the growth rate and which, hence, controls the strength of the interaction between the dune and the vegetation. We found that the final shape of the parabolic dune evolving from a barchan depends strongly on the growth rate of the vegetation. Slow-growing plants only slow down the arms of the barchan and do not transform it completely into a parabolic dune. The faster the plants grow, the faster the transformation is completed and the shorter are the arms of the resulting parabolic dune.

A quantitative comparison of the results from our vegetation model with data on parabolic dunes measured our field trip to a parabolic dune field in Northeastern Brazil gave excellent results.

5 Mars dunes

There are also dunes on the Planet Mars. Sand dunes have been found on Mars for the first time in Mariner 9 images of the Proctor Crater, within the southern highlands of Mars. Since then, other Missions sent to Mars provided us with thousands of images

which revealed a rich diversity of dune shapes including barchans, transverse dunes, and also linear and star dunes. With the high resolution images available of Mars, e.g. those from the Mars Global Surveyor (MGS) Mars Orbiter Camera (MOC), the study of the Martian surface has become an essentially geologic issue.

Barchan dunes are certainly the simplest and best understood type of dune. Therefore, we started our exploration of Mars dunes with the investigation of a field of barchan dunes located in the Arkhangelsky Crater on Mars (41.2° S, 25.0° W), one image of which is shown in fig. 3. Our goal is to use the dune model to reproduce the dune shape observed in fig. 3 using parameters for Mars. We are interested in answering the following question: Has it been possible that these dunes formed under the present atmospheric conditions of Mars? Using the values of martian atmospheric density and gravity, our first aim is to find the conditions of wind and sand flux which define the dune shape observed in fig. 3.

Many of the model parameters we need to calculate dunes on Mars are known from the literature. Some of these parameters have been mentioned above — the gravity g and atmospheric density ρ_{fluid}, pressure P and temperature T. Recent Mars Missions obtained important data on sand and wind conditions on Mars, as detailed below, which we use in our calculations.

We performed simulations with open boundaries and a small influx q_{in} at the inlet, with values typically less than 30% of the saturated flux q_{s}. Such low values for $q_{\text{in}}/q_{\text{s}}$ are characteristic of the interdune in terrestrial dune fields developing on bedrock. A small value of $q_{\text{in}}/q_{\text{s}}$ is also reasonable for the Arkhangelsky dunes since sediment access in craters is commonly restricted. In this way, we need to find for which values of γ and the shear velocity u_* — which is set of course larger than $u_{*\text{t}} = 2.0$ m/s — the model reproduces the dune shape in the Arkhangelsky Crater. The initial surface is a gaussian sand hill with dimensions of the order of the dune sizes observed .

We find that the elongated shape of the Arkhangelsky dunes is in general obtained for a shear velocity close to the threshold. As u_* increases, for a constant value of γ, the dune shape deviates from the Arkhangelsky dunes. One conclusion we get from our calculations, thus, is that the shear velocity in the Arkhangelsky Crater must be close to the threshold friction speed, and probably around 3.0 m/s. Figure 3 shows one dune calculated with this u_* value together with a MOC image of one Arkhangelsky dune. Most interestingly, however, we discovered that γ must be ten times larger on Mars than on Earth to produce the observed dunes. Concluding, we found that martian dunes may have been formed by winds close to the threshold, under the present atmospheric conditions of Mars, and our calculations reveal that larger splashes on Mars are relevant to explain the size of martian dunes. Finally, simulating our model to study north polar dunes on Mars support the hypothesis that the unusual dune shapes observed in the Chasma Boreale region are a result of induration.

6 Conclusions

We have presented simulations of the dune model originally introduced by Sauermann et al. (2001) and later improved by Schwämmle and Herrmann (2005) and extended them to study dunes with vegetation, and we tested the model to calculate dunes on Mars.

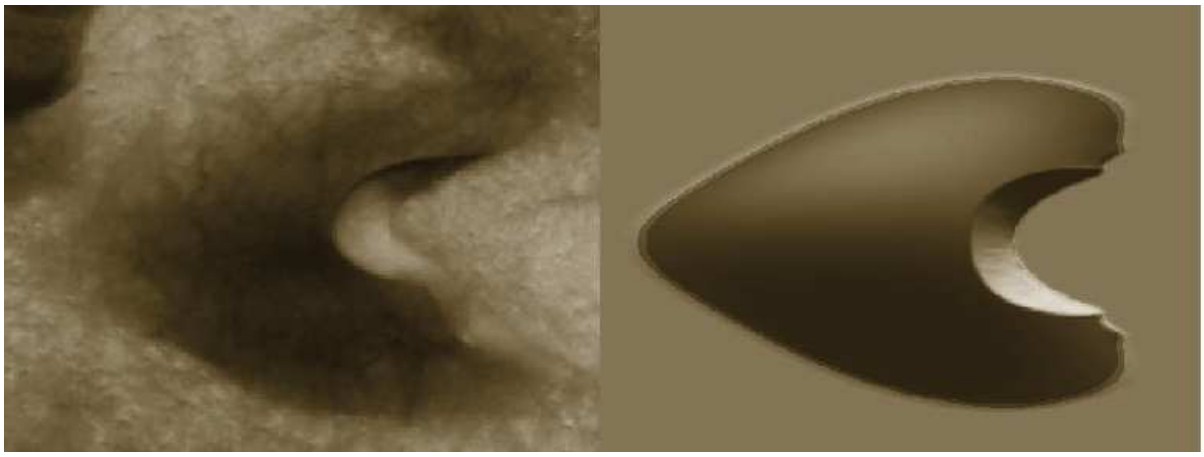

Figure 3: MOC image (left) and calculation (right) of barchan dune of width 650 m in the Arkhangelsky Crater on Mars. Calculation was performed with $u_* = 3.0$ m/s and $\gamma = 10\,\gamma_{\mathrm{Earth}}$.

We could simulate the transformation of barchans into parabolic dunes, as observed by Tsoar and Blumberg (2002). Furthermore, we have applied our dune model to calculate the shape of the barchan dunes on Mars.

Our results are of extreme relevance to understand the formation and evolution of sand dunes in coastal areas, where vegetation very often appears to compete against saltation transport and dune mobility. Furthermore, from calculations of Mars barchan dunes, we gained important insight about the role of the saturation length for the selection of dune size and shape, which is crucial to explain the natural appearence of dunes on Mars. A complete modelling of the formation of dune fields using the methods presented here will be subject of future research.

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5

CSE Research Projects

Title: Dynamics of premixed hydrogen/air flames in microchannels

Researchers: Gianmarco Pizza[1,2], Christos E. Frouzakis[1], Ioannis Mantzaras[2], Ananias G.Tomboulides[3], Konstantinos Boulouchos[1]

Institute/ Group: [1]Aerothermochemistry and Combustion Systems Laboratory
[2]Paul Scherrer Institute, Villigen PSI
[3]University of Western Macedonia, Kozani, Greece

Combustion at the meso- and micro-scale has attracted a lot of interest in recent attempts to harness the high specific energy of fuels in miniaturized devices for portable power generation. Progress in the fundamental knowledge of micro- and meso-scale combustion and in the understanding of reactor thermal management is essential for the further development of such systems.

The stabilization and dynamics of lean (equivalence ratio, ϕ= 0.5) premixed hydrogen/air atmospheric pressure flames in planar microchannels of prescribed wall temperature were investigated with respect to the inflow velocity and channel height (0.3 to 1.0 mm) using direct numerical simulation with detailed chemistry and transport. Rich dynamics starting from periodic ignition and extinction of the flame and further transitioning to symmetric V shaped flames, asymmetric flames, oscillating and pulsating flames and finally again to asymmetric flames are observed as the inlet velocity is increased. The richest behavior is observed for the 1.0 mm height channel. For narrower channels, some of the dynamics are suppressed. The asymmetric flames, in particular, vanish for channel heights roughly less than twice the laminar flame thickness. Stability maps delineating the regions of the different flame types in the inlet velocity/channel height parameter space are constructed.

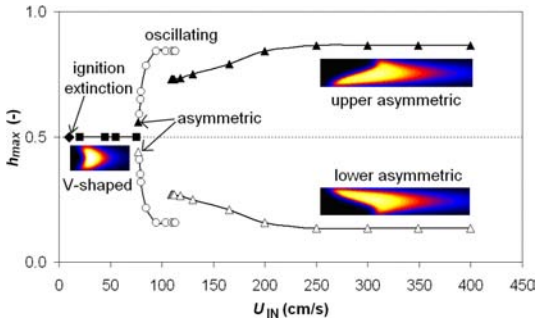


Figure 1: Flame stability diagram for the h=1.0 mm height channel. The images show the OH radical mass fraction.

References: In press in *Combustion and Flame*.

Title: Stationary and rotating cells in hydrogen/air jet diffusion flames

Researchers: Luzi A. Valär[1], Christos E. Frouzakis[1], Ananias G.Tomboulides[2], Konstantinos Boulouchos[1]

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

Description:

Direct numerical simulation with detailed chemistry and transport are used to study instabilities of CO_2-diluted-hydrogen/air jet diffusion flames close to extinction. Experiments have shown a variety of different cellular patterns (rotating single-, 2-, and 3-cell states as well as stationary 4- and higher-number cellular flames). Several states were found to co-exist, and the particular state realized was determined by the initial conditions.

A spectral-element based parallel code that solves the conservation equations of mass, momentum, species and energy in the low Mach number limit was employed for the 3-D simulations. In agreement with the experiments, the simulations captured stationary (5, 7 and 8 cells) and rotating (3 cells) flames by varying the fuel-jet velocity and composition and provide the details of the fast transitions between the different states.

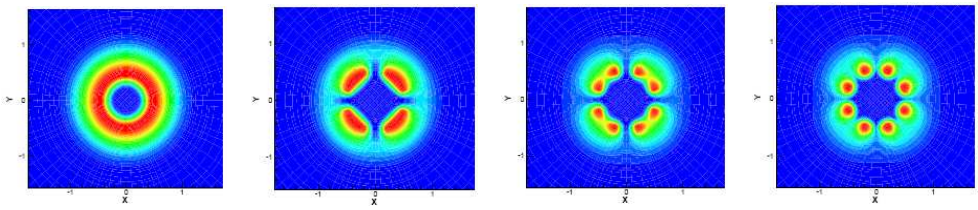


Figure 2: Transition from a strongly burning flame to an 8-cell cellular flame (temperature isocontours in the range $300K \leq T \leq 1500K$ on a plane half a nozzle diameter above the jet exit).

References: Manuscript in preparation.

Title: Hydrodynamics beyond Navier-Stokes: Exact Solution to the Lattice Boltzmann Hierarchy

Researchers: S. Ansumali[1], I. V. Karlin[2], S. Arcidiacono[3], A. Abbas[1], N. I. Prasianakis[2]

Institute/ Group: [1] Nanyang Technological University, Singapore
[2] Aerothermochemistry and Combustion Systems Laboratory, ETH
[3] Paul Scherrer Institute, Villigen

Description: The exact solution to the hierarchy of nonlinear lattice Boltzmann (LB) kinetic equations in the stationary planar Couette flow is found at nonvanishing Knudsen numbers. A new method of solving LB kinetic equations which combines the method of moments with boundary conditions for populations enables us to derive closed-form solutions for all higher-order moments. A convergence of results suggests that the LB hierarchy with larger velocity sets is the novel way to approximate kinetic theory.

References: Phys. Rev. Letters **98**, 124502 (2007).

Title: Quasi-equilibrium lattice Boltzmann method

Researchers: S. Ansumali[1], S. Arcidiacono[2], S. S. Chikatamarla[3] N. I. Prasianakis[3], A. N. Gorban[4],I. V. Karlin[3],

Institute/ Group:
[1] Nanyang Technological University, Singapore
[2] Paul Scherrer Institute, Villigen
[3] Aerothermochemistry and Combustion Systems Laboratory, ETH
[4] University of Leicester, UK

Description: A general lattice Boltzmann method for simulation of fluids with tailored transport coefficients is presented. It is based on the recently introduced quasi-equilibrium kinetic models, and a general lattice Boltzmann implementation is developed. Lattice Boltzmann models for isothermal binary mixtures with a given Schmidt number, and for a weakly compressible flow with a given Prandtl number are derived and validated.

References: Eur. Phys. J. B **56**, 135139 (2007).

Title: From hyperbolic regularization to exact hydrodynamics for linearized Grads equations

Researchers: M. Colangeli[1], I. V. Karlin[2], M. Kröger[1]

Institute/ Group: [1] Polymer Physics, ETH
[2]Aerothermochemistry and Combustion Systems Laboratory, ETH

Description:

Inspired by a recent hyperbolic regularization of Burnetts hydrodynamic equations [A. Bobylev, J. Stat. Phys. 124, 371 (2006)], we introduce a method to derive hyperbolic equations of linear hydrodynamics to any desired accuracy in Knudsen number. The approach is based on a dynamic invariance principle which derives exact constitutive relations for the stress tensor and heat flux, and a transformation which renders the exact equations of hydrodynamics hyperbolic and stable. The method is described in detail for a simple kinetic modela 13 moment Grad system.

References: Phys. Rev. E **75**, 051204 (2007).

Title: Hyperbolicity of exact hydrodynamics for three-dimensional linearized Grads equations

Researchers: M. Colangeli[1], I. V. Karlin[2], M. Kröger[1]

Institute/ Group: [1] Polymer Physics, ETH
[2]Aerothermochemistry and Combustion Systems Laboratory, ETH

Description:

We extend to the three-dimensional situation a recent proof of hyperbolicity of the exact (to all orders in Knudsen number) linear hydrodynamics obtained from Grads moment system [M. Colangeli, I. Karlin, M. Krger, Phys. Rev. E 75, 051204 (2007)]. Proof of an H theorem is also presented.

References: Phys. Rev. E **76**, 022201 (2007).

Title: Lattice Boltzmann model for the simulation of multicomponent mixtures

Researchers: S. Arcidiacono[1], I. V. Karlin[2], J. Mantzaras[1], C. E. Frouzakis[2]

Institute/ Group: [3] Paul Scherrer Institute, Villigen
[2] Aerothermochemistry and Combustion Systems Laboratory, ETH

Description:

A lattice Boltzmann (LB) model for the simulation of realistic multicomponent mixtures is constructed. In the hydrodynamic limit, the LB model recovers the equations of continuum mechanics within the mixtureaveraged diffusion approximation. The present implementation can be used to simulate realistic mixtures with arbitrary Schmidt numbers and molecular masses of the species. The model is applied to the mixing of two opposed jets of different concentrations and the results are in excellent agreement with a continuum model. An application to the simulation of mixtures in microflows is also presented. Results compare well with existing kinetic theory predictions of the slip coefficient for mixtures in a Couette flow.

References: Phys. Rev. E **76**, 046703 (2007).

Title: Optimization strategies for the entropic lattice Boltzmann method

Researchers: F. Tosi[1], S. Ubertini[2], S. Succi[3], I. V. Karlin[4]

Institute/ Group:
[1] Universita degli studi di Firenze, Italy
[2] Universita degli studi di Roma Tor Vergata, Italy
[3] Istituto Applicazioni del Calcolo CNR, Roma, Italy
[4] Aerothermochemistry and Combustion Systems Laboratory, ETH

Description:

The entropic formulation of the lattice Boltzmann method (LBM) features enhanced numerical stability due to its compliance with the Boltzmann H-theorem. This stability comes at the price of some computational overhead, associated with the need of adjusting the local relaxation time of the standard LBM in such a way as to secure compliance with the H-theorem. In this paper, we discuss a number of possible optimization strategies to reduce the computational overhead of entropic LBMs.

References: Journal of Scientific Computing **30(3)**, 369-287 (2007).

Title: Lattice Boltzmann method for thermal flow simulation on standard lattices

Researchers: N. I. Prasianakis[1], I. V. Karlin[1]

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

Description:

The recently introduced consistent lattice Boltzmann model with energy conservation [S. Ansumali and I. V. Karlin, Phys. Rev. Lett. 95, 260605 (2005)] is extended to the simulation of thermal flows on standard lattices. The two-dimensional thermal model on the standard square lattice with nine velocities is developed and validated in the thermal Couette and Rayleigh-Benard natural convection problems.

References: Phys. Rev. E **76**, 016702 (2007).

Title: Renormalization of the lattice Boltzmann hierarchy

Researchers: I. V. Karlin[1], S. Ansumali[2]

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory, ETH
[2] Nanyang Technological University, Singapore

Description:

Is it possible to solve Boltzmann-type kinetic equations using only a small number of particle velocities? We introduce a technique of solving kinetic equations with a (arbitrarily) large number of particle velocities using only a lattice Boltzmann method on standard, low-symmetry lattices. The renormalized kinetic equation is validated with an exact solution of the planar Couette flow at moderate Knudsen numbers.

References: Phys. Rev. E **76**, 025701 (Rapid Communication) (2007).

Title: Comparison of invariant manifolds for model reduction in chemical kinetics

Researchers: E. Chiavazzo[1], A. N. Gorban[2], I. V. Karlin[1]

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory, ETH
[2] University of Leicester, UK

Description:

A modern approach to model reduction in chemical kinetics is often based on the notion of slow invariant manifold. The goal of this paper is to give a comparison of various methods of construction of slow invariant manifolds using a simple Michaelis-Menten catalytic reaction. We explore a recently introduced Method of Invariant Grids (MIG) for iteratively solving the invariance equation. Various initial approximations for the grid are considered such as Quasi Equilibrium Manifold, Spectral Quasi Equilibrium Manifold, Intrinsic Low Dimensional Manifold and Symmetric Entropic Intrinsic Low Dimensional Manifold. Slow invariant manifold was also computed using the Computational Singular Perturbation (CSP) method. A comparison between MIG and CSP is also reported.

References: Commun. in Comput. Phys. **2(5)**, 964-992 (2007).

Title: Elements of the Lattice Boltzmann Method II: Kinetics and Hydrodynamics in One Dimension

Researchers: I. V. Karlin[1], S. S. Chikatamarla[1], S. Ansumali[2]

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory, ETH
[2] Nanyang Technological University, Singapore

Description:

Concepts of the lattice Boltzmann method are discussed in detail for the one-dimensional kinetic model. Various techniques of constructing lattice Boltzmann models are discussed, and novel collision integrals are derived. Geometry of the kinetic space and the role of the thermodynamic projector is elucidated.

References: Commun. in Comput. Phys. **2(2)**, 196-238 (2007).

Title: Kinetically reduced local Navier-Stokes equations for simulation of incompressible viscous flows

Researchers: S. Borok[1], S. Ansumali[1], I. V. Karlin[2]

Institute/ Group: [1] Nanyang Technological University, Singapore
[2] Aerothermochemistry and Combustion Systems Laboratory, ETH

Description:

Recently, a new approach to study incompressible fluid flow was suggested in [S. Ansumali, I. Karlin, H.C. Öttinger, PRL 94, 080602 (2005)] - the kinetically reduced local Navier-Stokes (KRLNS) equations. We consider a simplified two-dimensional KRLNS system and compare it with Chorin's artificial compressibility method. A comparison of the two methods for steady state computation of the flow in a lid-driven cavity at various Reynolds number shows that the results from both methods are in good agreement with each other. However, in the the transient flow, it is demonstrated that the KRLNS equations correctly describe the time evolution of the velocity and of the pressure, unlike the artificial compressibility method.

References: Phys. Rev. E, accepted for publication (2007).

Title: Computational Solid State Electronics

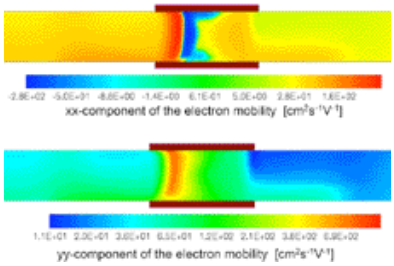
Researchers: Wolfgang Fichtner
Andreas Schenk
Simon Brugger
Stefan Röllin
Beat Sahli
Mathieu Luisier
Dölf Aemmer

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

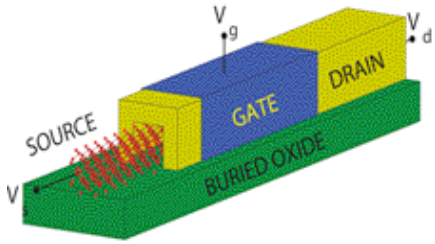
Description:

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 20 nm with structures down to 1 nm) effects at the atomistic or quantum-mechanical level are becoming dominant.

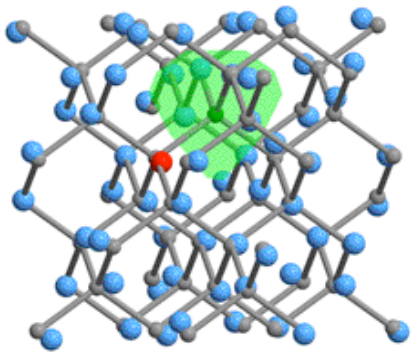
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulation tools for molecular dynamics studies in material diffusion, novel devices such as nanowire transistors, and quantum devices. For all of our projects, the main emphasis lies in the exploration how accurate physical models can be combined with advanced numerical algorithms including OpenMP and MPI parallelization. These simulations were carried out on high-end compute-servers of our laboratory. We also use the IBM Cray XT3 and the IBM P575 systems at CSCS Manno in a *Large User Project*. The following pictures illustrate some of our activities:



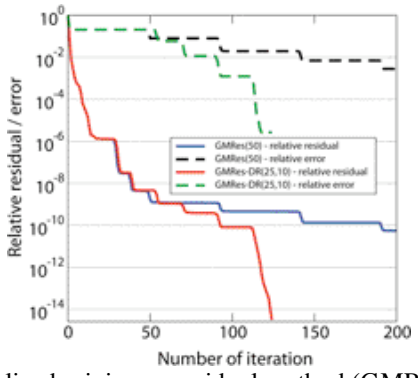
One-particle Monte-Carlo Simulation of CMOS devices of 2015 (year of production).



Full band simulations of silicon nanowire transistors: schematic view of a triple-gate device on a buried oxide.



Ab initio simulation of the diffusion mechanisms of As and Sb in silicon.



Generalized minimum residual method (GMRes) with deflating restarting in device simulation.

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

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

Institute/ Group: [⋆]Institute of Computational Science, ETH Zürich
[†]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 (μFE) 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 μFE 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 μFE 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.

References:

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. (2007), in press. doi:10.1002/nme.2101.

P. Arbenz and C. Flaig: *On Smoothing Surfaces in Voxel Based Finite Element Analysis of Trabecular Bone*. Proceedings of LSSC'07: Large Scale Scientific Computing. Sozopol, Bulgaria, June 4-9, 2007. To appear in Lecture Notes in Computer Science 4818. Springer 2007, Berlin.

A. Cohen, D. Dempster, R. Müller, E. Guo, X. H. Zhang, A. J. Wirth, G. H. van Lenthe, X. D. McMahon, H. Zhou, M. R. Rubin, J. P Bilezikian, R. R. Recker, E. Shane. *High resolution peripheral quantitative CT (HRpQCT) of the radius reflects iliac crest biopsy measures of microstructure and mechanical competence*. Annual Meeting of the American Society for Bone and Mineral Research; Honolulu, USA; 2007.

A. Wirth, T. L. Mueller, U. Mennel, M. Sala, P. Arbenz, G. H. van Lenthe, R. Müller: *Stability Of Bone-Implant Constructs: A Computational Mechanics Approach Based On High Resolution Computed Tomography*. 15th Annual Symposium on Computational Methods in Biomechanics Pre-ORS, UCSD, San Diego, CA, February 2007.

A. Wirth, T. L. Mueller, G. H. van Lenthe, J. Goldhahn, J. Schense, J. Watson, V. Jamieson, P. Messmer, O. Trentz, D. Uebelhart, D. Weishaupt, M. Egermann, and R. Müller. *In vivo assessment of mechanical stability during fracture healing in humans*. 53rd Annual Meeting of the Orthopaedic Research Society; San Diego, USA; p. 1273, 2007.

A. Wirth, T. L. Mueller, G. H. van Lenthe, J. Goldhahn, J. Schense, J. Watson, V. Jamieson, P. Messmer, O. Trentz, D. Uebelhart, D. Weishaupt, M. Egermann, and R. Müller. *Computational assessment of mechanical stability during fracture healing in humans based on high-resolution medical images*. European Society of Biomechanics Workshop 2007; Dublin, Ireland; 2007.

A. J. Wirth, T. L. Mueller, R. Müller, P. Arbenz, G. H. van Lenthe. *Fast and automated analyses of bone-implant function from medical images using high-performance computing*. 2007 Annual Meeting, Swiss Society for Biomedical Engineering; Neuchâtel, Switzerland, 2007.

Title: Visualization Tools for Vorticity Transport Analysis in Incompressible Flow

Researchers: Filip Sadlo
Ronald Peikert

Institute/ Group: Institute of Computational Science
Computer Graphics Laboratory

Description:

Vortices are undesirable in many applications while indispensable in others. It is therefore of common interest to understand their mechanisms of creation. This paper aims at analyzing the transport of vorticity inside incompressible flow. The analysis is based on the vorticity equation and is performed along pathlines which are typically started in upstream direction from vortex regions. Different methods for the quantitative and explorative analysis of vorticity transport are presented and applied to CFD simulations of water turbines. Simulation quality is accounted for by including the errors of meshing and convergence into analysis and visualization. The obtained results are discussed and interpretations with respect to engineering questions are given.

References:

IEEE Transactions on Visualization and Computer Graphics, Vol. 12, No. 5, pp. 949-956, 2006.

Title: Efficient Visualization of Lagrangian Coherent Structures by Filtered AMR Ridge Extraction

Researchers: Filip Sadlo
Ronald Peikert

Institute/ Group: Institute of Computational Science
Computer Graphics Laboratory

Description:

This paper presents a method for filtered ridge extraction based on adaptive mesh refinement. It is applicable in situations where the underlying scalar field can be refined during ridge extraction. This requirement is met by the concept of Lagrangian coherent structures which is based on trajectories started at arbitrary sampling grids that are independent of the underlying vector field. The Lagrangian coherent structures are extracted as ridges in finite Lyapunov exponent fields computed from these grids of trajectories. The method is applied to several variants of finite Lyapunov exponents, one of which is newly introduced. High computation time due to the high number of required trajectories is a main drawback when computing Lyapunov exponents of 3-dimensional vector fields. The presented method allows a substantial speed-up by avoiding the seeding of trajectories in regions where no ridges are present or do not satisfy the prescribed filter criteria such as a minimum finite Lyapunov exponent.

References:

To appear in: IEEE Transactions on Visualization and Computer Graphics, Vol. 13, No. 5, 2007.

Title: General characteristic-based algorithm for off-lattice Boltzmann simulations

Researchers: André Bardow, Ilya V. Karlin, Andrei A. Gusev

Institute/ Group: Institute of Polymers and Institute of Energy Technology

Description:

The Lattice Boltzmann method offers an appealing potential for simulation of fluid flows. However, the intrinsic coupling of momentum and space discretization restricts the applicability of the traditional Lattice Boltzmann method to uniform, regular lattices which is often disadvantageous in practice. Available off-lattice Boltzmann algorithms have stability problems which are to be handled at the expense of additional computational cost. Here, we propose and validate a general characteristic-based algorithm for off-lattice Boltzmann simulations that preserves all appealing properties of the standard Lattice Boltzmann method while extending the method to unstructured grids. Both, finite-element and finite-difference implementations of the algorithms are exemplified.

References: EUROPHYSICS LETTERS **75** (2006) 434-440

Title: Micromechanical mechanism of reinforcement and losses in filled rubbers

Researchers: Andrei A. Gusev

Institute/ Group: Institute of Polymers

Description:

We study a model system composed of a rubber matrix reinforced by a percolating diamond network of non-overlapping, almost touching identical spheres joined by coating layers of immobilized glassy polymer. We have developed a novel periodic mixed formulation solver for multiphase materials with nearly incompressible phases. We use serendipity family cubic shape brick elements with an incomplete cubic interpolation for the displacements and an element-based discontinuous interpolation for the pressure. Our numerical results indicate that a simple micromechanical mechanism can explain the observed relationship between the reinforcement and the energy dissipation in filled rubbers. We have observed a remarkable localization of both storage and dissipation energy, found to occur primarily in the coating layers of immobilized polymer. These findings put a new emphasis on the role of the interfacial phenomena and suggest that the physical (van der Waals) forces responsible for the filler network formation may not necessarily directly affect the reinforcement and the losses but rather indirectly, by way of adhesive joints formed from the coating layers of immobilized polymer.

References: MACROMOLECULES **39** (2006) 5960-5962

Title: On the glassy state of multiphase and pure polymer materials

Researchers: Stephan A. Baeurle
Atsushi Hotta
Andrei A. Gusev

Institute/ Group: Institute of Polymers & Materials Research Laboratory, UCSB, U.S.A.

Description:

In this work we formulate a new glass theory and investigate its suitability for describing the mechanical response of thermoplastic elastomers composed of styrenic-block copolymers. These materials are composed of glassy domains of polystyrene, which physically link soft rubbery chain segments made of either polybutadiene or polyisoprene. We demonstrate that the crossover in the shift factors, observed experimentally to change from Williams–Landel–Ferry to Arrhenius behavior passing through a characteristic crossover temperature T^* from below, coincides with the crossover from power-law to stretched-exponential behavior of the stress relaxation found in recent tensile experiments. Moreover, we show that the characteristic crossover temperature T^* is identical with the underlying true equilibrium second-order phase transition temperature T_2 of the polystyrene crosslinks, predicted by the thermodynamic theory of Gibbs and Di Marzio for pure glassy polystyrene in the infinite-time limit. By combining the recently introduced theory of Di Marzio and Yang with the significant-structure theory of Eyring and Ree, we develop a new glass theory, which is capable of explaining the mechanical response of multiphase as well as pure glassy materials. Moreover, we show a clear evidence for the existence of T_2 postulated in 1950s for pure glasses and hotly debated since then.

References: POLYMER **47** (2006) 6243-6253

Title: Physically admissible rules of evolution for discrete representations of continuous media

Researchers: Andrei A. Gusev

Institute/ Group: Institute of Polymers

Description:

We propose a weighted residual procedure for defining physically admissible evolution rules for discrete models of generally anisotropic continuous media. The procedure is used to define 2D isotropic square Lattice Spring Models (LSM) of the Laplace, Maxwell, and Cauchy-Poisson equations. The latter LSM is employed to simulate the power law acoustic emission accompanying the microfracturing phenomenon in heterogeneous solids. We demonstrate the necessity and the advantages of physically admissible evolution rules, in comparison with commonly employed, ad hoc defined and empirically adjusted evolution rules.

References: JOURNAL OF NON-CRYSTALLINE SOLIDS **352** (2006) 4880-4883

Title: A new multiscale modeling approach for the prediction of mechanical properties of polymer-based nanomaterials

Researchers: Stephan A. Baeurle
Takao Usami
Andrei A. Gusev

Institute/ Group: Institute of Building Materials, Institute of Polymers, and Materials Research Laboratory, UCSB, U.S.A.

Description:

A detailed knowledge about the physics and chemistry of multiphase materials on different length and time scales is essential to tailor their macroscopic physical and mechanical properties. A better understanding of these issues is also highly relevant to optimize their processing and, thus, their elucidation can be decisive for their final industrial application. In this paper, we develop a new multiscale modeling method, which combines the self-consistent field theory approach with the kinetic Monte Carlo method, to simulate the structural-dynamical evolution taking place in thermoplastic elastomers, where hard glassy and soft rubbery phases alternate. Since the early seventies, it is well established that the properties of the core nanophases in these multiphase materials considerably affect their overall mechanical properties. However, recent experimental studies have clearly demonstrated that, besides the efficient handling of the core nanophases, the appropriate treatment of their interfacial region is another major challenge one has to face on the way of target-oriented development of these materials. In this work, we set a particular focus on the complex structural-dynamical processes occurring at the interphases, and study their influence on the local structural and mechanical properties. To reach our objectives, we apply the new methodology on a thermoplastic elastomer composed of ABA triblock copolymers, subjected to a sizeable external perturbation, and determine its time-averaged internal stress and composition profile. We deduce from this investigation that, to obtain the correct local mechanical properties of these multiphase materials, their structure and dynamics need to be taken into account on an equal footing. Finally, our investigation also provides an explanation and confirms the importance of the chain-pullout mechanism in the viscoelastic and stress relaxation behavior of these materials.

References: POLYMER **47** (2006) 8604-8617

Title: Asymptotic back strain approach for estimation of effective properties of multiphase materials

Researchers: Andrei A. Gusev

Institute/ Group: Institute of Polymers

Description:

Estimation of the effective properties of composite materials from those of the constituents and the material's morphology is a classical problem of both theoretical and technological interest, and many specific homogenization approaches have been proposed in the literature. Interesting methods have been developed for numerical estimation of the effective properties, for a survey and references see. In particular, boundary integral equation methods have been shown to yield incredibly accurate estimates for 2D composites. However, much less progress has been made with these methods for 3D composites. Finite element methods have been shown to deliver engineering accuracy predictions for the effective properties of realistic 3D random composites, on the basis of periodic multi-inclusion computer models represented by morphology adaptive unstructured meshes. However, the unstructured mesh finite element approach involves a demanding, generally system specific meshing effort, so reliable numerical estimates for many realistic problems still remain outstanding. Linear response effective properties (stiffness, dielectric constants, etc.) relate the average responses (stress, electric induction, etc.) to the average perturbations (strain, electric field, etc.). It is tempting to think that such low order moments should start converging asymptotically already when estimated based on relatively poor resolved computer models. In this work we present a specific, pixel based finite element approach that extracts effective stiffness estimates from the asymptotic stress responses of periodic cells comprised of representative morphological fragments subjected to back strain deformation fields. For illustration, we study variable resolution pixel based computer models of a 3D composite consisting of a matrix reinforced by a random dispersion of rigid none-overlapping spheres and show that the approach can indeed deliver reliable estimates for the effective stiffness of 3D random composites.

References: ADVANCED ENGINEERING MATERIALS 9 (2007) 117-120

Title: Rapid Mass Transport in Mixed Matrix Nanotube/Polymer Membranes

Researchers: Andrei A. Gusev
Olga Guseva

Institute/ Group: Institute of Polymers, MatSim GmbH, and EMPA-Dübendorf

Description:

Many potential applications have been proposed for carbon nanotubes. The possibility of using carbon nanotubes (CNT) for chemical and biological separations has also been recognized for some time. The first molecular dynamics simulations predicted that the transport of light gases inside CNTs should be orders of magnitude faster than in any other known material, in fact as fast as in gases. It was shown that the rapid transport can originate in the intrinsic smoothness of the walls of nanotubes. Following on from experiments with devices composed of multiwalled nanotubes incorporated across polymer films, a recent experimental study of gas permeation through single- and double-walled CNTs in silicon nitride matrix membranes has revealed enhanced transport rates of one to two orders of magnitude compared the Knudsen diffusion model. However, the observed selectivity was low and followed the inverse-square-root scaling of molecular mass of the Knudsen model. In these membrane devices, the nanotubes constituted the only possible path for molecular transport across the membrane. It has been suggested that using composite membranes composed of nanotubes dispersed in a polymer matrix may prove an appealing route for fabrication of fast mixed matrix membranes. In this work, we have used the finite element method to access the potential of mixed matrix nanotube/polymer membranes. We introduced a coupled-form finite element approach to estimate permeability performance of mixed matrix nanotube/polymer membranes. It appeared that the universal approximation of perfectly permeable nanotubes was appropriate for predicting the overall rates of single gas transport through CNT/polymer membranes. Based on direct finite element predictions, we developed a set of simple design equations and demonstrated that mixed matrix CNT/ polymer membranes can favorably combine the high-flux performance of nanotubes with the intrinsic selectivity of polymer matrix.

References: A manuscript in press in ADVANCED MATERIALS

Title: Rapid exponential convergence of finite element estimates of the effective properties of heterogeneous materials

Researchers: Andrei A. Gusev

Institute/ Group: Institute of Polymers

Description:

Heterogeneous materials are widely used in various applications. They are also abundant in nature, defining structural performance and thus enabling functions of living cells, bones, plants, trees, etc. On a local scale, the properties of heterogeneous materials may considerably vary from point to point. However, on larger scales their overall, effective responses can usually be described by homogeneous constitutive equations. Various theoretical homogenization approaches have been proposed in the literature. In the last decade, they have been supplemented by direct numerical predictions, with the finite element method (FEM) and the boundary equation method (BEM) being by far most frequently employed. Real materials have a 3D random microstructure. Consequently, for realistic numerical studies one should generally use random-microstructure computer models with very large volume (FEM) or surface (BEM) meshes. It is then difficult to extract reliable property estimates from such models with confidence. Therefore, a serious but commonly ignored problem is to assess the adequacy of the resulting property predictions. In our recent work, we employed uniform, pixel-based grid representations and showed that upon increasing grid resolution, numerical FEM estimates can actually enter into asymptotic convergence already at surprisingly low grid resolutions. For example, for a composite comprised of a random dispersion of identical spheres, a resolution of a few pixels per sphere was found to be already sufficient. However, for materials with more complex morphologies involving variable size and/or large aspect ratio inclusions (fibers, platelets, etc.), the uniform grid route obviously becomes less efficient. It is the unstructured mesh approach which offers an appealing route to extract reliable finite-element estimates of the effective properties of complex morphology heterogeneous materials. Here, by realizing the common mathematical structure of the governing equations we develop and validate a general-purpose error estimator for the finite element solutions for the effective properties of heterogeneous materials. We show that the error should generally decrease exponentially upon increasing order of the polynomial interpolation. We use this finding to demonstrate the practical feasibility of reliable property predictions for a majority of particulate-morphology heterogeneous materials.

References: A manuscript accepted for publication in ADVANCED ENGINEERING MATERIALS

Title: An agent model for friendship networks

Researchers: Dr. Herman M. Singer
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The evaluation of statistical properties and the modeling of social networks have become a major research topic in the field of complex networks. While many complex networks show a scale free behavior, it is found that social networks of contacts and friendships are inherently single scale. We propose a new agent based model to understand the structuring of social networks in a fixed setting such as for example enrolling at a university. The friendship formation is based on mutual interest and the frequency of encounters. The model shows distinctive single scale behavior and reproduces accurately the measurable experimental quantities like clustering coefficients, degree distributions, degree correlations and the friendship distribution. The model produces self-organized local community structures of common interest and can be described as a network of densely interconnected networks. For the friendships it is found that the mutual interest is the dominant factor and that the number of encounters plays only a minor role.

Title: Simulation of Fragmentation Processes

Researchers: Dr. Falk K. Wittel
Prof. Humberto A. Carmona

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We study the brittle fragmentation of spheres by using a three-dimensional Discrete Element Model. Large scale computer simulations are performed with a model that consist of agglomerates of many particles, interconnected by beam-truss elements. We focus on the detailed development of the fragmentation process and study several fragmentation mechanisms. The evolution of meridional cracks is studied in detail. These cracks are found to initiate in the inside of the specimen with quasi-periodic angular distribution. The fragments that are formed when these cracks penetrate the specimen surface give a broad peak in the fragment mass distribution for large fragments that can be fitted by a two-parameter Weibull distribution. This mechanism can only be observed in 3D models or experiments. The results prove to be independent of the degree of disorder in the model. Our result significantly improves the understanding of the fragmentation process for impact fracture since besides reproducing the experimental observations of fragment shapes, impact energy dependence and mass distribution, we also have full access to the failure conditions and evolution.

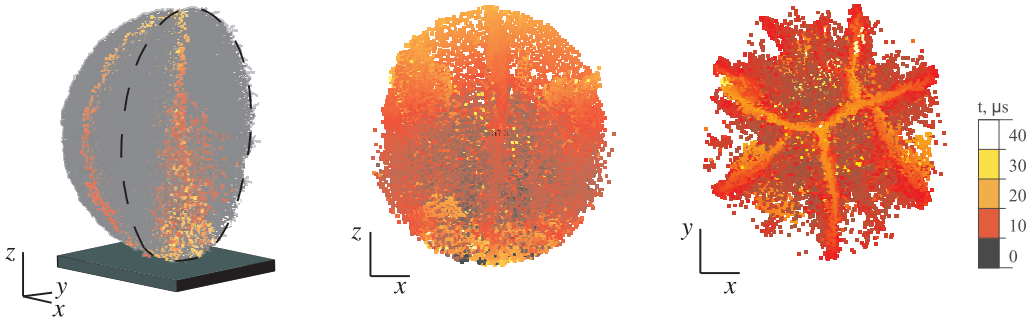


Figure 1: Visualization of the fragmentation process. Colored dots display the positions of the broken bonds according to the time of breaking.

References:

[1] H. A. Carmona, F. K. Wittel, F. Kun, and H. J. Herrmann *Fragmentation processes in impact of spheres*, submitted to Physical Review E (2007).

Title: The Nature of Quicksand

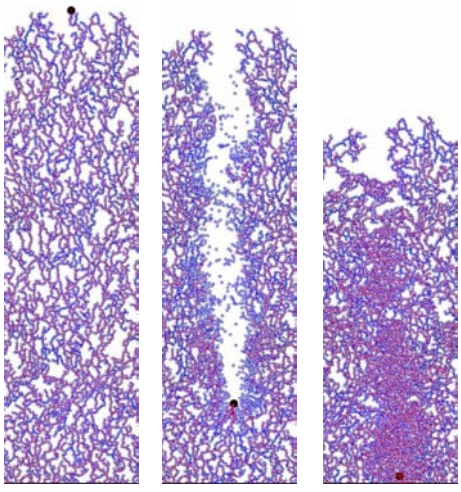
Researchers: Dr. Dirk Kadau
Prof. José S. Andrade
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The nature and danger of quicksand has been disputed since a long time. Researchers of the Computational Physics of Engineering Materials group investigated a specific type of quicksand at the shore of drying lagoons. Cyanobacteria form an impermeable crust, giving the impression of stable ground. After breaking the crust a person rapidly sinks to the bottom of the field (upper figure). Before destroying the crust the measured shear strength is essentially constant up to the bottom of the basin and then it rapidly increases. After the system collapsed the shear strength linearly increases with the depth. To undermine our point that objects lighter than water can be swallowed in the quicksand, we simulated a model in which we constructed a tenuous granular structure representing the unperturbed soil (lower figure, a)). The initial structure consists of cohesive disks put together by ballistic deposition and settled by gravity using Contact Dynamics. Pushing in an object leads to breaking of cohesive bonds. The soil collapses irreversibly and traps the intruder inside a dense soil (lower figure, c)). Unlike quicksand fluidized by an increase of pore pressure, in this specific soil no lifting force or buoyancy can push the object to the surface again. Instead, a high force for pulling out is needed. In particular, we investigated how deep the object can be pushed in and how well the intruder is captured by the soil.

Quicksand in the Lencois Maranhenses, a natural park in the North-East of Brazil.



Computer model of experimentally investigated quicksand. An object pushed inside gets trapped under the collapsing grain structure.

Title: Random turbulent velocity field

Researchers: Dr. Reza Mahmoodi Baram
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The number of degrees of freedom in a turbulent flow increases as $Re^{9/4}$, Re being the Reynolds number. This makes it nearly impossible to simulate flows in nature, for which Re often exceeds 10^8, using current computers. However, the exact details of the motion of the flow are unimportant since all measured physical quantities are statistical averages.

Although the statistical properties of turbulence are well-known and reproducible, no theory of turbulence has been found yet, which fully describes them. In this work we propose a way of generating instances of divergence-free velocity fields in a three-dimensional periodic box whose statistical properties match that of real flows. Some orthonormal divergence-free bases are used to generate arbitrary instances of a velocity field in Fourier space, which is then transformed to real space. By choosing the amplitude of the modes from a properly-chosen random distribution, it is possible to impose the Kolmogorov's scaling into the field. However, other properties like PDF of velocities are not reproduced just by imposing the Kolmogorov's scaling. This means there is much more happening in a flow, which cannot be deduced from Kolmogorov's theory. We strongly believe, that in order to capture all features of a real turbulent flow, we need to invoke the dynamics of the flow governed by the Navier-Stokes equations. This is the subject of on-going research.

Title: River Delta Formation

Researchers: Hansjörg Seybold
Prof. José S. Andrade
Prof. Hans J. Herrmann
Dr. Peter Molnar
Prof. Wolfgang Kinzelbach

Institute: Computational Physics for Engineering Materials, IfB
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. We develop a model to describe the time evolution of the landscape by erosion and deposition in river beds. The model is based on a resistor network lattice where the landscape and the water height are discretized on the nodes and the flow on the bonds. The 'resistance' of the landscape to the water flow is changed according to the water flow. If the flow is fast, the landscape is eroded and if it is slow we obtain deposition. Using the model the formation of braided rivers and river deltas is studied and compared with existing formations. According to different parameters in the erosion laws surprisingly realistic patterns have been obtained and different delta type could be reproduced. Furthermore several phenomena of real deltas like the switching of the delta lobe could be observed and characterized.

References:

[1] H. Seybold, J. S. Andrade, H.J. Herrmann, *River Delta Modeling* PNAS (2007), accepted.

Title: Reaction-diffusion processes under particle flows

Researchers: Atsushi Kamimura[1,2]
Prof. Hans J. Herrmann[1]
Prof. Nobuyasu Ito[2]

Institute: [1]Computational Physics for Engineering Materials, IfB
ETH Zürich
[2]Department of Applied Physics, University of Tokyo

Description:

In reaction-diffusion systems, fluctuations can play an important role in their macroscopic behavior even for simple reactions such as $A + B \to C + D$ in low dimensional systems. For the reaction, fluctuations between the reactants A and B often cause domain formations of single species A or B, and reactions occur between the two domains of A and B. Therefore, the behavior is essentially different from mean-field analytical approaches and computational simulations are powerful tools for the investigations under certain conditions. In this project, a reaction-diffusion system under a particle flow is investigated by using molecular dynamics simulation of hard sphere particles in 2D. In our systems, the reactants are flowing in at one end $x = 0$ and particles are moving out at the other end $x = L_x$.

We obtain that, at some snapshots, reactants clearly show the formation of domains of a single reactant. In fact, we obtain that the average distributions of reactants in a steady state show slower decays than those of the mean-field analytical solutions. Further, because the flow of particles $J_x = \rho(x)V_x$ is conserved along x, distributions of products and reaction events can be calculated by the distributions of reactants, which are in good agreements with the simulation results.

Title: Morphogenesis in Constrained Spaces

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

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

How does a membrane fold when it grows inside a finite volume? The main scientific interest of our project lies in a theoretical understanding of the underlying processes like symmetry breaking/buckling, and the dependence on system parameters (friction, growth criteria etc.). For a mechanically accurate simulation, two aspects need to be considered: First, elastic media are described by highly non-linear differential equations. For strongly crumpled surfaces, we cannot - as is often done - neglect higher order terms, and have to resort to sophisticated, computationally demanding shell models. Second, when a membrane buckles, it has a strong dynamical character with high frequency modes. Their simulation therefore requires small time-steps and a fine discretization grid. These problems are best overcome by parallelization and adaptive meshing of the membrane surface. The latter has already been employed for our preliminary work on a similar 2D system (Figure 2). Here, the discretization is adapted according to the local curvature in a way that also preserves the local deformation history stemming from plastic yielding.

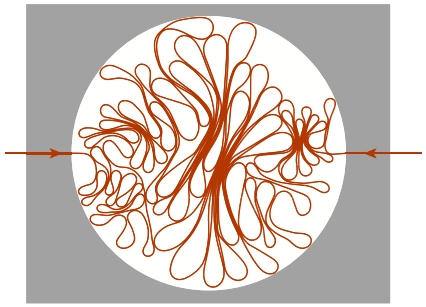


Figure 2: Numerical simulation of a long wire injected into a 2D cell.

References:

[1] N. Stoop, F. K. Wittel, H. J. Herrmann, *Stiffness Divergence of Strongly Crumpled Wires*, Phys. Rev. E, submitted (2007).

Title: Molecular based Models of Non-Newtonian Microfluids

Researchers: Lukas D. Gamper
Dr. Falk K. Wittel
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

The failure of bond lines in wood constructions under load can lead to tragic accidents like the collapse of buildings under snow load. Compared to engineering materials, good numerical models for wood failure and wood bond line failure are rare. To predict bond line failure, one has to consider the whole production history, including for example flow processes of various complex fluids (glues) into the capillary wood microstructure. We approach the problem by considering the glue as a non-Newtonian fluid. These are fluids, in which the viscosity depends on the strain rate (e. g. corn starch), whereas Newtonian fluids have constant viscosity. Microfluidics of non-Newtonian fluids is a field of broad interest, however due to the complexity of modeling, studies in the field are rare.

Within this project we simulate the glue as a non-Newtonian microfluid based on molecular dynamics simulations. First we study the rheologic behavior of glue, modeled as a non-Newtonian fluid. Subsequently we introduce walls with various properties, representing technical surfaces. Finally we study the dynamics of the non-Newtonian fluid in capillary flow. Currently Lennard-Jones type potentials are used to calculate droplet formation, droplet evolution, wetting of smooth bounding walls and subsequent determination of wetting angles. Extensions of the molecular dynamics simulation to more realistic, non Newtonian fluids compressed between rough walls are on the way.

Title: Simulation of fragmentation of plastic materials

Researchers: Gabor Timar
Prof. Hans J. Herrmann

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

We study the plastic fragmentation of spheres by using three-dimensional Discrete Element Models. Large scale computer simulations are performed with models that consist of agglomerates of many spherical particles, connected by beam-truss elements. A plastic constitutive law is introduced to the bonds, enabling us to simulate the fragmentation of ductile materials. The main goal is to compare the properties of plastic fragmentation with the results acquired from simulations of brittle materials. Focus is put on the detailed development of the fragmentation process and the dependence of the critical velocity on parameters such as the yield strength of the beams. The resulting fragment mass distribution in plastic fragmentation is investigated as well.

References:

[1] H. A. Carmona, F. K. Wittel, F. Kun and H. J. Herrmann, *Fragmentation processes in impact fracture*, Phys. Rev. E (2007), submitted.

Title: A numerical and experimental study of flow and instabilities in concentrated colloidal suspensions

Researchers: Dr. Jan Ludvig Vinningland
Prof. Hans J. Herrmann
Prof. Eirik G. Flekkøy
Prof. Knut Jørgen Måløy
Dr. Renaud Toussaint

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich
Complex group, University of Oslo

Description:

As grains become smaller than about 1 μm in diameter the dynamics of the grains and their interactions with the interstitial fluid change significantly. Brownian motion must be included in the description as well as attractive Van-der-Waals forces and repulsive Coulomb forces. This interesting interplay of forces make way for a plethora of different structures and properties, which depend strongly on the strength of these forces. Such colloidal systems will be investigated numerically by means of a numerical model originally tailored to describe the hydrodynamic interactions of a granular phase with the ambient fluid. This model must be extended with relevant interactions in order to describe colloids. The model has recently provided insights into granular Rayleigh-Taylor instability [1], plug flow [2], fluidized beds [3], and the bubble-instability in a tube of sand [4].

References:

[1] J. L. Vinningland, Ø. Johnsen, E. G. Flekkøy, R. Toussaint, and K. J. Måløy. Granular Rayleigh-Taylor Instability: Experiments and simulations. *Phys. Rev. Lett.*, 99(4):048001, 2007.

[2] M. Strauß, S. McNamara, H. J. Herrmann, G. Niederreiter, and K. Sommer. Plug conveying in a vertical tube. *Powder Tech.*, 162:16, 2006.

[3] S. McNamara, E. G. Flekkøy, and K. J. Måløy. Grains and gas flow: Molecular dynamics with hydrodynamic interactions. *Phys. Rev. E*, 61(4):4054–4059, 2000.

[4] E. G. Flekkøy, S. McNamara, K. J. Måløy, and D. Gendron. Structure formation and instability in a tube of sand. *Phys. Rev. Lett.*, 87(13):134302, 2001.

Title: Computational resources at the Institute for Building Materials

Researchers: Markus Künstner, System-Administrator ComPhys-Group

Institute: Computational Physics for Engineering Materials, IfB
ETH Zürich

Description:

To provide the requested computational power for the simulations done by our group-members, we decided to build a high-performance computing cluster (HPC).

This cluster consists of one master node as well as 30 computational nodes. Each node has two Intel Woodcrest 3.0 GHz CPU's inside. Along with the processor, each node is equipped with 6GB of RAM. This results in 120 cores or 1'440 GigaFLOPS (Floating Point Operations Per Second). As for the storage of the cluster, a RAID-System (Redundant Array of Independent Discs) providing approximately 5TB of disc-space is used.

The big advantage of this cluster, a single job being able to run on more than one node at the same time. This parallelisation leads to an enormous increase in speed, it has to be properly implemented in the source-code though. Even non-parallelised code runs faster due to the fast Intel Woodcrest server-processors combined with the proprietary Intel-compilers. With this cluster, the users won't be restrained working on their local computers since all the CPU-intensive tasks are executed on the cluster.

For the time being, the main purpose of using the cluster is running self-written code, most of it in C++ and C. To analyse the calculated data, Matlab (R2007a) is the preferred program on the system. Other important references are the Intel Compilers for C and Fortran. Compared to the gcc-compiler, not only the compilation itself finishes earlier, the produced binaries run up to 30% faster compared to the standard Linux compilers.

Title: Simulations for High Current Arc Plasmas

Researchers: Prof. Rolf Jeltsch
Prof. Christoph Schwab
Prof. Ralf Hiptmair
Prof. Manuel Torrihon
Dr. Vincent Wheatley
Patrick Huguenot
Harish Kumar
Gisela Widmer

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 a 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.

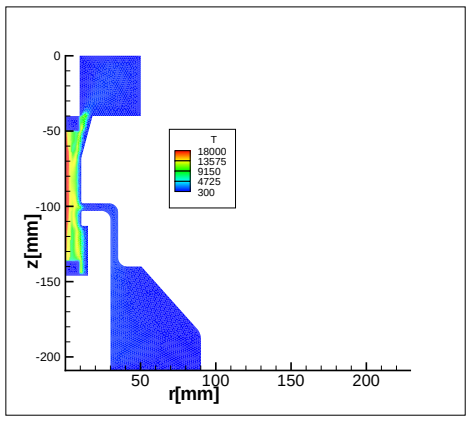


Figure 1: Temperature distribution in an axisymmetric circuit breaker simulation.

In this project we are attempting to model these phenomena. We consider the equations of magnetohydrodynamics, these describe the flow of plasma in the presence of a magnetic field along with evolution of that field. These equations are to be solved numerically in realistic, complex circuit breaker geometries using Discontinuous-Galerkin methods. The domain is initially filled with SF6. We begin our computations after anode and cathode are fully separated and a core of ionized gas exists between these two. The strong electric field between the contacts drives the high arc current, which dissipates large amount of energy further ionizing the gas and raising the pressure in the heating volume. When the current decays during the AC cycle, the high pressure in the heating volume drives the plasma flow which extinguishes the arc.

In order to successfully simulate this process, we must establish what physical mechanisms are important in the flow. For example, the importance of radiation, turbulence and real gas effects must be studied. We must then assess what numerical methods can best be used to capture these mechanisms. Finally these methods will be implemented to develop a simulation tool that can be used to study the details of the operation of gas circuit breakers.

Title: Estimating the eddy-current modelling error

Researchers: Kersten Schmidt
Oliver Sterz (CST GmbH, Darmstadt)
Ralf Hiptmair

Institute/ Group: Seminar for Applied Mathematics
Department of Mathematics

Description:

In many low-frequency applications the eddy current model is used to describe the electromagnetic fields. It is well-known by heuristic arguments that the eddy-current approximation is meaningful if

1. the diameter of the computational domain is small compared to the wavelength, (quasi-static limit),
2. and the conductivities are high, $\omega\varepsilon \ll \sigma$,

where $\omega > 0$ is the fixed angular frequency, and ε and σ designate the permittivity and the conductivity, respectively. We worked out improved estimates of the modelling error as well as an improved asymptotic analysis when the angular frequency tends to zero. Furthermore, we showed that under certain assumptions on the geometry the above conditions are indeed sufficient for a meaningful approximation of the Maxwell equations by the eddy-current model.

The theoretical results are complemented by numerical examples using high order finite elements (*hp-FEM* with C++-library Concepts). These demonstrated that the estimates are sharp (see Fig. 1). Hence, this work delivers a mathematical basis for assessing the scope of the eddy-current model.

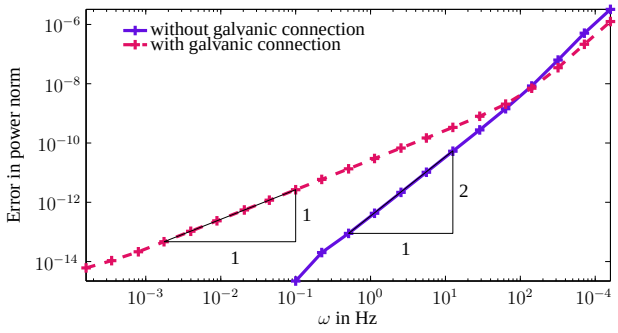
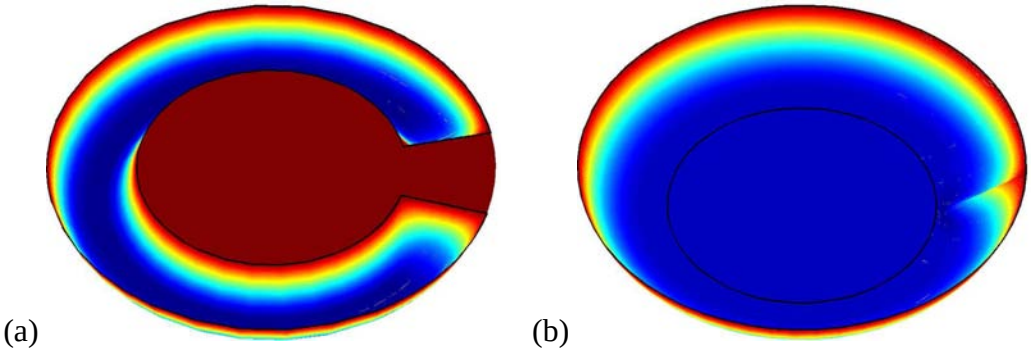


Figure 1: Error in power norm for a conductive half ring. The blue solid line is without galvanic connection, the red dashed line with galvanic connection.

Finally, we considered a conducting cylinder with a slit of width $d > 0$, see Fig, 2. This geometry foil eddy current modelling for small d. We investigated the impact of varied d on the modelling error. For a wide slit the exact magnetic field is expected to penetrate into the ring, where it will be almost constant. For a very narrow slit capacitive coupling will allow a current to flow around the ring, which effectively shields the exterior magnetic field. The full Maxwell solutions depicted in Fig. 2 mirror this expected behavior. The numerical results showed, that the eddy current solution will be utterly wrong for d below a critical value d_c and that the modeling error behaves like $O((d - d_c)^{-1})$ for larger d.



(a) (b)

Figure 2: Amplitute of the magnetic field for a ring with a wide slit ($d = 1\,\mathrm{m}$) (a) and a very narrow slit ($d = 0.92\,\mathrm{nm}$) (b).

References:

[1] K. Schmidt, O. Sterz, and R. Hiptmair, *Estimating the eddy-current modelling error*, IEEE Trans. Magn. (2007), to appear

[2] Concepts Development Team, *Concepts Homepage*, http://www.concepts.math.ethz.ch

Title: Efficient Algorithms for solving the Radiative Transfer Equation

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

Institute: Seminar for Applied Mathematics
ETH Zürich
in collaboration with ABB Corporate Research

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 aim is solve the radiative transfer equation at overall computational costs that are proportial 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*, Research Report 2007-01 (2007), in review

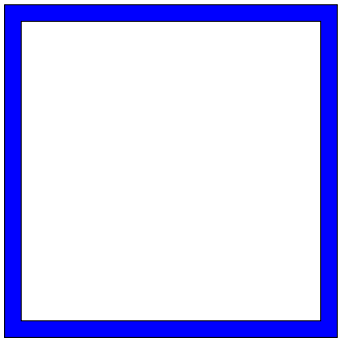
Title: Computation of the band structure of two-dimensional Photonic Crystals with *hp* Finite Elements

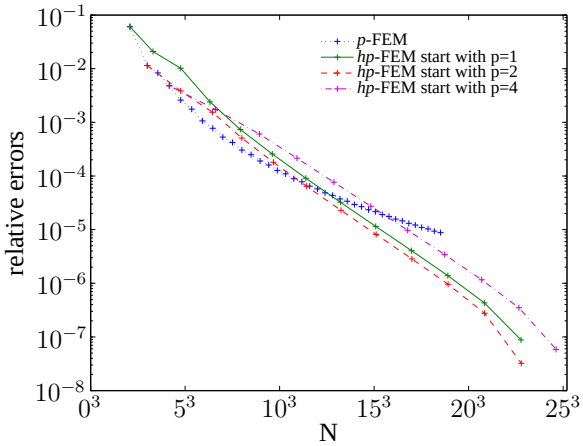
Researchers: Kersten Schmidt
Peter Kauf

Institute/ Group: Seminar for Applied Mathematics
Department of Mathematics

Description:

Photonic crystals are refractive objects with a certain periodic structure. One can construct them such that the behaviour of incoming light is different for varying wavelengths, which makes applications in photonics like optical mirrors and switches possible. For the prediction of photonic crystal properties one consults a model of an infinte crystal with ideal periodicity in two or three directions. By the Floquet-Bloch transformation the eigenvalue problem for the allowed frequencies in an infinite domain is reformulated into a set of eigenvalue problems in a periodicity cell, ordered by the quasi-momemtum $\mathbf{k}$. The relation between quasi-momentum and frequency is the well-known *band structure*. We show the application of *p*-FE and *hp*-adaptive FE of our software package Concepts for two-dimensional photonic crystals. With the implemented quasi-periodic boundary conditions the system matrices for different $\mathbf{k}$ only vary in entries belonging to the boundary. Most of the entries thus stay the same for all the eigenvalue problems. Using *hp* FEM, the numerical examples exhibit exponential convergence in the eigenvalues both for smooth and polygonal interfaces.





The elementary cell with dielectric veins (*left*). The convergence of the relative error for the TE mode for $\varepsilon = 8.9$, vein thickness 0.2 at each side (*right*). We use *p*-FEM and *hp*-FEM, the latter with different initial polynomial degree. For *hp*-FEM one clearly sees the exponential convergence.

References:

[1] K. Schmidt, P. Kauf *Computation of the band structure of two-dimensional Photonic Crystals with* hp *Finite Elements*, SAM Report 2007-05. ETH Zurich, Seminar for Applied Mathematics, July 2007.

[2] Concepts Development Team, *Concepts Homepage*, http://www.concepts.math.ethz.ch

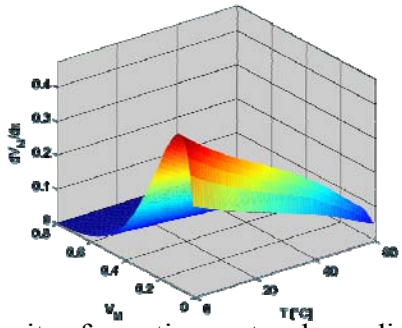
Title: Forming Limit Prediction of Metastable Materials with Temperature and Strain Induced Martensite Transformation

Researchers: Jürg Krauer
Pavel Hora

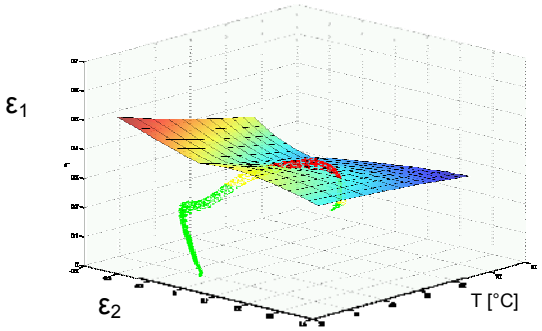
Institute: Institute of Virtual Manufacturing

Description:

Stainless steels as well as TRIP and TWIP steels show a hardening behavior, which can be described only in dependency on the deformation and temperature history during the real forming process. Because the hardening behavior is the determinate factor for the necking phenomenon, the prediction of rupture becomes also deformation path and temperature dependent. As a consequence, the common FLC-method, using a single curve for the prediction of the failure state is not accurate enough.
Phase transformation is another important phenomenon during the forming processes of these kinds of steel. Due to the form of the hard phases like austenite, ferrite or martensite, the material properties are strongly affected. Effects like the temperature dependent behavior of the α-martensite formation or the sensitivity in terms of material properties of different charges have very much influence on the phase transformation and therefore on the necking process. In order to predict the necking in the sheet forming processes for metastable steels with reasonable precision, the thermal computation must be performed and the criterion for the phase transformation must be checked according to the deformation history and the temperature distribution. The deformation, temperature and phase structure are the three essential factors for a proper description of the material properties of these steels.
For this project, standard tensile-tests and stretch-drawing tests were simulated. The simulations were done with the IVP-software StreckForm^{TM}. In the current version, both the Hänsel model for the martensite description and the eMMFC model for the description of the failure are implemented. The experimental data allows to determinate a temperature dependent FLC. With the description for the hardening from the eMMFC, a forming limit surface can be evaluated under the assumption of linear strain paths. For a continuous temperature dependent failure criterion, a surface can be laid over the nonisothermal failure curves.



Martensite formation rate depending on temperature and actual martensite content



3D-Deformation path of the simulated stretch-drawing test in the FLC-T

References:

J. Krauer, P. Hora, L. Tong, *Forming Limit Prediction of Metastable Materials with Temperature and Strain Induced Martensite Transformation*, Proc. of the Numiform'07 Conf.

Title: A dislocation based material model for warm forming simulation

Researchers: Bekim Berisha
Pavel Hora

Institute: Institute of Virtual Manufacturing

Description:

This work deals with high strength low carbon steels. If such a steel is formed at a certain temperature, the strength after cooling to room temperature is very high. The increase of the strength is caused by the effect of dynamic strain ageing. Besides temperature dependence, the dynamic strain ageing effect depends on the material composition and especially on the free-nitrogen and/or carbon concentration.
Based on experimental results, a dislocation material model describing the influence of dynamic strain ageing on the deformation behavior at ordinary conditions has been developed. In order to simulate the warm forming process and to predict the material properties at room temperature, one stage compression tests of cylindrical samples have been performed at a constant strain rate and constant temperature, in a temperature range of 25-500 °C.
Bergström's theory of work hardening is used as a basis for the model development. In the developed model a relationship between material coefficients of the Bergström model and temperature is investigated. The new material model is implemented in an in-house FE-Code.
The fit of the experimental data of the warm compressed specimens are shown in Figure 1 (left). The results of the simulation and experimental data of two stage compression tests are shown in Figure 1 (right). The prediction of the yield strength of the second stage has a high accuracy, independent from the strain of the first deformation, Figure 1 (right). If the first and the second deformation is done at room temperature, or almost at room temperature, no dynamic strain ageing effect is possible, Figure 2 (right).

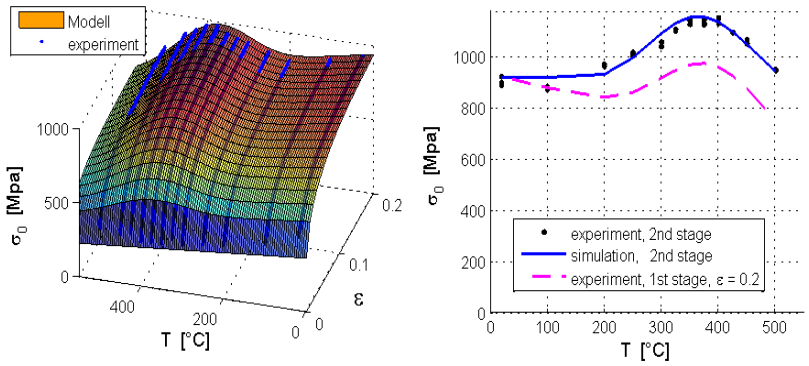


Figure 1: The fit of the first stage compression tests with the new model (left); Yield strength vs. temperature and pre-deformation at ε = 0.2 (right)

Simulation of the forming process provides data for optimizing strength properties and enables process control.

References:

B. Berisha, P. Hora, F. Vanini, L. Tong, "A dislocation based material model for warm forming simulation", Proc. International Conference on Computational Plasticity 2007

Title: Damage Model for the Failure Prediction in Bulk Forming Processes

Researchers: Longchang Tong
Pavel Hora

Institute: Institute of Virtual Manufacturing

Description:

The numerical Simulation for the forming processes is remarkably enhanced by the implementation of failure prediction modulus. In contrast to the FEM simulation for sheet forming processes, where the concept of FLC have been successfully used, the failure prediction for the bulk forming processes remains a large obstacle despite of many models to handle this problem. Most existing models for the failure prediction of bulk forming processes are empirical formulas or use a scale damage factor. If certain condition is fulfilled or the damage factor reaches a critical value, the necking or rupture is indicated.
Experiments showed that the damage inside the material is strongly orientation dependent. A specimen undergoes compressive deformation can be further compressed without noticeable damage. However, as soon as the load changes the direction to tensile, rupture appears immediately. The material behaves just as completely damaged.
Based on the foundation of experiments, a direction oriented damage model for the failure prediction in the FE simulation of bulk forming processes is presented in this paper. This model assumes that all kinds of plastic deformation cause material damages. These damages are strongly oriented according to the plastic deformations. The damages keep hideaway if the compressive stress is applied. As the tensile stress is applied, the damages become active. As soon as the tensile stress exceeds a limit value, rupture appears and the material fails.
The initial limit stresses in different direction form a spherical surface for isotropic materials or an ellipsoid surface for anisotropic materials. The damages caused by the plastic deformations lead to the change of the limit surface. The current stress limit surface is obtained by taking account of the accumulated deformations as well as the hydrostatic pressure accompanied with the deformations. During the FE simulation, the principal stresses in each element are evaluated and compared with the limit stresses. In case the stresses in the workpiece exceed the limit value, failure can be predicted.
The influence of the deformation on the limit stresses can be determined by combining the experiments with the numerical computation.

References

L. Tong, P. Hora, L. Tong, *Damage Model for the Failure Prediction in Bulk Forming Processes*, Proc. of the Numiform’07 Conf. (Porto, P, 2007)

Title: Application of Regression Models in Fineblanking Process Simulations

Researchers: Marc Vinzens
Niko Manopulo
Pavel Hora

Institute: Institute of Virtual Manufacturing

Description:

Today mostly the Finite Element Method (FEM) is applied to fineblanking processes, which allows a well trained and experienced development engineer to simulate the process and decide about the producibility of the required part. The decision of the engineer is mainly based on experience. This experience is founded on previous tasks that have been solved, which can be based on knowledge acquired by experiment or simulation. For this reason the conservation and accessibility of experience is vital to firstly, enable new staff to be trained faster, secondly, to enable an information flow between experts, and thirdly, conserve knowhow in a company.
To allow conservation and accessibility of knowhow of the fineblanking process, a methodology is proposed to allow the approximation of the forming behavior by building a regression model on a series of FE simulation results. This regression model represents an approximation of a specific target function (e.g. risk of failure) based on a limited set of parameters (e.g. cutting radius, V-ring angle etc.). The aim is to provide the user with an interface which allows to predict the value of the target function by providing the values for the parameters thus using the model as a “producibility guideline” for similar processes. Figure 1
At the moment research is manly focused on creating a database of FE results for a specific test example which must be available to create a good regression model. For creating such a database different tasks have been solved to allow automated FE simulation generation. These are a parameter reducing volume model, automated tool surface generation with CATIA V5 and automated surface meshing by using Altair Hypermesh.

Future research focus will be set on selection of appropriate parameters and target functions, and the choice of regression models which meet the required specifications.

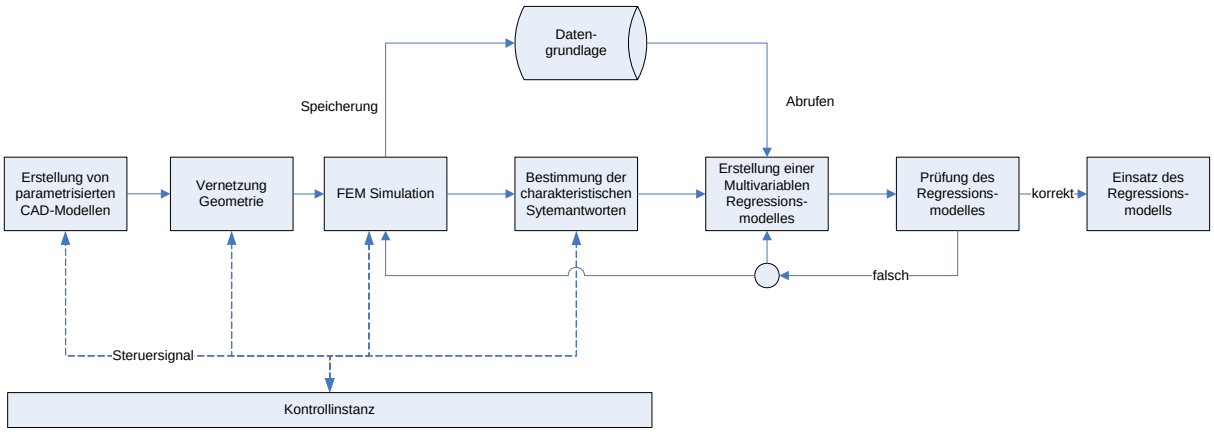


Figure 1 Database generation and modelling process

Title: Relative stabilities of the alkali cations 222 cryptates in the gas phase and in water-methanol solution.

Researchers: Elisa S. Leite[**,***]
Sidney R. Santana[**]
Philippe H. Hünenberger[*]
Luiz C.G. Freitas[**,***]
Ricardo L. Longo[**]

Institute/ Group:
[*] Laboratory of Physical Chemistry
[**] Departamento de Química Fundamental, Universidade Federal de Pernambuco, Recife (Brazil)
[***] Departamento de Química, Universidade Federal de São Carlos, São Carlos (Brazil)

Description :

The relative stabilities of the alkali $[M \subset 222]^+$ cryptates (M = Na, K, Rb and Cs) in the gas phase and in solution (80:20 v/v methanol:water mixture) at 298 K are computed using a combination of *ab initio* quantum-chemical calculations (HF/6-31G and MP2/6-31+G*//HF/6-31+G*) and explicit-solvent Monte Carlo free-energy simulations. The results suggest that the relative stabilities of the cryptates in solution are due to a combination of steric effects (compression of large ions within the cryptand cavity), electronic effects (delocalization of the ionic charge onto the cryptand atoms) and solvent effects (dominantly the ionic dessolvation penalty). Thus, the relative stabilities in solution cannot be rationalized solely on the basis of a simple match or mismatch between the ionic radius and the cryptand cavity size as has been suggested previously. For example, although the $[K \subset 222]^+$ cryptate is found to be the most stable in solution, in agreement with experimental data, it is the $[Na \subset 222]^+$ cryptate that is the most stable in the gas phase. The present results provide further support to the notion that the solvent in which supramolecules are dissolved plays a key role in modulating molecular recognition processes.

References: E.S. Leite, S.R. Santana, P.H. Hünenberger, L.C.G. Freitas and R.L. Longo
J. Mol. Model. **13** (2007) 1017-1025.

Title: Explicit-solvent molecular dynamics simulations of a DNA tetradecanucleotide duplex: lattice-sum versus reaction-field electrostatics.

Researchers: Vincent Kräutler*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Five long-timescale (10 ns) explicit-solvent molecular dynamics simulations of a DNA tetradecanucleotide dimer are performed using the GROMOS 45A4 force field and the SPC water model, in order to investigate the effect of the treatment of long-range electrostatic interactions as well as of the box shape and size on the structure and dynamics of the molecule (starting from an idealized B-DNA conformation). Long-range electrostatic interactions are handled using either a lattice-sum method (particle-particle–particle-mesh; one simulation performed within a cubic periodic box) or a cutoff-based reaction-field method (four simulations, with long-range cut-off distances of 1.4 or 2.0 nm, and performed within cubic or truncated-octahedral periodic boxes). The overall double-helical structure, including Watson-Crick base pairing, is well conserved in the simulation employing the lattice-sum scheme. In contrast, the Watson-Crick base pairing is nearly completely disrupted in the four simulations employing the reaction-field scheme. These four simulations result in highly distorted compact (cutoff distance of 1.4 nm) or extended (cutoff distance of 2.0 nm) structures, irrespective of the shape and size of the computational box. These differences observed between the two schemes appear to be correlated with large differences in the radial distribution function between charged entities (backbone phosphate groups and sodium counterions) within the system.

References: V. Kräutler and P.H. Hünenberger
Mol. Simul. (2007) submitted.

Title: The effect of trehalose on a phospholipid membrane under mechanical stress.

Researchers: Cristina S. Pereira*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Explicit-solvent molecular dynamics simulations are used to investigate at atomic resolution the effect of trehalose on a hydrated phospholipid bilayer under mechanical stress (stretching forces imposed in the form of negative lateral pressure). Simulations are carried out in the absence or in the presence of trehalose at 325 K and with different values for the negative lateral pressure. In the concentration regime (2 molal) and range of lateral pressures (1 to -250 bar) investigated, trehalose is found to interact directly with the membrane, partially replacing water molecules in the formation of hydrogen bonds with the lipid headgroups. Similar to previous findings in the context of thermal stress, the number, degree of bridging and reaching depth of these hydrogen bonds increases with the magnitude of the perturbation. However, at the concentration considered, trehalose is not sufficient to preserve the integrity of the membrane structure and to prevent its extreme elongation under the effect of stretching forces.

References: C.S. Pereira and P.H. Hünenberger
Biophys. J. (2007) submitted.

Title: The influence of polyhydroxylated compounds on a hydrated phospholipid bilayer: a molecular dynamics study.

Researchers: Cristina S. Pereira*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Molecular dynamics simulations are used to investigate the interaction of the polyhydroxylated cosolutes methanol (MET), ethylene glycol (ETG), glycerol (GLY), glucose (GLU) and trehalose (TRH) with a hydrated phospholipid bilayer in the liquid-crystalline phase at 325 K. The comparison is performed at constant effective concentration of cosolute hydroxyl groups. The results (along with available experimental data) lead to the formulation of two distinct mechanisms for the interaction of polyhydroxylated compounds with lipid bilayers. The alcohol-like mechanism (active for MET and ETG) involves preferential affinity of the cosolute for the superficial region of the bilayer interior and is driven by the hydrophobic effect. It results in a lateral expansion of the membrane, a disorder increase within the bilayer, and a partial substitution of water by cosolute molecules at the hydrogen-bonding sites provided by the membrane (predominantly at the level of the ester groups). The sugar-like mechanism (active for GLU and TRH) involves preferential affinity of the cosolute for the bilayer surface (formation of a coating layer) and is driven by entropic effects. It results in the absence of lateral expansion and change in disorder within the bilayer, and a partial substitution of water by cosolute molecules (predominantly at the level of the phosphate groups). It also involves the bridging of lipid molecules via hydrogen-bonded cosolute molecules, a phenomenon that may have implications in the context of membrane stabilization by sugars. Hydrogen bonding itself is not viewed as a driving force for these two mechanisms, which only involve the (partial) substitution of water-lipid by cosolute-lipid hydrogen bonds (the sum of the two remaining essentially constant, irrespective of the nature and concentration of the cosolute).

References: C.S. Pereira and P.H. Hünenberger
Mol. Simul. (2007) submitted.

Title: Conformation, dynamics and ion-binding properties of single-chain polyuronates: a molecular dynamics study.

Researchers: Lovorka Perić *
Cristina S. Pereira*
Serge Pérez**
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry
** Centre de Recherche sur les Macromolécules Végétales, Grenoble (France)

Description :

We report and compare the results of sixteen explicit-solvent molecular dynamics simulations (10 ns) of homopolyuronate single chains corresponding to poly-$\beta(1\rightarrow4)$-D-glucuronate (pGlcU), poly-$\beta(1\rightarrow4)$-D-mannuronate (pManU), poly-$\alpha(1\rightarrow4)$-D-galacturonate (pGalU) and poly-$\alpha(1\rightarrow4)$-L-guluronate (pGlcU). The chains are made formally infinite by application of artificial periodicity along the chain axis (octameric or nonameric repeat unit). Eight main simulations are performed at 300 K in the presence of Ca^{2+} counter-ions (neutralizing amount), and starting from alternative regular two- and three-fold helical structures. Eight simulation variant probe the effect of an elevated temperature or of a different counter-ion environment. The main observations made in these simulations are: (*i*) the glycosidic linkages (and local helical parameters) show an important flexibility (in time) and variability (along the chains), and regular helical structures only account for a limited fraction of the conformational ensembles populated at 300 K; (*ii*) for all system considered, the binding of Ca^{2+} counter-ions is essentially non-specific, with the formation of a dense counter-ion atmosphere around the chains (condensation), but no specific (tight-binding) interactions at well-defined coordination sites; (*iii*) the 3_2-, 9_5-, 2_1- and 2_1-helices appear to be the preferential regular helical forms for single chain pGlcU, pManU, pGalU and pGulU in aqueous solution, with the possibility of an alternative 3_1-helix for pGalU (these forms should be viewed in the sense of helical propensities). Taken together, these observations suggest that if chain dimers are appropriately described by the egg-box model (or any other structural model with similar qualitative features) chain-chain association within junction zones in gels must be accompanied by a substantial chain rigidification and a dramatic change in the ion-binding mode.

References: L. Perić, C.S. Pereira, S. Pérez and P.H. Hünenberger
Mol. Simul. (2007) submitted.

Title: Residual structure in a fragment of urea-denatured outer membrane protein X: a molecular dynamics study

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

Institute/ Group:
* Laboratory of Physical Chemistry
** Institut für Molekularbiologie und Biophysik

Description :

Motivated by an experimental (NMR) study (Tafer et al., Biochemistry 43:860-869 (2004)) reporting the identification and characterization of non-random residual structure in two domains of urea-denatured Escherichia coli outer m embrane protein X (OmpX), we report the results of two long-timescale (0.4 μs) unrestrained explicit-solvent molecular dynamics simulations of a tetradecapeptide representative of one of these domains under strongly denaturing conditions (8 M urea). The two simulations are initiated from different starting structures (configuration of the corresponding segment in an NMR model structure of the urea-denatured protein or arbitrary extended configuration). Both simulations show the reversible formation and disruption of helical content (characteristic of the urea-denatured state) and β-turn (characteristic of the native state) secondary structure in multiple events. Events of helix formation are correlated with the formation of hydrogen bonds between two sidechains and the presence of a stable hydrophobic contact, and evidence a peculiar helix stabilization and N-terminal capping role for a negatively charged residue. These features are in qualitative agreement with the NMR model structure, and provide insight into the structure and dynamics of the peptide at atomic resolution. However, the quantitative agreement with experimental inter-proton distance upper bounds is at best acceptable, suggesting that a number of relevant configurations have not been sampled. Furthermore, major conformational transitions occur on the 100 ns timescale and the conformational ensembles sampled in the two simulations only overlap to a limited extent. Thus, in spite of the considerable computational effort invested in this study, the 0.4 μs timescale reached here seems still insufficient to permit an exhaustive sampling of the configurational space accessible to the peptide, and to clearly disentangle sampling, force-field and (possibly) experimental errors.

References: V. Kräutler, S. Hiller, K. Wüthrich and P.H. Hünenberger
Manuscript in preparation.

Title: Computation of methodology-independent ionic solvation free energies from molecular simulations: III. A new parameter set for alkali and halide ions.

Researchers: Maria Reif*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Three new sets of ion-water Lennard-Jones interaction parameters are proposed for the alkali (Li^+, Na^+, K^+, Rb^+) and halide (F^-, Cl^-, Br^-, I^-) ions, to be used in (explicit-solvent) molecular dynamics simulations together with the SPC water model, each of which was established to reproduce a set of "experimental" absolute ionic hydration free energies. The latter values were obtained by combining the conventional hydration free energies of Tissandier *et al.* (J. Phys. Chem. A 102, 7787, 1998) together with three possible values for the absolute hydration free energy of the proton [$\Delta G^\circ_{hyd}(H^+) = -1100$, -1075 or -1050 kJ·mol^{-1}], chosen over the expectation range suggested by different experimental approaches. Prior to parameter refinement, the raw simulation data was corrected for any methodological dependence on the boundary conditions (finite or periodic system, system shape, and size), treatment of electrostatic interactions (Coulombic, lattice sum, or cutoff based) and summation convention for the electrostatic potential at the ion site (by solvent charges or by solvent molecules), following the procedure described by Kastenholz *et al.* (J. Chem. Phys. 124, 224501, 2006). Due to the large uncertainty in the experimental value for the absolute hydration free energy of the proton, it is not possible to determine on the sole basis of the present simulations which of the three sets is the most accurate. Possible independent observables to perform such an assessment could include the structural and energetic properties of ionic crystals and melts, the hydration entropies of the ions or the structural and colligative properties of ionic solutions.

References: M. Reif and P.H. Hünenberger
Manuscript in preparation.

Title: Simulations for High Current Arc Plasmas

Researchers: Prof. Rolf Jeltsch
Prof. Christoph Schwab
Prof. Ralf Hiptmair
Prof. Manuel Torrihon
Dr. Vincent Wheatley
Patrick Huguenot
Harish Kumar
Gisela Widmer

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 a 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.

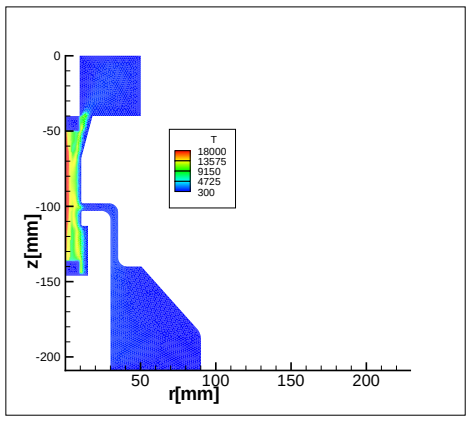


Figure 1: Temperature distribution in an axisymmetric circuit breaker simulation.

In this project we are attempting to model these phenomena. We consider the equations of magnetohydrodynamics, these describe the flow of plasma in the presence of a magnetic field along with evolution of that field. These equations are to be solved numerically in realistic, complex circuit breaker geometries using Discontinuous-Galerkin methods. The domain is initially filled with SF6. We begin our computations after anode and cathode are fully separated and a core of ionized gas exists between these two. The strong electric field between the contacts drives the high arc current, which dissipates large amount of energy further ionizing the gas and raising the pressure in the heating volume. When the current decays during the AC cycle, the high pressure in the heating volume drives the plasma flow which extinguishes the arc.

In order to successfully simulate this process, we must establish what physical mechanisms are important in the flow. For example, the importance of radiation, turbulence and real gas effects must be studied. We must then assess what numerical methods can best be used to capture these mechanisms. Finally these methods will be implemented to develop a simulation tool that can be used to study the details of the operation of gas circuit breakers.

Title: Explicit Multi-Scale Time-Integration Using Stabilized Runge-Kutta-Methods

Researchers: Prof. Manuel Torrilhon
Prof. Rolf Jeltsch

Institutes: Seminar for Applied Mathematics,
ETH Zürich

Description: Stabilized explicit Runge-Kutta methods use more stages which do not increase the order, but, instead, produce a bigger stability domain for the method. In that way stiff problems can be integrated by the use of simple explicit evaluations for which usually implicit methods had to be used. Ideally, the stability domain is adapted precisely to the spectrum of the problem at the current integration time in an optimal way, i.e., with minimal number of additional stages. This idea demands for constructing Runge-Kutta methods from a given family of flexible stability domain. Typically, these are given by a disk, real or imaginary intervals.

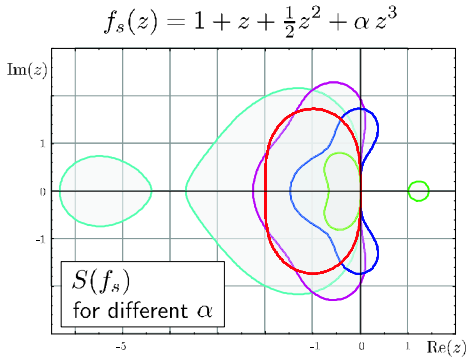


Figure 1: Variations of the stability domain of an explicit second order 3-stage Runge-Kutta Method.

In this project the results for real line spectra, are generalized to more general spectra in the form of a thin region. In thin regions the eigenvalues may extend away from the real axis into the imaginary plane. Semi-discretizations of hyperbolic-parabolic equations are a relevant application which exhibit a thin region spectrum. As a model, linear, scalar advection-diffusion is investigated. The second order stabilized explicit Runge-Kutta methods derived from the stability polynomials are applied to advection-diffusion and compressible, viscous fluid dynamics in numerical experiments. Due to the stabilization the time step can be controlled solely from the hyperbolic CFL condition even in the presence of viscous fluxes.

References:

[1] M. Torrilhon and R. Jeltsch, *Essentially Optimal Explicit Runge-Kutta Methods with Application to Hyperbolic-Parabolic Equations*, Num. Math. **106**, (2007), pp.303-334

Title: Two-phase Debris Flow Modeling

Researchers: Julia Kowalski
Prof. Manuel Torrilhon
Dr. Perry Bartelt
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics, ETH Zürich
Snow and Avalanche Research Institute (SLF), Davos

Description:

Debris flows constitute a major hazard in mountainous areas. They consist of mobilized sediments spanning a wide range of grain sizes and the flows are typically fully or partly saturated with water.

In the last decade shallow flow models have been successfully applied to simulate debris flows, however these models fail in regimes of dominant sedimentation and separation of components. The aim of this project is to derive a debris flow model that accounts for these effects. In a first step existing models have been generalized to allow for varying mixture densities. The resulting system is conditionally hyperbolic. A rigorous analysis of has been carried out to ensure, that regions of complex characterstics in the phase space are irrelevant for realistic flow situations. In a final step the developed numerical solver will be implemented into a GIS environment to simulate flow over complex terrain. Real scale data of debris flow events in the Illgraben (VS) provided by the Swiss Federal Institute for Forest, Snow and Landscape Research motivates and verifies the theory.

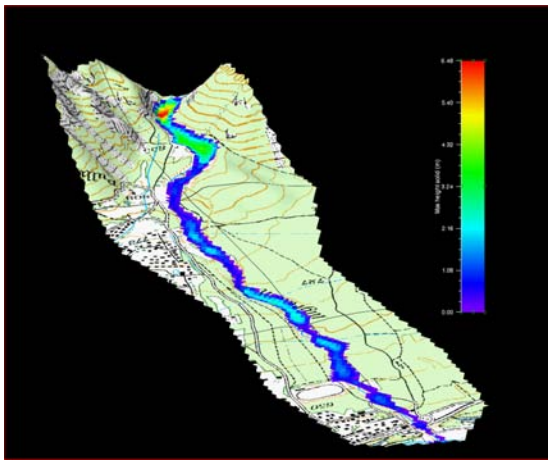


Figure 1: Simulation results of a debris flow event in the Illgraben. The plot shows the maximum height throughout the flow.

References:

[1] B. McArdell and P. Bartelt and J. Kowalski, *Field observations of basal forces and fluid pore pressure in a debris flow*, Geophysical Research letters (34) L07406 (2007)

Title: Compact Third Order Limiting for Conservation Laws

Researcher: Miroslav Čada
Prof. Manuel Torrilhon
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

In this study, we employ and generalize the idea of double-logarithmic reconstruction for the numerical solution of hyperbolic equations, as proposed recently by Artebrandt and Schroll. The result is a class of efficient third order schemes with a compact three-point-stencil and a single limiter. An identification of the basic properties of the double-logarithmic reconstruction led to conditions for the construction of new non-oscillatory third-order limiter functions. The resulting methods handle discontinuities as well as local extrema within the standard semi discrete MUSCL algorithm using only a single limiter function. Well known drawbacks of classical second order limiters, such as "squaring" effects and "clipping-off" of smooth extrema are healed [1] and computational results indicate a very good performance, accuracy proportion.

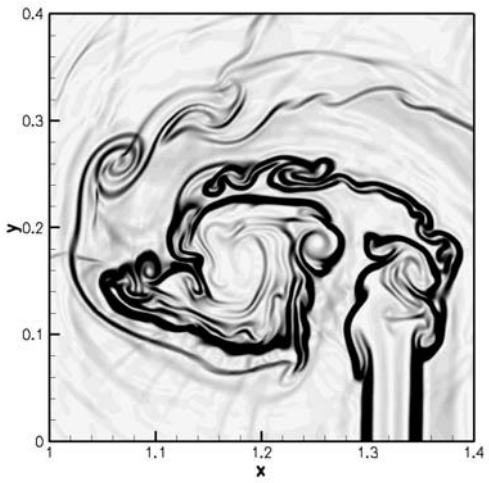


Figure 1: Emulated Schlieren image of shock bubble interaction computed on a 1700×500 grid with reflecting boundary conditions at $t = 0.4$ and CFL $= 1.5$.

The figure shows the result for shock-bubble interaction. The Euler equation of compressible gas dynamics are solved using the new third-order limiter function with the explicit third-order Runge-Kutta scheme for time integration.A stability analysis of the new scheme shows an improved CFL condition. We observe well resolved contact discontinuities with the new method. This results in considerably sharper resolved vortex structure with more small scale features. Due to the higher CFL number, the computational efficiency, i.e. the work per cell and timestep, of the new method is identical to second order methods.

References:

[1] M. Čada, M. Torrilhon and R. Jeltsch, *Compact Third Order Logarithmic Limiting for Non-Linear Hyperbolic Conservation Laws*, Proc. Eleventh Intl. Conf. Hyperbolic. Problems, Theory, Numerics and Applications (2007), in press

Title: Non-Equilibrium Gas Flow Computations based on Advanced Continuum Models

Researchers: Prof. Manuel Torrilhon
Prof. Henning Struchtrup

Institutes: Seminar for Applied Mathematics, ETH Zürich
Dept. Mechanical Engineering, Univ. Victoria, Canada

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 is built around a mathematical model based on Boltzmann's equation in kinetic theory and the derivation of suitable numerical methods. The model consists of moment equations with a special closure procedure. The standard closure relations are expanded around a non-equilibrium allowing for a multi-scale relaxation.

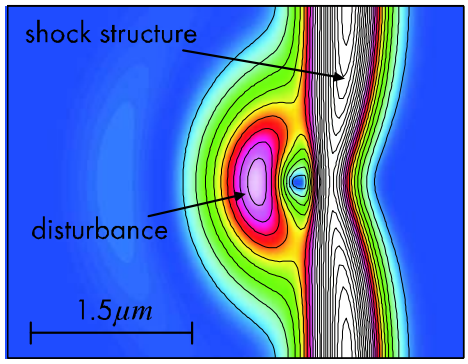


Figure 1: Micro-scale interaction of a density disturbance with a shock wave. The figure shows contours of heat flux computed with the R13-model.

The new system, called regularized 13-moment system (R13), is formed by relaxational partial differential equations of hyperbolic-parabolic type. It contains first order equations for the thermodynamic flow 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. Thus, the derivation of the numerical method is based on a finite-volume approach, but needs to include the relaxational and dissipative, second order parts. The characteristic properties of the R13 system are more complex than in traditional fluid dynamics due to the higher number of equations. For instance, the signal speed depend on the value of nonequilibrium quantities, like stress and heat flux.

References:

[1] M. Torrilhon, *Two-Dimensional Bulk Microflow Simulations Based on Regularized 13-Moment-Equations*, SIAM Multiscale Model. Simul. **5**(3), 695-728 (2006)

[2] H. Struchtrup and M. Torrilhon, *H-theorem, regularization, and boundary conditions for linearized 13 moment equations*, Phys. Rev. Lett. **99**, (2007), 014502

Title: 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

$$\partial_t f + c_k \partial_k f = \mathcal{S}(f).$$

The solution of this equation is a function

$$f : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \ni (\mathbf{x}, \mathbf{c}, t) \longmapsto f(\mathbf{x}, \mathbf{c}, t) \in \mathbb{R}_+$$

associating 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.

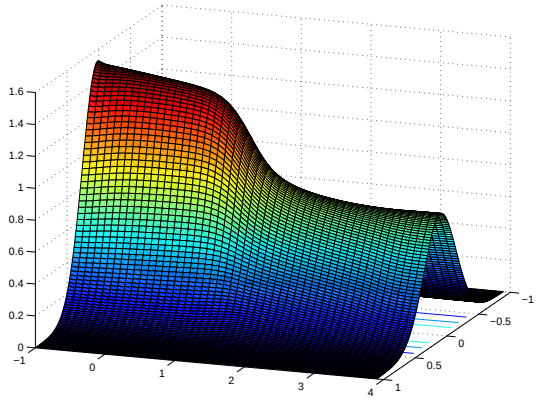


Figure 1: Example of a velocity distribution in a Riemann-Problem. The figure shows the projection to one velocity and one space dimension.

The aim of this project is an approach to Boltzmann's equation that combines the methods which are physically substantiated with state of the art numerical approaches to high dimensional problems.

Title: Turbulent reactive flow

Researchers: Daniel W. Meyer
Michael Hegetschweiler
Gaurav Anand
Michael Wild
Mathias Hack
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 nor chemical 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 in- and outflow boundary conditions. Especially for high turbulent intensities, i.e. if the rms velocity is large, standard boundary conditions can lead to significant particle losses. With a very simple approach, which is easy to implement, this problem could be cured. The second issue is related to particle number control. It is preferable to employ approximately the same number of particles in each grid cell. A common approach to achieve this is based on particle cloning and elimination. It was found that standard methods are inconsistent and therefore a completely new scheme for statistically stationary cases was devised. In large grid cells, the particles move with an elevated velocity, which results in a particle number density distribution inversely proportional to the local grid resolution. Moreover, if the particle velocity is included in this scheme, test cases with slow co-flows (very common) can be treated much more efficiently. In order to achieve consistency, care has to be taken when statistical information is extracted from the particle field. This local particle time stepping algorithm has been validated and currently it is under examination for reactive flow applications.

Turbulent combustion modeling: In terms of modeling, we focus on five topics: multi-scalar mixing, non-premixed turbulent combustion with local extinction and re-ignition, premixed turbulent combustion, spray combustion and NO_x formation.

References:

Rembold and M. Grass and P. Jenny. Parallel Hybrid Particle/Finite Volume Algorithm for Transported PDF Methods Employing Sub-Time Stepping. Accepted for publication in Computers & Fluids, 2007

Meyer and P. Jenny. Consistent Inflow and Outflow Boundary Conditions for Transported Probability Density Function Methods. Accepted for publication in Journal of Computational Physics, 2007

Title: Multi-phase flow in porous media

Researchers: Manav Tyagi
Hadi Hajibeygi
Patrick Jenny

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

Description:

Flow and transport in porous media has many applications in energy science, e.g. for catalytic processes, oil and gas recovery, and CO_2 storage in geological sub-surface formations.

Multi-scale modeling: 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. With the MSFV method it was demonstrated for the first time that large, realistic studies can be computed much faster than with conventional simulators. At the same time, the accuracy of the solution is hardly compromised. Recently, an efficient and general model to treat complex wells within the MSFV framework. Moreover, an iterative procedure which allows to converge MSFV solutions. Both contributions are relevant for the practical use of the MSFV method.

CO_2 sequestration: A related topic with high relevance is motivated by CO_2 sequestration. Currently, storing CO_2 in geological sub-surface formations seems to be one of the most promising feasible technologies to stabilize the CO_2 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 we believe that it allows to describe various complex non-equilibrium processes in a more general and natural way than in a classical Eulerian framework. Recently, it has been demonstrated that the method can be employed to model non-equilibrium two-phase behavior.

References:

Lunati and P. Jenny. Multi-Scale Finite-Volume Method for Density-Driven Flow in Porous Media. Accepted: Journal of Computational Geosciences, 2007

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: 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. In collaboration with Tobias Stamm and Dres. Safer Mourad and Markus Vöge from EMPA, 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, spatially varying absorption characteristics and a second multi-scale level to deal with realistic halftone print have been developed .

References:

P. Jenny and S. Mourad and T. Stamm and M. V{$\backslash$$}"oge and K. Simon. Computing light statistics in heterogeneous media based on a mass weighted probability density function method. JOSA A, Vol. 24, Issue 8, pp. 2206-2219, 2007

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 biology 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 science, which necessarily involves tight collaborations between life scientists, physicists and engineers.

Modeling the cerebral blood flow: This is a collaboration with Profs. Bruno Weber and Alfred Buck from the University of Zurich. 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. It will be investigated how local alterations affect the global CBF. Among others, insights gained from the simulations are valuable for the correct interpretation of data acquired by magnetic resonace imaging modalities.

Title: Incompressible Navier-Stokes flow

Researchers: Giuseppe Bonfigli
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.

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. Recently, this framework was combined with a novel immersed boundary technique to treat complex geometries. Currently it's efficiency is investigated and comparisons with classical multi-grid methods are made.

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

Researchers: Andreas Jocksch, Leonhard Kleiser, and Jörg Ziefle

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

Description:

Most engineering and geophysical flows occur at high Reynolds numbers and are turbulent. While it is theoretically possible to directly simulate turbulent flows by resolving all relevant length and time scales (direct numerical simulation, DNS), this approach is practicable only for very low Reynolds numbers. For larger Reynolds numbers the computational cost is prohibitive. As of today, the Reynolds numbers of most industrial flows are far beyond what is possible for DNS, and will continue to do so for a long time. 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, known as large-eddy simulations (LES), are able to predict unsteady flow processes at a relatively low computational cost (compared to DNS). 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 (in the order of one percent) of the cost needed for a DNS.
In a recent project, we implemented ADM in the semi-industrial finite-volume code NSMB with full support of domain decomposition and parallel computing. After the successful validation with the the canonical periodic-hill channel configuration, the setup was applied to flows belonging to the family of "jets-in-crossflow". The jet-in-crossflow configuration can be found in a variety of technical applications such as fuel injection in combustors, plumes of smoke stacks or vertical/short take-off and landing (V/STOL) aircraft. We used NSMB with ADM to investigate the film cooling of turbine blades. In this application a large isobaric plenum feeds cool fluid through a short inclined nozzle into a hotter turbulent boundary layer. This investigation allowed the analysis of the secondary flows within the coolant nozzle, and the dominant vortex structures in the mixing region, both of which are crucial for the understanding and the efficiency of the film-cooling process.
Another project covers transition of high-speed boundary layers. Localised transition, i.e., the growth of turbulent spots, is investigated by means of LES using ADM. Again, the code was designed to support large-scale parallel computing. Validation tests for this kind of transition showed a good agreement between DNS and LES. Our LES results can deliver reference values for this special type of transition modelling.

References: See separate list.

Title: Nonlinear Instabilities in Swirling Mixing Layers

Researchers: Felix Keiderling, Leonhard Kleiser, Sebastian Müller

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

Description:
Swirling mixing layers occur in many technical applications. Typical examples are leading-edge vortices on delta wings or flame holders in combustion devices. Good mixing is crucial for the design of combustion systems for different applications. A detailed understanding of the physics of swirling jet flows and mixing layers is essential for the development of new turbulence and mixing models. To improve the understanding of the underlying flow physics, substantial research efforts have been undertaken in the past decades. These efforts primarily aimed at modeling basic elements of swirling motion and to determine the associated stability characteristics. The addition of swirl can enhance the mixing of circular mixing layers and jet flows. In this project, the nonlinear disturbance evolution and transition to turbulence in a subsonic swirling circular mixing layer has been studied. Our simulations were designed for capturing the nonlinear and nonparallel evolution of initially linear instabilities as well as their nonlinear interactions. In a first step, direct numerical simulations (DNS) were performed using different instability forcings imposed at the inflow. Each forcing consisted of a mix of distinct spatially amplifying harmonic waves which were assembled to be among one group out of three distinct instability families. The associated highly resolved DNS revealed a transition to turbulence in two cases (out of three) which are not present (to our knowledge) in swirl–free mixing layers. The simulation code used for this study relies on high order approximations with spectral resolution properties for spatial discretization. The implementation of the cylindrical-coordinate Navier–Stokes solver has been supplemented by extensive validation studies. Furthermore, we applied large-eddy simulation (LES) to simulate the nonlinear evolution of a swirling mixing layer. LES results were assessed at different resolutions and compared with reference results from DNS.

References: See separate list.

Title: Prediction of Aeroacoustic Jet Noise using LES

Researchers: Felix Keiderling, Leonhard Kleiser, Dominik Obrist

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

Description:

Because of tightening noise emission regulations the reduction of jet noise is a research field of growing interest. The noise generation mechanisms in subsonic jet flow are far from being fully understood and, therefore, noise reduction approaches have remained largely empirical. Numerical tools for the prediction of aerodynamically generated noise which support the early design process of future jet engines are still to be developed. Because of the unsteady nature of the flow these predictions are inherently tied to time-dependent flow simulations. With the continued increase of computer power, simulations for relevant Reynolds numbers come into reach of time-dependent large-eddy simulations (LES). Our contribution in this field of research focuses on the direct noise computation of jet flows using LES as well as on the development of acoustic far-field solvers to predict the emitted far-field noise accurately and efficiently.
As a subgrid-scale model for the LES we use the Approximate Deconvolution Model (ADM). In previous work, a comparative study of DNS and LES with ADM of a compressible transitional rectangular jet at a subsonic Mach number was performed and very good predictive capabilities of the LES was demonstrated. Following this, we started a study of a round, high subsonic jet configuration in the intermediate as well as the high Reynolds number regime.
To this end, we use a DNS/LES code developed for cylindrical geometries for simulations of circular jet flows and its associated noise. Results for the aerodynamic region are found to be in excellent agreement with experimental data and other numerical simulations. The directly computed noise spectra exhibit minor deviations from other data which may be linked to different inflow treatment.
The perceived noise at remote observer locations can be determined most efficiently with an acoustic far-field solver. Far-field solvers extrapolate the information of an underlying DNS/LES to the acoustic far-field and thereby couple the fluid flow with an acoustic field. We developed two different acoustic far-field solvers to get a better understanding of the numerical quality and performance of the different formulations proposed in the literature. Both solvers directly interface with the previously described DNS/LES solver. One far-field solver is based on a surface integral formulation by Ffowcs Williams & Hawkings. The second solver is based on spatially spectral formulation of Lighthill's acoustic analogy which results in a Fourier volume integral. These two methods are examined for their computational efficiency, their numerical accuracy and their robustness to perturbed initial data.

References: See separate list.

Title: Simulation of Particle-laden Flows

Researchers: Rolf Henniger, Leonhard Kleiser

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

Description:

This project is concerned with the direct numerical simulation and the large eddy simulation of miscible fluid flows with steep concentration gradients. Our focus is on particle-driven gravity currents which form when a heavier fluid propagates into a lighter one. In the case of particle-driven gravity currents, the density difference is caused by a differential loading of the fluid with small suspended particles. The prediction of such flows is important not only from a fundamental scientific point of view, but also with respect to environmental and industrial applications such as turbidity currents in lakes or oceans, powder snow avalanches, or settling of particles in sedimentation tanks.
For this purpose, a high-order accurate simulation code for the incompressible Navier-Stokes equations has been developed which is suitable for massively parallel computers. It is based on a finite-difference discretization in space and a semi-implicit integration scheme in time. Velocity components and pressure are calculated on a staggered grid. The elliptical problem is solved in an iterative manner, split into inner and outer iteration cycles, such that the momentum and continuity equations are accurately satisfied. The inner iteration cycle is similar to a discrete Poisson problem with Neumann boundary conditions. We employ a multigrid procedure with Processor Block Gauss-Seidel smoothing. In addition, the rate of convergence is accelerated by a Krylov subspace method (BiCGStab) which utilizes the multigrid algorithm as a preconditioner.
The particles are described in an Eulerian framework and are represented as a concentration field, for which a transport equation is solved. Similar to the fluid phase, the transport equation is discretized with finite differences in space and a semi-implicit integration scheme in time.

References: See separate list.

Title: Fluid mechanics of benign paroxysmal positional vertigo (BPPV)

Researchers: Leonhard Kleiser, Dominik Obrist, Stefan Hegemann*

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

* Dept. of Otorhinolaryngology, University Hospital Zurich

Description:

Sedimenting particles in the semicircular canals 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.
We developed an analytical model for BPPV in an idealized representation of a semicircular canal. This model was studied extensively by numerical and analytical methods. Based on these results we devised a concept for the numerical simulation of the full fluid mechanics of BPPV. This concept includes the simulation of following aspects of BPPV:

- The three-dimensional Stokes flow in a morphologically accurate model of a human semicircular canal.
- The particle dynamics and their interaction with each other, with the fluid and with the canal walls.
- The deflection of the cupula (a gelatinous structure inside the canal) due to the particulate flow.

Over the course of the past year we performed several studies to investigate whether the proposed numerical methods yield satisfying results in terms of numerical accuracy and robustness.
We proposed to use the method of fundamental solutions (MFS) for the three-dimensional simulation of the Stokes flow. On the one hand, this method yields spectral convergence. On the other hand, we found that MFS exhibits a numerical instability which appears to contradict some of the results reported in the literature. We were able to derive an explicit upper bound which characterizes this instability. This error bound shows that the instability is tightly connected to the singular value decomposition of the MFS system matrix. We found that the boundary condition must be well contained in the space spanned by the left singular vectors. Otherwise, truncation errors will occur and the numerical instability will be triggered.
Apart form this, we investigated ways to regularize MFS and we tested the quality of the proposed particle model in connection with MFS. A physical experiment for BPPV (developed simultaneously at IFD) serves as a guidance and tool for the development and validation of our numerical simulation of BPPV.

References: See separate list.

Title: Models for entangled polymeric systems, filamentous physical and chemical gels

Researchers: Prof. Martin Kröger [1]
Prof. Yitzhak Rabin [2]
Prof. Vlasis Mavrantzas [3]
Prof. Sachin Shanbhag [4]

Institutes: [1] Computational Polymer Physics, D-MATL, ETH Zürich
[2] Tel Aviv University, Israel
[3] University of Patras, Greece
[4] School of Computational Science, Florida, U.S.A.

Description:

We established a buttom-up multiscale approach for dendronized polymers by introducing the Janus Chain model [1], which adds a vectorial degree of freedom (Janus vector) - related to the sectorial amphiphilicity - to each segment of the linear backbone of a (classical) uncharged, semiflexible, multibead chain representation of a polymer. The JC features induced-spontaneous polymeric curvature ultimately triggering complexation. JC parameters related to the topology and chemical details are obtained from the atomistic level. The model exhibits the formation of superstructures and double-helical conformations; it is efficiently solved via Brownian dynamics simulation, and can be seen as a member of a universality class which is one (two) levels above the magnetic (semiflexible) chain model. It therefore should allow to model not only dendronized polymers, but also structures belonging to the same class - exhibiting spontaneous curvature - such as single stranded DNA. Existing methods to obtain the primitive path network for monodisperse, linear polymers in the molten state have been applied and critically compared [2,3]. We introduced a toy model that contains the basic features of microphase separation in polymer gels: a stretched elastic network of Lennard-Jones particles, studied in two dimensions [4].

References:

[1] Y. Ding, H.C. Öttinger, A.D. Schlüter, M. Kröger, From atomistic simulation to the dynamics, structure and helical network formation of dendronized polymers: The Janus chain model, J. Chem. Phys. **127** (2007) 094904.

[2] S. Shanbhag, M. Kröger, Primitive path networks generated by annealing and geometrical methods: Insights into differences, Macromolecules **40** (2007) 2897.

[3] K. Foteinopoulou, N.C. Karayiannis, V.G. Mavrantzas, M. Kröger, Primitive path identification and entanglement statistics in polymer melts: Results from direct topological analysis on atomistic polyethylene models, Macromolecules 39 (2006) 4207.

[4] O. Peleg, M. Kröger, I. Hecht, Y. Rabin Filamentous networks in phase-separating two-dimensional gels, EPL 77 (2007) 58007.

Title: Suitability of IBM CELL and other multi-core processors for numerical simulations

Researcher: Wes Petersen

Institute: Seminar for Applied Mathematics

ETH Zürich

Description:

In quickly changing technologies, we must strive to understand which developments will serve our needs in scientific computing. Just as microprocessors, largely developed for a business environment, subsumed custom designed processors by 1990, parallelism and power costs push us to examine other strategies for the future. In particular, IBM **CELL** processors and Intel and AMD multi-core chips offer high performance, low cost, and low power consumption.

A group of RW (Rechnergestutzte Wissenschaft), and physics undergraduate/graduate students are now experimenting with CELL processors in the form of PlayStation-3's. With evolving degrees of participation, students Christine Tobler, Denis Nordmann, Franois Gaignat, Stephan Gammeter, Kaspar Mller, Lukas Gamper, Mauro Calderara, Patrick Mchler, Robin Krom from ETH; Jonathan Coles and Alessandro Viretta from Univ. Zürich have been meeting and discussing work on our little 4-PS3 cluster. A website `cubits.ch` was set up, and at least two projects have been completed.

In a test project, three of the above student group, Mauro Calderara, Jonathan Coles, and Franois Gaignat, wrote some high-precision (128-bit) arithmetic primitives for the CELL slave processors (SPUs, there are 8). Coles wrote the $(+, -)$ operations and Gaignat wrote the multiply. Reports on these results are being written, and one, Gaignat's, is done. Calderara, who put together some tests for the arithmetic, also ported `Open MPI` to the cluster, connected by Ethernet.

Encouragement and support for these activities come from professors Rolf Jeltsch, Daniel Kressner, Wes Petersen, and Jörg Waldvogel of SAM; Matthias Troyer from ITP; and George Lake from Univ. Zürich. Other interested parties now involved are from the WR program in Informatik.

Reference:

Franois Gaignat *Multiplication of hfn numbers*, project report, Oct. 2007.

Title: Asset pricing for idiosyncratically incomplete markets

Researchers: Semyon Malamud
Eugene Trubowitz
Wesley P. Petersen

Department: Dept. of Mathematics, ETHZ

Description:

A model of idiosyncratically incomplete markets with heterogeneous agents has been produced by Malamud and Trubowitz. Their approximate solutions are based on a perturbation approach with an expansion parameter ϵ which measures the degree of inhomogeneity. Their model is an extension of work by Constantinides and Duffie from 1996, but one which allows for trade and other generalizations.

Numerical Monte-Carlo calculations permit non-perturbative solutions while allowing us to study the limits of $O(\epsilon^2)$ results. Our simulations compute explicit economic parameters from both perturbation formulae and non-perturbative numerical solutions of the model. We find good agreement to $\epsilon \approx 1/10$ and qualitative agreement to about twice this value. The model and its computed solutions also permit study of certain *stylized facts* (e.g. Campbell and Cochrane, 1999) taken from market observations. Our tests are being run on the ETH Beowulf clusters *Hraidar* and *Gonzales*.

References: S. Malamud, W. Petersen and E. Trubowitz, *Asset Pricing in Strongly Heterogeneous Economies*, ETHZ (2006-7), in preparation.
G. M. Constantinides and D. Duffie, J. of Political Economy, 104 (2), p.219–240 (1996).

Title: Theory and Molecular Spectroscopy of the Parity Violating Electroweak Interaction: Signatures in Rovibrational Spectra of Polyatomic Molecules

Researchers: J. Stohner*
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Institute/Group: * Zürich University of Applied Sciences (ZHW), Institute of Chemistry and Biotechnology ICB, Winterthur
** Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Different from previous assumptions we know now, that the energy of enantiomers in an achiral environment is not identical. The status of calculations on such parity violating energy differences between enantiomers is reviewed briefly. [1, 2]

References:

[1] M. Quack und J. Stohner, Trendbericht Physikalische Chemie 2005, Nachrichten aus der Chemie **54**, 282 – 284
[2] J. Stohner and M. Quack, in "Recent Progress in Computational Sciences and Engineering", Lecture Series on Computer and Computational Sciences, (Proceedings of the ICCMSE, Chania, Crete, 26.10.-12.11.2006), Vol. **7B**, pages 968 – 972, (Theodore Simos and George Maroulis eds), Brill Academic Publishers, Leiden 2006 (ISBN 10: 90 04 15542 2, ISBN 13: 978 9004155 42 2)

Title: Mode selective tunneling dynamics observed by high resolution spectroscopy of the bending fundamentals of $^{14}NH_2D$ and $^{14}ND_2H$

Researchers: M. Snels*
H. Hollenstein**
M. Quack**

Institute/Group: * Istituto di Scienze dell'Atmosfera e del Clima, Sezione di Roma, CNR, Roma, Italy
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

High resolution (0.004 and 0.01 cm^{-1} instrumental bandwidth) interferometric Fourier transform infrared spectra of $^{14}NH_2D$ and $^{14}ND_2H$ were measured on a Bomem DA002 spectrometer in a supersonic jet expansion and at room temperature. We report the analysis of the bending fundamentals of $^{14}NH_2D$ with term values $T_v(s)$ = 1389.9063(2) cm^{-1} and $T_v(a)$ = 1390.4953(2) cm^{-1} for the ν_{4b} fundamental and $T_v(s)$ = 1605.6404(7) cm^{-1} and $T_v(a)$ = =1591.0019(7) cm^{-1} for the ν_{4a} fundamental, and of $^{14}ND_2H$ with term values of $T_v(s)$ = 1233.3740(2) cm^{-1} and $T_v(a)$ = =1235.8904(2) cm^{-1} for the ν_{4a} fundamental and $T_v(s)$ = 1461.7941(9) cm^{-1} and $T_v(a)$ = 1461.9918(19) cm^{-1} for the ν_{4b} fundamental. In all cases $T_v(s)$ gives the position of the symmetric inversion sublevel (with positive parity) and $T_v(a)$ the position of the antisymmetric inversion sublevel (with negative parity). The notation for the fundamentals ν_{4a} and ν_{4b} is chosen by correlation with the degenerate ν_4 mode in the C_{3v} symmetric molecules NH_3 and ND_3. The degeneracy is lifted in C_s symmetry and *a* indicates the symmetric, *b* the antisymmetric normal mode with respect to the C_s symmetry plane in NH_2D and ND_2H. Assignments were established with certainty by means of ground state combination differences. About 20 molecular parameters of the effective *S*-reduced Hamiltonian could be determined accurately for each fundamental. In particular, the effect of Fermi resonances of the $2\nu_2$ overtone with the ν_{4a} bending mode was observed, leading to an increased inversion splitting in the case of ND_2H and to a strongly increased inversion splitting and an inverted order of the two inversion levels in NH_2D. Rotational perturbations observed with the ν_{4b} bending fundamentals are probably due to Coriolis interactions with the inversion overtone $2\nu_2$. The results are important for understanding isotope effects on the inversion in ammonia as well as its selective catalysis and inhibition by excitation of different vibrational modes, as treated by quantum dynamics on high dimensional potential hypersurfaces of this molecule. Extensive computations are necessary for the analyses of such processes.

References:

[1] . M. Snels, H. Hollenstein, M. Quack, J. Chem. Phys. **125**, 194319-1 – 194319-12 (2006)

Title: High-resolution rovibrational analysis of vibrational states of A_2 symmetry of the dideuterated methane CH_2D_2: the levels ν_5 and $\nu_7 + \nu_9$

Researchers: O. N. Ulenikov*
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S. V. Grebneva*
H. Hollenstein**
M. Quack**

Institute/Group: * Laboratory of Molecular Spectroscopy, Department of Physics, Tomsk State University, RU - 634050 Tomsk
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

The infrared spectrum of the CH_2D_2 molecule has been measured in the region 900 – 1500 cm^{-1} on a Bomem DA002 Fourier transform spectrometer with a resolution of 0.0024 cm^{-1} (FWHM, unapodized). Transitions belonging to the hot bands $\nu_7 + \nu_9 - \nu_7$, $\nu_7 + \nu_9 - \nu_9$, $\nu_5 + \nu_7 - \nu_5$ and $\nu_5 + \nu_9 - \nu_5$ were extracted from the recorded spectra to determine the rovibrational energies of the A_2 symmetry vibrational states ($\nu_7 = \nu_9 = 1$) at 2329.698 cm^{-1} and ($\nu_5 = 1$) at 1331.409 cm^{-1}. Vibrational energies as well as rotational and centrifugal distortion parameters of the ($\nu_7 = \nu_9 = 1$) and ($\nu_5 = 1$) states were determined that reproduce the experimental rovibrational energy levels of the ($\nu_7 = \nu_9 = 1$) and ($\nu_5 = 1$) vibrational states with a d_{rms} deviation of 0.0017 and 0.0006 cm^{-1}, respectively. The results are discussed in relation to the equilibrium structure of methane, which is redetermined here from the experimental data, and in relation to its potential hypersurface and anharmonic vibrational dynamics. Extensive computations are necessary in the analyses of the data.

References:

[1] O. N. Ulenikov, E. S. Bekhtereva, S. V. Grebneva, H. Hollenstein, and M. Quack, Mol. Phys. **104**, 3371 – 3386 (2006)

Title: High sensitivity femtosecond gas phase pump-probe experiments using a hollow waveguide: intramolecular redistribution processes in CH_3I

Researchers: V N. Krylov*
A. Kushnarenko**
E. Miloglyadov**
M. Quack**
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** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Pump-probe experiments using a delay line are one important approach in the investigation of molecular dynamics on the femtosecond to picosecond time scale. As the pulse energies for femtosecond pulses are usually small, the measured signal has to be obtained from the overlap region of two focused laser beams. Due to the low density in the gas phase high sensitivity experiments are essential, particularly if one or both laser pulses are in the infrared (IR) or near-IR range with much smaller absorption cross section as compared to the visible or ultraviolet (UV). To increase the interaction volume between pump- and probe-pulse, the two laser beams can be focused into a hollow waveguide with an inner diameter d_{ID} = 100 to 500 μm. We have calculated the focusing condition for a near-IR pump- and an ultraviolet (UV) probe-beam to excite nearly exclusively the lowest HE_{11}-mode within the waveguide. For molecular samples with a low absorption coefficient ($\alpha < 0.1$ m^{-1} for the probe beam in the ultraviolet) an enhancement of the measured probe signal of a factor of 9 – 10, relative to a confocal arrangement in a cell is calculated from the intensity distribution within a hollow waveguide with an inner diameter d_{ID} = 250 μm and length L_{wg} = 500 mm. The theoretical calculations were confirmed in pump- probe experiments of intramolecular vibrational energy redistribution (IVR) in CH_3I vapour. In the experiments the first overtone of the CH-stretching vibration is excited with a near-IR pump-pulse and the redistribution of the vibrational energy to other vibrational degrees of freedom, especially to the CI-stretching vibration, is detected through a change of the UV-spectrum by a probe pulse around 310 nm.

References:

[1] V N. Krylov, A. Kushnarenko, E. Miloglyadov, M. Quack, G. Seyfang, In "Commercial and Biomedical Applications of Ultrafast Lasers VII", (Proceedings, Photonics West 2007; 20 – 25 Jan 2007, San Jose California), Proceedings of SPIE Volume 6460, Nr. 64601D-1 – 64601D-11 (Joseph Neev, Stefan Nolte, Alexander Heisterkamp, Christopher B. Schaffer Editors, SPIE, ISBN 9780819465733).

Title: Rovibrational analysis of the $2\nu_3$, $3\nu_3$ and ν_1 bands of $CHCl_2F$ measured at 170 and 298 K

Researchers: S. Albert*
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M. Quack*
Andreas Steinlin***

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

We report the infrared spectrum of fluorodichloromethane ($CHCl_2F$, HCFC21), measured with the Bruker IFS 125 HR Zürich~Prototype (ZP) 2001 interferometric Fourier transform infrared (FTIR) spectrometer at room temperature, and at 170 K in a collisional and enclosive temperature adjustable cooling cell designed with White-type multireflection optics and effective optical path lengths of 10 to 17.5 m. The spectra were recorded with effective resolutions of 0.0011 to 0.0017 cm^{-1} (maximum optical path difference (MOPD) is 10 m) in the range 1900 – 3600 cm^{-1}. The spectrum was analysed using an effective Hamiltonian in the $2\nu_3$ region of $CH^{35}Cl_2F$ (band center $\tilde{\nu}_0$ = 2140.084 6 cm^{-1}) and $CH^{35}Cl^{37}ClF$ ($\tilde{\nu}_0$ = 2139.991 8 cm^{-1}, the $3\nu_3$ region of $CH^{35}Cl_2F$ ($\tilde{\nu}_0$ = 3182.361 8 cm^{-1}) and $CH^{35}Cl^{37}ClF$ ($\tilde{\nu}_0$ = 3182.166 2 cm^{-1}) and in the ν_1 region of $CH^{35}Cl_2F$ ($\tilde{\nu}_0$ = 3024.016 2 cm^{-1}). About 14000 rovibrational lines were assigned overall. These are tabulated separately in a supplementary publication. Local perturbations have been identified in most of the bands. A dark state coupled through a *c*-type Coriolis resonance to the $3\nu_3$ state of $CH^{35}Cl_2F$ has been identified with a band center of $\tilde{\nu}_0$ = 3189.62 cm^{-1} and a coupling constant of ξ_c = 0.0103 cm^{-1} ($3\nu_3$/dark state). The results are discussed in relation to atmospheric trace gas absorption, intramolecular vibrational-rotational redistribution processes and to molecular parity violation in the case of the isotopically chiral isotopomer $CH^{35}Cl^{37}ClF$. Extensive computations are carried out in the analyses of the data.

References:

[1] S. Albert, S. Bauerecker, M. Quack, Andreas Steinlin, Mol. Phys. **105**, 541 – 558 (2007)

Title: High resolution rovibrational spectroscopy of chiral and aromatic compounds

Researchers: S. Albert
M. Quack

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

Description:

The analysis of selected rovibrationally resolved infrared spectra of some relatively heavy and large polyatomic molecules is reviewed. A short historical summary of the development of high resolution interferometric Fourier transform infrared (FTIR) spectrometers is given and the possibilities of the currently most highly resolving FTIR spectrometer, which is commercially available in the Bruker IFS 125 series, are discussed. The computational tools necessary to analyse FTIR spectra are described briefly. As examples of rovibrational analysis the spectra of three selected molecules $CHCl_2F$, CDBrClF, and pyridine (C_5H_5N) are discussed.
The spectrum of $CHCl_2F$, a fluorochlorohydrocarbon, is of interest for a better understanding of the chemistry of the Earth's atmosphere. CDBrClF is a chiral molecule and therefore the analysis of its rovibrational spectra provides the basis for carrying out further experiments towards the detection of molecular parity violation. The analysis of the pyridine FTIR spectra illustrates the potential of the new generation of FTIR spectrometers in the study of spectra and rovibrational dynamics of aromatic systems and molecules of potential biological interest.

References:
[1] S. Albert and M. Quack, ChemPhysChem **8**, 1271 – 1281 (2007)

Title: High resolution rovibrational spectroscopy of pyrimidine. Analysis of the B_1 modes ν_{10b} and ν_4 and the B_2 mode ν_{6b}.

Researchers: S. Albert
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Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

We report the first high resolution rovibrational analysis of the infrared spectrum of pyrimidine ($C_4H_4N_2$) based on measurements using our Fourier transform spectrometer, the Bruker IFS 125 HR Zürich Prototype (ZP) 2001. Measurements were conducted at room temperature in a White-type cell with effective optical pathlengths between 3.2 and 9.6 m and with resolutions ranging from 0.0008 to 0.0018 cm^{-1} in the region between 600 and 1000 cm^{-1}. The spectrum was analyzed in the ν_4 ($\tilde{\nu}_0$ = 718.5411 cm^{-1}), ν_{10b} ($\tilde{\nu}_0$ = 803.97948 cm^{-1}) and ν_{6b} regions of pyrimidine ($\tilde{\nu}_0$ = 620.54970 cm^{-1}) using an effective Hamiltonian. A total of about 15000 rovibrational transitions were assigned. The root mean square deviations of the fitted data are in the ranges d_{rms} = 0.00018 – 0.00024 cm^{-1}, indicating an excellent agreement of experimental line data with the calculations. The results are discussed briefly in relation to possible extensions to spectra of DNA bases and to intramolecular vibrational redistribution at higher energy. The analysis of the ν_{10b} and ν_4 bands will also be useful in the interstellar search for pyrimidine in the infrared region. Extensive computations are needed in the analyses of the data.

References:

[1] S. Albert and M. Quack, J. Mol. Spectrosc. **243**, 280 – 291 (2007)

Title: Quantities, Units and Symbols in Physical Chemistry, Third Edition
IUPAC and Royal Society of Chemistry, RSC, Cambridge (2007)
(Book with 250 pages, ISBN 978-0-85404-433-7)

Researchers: E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack*, J. Stohner*, H. L. Strauss, M Takami, A. Thor

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

Description:
This book with contributions from numerous authors all over the world in institutions, which are not all listed here, summarizes a most up to date set of data, nomenclature, definitions and recommendations important for physical chemistry and chemical physics, including computational chemistry and physics.

References:
[1] E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. Thor
Quantities, Units and Symbols in Physical Chemistry, Third Edition
IUPAC and Royal Society of Chemistry, RSC, Cambridge (2007)
(Book with 250 pages, ISBN 978-0-85404-433-7)

Title: Spectroscopic properties of trichlorofluoromethane CCl_3F calculated by density functional theory

Researchers: O. A. von Lilienfeld*
C. Léonard**
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M. Willeke*****
M. Quack *****

Institute/Group:
* New York University, Department of Chemistry, New York, New York 10003
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*** University of Cambridge, Dept. of Theoretical Chemistry, Lensfield Road
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***** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Trichlorofluoromethane is one of the most important anthropogenic pollutants in the earth's atmosphere. It acts both in the destruction of the ozone layer and, because of its strong "atmospheric window" band in the infrared arount 1100 cm^{-1} as a greenhouse gas with enormous global warming potential.

Density functional theory is used to generate local potential energy surfaces in normal coordinates for several chlorine isotopomers of trichlorofluoromethane (CCl_3F,CFC11). An examination of predicted structures suggested that the PBE0 functional would be suitable. Anharmonic surfaces around the equilibrium geometries are reported, as determined by energies, gradients, and second derivatives. Vibrational levels for fundamentals, overtones and combination bands are reported, as well as harmonic frequencies, anharmonic constants, rotational constants, isotope shifts, and infrared intensities. These are compared with experimental information.

References:

[1] O. A. von Lilienfeld, C. Léonard, N. C. Handy, S. Carter, M. Willeke, and M. Quack, Phys. Chem. Chem. Phys. (PCCP) 9, 5027 – 5035 (2007)

Title: Stereomutation Dynamics in Hydrogen Peroxide

Researchers: B. Fehrensen
D. Luckhaus*
M. Quack

Institute/Group: * University of British Columbia, Department of Chemistry, Vancouver, B.C. V6T 1Z1, Canada
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich

Description:

Hydrogen peroxide (H–O–O–H) is among the simplest prototype molecules showing a chiral equilibrium geometry with the possibility of fast quantum stereomutation in the low barrier limit. We report full dimensional quantum dynamical tunneling calculations on a semi-global fully six-dimensional empirically adjusted potential hypersurface for H_2O_2, which is realistically close to spectroscopic and thermochemical accuracy [1]. Solutions of the time independent Schrödinger equation lead to levels of well defined parity (but undefined chirality), which compare well with available spectroscopic results and provide numerous predictions. Solutions of the time-dependent Schrödinger equation with initial conditions of well defined chirality for P and M enantiomers show the time dependent wavepacket motion and periodic change of chirality for time scales between picoseconds and hundreds of picoseconds. Complete six-dimensional dynamics and adiabatic separation of the torsional mode from the high-frequency modes leads to essentially identical results for the stereomutation dynamics in terms of the relevant time dependence. Mode selective inhibition and catalysis of stereomutation by exciting various vibrationally excited levels are reported and discussed in relation to the concept of quasiadiabatic above barrier tunneling. The transition to relaxation behaviour and racemisation is demonstrated with quasithermal wavepackets and analysed in terms of a simple statistical model. At 3000 K the racemisation relaxation time is calculated to be 30 fs. We also discuss the results in the context of recent results on hydrogen peroxide as a prototype system for parity violation in chiral molecules.

References:

[1] B. Kuhn, T. R. Rizzo, D. Luckhaus, M. Quack, M. A. Suhm, J. Chem. Phys. **111,** 2565 – 2587 (1999)
[2] B. Fehrensen, D. Luckhaus, M. Quack, Chem. Phys. **338**, 90 – 105 (2007)

Title: High Resolution FTIR and Diode Laser Supersonic Jet Spectroscopy of the $N = 2$ HF-stretching polyad in $(HF)_2$ und (HFDF): Hydrogen Bond switching and Predissociation Dynamics

Researchers: Y. He*
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M. Quack**
M. A. Suhm***

Institute/Group: * Macquarie University, Department of Physics, Centre for Lasers & Applications, Sydney, NSW 2109
** Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
*** Universität Göttingen, Institut für Physikalische Chemie, DE - 37077 Göttingen

Description:

We report Fourier Transform Infrared (FTIR) and high resolution diode laser spectra (~ 1 MHz} instrumental bandwidth) obtained in cooled absorption cells as well as in a supersonic jet expansion for the $N = 2$ polyad region of the HF-stretching vibrations of $(HF)_2$, HFDF and DFHF. Three vibrational transitions have been observed for $(HF)_2$ and two for both monodeuterated isotopomers. For $(HF)_2$ we have identified and analysed the observed transitions of the polyad member 2_2 of the type $\Delta K_a = 0$ and $\Delta K_a = \pm 1$ up to rotational sublevel $K_a = 3$. Band centers as well as rotational constants of all three K_a states have been determined. The tunneling splittings due to hydrogen bond switching for these four K_a states have been investigated, with the $K_a = 0$ up to $K_a = 2$ sublevels having tunneling symmetry $\Gamma_{vt} = A^+$ for the lower tunneling states, and switching periods ranging from 158 ps for $K_a = 0$ to 1.35 ns for $K_a = 2$. A tunneling level inversion is found at $K_a = 3$, leading to a symmetry $\Gamma_{vt} = B^+$ for the lower tunneling state of this K_a-sublevel. The vibrational assignment of the measured spectra of $(HF)_2$ was established by comparison with the monodeuterated isotopomers HFDF and DFHF. For HFDF we have identified and analysed five subbands between 7600 cm^{-1} and 7730 cm^{-1}. We have determined the spectroscopic constants of the rotational levels $K_a = 0$ and $K_a = 1$ for the vibrationally excited state and of the levels of $K_a = 1$ and $K_a = 2$ of the ground state, the latter from combination differences. From the measurements in a supersonic jet expansion we determined the predissociation line width of the $N = 2_2$, $K_a = 1$ to be about 120 MHz for the $\Gamma_{vt} = A^+$ tunneling state of $(HF)_2$ and about 90 MHz for $\Gamma_{vt} = B^+$. For the $K_a = 0$ level of $N = 2_2$ we obtained a predissociation line widths ranging around 100 MHz, similar to those of the $K_a = 1$ level. In the case of HFDF, the predissociation line width of $K_a = 1$ is about 80 MHz. Predissociation lifetimes for these levels with the unbounded HF stretching excited thus are in the range of about 1 to 2 ns. The predissociation width in the $N = 2_1$ level is uncertain by about a factor three with $\lg(\Delta\nu / \text{MHz}) = (3 \pm 0.5)$ and in $N = 2_3$ it is about 600 MHz corresponding to rounded lifetimes of 0.1 ns and 0.3 ns when the bounded HF stretching is excited thereby demonstrating strongly mode selective predissociation rates in the $N = 2$ polyad. Under thermal equilibrium conditions we derived the pressure broadening coefficient for $(HF)_2$ ($\gamma = 6 \pm 1 \cdot 10^{-4}$ cm^{-1}/mbar in the frequency range between 7713 cm^{-1} and 7721 cm^{-1} for total gas

pressures between 10 and 60 mbar, all values as full widths half maximum). For absolute frequency calibrations we have remeasured the first overtone transitions of the monomer HF with much improved precision between P(5) (7515.80151 cm^{-1}) and R(7) (7966.22188 cm^{-1}).

References:

[1] Y. He, H. B. Müller, M. Quack, M. A. Suhm, Z. Phys. Chem. **221**, (2007) in press

Title: Studies on the Emergence of Structure in Quantum Mechanics

Researchers: C. Scherrer*
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J. Hutter**
U. Müller-Herold***

Institute/Group: * Laboratory of Physical Chemistry, ETH Zurich
** Institute of Physical Chemistry, University of Zurich
*** Chair of Material Flux and Waste Management, ETH Zurich

Description:

The Schrödinger equation discriminates particles interacting via Coulomb's law only by their masses and charges. Hence, the form of the equation is the same for two protons and an electron (the He^+ ion and the H_2^+ molecule) and for two electrons and one proton (the H^- ion). The structural transition visible in the mass-density when changing the relative magnitude of the masses of two identical particles plus one different particle was investigated. For this purpose, the wave functions of such systems were calculated using a very general formailism and a program that implements the theory of the stochastic variational method (SVM). The SVM allows to compute the wave functions of quantum few-body problems with almost arbitrary accuracy without making any structural assumptions like the Born-Oppenheimer approximation. Results of change of mass density for the transition from H^- to H_2^+ in the $(1s)2$ state were compared with reference results. In the literature, the mass-density calculations for these systems and the transition were carried out analytically[1] while modelling the Coulombic potentials by the $1/r^2$ harmonium model in Born-Oppenheimer approximation.

References: [1] U. Müller-Herold, J. Chem. Phys. 124, 014105 (2006).

Title: Structures of Aryl Calcium Compounds in Ether Solvents

Researchers: Lian Yu*
Markus Reiher*
Matthias Westerhausen**
Martin Gärtner**
Reinald Fischer**
Jens Langer**

Institute/Group: * Laboratorium für Physikalische Chemie, ETH Zürich, Hönggerberg Campus HCI, Wolfgang-Pauli-Str. 10, 8093 Zürich
** Institute of Inorganic and Analytical Chemistry, Friedrich-Schiller-Universität Jena, Germany

Description:

Ogano-alkali-metal chemistry has a long tradition. In 1900 Grignard discovered that organic magnesium compounds are easily accessible through the direct synthesis of organic halides with magnesium metal. Aryl calcium compounds show a very high reactivity and tend to cleave ether solvents already above −35 °C. From NMR spectroscopic data it was concluded that the THF uptake was too low to dissolve the aryl calcium derivatives as monomeric THF adducts. To investigate possible structures of oligomeric aryl calcium iodides and diaryl calcium compounds with respect to solvent effects, we employed quantum chemical DFT and MP2 calculations. The results show that the bridging σ-bound phenyl groups are coordinated in a η^6 mode to the other calcium atom in the optimized dimer and tetramer structures. The tendency of calcium cations to bind to π-electron systems has been shown experimentally for the benzylcalcium derivatives and metallocenes. Regarding the possible structures of diaryl dicalcium, in view of the results obtained for organic metal(I) compounds of zinc and cadmium with metal-metal bonds, we investigated Ca–Ca bonds with correlated ab initio methods like MP2, CC2 and CCSD(T). Our results indicate that the Ca(I)–Ca(I) bond stabilizes the diaryl dicalcium(I) compounds not only for steric but also for electronic reasons. These findings in turn motivated experimental colleagues to look for Ca–Ca bonds.

References: [1] R. Fischer, M. Gärtner, H. Görls, L. Yu, M. Reiher, M. Westerhausen, *Angew. Chem.* **2007**, *119*, 1642–1647, *Angew. Chem. Int. Ed.* **2007**, *46*, 1618–1623.
[2] M. Westerhausen, M. Gärtner, R. Fischer, J. Langer, L. Yu, M. Reiher, *Chem. Eur. J.* **2007**, *13*, 6292–6306.

Title: Topological Analysis of Electron Densities from Kohn–Sham and Subsystem Density Functional Theory

Researchers: Karin Kiewisch
Georg Eickerling
Markus Reiher
Johannes Neugebauer

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, Hönggerberg Campus HCI, Wolfgang-Pauli-Str. 10, 8093 Zürich

Description:

Electron densities for a set of hydrogen-bonded complexes were calculated using either conventional Kohn–Sham density-functional theory (DFT) or the frozen-density embedding (FDE) method, which is a subsystem approach to DFT. For a detailed analysis of the differences between these two methods within DFT we compared the topology of the electron densities obtained in these ways in terms of deformation densities, bond critical points, and the negative Laplacian of the electron density [1]. Different kinetic-energy functionals as needed for the frozen-density embedding method were tested and compared to a purely electrostatic embedding. The results demonstrate that FDE is able to reproduce the characteristics of the density in the bonding region in rather strongly bonded systems like the $F{-}H{-}F^-$ molecule, which contains one of the strongest hydrogen bonds. Basis functions on the frozen system are usually required to accurately reproduce the electron densities of supermolecular calculations. However, we could show that it is in general sufficient to provide just a few basis functions in the boundary region between the two subsystems so that the use of the full supermolecular basis set can be avoided. It also turned out that electron-density deformations upon bonding predicted by FDE lack directionality with currently available functionals for the non-additive kinetic energy contribution.

References: [1] K. Kiewisch, G. Eickerling, M. Reiher, J. Neugebauer, *to be submitted* **2007**.

Title: The Density Matrix Renormalization Group Method Facing the Spin State Problem in Quantum Chemistry

Researchers: Konrad H. Marti
Gerrit Moritz
Irina Malkin Ondík
Markus Reiher

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Description:

In transition metal catalysis, the precise characterization of relative energies is of paramount importance. It is still a challenging task to predict, in particular, energy differences between states of different spin accurately using a wide variety of today's standard quantum chemical methods. To tackle the calculation of relevant transition metal catalysts one is limited to the application of broken-symmetry DFT since other methods are no longer feasible. However, broken-symmetry DFT often exhibits deficiencies in accuracy — apart from conceptual difficulties. In multi-configuration methods, on the other hand, one usually needs a large (often prohibitively large) active space for a qualitatively correct description of the electronic structure. This is highlighted especially in bi- or polynuclear transition metal compounds. The density matrix renormalization group (DMRG) algorithm allows the treatment of a large active space which is by far not reachable using standard ab-initio quantum chemical methods. We investigated the DMRG algorithm as a substitute for CASSCF in cases where CASSCF fails to produce a qualitatively correct electronic structure, i.e., if the required active space is larger than say 18 electrons in 18 spatial orbitals.
For validation purposes, we have studied the relative energies of the spin state splitting between the singlet and triplet state of NiCO and CoH. We have observed for both systems that the relative error of the spin splitting is converging to a constant value by increasing the number of DMRG states [1]. We also showed that DMRG is capable of properly describing the energetics of the binuclear μ-η^2:η^2 peroxo and bis(μ-oxo) copper-oxygen isomers [1]. DMRG calculations were performed for the dicopper-oxygen cores and even for the dicopper-oxygen isomers with six ammine ligands.
The convergence of the DMRG algorithm is difficult to analyze because of the many numerical transformation steps involved. Therefore, our new implementation provides a decomposition of the intermediate and converged DMRG many-particle states in a Slater determinant many-particle basis. We showed that inspecting the total energy alone can be misleading as a decrease of this observable may not necessarily be taken as an indication for the pickup of essential configurations in the CI expansion [2].

References:
[1] K. H. Marti, I. Malkin Ondík, G. Moritz, M. Reiher, *J. Chem. Phys.* **2007**, submitted.
[2] G. Moritz, M. Reiher, *J. Chem. Phys.* **2007**, *126*, 244109.

Title: Analytic High-Order Douglas–Kroll–Hess Electric Field Gradients

Researchers: Remigius Mastalerz[†]
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Markus Reiher[†]

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Description:

The calculation of molecular properties within a scalar-relativistic Douglas–Kroll–Hess (DKH) framework leads to inaccurate results when calculating the desired property from non-DKH-transformed (i.e. non-relativistic) property integrals. An efficient implementation of DKH-transformed property integrals is therefore required to account for this so-called picture change error. In particular the electric field gradient, as a property calculated within a numerical or low-order analytical DKH approach has received special attention in the past few years.
We presented a comprehensive study of analytical electric field gradients in hydrogen halides calculated within the high-order Douglas–Kroll–Hess scalar-relativistic approach taking picture-change effects analytically into account. We demonstrated the technical feasibility and reliability of a high-order DKH unitary transformation for the property integrals. The convergence behavior of the DKH property expansion was discussed close to the basis set limit and conditions ensuring picture-change-corrected results are determined. Numerical results were presented, which show that the DKH property expansion converges rapidly towards the reference values provided by four-component methods. This demonstrates that in closed-shell cases the scalar-relativistic DKH(2,2) approach which is of second order in the external potential for both orbitals and property operator yields a remarkable accuracy. Moreover, the effect of a finite-nucleus model, different parameterization schemes for the unitary matrices and the reliability of standard basis sets were investigated.

References: [1] R. Mastalerz, G. Barone, R. Lindh, M. Reiher, *J. Chem. Phys.* **2007**, *127*, 074105.

Title: Coupled Excitations within a Subsystem Formulation of TDDFT

Researcher: Johannes Neugebauer

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, Hönggerberg Campus HCI, Wolfgang-Pauli-Str. 10, 8093 Zürich

Description:

The investigation of chromophores in functional aggregates, e.g. in light-harvesting complexes, requires the characterization of excited states of very large systems. Subsystem density-functional theory, in particular the frozen-density embedding method, can be applied to efficiently describe a chromophore in a complex environment. However, this method was until recently restricted to local transitions of the embedded molecule, whereas the description of systems with several chromophores requires to consider excitation energy couplings between the subunits [1]. A general subsystem approach to time-dependent density functional theory (TDDFT) was developed, which includes such couplings based on local electronic transitions of the subunits, so that the interpretation of the excitations is greatly simplified. The algorithm can be implemented efficiently, so that couplings are selectively calculated for interacting chromophores [2]. It can thus bridge the gap between TDDFT and model descriptions of excitonic couplings and excitation energy transfer, so that studies of photophysical properties of natural light-harvesting complexes are within reach of this approach [3].

References:

[1] J. Neugebauer, E. J. Baerends, *J. Phys. Chem. A* **2006**, *110*, 8786.
[2] J. Neugebauer, *J. Chem. Phys.* **2007**, *126*, 134116.
[3] J. Neugebauer, *to be submitted* **2007**.

Title: QM/MM modetracking

Researchers: Carmen Herrmann
Johannes Neugebauer
Markus Reiher

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Description:

Our goal was to calculate selected vibrational normal modes and frequencies directly and thus efficiently for extended molecular systems described by quantum mechanics / molecular mechanics (QM/MM) embedding methods [1]. Vibrational spectroscopy, in particular in combination with theoretical predictions, may provide a valuable tool to elucidate the binding of small molecules such as CO, NO, or O2, to the active centers of enzymes. However, a conventional vibrational analysis yields all vibrational normal modes and frequencies of the molecular system under study, and may require an enormous computational effort in case of large molecules, or even make these calculations impossible at all. While the problem of calculating molecular energies for such systems may be solved by using QM/MM techniques, the vibrational problem requires additional methodological concepts. The modetracking protocol [2,3] provides a direct means to calculate only those normal modes which are really of interest, without ever computing the full Hessian matrix. This algorithm has been applied successfully to different problems in theoretical vibrational spectroscopy [3]. It is based on a Davidson-type algorithm, which refines one or several initial, chemically reasonable, guess vibration(s) iteratively up to arbitrary accuracy. The algorithm is implemented in the program AKIRA [4], a parallel meta-program processing energy gradients provided by different quantum chemistry packages such as ADF [5]. For the QM/MM calculations, the AKIRA/ADF interface has been extended. The new implementation was validated for small test molecules by comparisons to full QM/MM vibrational analyses performed with the SNF program [6]. As a proof-of-principle, the new implementation was applied to the CO stretching mode in CO-myoglobin. Furthermore, some technical aspects needed to be addressed, such as the consequences of different QM/MM implementations for the efficiency of mode-tracking calculations and a double-parallel version of the AKIRA/ADF interface.

References:

[1] C. Herrmann, J. Neugebauer, M. Reiher, to be submitted.
[2] M. Reiher, J. Neugebauer, J. Chem. Phys., 2003, 118, 1634-1641.
[3] C. Herrmann, J. Neugebauer, M. Reiher, New J. Chem., 2007, 31, 818-831.
[4] http://www.theochem.ethz.ch/software/akira
[5] Amsterdam Density Functional Program; Theoretical Chemistry, Vrije Universiteit: Amsterdam. http://www.scm.com
[6] http://www.theochem.ethz.ch/software/snf

Title: Relativistic Effects on the Topology of the Electron Density

Researchers: Georg Eickerling[†]
Remigius Mastalerz[†]
Verena Herz[‡]
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Hans-Jörg Himmel[◇]
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Description:

The topological analysis of electron densities obtained either from X-Ray diffraction experiments or from quantum chemical calculations provides detailed insight into the electronic structure of atoms and molecules. Of particular interest is the study of compounds containing (heavy) transition metal elements, which is still a challenge for experiment as well as from a quantum-chemical point of view. Accurate calculations need to take relativistic effects into account explicitly. Regarding the valence electron density distribution, these are often only included indirectly through relativistic effective core potentials. But as different variants of relativistic Hamiltonians have been developed all-electron calculations of heavy elements in combination with various electronic structure methods are feasible. Yet, there was no systematic study of the topology of the total electron density distribution calculated in different relativistic approximations available. We therefore compared different relativistic Hamiltonians with respect to their effect on the electron density in terms of a topological analysis. The Hamiltonians chosen were the four-component Dirac–Fock–Coulomb, the quasi-relativistic two-component zeroth-order regular approximation and the scalar-relativistic Douglas–Kroll–Hess operators.

References: [1] G. Eickerling, R. Mastalerz, V. Herz, W. Scherer, H.-J. Himmel, M. Reiher, *J. Chem. Theory Comput.* **2007**, *in press*

Title: Tracing Products of Photochemical Reactions by Theoretical Resonance Raman Spectroscopy

Researchers: Karin Kiewisch[1]
Stephan Laimgruber[2]
Peter Gilch[2]
Johannes Neugebauer[1]

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Description:

Raman spectroscopy is a powerful technique for the identification of transient species if applied in a time-resolved, resonance-enhanced manner [1,2]. In order to assign the spectra thus obtained to possible intermediates, comparison with calculated spectra is essential. Several approximate approaches to the calculation of resonance Raman spectra exist, all of which can be employed in connection with time-dependent density functional theory (TDDFT) methods [3]. In our work, we compared different approximations for these calculation, e.g., sum-over-states approaches as well as short-time approximations to the excited-state wave-packet dynamics [4,5].
As a model system we considered *o*-Nitrobenzaldehyd (*o*-NBA) and its photochemical products after laser excitation, for which detailed experimental spectra are available [1,2]. Upon photoexcitation of *o*-NBA, the first intermediate observed was identified as a ketene, after which a second intermediate occurs, that finally evolves into a molecule containing a nitroso group. Structure, vibrational frequencies, excitation energies and resonance Raman intensities within the framework of the short-time approximation for *o*-NBA and the intermediate reaction products were obtained from TDDFT calculations. The impact of different assumptions and approximations in the evaluation of the scattering tensor elements was tested for *o*-NBA. Calculated resonance Raman spectra of possible intermediates were then employed to draw conclusions about the identity of the transient photochemical products [5].

References: [1] S. Laimgruber, H. Schachenmayr, B. Schmidt, W. Zinth, P. Gilch, *Appl. Phys. B–Lasers Opt* **2006**, *85*, 557.
[2] S. Laimgruber, W. J. Schreier, T. Schrader, F. Koller, W. Zinth, P. Gilch, *Angew. Chem. Int. Ed.* **2005**, *44*, 7901.
[3] J. Neugebauer, B. A. Hess, *J. Chem. Phys.* **2004**, *120*, 11564.
[4] C. Herrmann, J. Neugebauer, M. Presselt, M. Schmitt, S. Rau, J. Popp, M. Reiher, *J. Phys. Chem. B* **2007**, *111*, 6078.
[5] S. Laimgruber, P. Gilch, K. Kiewisch, J. Neugebauer, *in preparation* **2007**.

Title: Relevance of the Electric-Dipole–Electric-Quadrupole Contribution to Raman Optical Activity Spectra

Researchers: Sandra Luber
Carmen Herrmann
Markus Reiher

Institute/Group: Laboratorium für Physikalische Chemie, ETH Zürich, Hönggerberg Campus HCI, Wolfgang-Pauli-Str. 10, 8093 Zürich

Description:

The determination of the absolute configuration of chiral molecules is of particular importance. In this regard, vibrational Raman Optical Activity (ROA) spectroscopy is a well-established technique, which measures the intensity difference between scattered right- and left-circularly polarized light. Since generally applicable rules about the relationship of the molecular structure to the corresponding measured intensity differences are missing, quantum chemical calculations of the ROA spectra are needed for the interpretation of the experimental spectra.
The theoretical description of ROA spectroscopy involves three generalized polarizability tensors, the electric-dipole–electric-dipole, the electric-dipole–magnetic-dipole, and the electric-dipole–electric-quadrupole polarizability tensors. Interestingly, not all of these tensors contribute to the spectrum after rotational averaging in equal shares. In the literature, different statements have been made concerning the relative importance of these tensors. We studied their mutual relationship and relative importance. For the contributions of the electric-dipole–electric-quadrupole tensor (so-called A-tensor), a comparison of ROA spectra calculated with and without the contribution of the A-tensor was performed. The statistical analysis of the corresponding data relied on a test set of organic molecules. The DFT calculations were carried out with the vibrational spectroscopy program package Snf in combination with the Dalton quantum chemistry package.
For all molecules, basically one common pattern was found. If the contributions of the electric-dipole–electric-quadrupole tensor are neglected, the spectra experience only a small change. This is especially valid for the wavenumber region below 2000 cm^{-1}, which is the one usually measured in ROA experiments. At higher wavenumbers stretching modes of hydrogen atoms bound to carbon atoms occur, which often show a sign inversion of the corresponding intensity differences or at least a remarkable change in the magnitudes of the intensity difference if the A-tensor contribution is dropped.

References: [1] S. Luber, C. Herrmann, M. Reiher, *J. Phys. Chem. A* **2007**, submitted.

Title: First–Principles Investigation of the Schrock Mechanism of Dinitrogen Reduction

Researchers: Stephan Schenk*
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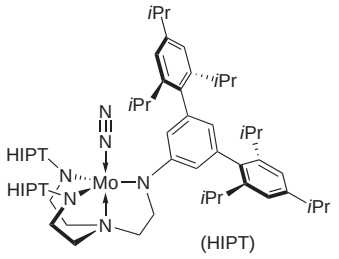
**Universität Leipzig, Lehrstuhl für Theoretische Chemie, Linnestr. 2, D-04103 Leipzig

Description:

Nitrogen plays a very important role in life. Unfortunately, it cannot be used in its most redundant form dinitrogen, N_2, but has to be reduced first to ammonia (a process that is called nitrogen fixation). Nature accomplishes this task by means of the nitrogenase enzymes. On an industrial scale, ammonia is consumed in the fabrication of fertilizers crucial for sustaining the world crop production. Ammonia is traditionally obtained by the Haber–Bosch process through reaction of molecular nitrogen and hydrogen at elevated pressure and temperature at metal oxide surfaces. Since this process requires huge amounts of energy, an efficient catalyst working at ambient conditions is desirable. In 2003, Schrock *et al.* reported the first successful catalytic cycle employing a molybdenum complex (see figure below) in the presence of an electron and proton source [1]. We investigated the intriguing details of this catalytic mechanism applying density functional methods [2]. Our data shows that replacement of the bulky HIPT substituent by smaller groups leads to errors up to $100\,\mathrm{kJmol^{-1}}$. During the generation of the first molecule of ammonia, protonation of the ligand plays an important role. With increasing number of hydrogens on the terminal nitrogen atom, the reduction becomes more and more difficult. The energetically most feasible step is the generation of the first molecule of ammonia. Reaction energies were not only reported for the usually applied reductant decamethyl chromocene but also for a series of other metallocenes. Furthermore, data has been provided in such a way as to allow for a convenient estimation of the feasibility of the catalysis with an arbitrary combination of proton and electron sources.



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.* **2007**, submitted.

Title: Modeling Weather and Climate on European and Alpine scales

Researchers: Bodo Ahrens, Peter Brockhaus, Erich Fischer, Martin Hirschi, Cathy Hohenegger, Simon Jaun, Eric Jäger, Daniel Lüthi, Christoph Schär, Reinhard Schiemann, Sonia I. Seneviratne, Reto Stöckli, Mark Verbunt

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

Description:

Our research is directed towards continental and Alpine-scale weather and climate, with special focus on the water cycle. A broad continuum of temporal scales (from short-range weather forecasting to climate change) and horizontal resolutions (horizontal grid spacing between 1 to 50 kilometers) is considered. Research on climate aspects is dedicated to the study of natural and anthropogenic climate variations on seasonal to centennial time scales. The main thrust of our recent work is dedicated to the understanding and simulation of the European summer climate. In recent work we have mostly used the CLM/COSMO limited-area atmospheric model. Specific studies involving HPC resources have addressed

- aspects of a comprehensive European-scale climate change scenario conducted at a horizontal resolution of 50 km,
- predictability studies for weather forecasting purposes at a cloud-resolving resolution of 2 km,
- ensemble experiments with a coupled meteorological / hydrological forecasting system addressing the forecasting of extreme flood events in the Alpine region, and
- process studies related to the European summer climate.

One of the key results of our climate modeling work relates to the dynamics of extreme European summer heat waves. Using a series of experiments, we have isolated and quantified the role of soil moisture conditions on the development of heat waves for a series of past heat wave events (including the summer 2003). The results of these studies are consistent with our earlier research using climate change scenarios. We are also studying the role of moist convection for the European summer climate using parameterized and explicit representations of convection.

In the area of weather forecasting, our results show that the atmospheric predictability in cloud-resolving short-range forecasting is fundamentally distinct from that in synoptic-scale medium-range forecasting, to the extent that the emergence of nonlinear effects in the two systems scales differently. This result is of considerable theoretical interest and has practical implications, but is not yet fully understood.

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

Title: Simulations for High Current Arc Plasmas

Researchers: Prof. Rolf Jeltsch
Prof. Christoph Schwab
Prof. Ralf Hiptmair
Prof. Manuel Torrihon
Dr. Vincent Wheatley
Patrick Huguenot
Harish Kumar
Gisela Widmer

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 a 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.

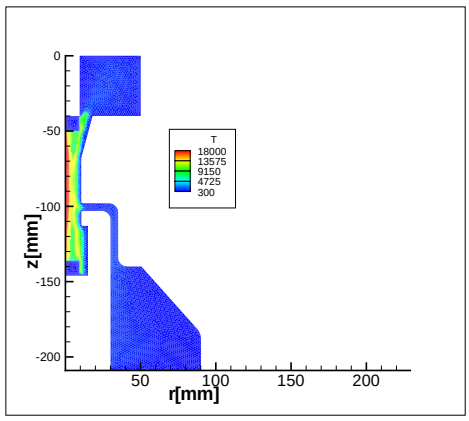


Figure 1: Temperature distribution in an axisymmetric circuit breaker simulation.

In this project we are attempting to model these phenomena. We consider the equations of magnetohydrodynamics, these describe the flow of plasma in the presence of a magnetic field along with evolution of that field. These equations are to be solved numerically in realistic, complex circuit breaker geometries using Discontinuous-Galerkin methods. The domain is initially filled with SF6. We begin our computations after anode and cathode are fully separated and a core of ionized gas exists between these two. The strong electric field between the contacts drives the high arc current, which dissipates large amount of energy further ionizing the gas and raising the pressure in the heating volume. When the current decays during the AC cycle, the high pressure in the heating volume drives the plasma flow which extinguishes the arc.

In order to successfully simulate this process, we must establish what physical mechanisms are important in the flow. For example, the importance of radiation, turbulence and real gas effects must be studied. We must then assess what numerical methods can best be used to capture these mechanisms. Finally these methods will be implemented to develop a simulation tool that can be used to study the details of the operation of gas circuit breakers.

Title: Efficient pricing under multiscale stochastic volatility models

Researchers: N. Hilber
Prof. C. Schwab

Institute/ Group: Seminar of Applied Mathematics
Department of Mathematics

Description:

The fast numerical valuation of financial derivatives under stochastic volatility is addressed.
In the standard Black-Scholes model the volatility of the risky asset is assumed to be constant or a function of time and explicit pricing formulas are available for European Vanillas. Such models are generally too crude to match observed log-return prices well. A more flexible class of models assumes that the volatility is a stochastic process. Such models lead to degenerate parabolic partial differential equations (or to parabolic partial integro differential equations, if jump processes are involved) in $d \geq 2$ space dimensions, which, in general, cannot be solved in closed form. Standard discretizations suffer form the so-called curse of dimension, i.e. the number of degrees of freedom grows like $O(h^{-d})$, where h is the mesh-width in one dimension. To reduce the number of the degrees of freedom, wavelet based sparse tensor product Finite Element spaces are used. We apply *hp*-discontinuous Galerkin time stepping to discretize in time, where the wavelet basis is used to precondition the iterative solver of the corresponding matrix equations in each time step. The resulting algorithm has log-linear complexity comparable to that of the best FFT-based methods for the usual Black-Scholes type model.

References: N. Hilber, A.-M. Matache and C. Schwab, *Sparse Wavelet Methods for Option Pricing under Stochastic Volatility* , Journal of Computational Finance, **8** (4) (2005),1–42.

Title: Computational Finance: Lévy Models in Finance - Numerical Analysis and Computation

Researcher: Nils Reich (SAM)
Christoph Winter (SAM)
Prof. Christoph Schwab (SAM)

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

In standard Mathematical Finance Brownian motion plays the dominating role as driving process for modeling price movements. It has been however observed that the Gaussian models do not fit very well the real-life data, e.g. do not allow so called fat tails and asymmetry of observed log returns.

One way to satisfy these conditions is to replace Brownian motion by Lévy processes which are jump processes. For non-Gaussian Lévy processes with jumps an appropriate theory is not a theory of local differential operators but that of non-local pseudo-differential operators.

In the d-dimensional Black-Scholes model the dependence structure is characterized entirely by its covariance matrix. Arbitrage free derivatives prices are the solution of parabolic partial differential equations in d dimensions. To break down the complexity sparse tensor product spaces are applied. Due to the local nature of the Black-Scholes operator, the resulting matrices are sparse.

We extend this to Lévy processes. Using Lévy copulas, d-dimensional Lévymodels can be constructed where the jumps are dependent. Derivative prices are now solutions of partial integro-differential equations. The domains of the corresponding infinitesimal generators are anisotropic Sobolev spaces. Since the multidimensional Lévy densities have singularities at the origin and on the axes, special numerical quadrature formulas are needed for the computation of the integral part. Again, applying sparse tensor products the computational complexity can be reduced significantly. The resulting matrices are of lower dimension but still dense. Therefore, we reduce their complexity further by applying wavelet compression for (anisotropic) tensor product wavelets.

References:

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[2] T. von Petersdorff and C. Schwab, *Numerical solution of parabolic equations in high dimensions*, M2AN Math. Model. Numer. Anal. 38 (2004)

Title: Numerical solution of operator equations with stochastic data

Researcher: Dr. Alexey Chernov*
Prof. Christoph Schwab*

Institute: * Seminar for Applied Mathematics, ETH Zürich.

Description:

We analyze numerical solution of operator equations $\mathcal{A}u = g$ in domains with stochastic load $g = g(\omega)$ and/or boundary perturbations $\Gamma = \Gamma(\omega)$. The aim is the computation of the moments $\mathcal{M}^k u := \mathbb{E}[\otimes_{i=1}^k u]$, $k \geq 1$, if the corresponding moments of the perturbation are known. The case of correlated stochastic load and boundary perturbations is of particular interest. The problem on the stochastic surface is reduced to a problem on the nominal deterministic surface Γ with the random perturbation parameter $\kappa(\omega)$. Note, that $u(\omega)$ depends nonlinearly on $\kappa(\omega)$.

Resulting formulation for the kth moment is posed in the tensor product Sobolev spaces and involve the k-fold tensor product operators $\mathcal{A}^{(k)} = \otimes_{i=1}^k \mathcal{A}$. In particular, in [4] we consider the case of single layer potential of the Laplacian $\mathcal{A} = \mathcal{V}$. The standard full tensor product Galerkin BEM requires $\mathcal{O}(N^k)$ unknowns for the kth moment problem, where N is the number of unknowns needed to discretize the surface Γ. Based on [3], we develop the sparse p-version Galerkin BEM to reduce the number of unknowns to $\mathcal{O}(N(\log N)^{k-1})$ (cf. [1], [2] for the wavelet approach). Note that the p-version of BEM is particularly advantageous in the case of regular solutions.

We analyze possible generalizations of the suggested method to the hypersingular integral equations as well to the Helmholtz and Maxwell problems.

References:

[1] H. Harbrecht, R. Schneider and Ch. Schwab, *Sparse second moment analysis for elliptic problems in stochastic domains*, Research Report No. 2007-06, Seminar for Applied Mathematics, ETH Zürich

[2] T. von Petersdorff and Ch. Schwab, *Sparse finite element methods for operator equations with stochastic data*, Appl. Math., Vol. 51, no. 2, pp. 145–180, (2006)

[3] V. N. Temlyakov, *Approximation of periodic functions*, Nova Science Publ., New York, (1994).

[4] A. Chernov and Ch. Schwab, *Sparse p-version BEM for first kind boundary integral equations with random loading*, Appl. Numer. Math., submitted

Title: Sparse techniques for elliptic sPDEs

Researchers: Marcel Bieri
Christoph Schwab

Institute: Seminar for applied mathematics (SAM)

Description:

The project describes the analysis and the implementation of algorithms for the deterministic numerical solution of elliptic boundary value problems with stochastic coefficients in a physical domain $D \subset \mathbb{R}^d$.

A separation of deterministic and stochastic parts of the input data is achieved by a so-called Karhunen-Loève expansion truncated after M terms. In the following, the stochastic problem is reduced to a deterministic but M-dimensional, parametric deterministic problem, whith M possibly large.

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

- sparse techniques for approximating the solutions random behavior.
- computer parallelism to efficiently overcome potential bottlenecks in our proposed algorithms.

By looking at sparse approximation techniques we focus on two methods, namely a *sparse stochastic Galerkin FEM* (sGFEM) and a *sparse stochastic collocation FEM* (sCFEM), see also [2]. Both offer the possibility 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. A special attention is given to the case where the random fields have a short correlation length since this arises naturally in many engineering applications and turns out to additionaly increase the complexity of the problem.

References

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[2] R.-A. Todor and C. Schwab. Convergence Rates for Sparse Chaos Approximations of Elliptic Problems with Stochastic Coefficients. *IMA Journal of Numerical Analysis*, 27: p.232-261, 2007.

Title: Sparse Wavelet FEM for Elliptic Problems with Stochastic Data

Researcher: Bastian Pentenrieder*
Prof. Christoph Schwab*

Institute: * Seminar for Applied Mathematics, ETH Zürich.

Description:

We consider linear elliptic SPDEs in product domains $D \subset \mathbb{R}^n\,(n = 1, 2, 3)$. Sources of randomness are stochastic coefficients or loadings, respectively. The particular focus here is on problems with short correlation length in the random fields modelling the uncertainties.
The aim is to approximate first and second moments of the solution using the corresponding moments of the random input data. This can be done for the k-th moment by solving *deterministic* PDEs in kn dimensions. The goal is to develop an efficient wavelet FE method for these ones. Due to the short correlation length, classical approaches like sparse grids of hyperbolic cross type turn out to be inappropriate. Instead, we employ a sparsification strategy linked to matrix compression techniques in BEM.
The properties of the derived algorithm (approximation and complexity estimates) are examined both theoretically and by experiment. A major part of the work is concerned with the implementation. Comparisons with other methods, such as *hp*-FEM and H-matrices, are also part of the research.

References:

[1] C. Schwab, R.A. Todor, *Sparse finite elements for elliptic problems with stochastic loading*, Numerische Mathematik (2003) 95: 707-734

[2] R.A. Todor, *Sparse Perturbation Algorithms for Elliptic PDE's with Stochastic Data*, Dissertation, ETH Zurich, 2005

[3] P.-A. Nitsche, *Sparse Tensor Product Approximation of Elliptic Problems*, Dissertation, ETH Zurich, 2004

Title: Anisotropic Multivariate Lévy Processes and their Kolmogorov Equation

Researcher: Nils Reich*
Prof. Christoph Schwab*
Christoph Winter*

* Seminar for Applied Mathematics, ETH Zürich.

Description:

In this work we consider the valuation of financial derivative contracts on baskets of risky assets whose prices are Lévy like Feller processes. The dependence among the marginals' jump structure is parameterized by copulas. For marginals of regular, exponential Lévy type we show that the infinitesimal generator $\mathcal{A}$ of the resulting Lévy copula process is a pseudo-differential operator whose principal symbol is a distribution of anisotropic homogeneity. We analyze the jump measure of the corresponding Lévy copula processes. We prove the domains of their infinitesimal generators $\mathcal{A}$ are certain anisotropic Sobolev spaces. In these spaces and for a large class of Lévy copula processes, we prove a Gårding inequality for $\mathcal{A}$.
We design a wavelet-based dimension-independent tensor product discretization for the efficient numerical solution of the parabolic Kolmogorov equation $u_t + \mathcal{A}u = 0$ arising in valuation of derivative contracts under possibly stopped Lévy copula processes. In the wavelet basis diagonal preconditioning yields a bounded condition number of the resulting matrices.

References:

[1] W. Farkas, N. Reich, C. Schwab, Anisotropic stable Lévy copula processes - analytical and numerical aspects, Math. Models and Methods in Appl. Sciences, 17, 2007, 1405–1443.

Title: Sparse Tensor Product-based Wavelet Compression for Anisotropic Operators

Researcher: Nils Reich*

* Seminar for Applied Mathematics, ETH Zürich.

Description:

For a wide class of non-local anisotropic operators we construct a new sparse tensor product-based wavelet compression scheme using anisotropic tensor product wavelets. The scheme (asymptotically) reduces the complexity of the corresponding Finite Element stiffness matrix from originally $\mathcal{O}(h^{-2d})$ to essentially optimal $\mathcal{O}(h^{-1}|\log h|^{2(d-1)})$, where h denotes the meshwidth of the Finite Element discretization. It is based on a combination of concepts from [1, 3] and the references therein.
To describe the operators under consideration, we introduce anisotropic symbol classes and study some of their analytical properties (e.g. relaxed smoothness requirements for sparse tensor product convergence).
The project is motivated by Finite Element-based derivatives pricing in multi-dimensional Lévy models as described in [2]. The compression techniques are neither limited to Lévy models nor to non-local operators only arising in finance.

References:

[1] W. Dahmen, H. Harbrecht, R. Schneider, Compression techniques for boundary integral equations - asymptotically optimal complexity estimates, SIAM J. Num. Anal., 43, 2006, 2251–2271.

[2] W. Farkas, N. Reich, C. Schwab, Anisotropic stable Lévy copula processes - analytical and numerical aspects, Math. Models and Methods in Appl. Sciences, 17, 2007, 1405–1443.

[3] M. Griebel, P. Oswald, T. Schiekofer, Sparse grids for boundary integral equations, Numer. Math., 83, 1999, 279–312.

Title: Wavelet methods for the Pricing of Derivatives with Additive Driving Processes – Analytical and Numerical Aspects

Researcher: Lukas Wampfler
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics, ETH Zürich.

Description:

In this work we consider the valuation of financial derivative contracts on risky assets whose prices are exponentials of additive stochastic processes.
When using Lévy models for option pricing, it has been observed that it is not possible to fit impilied volatility surfaces across both strikes and maturities. Therefore, we use models with time-inhomogeneous increments.

We want to develop a framework for the pricing of derivatives where the underlying process is an additive stochastic process, i.e. a stochastically continuous process with independent but in general instationary increments.

We shall derive a partial integro-differential equation (PIDE) for different types of contracts (European, American, Barrier), where the background driving process is additive. Special attention has to be paid to the characteristic triple of the additive process which may have singularities as time approaches the maturity of the contract, but is analytic in time elsewhere. Thus a uniform time step will not be optimal. One of the tasks will be to find the optimal time stepping method for the resulting parabolic equalities or inequalities. Furthermore we want to find suitable function spaces for the variational formulation and for the solution of the above PIDEs, i.e. prove unique existence and regularity of the price of the contract and identify necessary conditions and assumptions on the generating triplet of the process for existence of a solution.

We want to efficiently solve the resulting parabolic problem with time-dependent coeficients using wavelet compression and different time-stepping schemes. In the future, we should also be able to extend this procedure to multi-dimensional models using a copula construction.

References:

[1] P.Carr, H.Geman, D.Madan and M.Yor, *Self Decomposability and Option Pricing*, Mathematical Finance, Vol. 17, pp. 31-57, 2007

Title: The ALPS project release 1.3:
open source software for strongly correlated systems

Researchers: A.F. Albuquerque, F. Alet, P. Corboz, P. Dayal, A. Feiguin, S. Fuchs, L. Gamper, E. Gull, S. Gürtler, A. Honecker, R. Igarashi, M. Körner, A. Kozhevnikov, A. Läuchli, S.R. Manmana, M. Matsumoto, I.P. McCulloch, F. Michel, R.M. Noack, G. Pawlowski, L. Pollet, T. Pruschke, U. Schollwöck, S. Todo, S. Trebst, M. Troyer, P. Werner, S. Wessel

Institute/Group: ALPS collaboration

Description:

We present release 1.3 of the ALPS (Algorithms and Libraries for Physics Simulations) project, an international open source software project to develop libraries and application programs for the simulation of strongly correlated quantum lattice models such as quantum magnets, lattice bosons, and strongly correlated fermion systems. Development is centered on common XML and binary data formats, on libraries to simplify and speed up code development, and on full-featured simulation programs. The programs enable non-experts to start carrying out numerical simulations by providing basic implementations of the important algorithms for quantum lattice models: classical and quantum Monte Carlo (QMC) using non-local updates, extended ensemble simulations, exact and full diagonalization (ED), as well as the density matrix renormalization group (DMRG). Changes in the new release include a DMRG program for interacting models, support for translation symmetries in the diagonalization programs, the ability to define custom measurement operators, and support for inhomogeneous systems, such as lattice models with traps. The software is available from our web server at http://alps.comp-phys.org/

References:

Journal of Magnetism and Magnetic Materials **310**, 1187 (2007)

Title: Absence of a structural glass phase in a monoatomic model liquid predicted to undergo an ideal glass transition

Researchers: C. Gils, H.G. Katzgraber and M. Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:

We study numerically a two-dimensional monodisperse model of interacting classical particles predicted to exhibit a static liquid-glass transition [Phys. Rev. E 72, 021502 (2005)]. Using a dynamical Monte Carlo method we show that the model does not freeze into a glassy phase at low temperatures. Instead, depending on the choice of the hard-core radius for the particles, the system either collapses trivially or a polycrystalline hexagonal structure emerges.

References:

J. Stat. Mech. P09011 (2007)

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:
Preprint, submitted to PRB

Title: Modernizing the C++ Interface to MPI

Researchers: P. Kambadur, D. Gregor, A. Lumsdaine, A. Dharurkar [*]
Matthias Troyer [**]

Institute/Group: Department of Computer Science, Indiana University [*]
Theoretische Physik, ETH Zürich[**]

Description:

The Message Passing Interface (MPI) is the de facto standard for writing message passing applications. Much of MPI's power stems from its ability to provide a high performance, consistent interface across C, Fortran, and C++. Unfortunately, with cross-language consistency at the forefront, MPI tends to support only the lowest common denominator of the three languages, providing a level of abstraction far lower than typical C++ libraries. For instance, MPI does not inherently support standard C++ constructs such as containers and iterators, nor does it provide seamless support for user-defined classes. To map these common C++ constructs into MPI, programmers must often write non-trivial boiler-plate code and weaken the type-safety guarantees provided by C++. This paper describes several ideas for modernizing the C++ interface to MPI, providing a more natural syntax along with seamless support for user-defined types and C++ Standard Library constructs. We also sketch the C++ techniques required to implement this interface and provide apreliminary performance evaluation illustrating that our modern interface does not imply unnecessary overhead.

References:

Preprint, submitted to Parallel Computing

Title: Optimized Broad-Histogram Ensembles for the Simulation of Quantum Systems

Researchers: E. Gull, M. Troyer[*]
N. Stoop [**]
S. Wessel [***]
S. Trebst [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] IfB, ETH Zürich
[***] Universität Stuttgart
[****] Station Q, Microsoft

Description:

The efficiency of statistical sampling in broad-histogram Monte Carlo simulations can be considerably improved by optimizing the simulated extended ensemble for fastest equilibration. Here we describe how a recently developed feedback algorithm can be generalized to the simulation of quantum systems in the context of a stochastic series expansion (SSE) quantum Monte Carlo simulations. Whenever the chosen update methods is efficient, such as loop cluster or directed loop updates for nonfrustrated quantum magnets, we find that a flat histogram in the expansion order is optimal if a new variable-length formulation of the SSE is used. Whenever the update method suffers from slowdown, such as at a first-order phase transition, the optimized ensemble reweights towards expansion orders in the transition region.

References:
Preprint, submitted to J. Stat. Mech.

Title: Performance analysis of continuous-time solvers for quantum impurity models

Researchers: E. Gull, M. Troyer[*]
P. Werner, A.J. Millis [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Columbia University, New York

Description:

Impurity solvers play an essential role in the numerical investigation of strongly correlated electrons systems within the "dynamical mean field" approximation. Recently, a new class of continuous-time solvers has been developed, based on a diagrammatic expansion of the partition function in either the interactions or the impurity-bath hybridization. We investigate the performance of these two complimentary approaches and compare them to the well-established Hirsch-Fye method. The results show that the continuous-time methods, and in particular the version which expands in the hybridization, provide substantial gains in computational efficiency.

References:

Preprint, submitted to Phys. Rev. B

Title: Recent results from the Gaussian Quantum Monte Carlo method for fermions with symmetry projection

Researchers: Fakher F. Assaad[*]
Phillipe Corboz, Matthias Troyer[**]
A. Kleine, I. P. McCulloch , U. Schollwöck [***]

Institute/Group: [*] Theoretische Physik und Astrophysik, Universität Würzburg
[**] Theoretische Physik, ETH Zürich
[***] Theoretische Physik, RWTH Aachen

Description:

Gaussian Quantum Monte Carlo (GQMC) is a stochastic phase space method for fermions with positive weights. In the example of the Hubbard model close to half filling it fails to reproduce all the symmetries of the ground state leading to systematic errors at low temperatures. In a previous work we proposed to restore the broken symmetries by projecting the density matrix obtained from the simulation onto the ground state symmetry sector. In this paper we present a systematic study of the method for 2 and 3 leg Hubbard ladders for different fillings and on-site repulsion strengths. We provide several indications that the systematic errors stem from non-vanishing boundary terms in the partial integration step in the derivation of the Fokker-Planck equation. Possible solutions to avoid boundary terms are discussed. Furthermore we compare results obtained from two different sampling methods: Reconfiguration of walkers and the Metropolis algorithm.

References:

Preprint, submitted to Phys. Rev. B

Title: Supersolidity in ^{4}He

Researchers: M. Boninsegni[*]
B. Svistunov[**, ***]
N. Prokof'ev[**, ***]
A. Kuklov[****]
Lode Pollet Matthias 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:

By large-scale quantum Monte Carlo simulations we show that grain boundaries in Helium-4 crystals are generically superfluid at low temperature, with a transition temperature of the order of about 0.5K at the melting pressure; insulating grain boundaries are found only for special orientations of the grains. We also find that close vicinity to the melting line is not a necessary condition for superfluid grain boundarie , and a grain boundary in direct contact with the superfluid liquid at the melting curve is found to be mechanically stable and the grain boundary superfluidity observed by Sasaki *et al.* [Science 313, 1098 (2006)] is not just a crack filled with superfluid.

We also find that the screw dislocation along the hexagonal axis of an hcp Helium-4 crystal features a superfluid (at T -> 0) core. This is the first example of a regular quasi-one-dimensional supersolid—the phase featuring both translational and superfluid orders, and one of the cleanest cases of a Luttinger-liquid system. In contrast, the same type of screw dislocation in solid H_2 is insulating.

References:

Phys. Rev. Lett. **98**, 135301 (2007)

Phys. Rev. Lett. **99**, 035301 (2007)

Title: Dimer-quadrupolar quantum phase transition in the quasi-one-dimensional Heisenberg model

Researchers: Kenji Harada[*]
Naoki Kawashima[**]
Matthias Troyer[***]

Institute/Group: Department of Applied Analysis and Complex Dynamical Systems, Kyoto University[*]
Institute for Solid State Physics, University of Tokyo[**]
Theoretische Physik, ETH Zürich[***]

Description:
The quasi-one-dimensional S=1 Heisenberg antiferromagnet with a biquadratic term is investigated at zero temperature by quantum Monte Carlo simulation. As the magnitude of the inter-chain coupling is increased, the system undergoes a phase transition from a spontaneously dimerized phase to a Néel ordered or spin nematic phase. The numerical results suggest the possibility of an unconventional second-order transition in which the symmetry group characterizing one phase is not a subgroup of the other.

References:

J. Phys. Soc. Jpn. 76, 013703 (2007)

Title: Breakdown of a topological phase:
Quantum phase transition in a loop gas model with tension

Researchers: S. Trebst, C. Nayak [*]
P. Werner [**]
M. Troyer [***]
K. Shtengel [***]

Institute/Group: [*] Station Q, Microsoft
[**] Columbia University
[***] Theoretische Physik, ETH Zürich
[****] University of California, Riverside

Description:

We study the stability of topological order against local perturbations by considering the effect of a magnetic field on a spin model—the toric code—which is in a topological phase. The model can be mapped onto a quantum loop gas where the perturbation introduces a bare loop tension. When the loop tension is small, the topological order survives. When it is large, it drives a continuous quantum phase transition into a magnetic state. The transition can be understood as the condensation of ''magnetic''vortices, leading to confinement of the elementary ''charge'' excitations. We also show how the topological order breaks down when the system is coupled to an Ohmic heat bath and relate our results to error rates for topological quantum computations.

References:

Phys. Rev. Lett. 98, 070602 (2007).

Title: Interacting anyons in topological quantum liquids: The golden chain

Researchers: A. Feiguin[*], S. Trebst, A. Kitaev, Z. Wang, M. Freedman [*]
A.W.W. Ludwig [**]
M. Troyer [***]

Institute/Group: [*] Station Q, Microsoft
[**] University of California, Santa Barbara
[***] Theoretische Physik, ETH Zürich

Description:

We discuss generalizations of quantum spin Hamiltonians using anyonic degrees of freedom. The simplest model for interacting anyons energetically favors neighboring anyons to fuse into the trivial ('identity') channel, similar to the quantum Heisenberg model favoring neighboring spins to form spin singlets. Numerical simulations of a chain of Fibonacci anyons show that the model is critical with a dynamical critical exponent $z = 1$,and described by a two-dimensional (2D) conformal field theory with central charge $c = 7/10$. An exact mapping of the anyonic chain onto the 2D tricritical Ising model is given using the restricted-solid-on-solid (RSOS) representation of the Temperley-Lieb algebra. The gaplessness of the chain is shown to have topological origin.

References:

Phys. Rev. Lett. 98, 160490 (2007).

Title: Quantum Monte Carlo study of a 1D phase-fluctuating condensate

Researchers: C. Gils, L. Pollet, M. Troyer [*]
A. Vernier, F. Hebert, G.G. Batrouni [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Nice

Description:

We study numerically the low temperature behaviour of a 1D Bose gas trapped in an optical lattice. For a sufficient number of particles and weak repulsive interactions, we find a clear regime of temperatures where density fluctuations are negligible but phase fluctuations are considerable, *i.e.* , a quasicondensate. In the weakly interacting limit, our results are in very good agreement with those obtained using a mean-field approximation. In coupling regimes beyond the validity of mean-field approaches, a phase-fluctuating condensate also appears, but the phase-correlation properties are qualitatively different. It is shown that quantum depletion plays an important role.

References:

Phys. Rev. A 75, 063631 (2007).

Title: Mixture of bosonic and spin-polarized fermionic atoms in an optical lattice

Researchers: L. Pollet, M. Troyer, [*]
C. Kollath [**]
U. Schollwöck [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Geneve
[***] RWTH Aachen

Description:

We investigate the properties of Bose-Fermi mixtures for experimentally relevant parameters in one dimension using numerical methods. We find that the strong attractive interaction between the bosons and fermions leads to the creation of polaronic particles. The effect of the fermions on the bosons is not only to deepen the parabolic trapping potential, but also to reduce the bosonic repulsion. This reduction would theoretically lead to an increase in the bosonic visibility. The opposite was observed however in the experimental 87Rb - 40K systems, most likely due to a sharp rise in temperature.

References:

Preprint, submitted to Phys. Rev. Lett.

Title: Ramping fermions in optical lattices across a Feshbach resonance

Researchers: H. G. Katzgraber, A. Esposito, M. Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:

We report results of quantum Monte Carlo simulations in the canonical and the grand-canonical ensemble of the two- and three-dimensional Bose-Hubbard model with quadratic and quartic confining potentials. The quantum criticality of the superfluid--Mott insulator transition is investigated both on the boundary layer separating the two coexisting phases and at the center of the traps where the Mott-insulating phase is first established. Recent simulations of systems in quadratic traps have shown that the transition is not in the critical regime due to the finite gradient of the confining potential and that critical fluctuations are suppressed. In addition, it has been shown that quantum critical behavior is recovered in flat confining potentials as they approach the uniform regime. Our results show that quartic traps display a behavior similar to quadratic ones, yet locally at the center of the traps the bulk transition has enhanced critical fluctuations in comparison to the quadratic case. Therefore quartic traps provide a better prerequisite for the experimental observation of true quantum criticality of ultracold bosonic atoms in optical lattices.

References:

H. G. Katzgraber, A. Esposito, M. Troyer, Phys. Rev. A **74**, 043602 (2006)

Title: Critical behavior of the three- and ten-state Potts glass

Researchers: Lik Wee Lee*,
Helmut Katzgraber**,
A. Peter Young*

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

Description:

We study the critical behavior of the short-range p-state Potts spin glass in three and four dimensions using Monte Carlo simulations. In three dimensions, for p = 3, a finite-size scaling analysis of the correlation length shows clear evidence of a transition to a spin-glass phase at T_c = 0.273(5) for a Gaussian distribution of interactions and T_c = 0.377(5) for a bimodal distribution. These results indicate that the lower critical dimension of the 3-state Potts glass is below three. By contrast, the correlation length of the ten-state (p = 10) Potts glass in three dimensions remains small even at very low temperatures and thus shows no sign of a transition. In four dimensions we find that the p = 3 Potts glass with Gaussian interactions has a spin-glass transition at T_c =0.536(3).

References:

Physical Review B **74**, 104416 (2006)

Title: Effective critical behavior of the two-dimensional Ising spin glass with bimodal interactions

Researchers: Helmut G. Katzgraber*,
Lik Wee Lee**,
Ian A. Campbell***

Institute/Group: * Theoretische Physik, ETH Zürich
** Physics Department, University of California Santa Cruz
*** Laboratoire des Verres, Universite Montpellier

Description:

Monte Carlo data of the two-dimensional Ising spin glass with bimodal interactions are presented with the aim of understanding the low-temperature physics of the model. An analysis of the specific heat, spin-glass susceptibility, finite-size correlation length, and the Binder ratio is performed to try to verify a recent proposal in which for large system sizes and finite but low temperatures the effective critical exponents are identical to the critical exponents of the two-dimensional Ising spin glass with Gaussian interactions. Our results show that with present system sizes the recently proposed scenario in which the two-dimensional Ising spin glass with bimodally distributed interactions is in the same universality class as the model with Gaussian-distributed disorder at low but finite temperatures cannot be reliably proven.

References:

Physical Review B **75**, 014412 (2006)

Title: Temperature and Disorder Chaos in three-dimensional Ising Spin Glasses

Researchers: Helmut G. Katzgraber*
Florent Krzakala**

Institute/Group: * Theoretische Physik, ETH Zürich
** Laboratoire PCT, CNRS, Paris, France

Description:

We study the effects of small temperature as well as disorder perturbations on the equilibrium state of three-dimensional Ising spin glasses via an alternate scaling ansatz. By using Monte Carlo simulations, we show that temperature and disorder perturbations yield chaotic changes in the equilibrium state and that temperature chaos is considerably harder to observe than disorder chaos.

References:

Physical Review Letters **98**, 01201 (2007)

Title: Typical versus average helicity modulus in the three-dimensional gauge glass: Understanding the vortex glass phase

Researchers: Helmut G. Katzgraber, Diethelm Würtz, and Gianni Blatter

Institute/Group: Theoretische Physik, ETH Zürich

Description:

We numerically compute the helicity modulus of the three-dimensional gauge glass by Monte Carlo simulations. Because the average free energy is independent of a twist angle, it is expected that the average helicity modulus, directly related to the superfluid density, vanishes when simulations are performed with periodic boundary conditions. This is not necessarily the case for the typical (median) value, which is nonzero, because the distribution of the helicity modulus among different disorder realizations is very asymmetric. We show that the data for the helicity modulus distribution are well described by a generalized extreme-value distribution with a nonzero location parameter (most probable value). A finite-size scaling analysis of the location parameter yields a critical temperature and critical exponents in agreement with previous results. This suggests that the location parameter is a good observable. There have been conflicting claims as to whether the superfluid density vanishes in the vortex glass phase, with Fisher et al. [Phys. Rev. B 43, 130 (1991)] arguing that it is finite and Korshunov [Phys. Rev. B 63, 174514 (2001)] predicting that it is zero. Because the gauge glass is commonly used to describe the vortex glass in high-temperature superconductors, we discuss this issue in light of our results on the gauge glass.

References:

Physical Review B **75**, 214511 (2007)

Title: Engineering exotic phases for topologically-protected quantum computing by emulating quantum dimer models

Researchers: A. Fabricio Albuquerque, Helmut G. Katzgraber, Matthias Troyer, and Gianni 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:

Preprint, submitted to Phys. Rev. B

Title: Finite- versus zero-temperature hysteretic behavior of spin glasses: Experiment and theory

Researchers: Helmut G. Katzgraber*
Didier Herisson, Michael Oesth, Per Nordblad**
Atsuko Ito, Hiroko Aruga Katori***

Institute/Group: * Theoretische Physik, ETH Zürich
* Department of Engineering Sciences, Uppsala University
* Riken, Japan

Description:

We present experimental results attempting to fingerprint nonanalyticities in the magnetization curves of spin glasses found by Katzgraber et al. [Phys. Rev. Lett. 89, 257202 (2002)] via zero-temperature Monte Carlo simulations of the Edwards-Anderson Ising spin glass. Our results show that the singularities at zero temperature due to the reversal-field memory effect are washed out by the finite temperatures of the experiments. The data are analyzed via the first order reversal curve (FORC) magnetic fingerprinting method. The experimental results are supported by Monte Carlo simulations of the Edwards-Anderson Ising spin glass at finite temperatures which agree qualitatively very well with the experimental results. This suggests that the hysteretic behavior of real Ising spin-glass materials is well described by the Edwards-Anderson Ising spin glass. Furthermore, reversal-field memory is a purely zero-temperature effect.

References:
Physical Review B **76**, 092408 (2007)

Title: Electromagnetic bandgap seal for microwave energy

Researchers: Rüdiger Vahldieck
Martin Gimersky
Matthew Mishrikey

Institute/ Group: Laboratory for Electromagnetic Fields and Microwave Electronics
Electromagnetic Field Theory Group

Description:

A novel concept for the sealing of microwave energy has been envisioned, and the required technology has been developed. Unlike conventional seals of microwave energy − which rely on aged technologies such as quarter-wave-deep electromagnetic chokes or voltage/current absorbers − the new concept utilizes simple, substantially periodic metallodielectric structures featuring one or more stop bands (bandgaps) in their forward-transmission characteristics. The concept is versatile, conformal, fully scalable and offers a number of advantages in comparison with conventional solutions. Demonstrator technology practically implementing the concept on the application of a household microwave oven has been developed and tested.

References:

R. Vahldieck, M. Gimersky, M. Mishrikey: Electromagnetic Bandgap Seal for Microwave Energy, European Patent Application 06011391.7, filed on 1 June 2006.

Title: Prediction of electromagnetic fields in the near-field region of antennas

Researchers: Martin Gimersky
Rüdiger Vahldieck

Institute/ Group: Laboratory for Electromagnetic Fields and Microwave Electronics
Electromagnetic Field Theory Group

Description:

In order to protect personnel operating radiating antenna structures, especially in high-power applications, hazard distances are determined by calculating the maximum radiated-power density at a given location. This can be done by using extrapolations from readily available far-field radiation values. In the near-field region of antennas, however, the power densities and safe distances obtained from the far-field formula are often excessive. As a result, applications of far-field approximations to near fields typically lead to overestimates in the near-field power densities and unnecessarily excessive − and costly − measures to guarantee the legal compliance of the emitter site.
The purpose of the project was therefore to accurately calculate near fields and, from the calculated field values, develop methods for quick predictions of the near fields (E- and H-field intensities and/or power density) for several types of antennas, namely:
¶ vehicle-mounted grounded half-loops in the 2−20 MHz frequency range;
¶ vehicle-mounted vertical monopoles;
¶ free-standing horizontal dipoles in the 20−100 MHz range;
¶ reflector-backed dipole array at 1.3 GHz;
¶ parabolic reflector in the 10−15 GHz range.
The predictions are worst-case approximations and more accurate than the predictions resulting from far-field approximations. Short computer codes to perform such calculations have been developed

References:

M. Gimersky, R. Vahldieck, "Prediction of electromagnetic fields in the near-field region of antennas – Phase 1," Technical Report to armasuisse (armasuisse (W+T) Rahmenvertrags-Nr. 4500314092, Aramis-Nr. R-3210/046-03), 27 November 2006.

M. Gimersky, R. Vahldieck, "Prediction of electromagnetic fields in the near-field region of antennas – Phase 2," Technical Report to armasuisse (armasuisse (W+T) Rahmenvertrags-Nr. 4500314092), to be submitted to armasuisse in October 2007.

Title: Electromagnetic simulations of complex structures with the Finite-Volume Time-Domain method.

Researchers: Christophe Fumeaux
Krishnaswamy Sankaran
Dirk Baumann
Rüdiger Vahldieck

Institute/ Group: Laboratory for Electromagnetic Fields and Microwave Electronics
Electromagnetic Field Theory Group

Description:

In this project, a general-purpose 3D solver for the accurate numerical simulations of electromagnetic (EM) fields is developed. The solver is based on the Finite-Volume Time-Domain (FVTD) method [5]. The FVTD method combines the advantage of an explicit time-stepping with an application in unstructured meshes (e.g. made of tetrahedrons). The geometrical flexibility of the method is beneficial for the modeling of complex structures, i.e. for the conformal approximation of curved or slanted surfaces, for the resolution of small details within larger structures and in connection with large dielectric contrasts. The simulation of scattering and low-level coupling problems has motivated the investigation - in the framework of FVTD - of accurate absorbing boundary conditions based on perfectly matched layers (PML) [2],[3]. Several flavors of PML have been implemented for FVTD and evaluated for efficiency and accuracy [6]. A PML with radial anisotropy has been developed in 2D for the truncation of cylindrical domains [3]. The concept has been subsequently extended to 3D spherical truncation [7]. In parallel to the algorithm development, the FVTD method has been applied to the solution of challenging electromagnetic problems. In particular, spiral antennas and dielectric resonator antennas have been considered [1],[4].

References:

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[2] K. Sankaran, C. Fumeaux, R. Vahldieck, "Cell-centered finite-volume based perfectly matched layer for time domain Maxwell system", IEEE Trans. Microwave Theory Techn. **54**(3), 1269 (2006)
[3] K. Sankaran, C. Fumeaux, R. Vahldieck, "Uniaxial and radial anisotropy models for finite-volume Maxwellian absorber", IEEE Trans. Microwave Theory Techn. **54**(12), 4297 (2006)
[4] G. Almpanis, C. Fumeaux, R. Vahldieck, "Novel broadband dielectric resonator antennas fed through double-bowtie-slot excitation scheme", ACES Journal, vol. **22**(1), 97 (2007)
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[6] T. Kaufmann, K. Sankaran, C. Fumeaux, R. Vahldieck, "A Review of Perfectly Matched Absorbers for the Finite-Volume Time-Domain Method", Accepted for publication in the ACES Journal (2007)
[7] C. Fumeaux, K. Sankaran, R. Vahldieck, "Spherical perfectly matched absorber for finite-volume 3-D domain truncation", Accepted for publication in the IEEE Trans. Microwave Theory Techn. (2007)

Title: Simulation of Optical Nano Structures

Reseachers: Christian Hafner
Kakhaber Tavzarashvili
Cui Xudong
Patrick Leidenberger
Rüdiger Vahldieck

Institute/ Group: Laboratory for Electromagnetic Fields and Microwave Electronics
Computational Optics, Electromagnetic Field Theory

Description:

We have developed a software package for the simulation of optical nano structures including lossy and dispersive material with or without electromagnetic band gaps. Field solvers based on boundary methods - the Multiple Multipole Program (MMP) and the Method of Auxiliary Sources (MAS) –, Method of Moments (MoM), as well as Finite Difference Time Domain (FDTD) are applied. This 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, FDTD is favorable as long as moderate accuracy of the results is sufficient.
The field solvers mentioned were applied to various cases, including metallic and metallo-dielectric photonic crystals, 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 2006 and 2007 three book chapters and sixteen papers in reviewed journals were published based on our field solvers.

Title: Simulation and Optimization of Metamaterials

Reseachers: Christian Hafner
Nicolas Guérin
Matthew Mishrikey
Arya Fallahi
Rüdiger Vahldieck

Institute/ Group: Laboratory for Electromagnetic Fields and Microwave Electronics
Computational Optics, Electromagnetic Field Theory

Description:

We have developed a software packages for both the simulation and optimization of metamaterials for low frequencies up to optical frequencies. 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, ani-reflective coatings, radar absorbing and shielding metamaterials, electrosmog protection, high temperature metamaterial shields, negative index metamaterials, photonic crystal structures, etc.

References:

In 2006 and 2007 two book chapters and eight papers in reviewed journals were published.

Title: A Comparison of Methods to Compute the Potential of Mean Force

Researchers: Daniel Trzesniak
Anna-Pitschna E. Kunz
Wilfred F. van Gunsteren

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

Description:

Most processes occurring in a system are determined by the relative free energy between two or more states because the free energy is a measure of the probability of finding the system in a given state. When the two states of interest are connected by a pathway, usually called reaction coordinate, along which the free-energy profile is determined, this profile or potential of mean force (PMF) will also yield the relative free energy of the two states. Twelve different methods to compute a PMF are reviewed and compared, with regard to their precision, for a system consisting of a pair of methane molecules in aqueous solution. We analyze all combinations of the type of sampling (unbiased, umbrella-biased or constraint-biased), how to compute free energies (from density of states or force averaging) and the type of coordinate system (internal or Cartesian) used for the PMF degree of freedom. The method of choice is constraint-bias simulation combined with force averaging for either an internal or a Cartesian PMF degree of freedom.

References: ChemPhysChem **8** (2007) 162-169 (DOI: 10.1002/cphc.200600527)

Title: Comparison of atomic-level and coarse-grained models for liquid hydrocarbons from molecular dynamics configurational entropy estimates

Researchers: Riccardo Baron[1]
Daniel Trzesniak[1]
Alex H. de Vries[1,2]
Andreas Elsener[1]
Siewert J. Marrink[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]Laboratory of Biophysical Chemistry, University of Groningen, The Netherlands

Description:

Thermodynamic data are often used to calibrate or test atomiclevel (AL) force fields for molecular dynamics (MD) simulations. In contrast, the majority of coarse-grained (CG) force fields do not rely extensively on thermodynamic quantities. Recently, a CG force field for lipids, hydrocarbons, ions, and water,[1] in which approximately four non-hydrogen atoms are mapped onto one interaction site, has been proposed and applied to study various aspects of lipid systems. To date, no extensive investigation of its capability to describe solvation thermodynamics has been undertaken. In the present study, a detailed picture of vaporization, solvation, and phase-partitioning thermodynamics for liquid hydrocarbons and water was obtained at CG and AL resolutions, in order to compare the two types of models and evaluate their ability to describe thermodynamic properties in the temperature range between 263 and 343 K. Both CG and AL models capture the experimental dependence of the thermodynamic properties on the temperature, albeit a systematically weaker dependence is found for the CG model. Moreover, deviations are found for salvation thermodynamics and for the corresponding enthalpy–entropy compensation for the CG model. Particularly water/oil repulsion seems to be overestimated. However, the results suggest that the thermodynamic properties considered should be reproducible by a CG model provided it is reparametrized on the basis of these liquid-phase properties.

References: J. Phys. Chem. B **110** (2006) 8464-8473

Title: Computational analysis of the mechanism and thermodynamics of inhibition of phosphodiesterase 5A by synthetic ligands

Researchers: Bojan Zagrovic
Wilfred F. van Gunsteren

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

Description:

Phosphodiesterases are a large class of enzymes mediating a number of physiological processes ranging from immune response to platelet aggregation to cardiac and smooth muscle relaxation. In particular, phosphodiesterase 5 (PDE5) plays an important role in mediating sexual arousal, and it is the central molecular target in treatments of erectile dysfunction. In this study, we look at the mechanism and thermodynamics of the binding of selective inhibitors sildenafil (Viagra) and vardenafil (Levitra) to PDE5 using molecular dynamics simulations. Our simulations of PDE5 with and without sildenafil suggest a binding mechanism in which two loops surrounding the binding pocket of the enzyme (H loop, residues 660-683, and M loop, 787-812) execute sizable conformational changes (~1nm), clamping the ligand in the pocket. Also, we note significant changes in the coordination pattern of the divalent ions in the active site of the enzyme, as well as marked changes in the collective motions of the enzyme when the ligand is bound. Using the thermodynamic integration approach we calculate the relative free energies of binding of sildenafil, vardenafil, and demethyl-vardenafil, providing a test of the quality of the force field and the ligand parametrization used. Finally, using the single-step perturbation (SSP) technique, we calculate the relative binding free energies of these three ligands as well. In particular, we focus on critical evaluation of the SSP technique and examine the effects of computational parallelization on the efficiency of the technique. As a technical improvement, we demonstrate that an ensemble of relatively short SSP trajectories (10 × 0.5ns) markedly outperforms a single trajectory of the same total length (1 × 5ns) when it comes to sampling efficiency, resulting in significant real-time savings.

References: J. Chem. Theory Comput. **3** (2007) 301-311, incl. supp. material

Title: Simulation of □-depsipeptides: The effect of missing hydrogen-bond donors on their folding equilibria

Researchers: Zrinka Gattin[1]
Alice Glättli[1]
Bernhard Jaun[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zurich, Switzerland
[2] Laboratory of Organic Chemistry, ETH Zurich, Switzerland

Description:

□-Depsipeptides are □-peptides in which one or more peptide linkages are replaced by ester linkages, resulting in a loss of a hydrogen-bond donor (N—H) and weakening of the corresponding carbonyl hydrogen-bond acceptor moiety. The effects of three of such peptide by ester substitutions in a hepta-□-peptide upon its (un)folding equilibrium in methanol solution are investigated using molecular dynamics simulations and compared to experimental data from NMR spectroscopy. The simulated conformational ensembles largely reproduce the experimentally measured NOE and ^{3}J-coupling constant data for the three different hepta-□-peptides, and confirm the relative stabilities of the 3_{14}-helical conformation, which is most weakened by substitution of the 4th peptide linkage and least by substitution of the 6th peptide linkage. The simulations are complementary to the experimental data by providing detailed insight into the conformational distributions that are compatible with the experimentally measured average values of observables.

References: Biopolymers 85 (2007) 318-332, incl. supp. mat.

Title: Analysis of neo-pentane-urea pair potentials of mean force in aqueous urea

Researchers: Daniel Trzesniak[1]
Nico F.A. van der Vegt[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zurich, Switzerland
[2]Max-Planck-Institute for Polymer Research, Mainz, Germany

Description:

Urea is often used as a denaturant in protein (un)folding studies because it alters the way hydrophobic solutes and water affect one another. The solvation structure of neo-pentane and urea in 6.9M urea aqueous solution are investigated by analysing the neo-pentane–urea potential of mean force (PMF) as a function of the neo-pentane–urea separation obtained from molecular dynamics simulations. The PMF is decomposed into its enthalpic (H) and entropic (S) contributions, which are further separated into solute (neo-pentane–urea pair) and solvent (urea, water) contributions. Statistical-mechanical, enthalpic and entropic contributions arising from solvent–solvent interactions do not contribute directly to the PMF because they exactly cancel each other. By excluding the solvent–solvent parts, it is seen that the first minimum in the PMF is due to a combination of contributions coming from the neo-pentane–urea pair self-enthalpy and from the entropy related to the interaction of the neo-pentane–urea pair solute with the remaining solvent molecules. The enthalpy of a neo-pentane–urea pair solute and the remaining urea and water molecules acts against neo-pentane–urea association because this association prohibits the remaining solvent from interacting with the urea molecule belonging to the solute. In addition, ranges of interest in the PMF are structurally and energetically characterized in terms of hydrogen bonding, non-bonded energies and number of neighbouring molecules of a given type. This leads to a consistent thermodynamic and structural picture of hydrophobic co-solvent interaction in aqueous urea.

References: Mol. Phys. **105** (2007) 33-39

Title: Mechanism and thermodynamics of binding of the polypyrimidine tract binding protein to RNA

Researchers: Nathan Schmid
Bojan Zagrovic
Wilfred F. van Gunsteren

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

Description:

The polypyrimidine tract binding protein (PTB) is involved in many physiological processes, including alternative splicing, internal ribosomal entry side (IRES)-mediated initiation of translation, and polyadenylation, as well as in ensuring mRNA stability. However, the role of PTB in these processes is not fully understood, and this has motivated us to undertake a computational study of the protein. PTB RNA binding domains (RBDs) 3 and 4 and their complexes with oligopyrimidine RNAs were simulated using the GROMOS simulation software using the GROMOS 45A4 force field. First, the stability and fluctuations of the tertiary fold and of the secondary structural elements in individual domains, the combined RBD34 domain, and their complexes with RNA were studied. Second, the simulation results were validated against the experimental NMR NOE data. The analysis of hydrogen bonding patterns, salt bridge networks, and stacking interactions of the RNA to the binding pockets of the protein domains showed that binding is not sequence-specific and that many RNA fragments can bind to them successfully. Further calculations of the relative free energy of binding for different polypyrimidine sequences were carried out using the thermodynamic integration (TI) and single-step perturbation (SSP) methods. It was not possible to calculate the relative free energies with high accuracy, but the obtained results do give qualitative insights into PTB's affinity for different RNA sequences. Furthermore, the low-energy conformations of the complexes that were found provided additional information about the mechanism of binding.

References: Biochemistry (2007) on-line (DOI: 10.1021/bi60626133)

Title: Enveloping Distribution Sampling: A method to calculate free energy differences from a single simulation

Researchers: Clara D. Christ
Wilfred F. van Gunsteren

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

Description:

The authors present a method to calculate free energy differences between two states *A* and *B* "on the fly" from a single molecular dynamics simulation of a reference state *R*. No computer time has to be spent on the simulation of intermediate states. Only one state is sampled, i.e., the reference state *R* which is designed such that the subset of phase space important to it is the union of the parts of phase space important to *A* and *B*. Therefore, an accurate estimate of the relative free energy can be obtained by construction. The authors applied the method to four test systems – dipole inversion, van der Waals interaction perturbation, charge inversion, and water to methanol conversion – and compared the results to thermodynamic integration estimates. In two cases, the enveloping distribution sampling calculation was straightforward. However, in the charge inversion and the water to methanol conversion, Hamiltonian replica-exchange molecular dynamics of the reference state was necessary to observe transitions in the reference state simulation between the parts of phase space important to *A* and *B*, respectively. This can be explained by the total absence of phase space overlap of *A* and *B* in these two cases.

References: J. Chem. Phys. (2007) on-line (DOI: 10.1063/1.2730508)

Title: Free energy calculations using flexible-constrained, hard-constrained and non-constrained MD simulations

Researchers: Markus Christen
Clara Christ
Wilfred F. van Gunsteren

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

Description:

A comparison of different treatments of bond-stretching interactions energies from simulations using rigid bonds maintained with the SHAKE algorithm, using partially rigid bonds maintained with a recently introduced flexible constraints algorithm, and using fully flexible bonds are compared in a multi-configurational thermodynamic integration calculation of changing liquid water into liquid methanol. The formula for the free energy change due to a changing flexible constraint in a flexible constraint simulation is derived. To allow for a more direct comparison between these three methods, three different pairs of models for water and methanol were used: a flexible model (simulated without constraints and with flexible constraints), a rigid model (simulated with standard hard constraints), and an alternative flexible model (simulated with flexible constraints and standard hard constraints) in which the ideal or constrained bond lengths correspond to the average bond lengths obtained from a short simulation of the unconstrained flexible model. The particular treatment of the bonds induces differences of up to 2% in the liquid densities, whereas (excess) free energy differences of up to 5.7 (4.3) $kJmol^{-1}$ are observed. These values are smaller than the differences observed between the three different pairs of methanol/water models: up to 5% in density and up to 8.5 $kJmol^{-1}$ in (excess) free energy.

References: Chem.Phys.Chem. (2007) on-line (DOI: 10.1002/cphc.200700176)

Title: On the calculation of velocity-dependent properties in molecular dynamics simulations using the leap-frog integration algorithm

Researchers: Michel A. Cuendet
Wilfred F. van Gunsteren

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

Description:

Widely used programs for molecular dynamics simulation of (bio)molecular systems are the Verlet and leap-frog algorithms. In these algorithms, the particle velocities are less accurately propagated than the positions. Important quantities for the simulation such as the temperature and the pressure involve the squared velocities at full time steps. Here, we derive an expression for the squared particle velocity at full time step in the leap-frog scheme, which is more accurate than the standardly used one. In particular, this allows to show that the full time step kinetic energy of a particle is more accurately computed as the average of the kinetic energies at previous and following half steps than as the square of the average velocity as implemented in various molecular dynamics codes. Use of the square of the average velocity introduces a systematic bias in the calculation of the instantaneous temperature and pressure of a molecular dynamics system. We show the consequences when the system is coupled to a thermostat and a barostat.

References: J. Chem. Phys. (2006) accepted

Title: A combined QM/MM molecular dynamics study on a condensed-phase S_N2 reaction at saturated nitrogen: the effect of explicitly including solvent polarization

Researchers: Daan P. Geerke[1]
Stephan Thiel[2]
Walter Thiel[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim, Germany

Description:

In a previous combined QM/MM molecular dynamics (MD) study from our laboratory on the identity S_N2 reaction between a chloride anion and an amino chloride in liquid dimethyl ether (DME), an increase in the free energy activation barrier was observed in the condensed phase when compared to the gas-phase activation energy. Here we reproduce these findings, but when comparing the condensed-phase potential of mean force (PMF) with the free energy profile in the gas phase (obtained from Monte Carlo simulations), we observe a smaller solvent effect on the activation barrier of the reaction. In the next step, we introduce an explicit description of electronic polarization in the MM (solvent) part of the system. A polarizable force field for liquid DME was developed based on the charge-on-spring (COS) model, which was calibrated to reproduce thermodynamic properties of the nonpolarizable model in classical MD simulations. The COS model was implemented into the MNDO/ GROMOS interface in a special version of the QM/MM software ChemShell, which was used to investigate the effect of solvent polarization on the free energy profile of the reaction under study. A higher activation barrier was obtained using the polarizable solvent model than with the nonpolarizable force field, due to a better solvation of and a stronger polarization of solvent molecules around the separate reactants. The obtained PMFs were subjected to an energy-entropy decomposition of the relative salvation free energies of the reactant complex along the reaction coordinate, to investigate in a quantitative manner whether the solvent (polarization) effects are mainly due to favorable QM-MM (energetic) interactions.

References: J.Chem.Theory Comput. (2007) accepted

Title: Calculation of the free energy of polarization: quantifying the effect of explicitly treating electronic polarization on the transferability of force-field parameters

Researchers: Daan P. Geerke
Wilfred F. van Gunsteren

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

Description:

The lack of an explicit description of electronic polarization in non-polarizable force fields usually results in an incomplete transferability of force-field parameter sets when applied in simulations of the system of interest in either a polar or an apolar environment. For example, the use of non-polarizable parameter sets optimized to reproduce experimental data on properties of pure liquids of polar compounds commonly yields too low solubilities in water for the corresponding compounds. The reason is that the fixed charge distributions calibrated for the pure liquid might correspond to too low molecular dipole moments in case of hydration. In the current study we quantitatively show that the inclusion of electronic polarization can improve the transferability of biomolecular force-field parameter sets. With this aim, free energies of polarization ΔG_{pola} have been calculated, with ΔG_{pola} corresponding to the free energy difference between identical systems described by a polarizable and a non-polarizable model. Using a non-polarizable model and a polarizable one (based on the charge-on-spring approach) for dimethyl ether (DME), which were both parameterized to reproduce experimental values for pure liquid properties, small values were found for ΔG_{pola} for the pure liquid or when a DME solute was solvated in the apolar solvent cyclohexane. For the solute hydrated in water, however, ΔG_{pola} was found to be of the same order of magnitude as the discrepancy between the free energy of hydration from simulation using a non-polarizable solute model and the experimental value. Thus, introducing polarizabilities clearly improves the transferability of the parameter set. Additionally, in calculations of an anion solvated in DME, ΔG_{pola} for the solvent adopted relatively large values. From an estimation of the errors in the calculated free energy differences, it was furthermore shown that the calculation of ΔG_{pola} offers an effective and accurate method to obtain differences in solvation (or excess) free energies between systems described by polarizable and non-polarizable models, when compared to a direct calculation of solvation (or excess) free energies.

References: J. Phys. Chem. B (2007) accepted

Title: Molecular dynamics simulation of human interleukin-4: comparison with NMR data and effect of pH, counterions and force field on tertiary structure stability

Researchers: Moritz Winger[1]
Haibo Yu[2]
Christina Redfield[3]
Wilfred.F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, WI 53706, U.S.A.
[3]Department of Biochemistry, University of Oxford, South Parks Road, Oxford OX1 3QU, United Kingdom

Description:

The human protein interleukin-4 (IL-4) has been simulated at two different pH values, 2.4 and 5.6, with different amounts of counterions present in the aqueous solution, and with two different force-field parameter sets using molecular dynamics simulation with the aim of validation of force field and simulation set-up by comparison to experimental NMR data, such as proton-proton NOE distance bounds, $^{3}J(HN,HC_{\alpha})$ coupling constants and backbone N-H order parameters. Thirteen simulations varying in the length from 3 to 7 ns are compared. At pH 5.6 both force-field parameter sets used do largely reproduce the NOE's and order parameters, the GROMOS 45A3 set slightly better than the GROMOS 53A6 set. 3J values predicted from the simulation agree less well with experimental values. At pH 2.4 the protein unfolds, unless counterions are explicitly present in the system, but even then the agreement with experiment is worse than at pH 5.6. When simulating a highly charged protein, such as IL-4 at pH 2.4, the inclusion of counterions in the simulation seems mandatory.

References: J. Biomol. NMR (2007) accepted

Title: The performance of non-polarizable and polarizable force-field parameter sets for ethylene glycol in molecular dynamics simulation of the pure liquid and its aqueous mixtures

Researchers: Daan P. Geerke
Wilfred F. van Gunsteren

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

Description:

Non-polarizable and polarizable force-field parameter sets for liquid ethylene glycol (EG) were developed for use in biomolecular simulation. In the polarizable models, electronic polarization effects were explicitly taken into account using the charge-on-spring method. The quality of the new force fields and two non-polarizable EG models taken from the literature was investigated by calculating relevant properties of the pure liquid and its aqueous mixtures, and comparing simulation results with experimental data. The performance of the EG models as a co-solvent in aqueous mixtures was additionally evaluated in a hydrophobic hydration study. The question was whether the experimentally known maximum in the solvation free enthalpy of argon at intermediate mixture compositions could be reproduced in the simulations. Values for the dielectric properties and excess free energy were found to be more off from experiment for the polarizable models than for the non-polarizable ones. However, a Kirkwood-Buff analysis of the aqueous mixtures and the hydrophobic hydration results exemplified that electronic polarization plays an important role in correctly describing attractive interactions between the EG and water co-solvent molecules. The *trans/gauche* ratio for ethylene glycol's O–C–C–O torsional angle was not found to systematically affect other important properties of the pure liquid and aqueous mixtures.

References: Mol. Phys. (2007) accepted

Title: Use of molecular dynamics simulation for optimising protein stability: Consensus designed ankyrin repeat proteins

Researchers: Moritz Winger
Wilfred F. van Gunsteren

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

Description:

In earlier work two highly homologous (87% sequence identity) ankyrin repeat (AR) proteins, E3_5 and E3_19, were studied using molecular dynamics (MD) simulation. Their stabilities were compared and it was found that the C-terminal capping unit is unstable in the protein E3_19, in agreement with CD-experiments. The different stabilities of these two very similar proteins could be explained by the different charge distributions among the AR units of the two proteins. Here another AR protein, N3C, with yet another charge distribution has been simulated using MD and its stability was analysed. In agreement with the experimental data, the N3C structure was found to be less stable than that of E3_5, but in contrast to E3_19, secondary structure was only slightly lost, while structurally N3C is closer to E3_19 than to E3_5. The results suggest that an equal charge distribution over the repeat units does enhance the stability of design AR proteins in aqueous solution, which however may be modulated by the bulkiness of amino-acid side chains involved in the mutations.

References: Prot. Eng. (2007) submitted

Title: On the calculation of the free energy of quantisation for molecular systems in the condensed phase

Researchers: Daan P. Geerke
Sandra Luber
Koni H. Marti
Wilfred F. van Gunsteren

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

Description:

Using the path-integral formalism, various expressions for the free energy of quantisation for a molecular system in the condensed phase are derived. These lead to alternative methods to compute quantisation free energies from molecular dynamics computer simulations, which were investigated with an eye to practical problems regarding their efficiency and the numerical precision of the obtained free-energy values. Use of the most practical method, which is based on free-energy perturbation, is demonstrated for a test system of liquid neon, for which the free energy of quantisation and its contribution to the excess free energy is evaluated.

References: J. Chem. Phys. (2007) submitted

Title: Validation of the GROMOS 53A6 force field for the study of beta-peptides in solution

Researchers: Bojan Zagrovic
Zrinka Gattin
Justin Kai-Chi Lau
Matthias Huber
Wilfred F. van Gunsteren

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

Description:

We have studied two different □□peptides in methanol using explicit solvent molecular dynamics simulations and the GROMOS 53A6 force field: a heptapeptide (peptide 1) expected to form a left-handed 3_{14}-helix, and a hexapeptide (peptide 2), expected to form a □-hairpin in solution. Our analysis has focused on identifying and analyzing the stability of the dominant secondary structure conformations adopted by the peptides, as well as on comparing the experimental NOE distance upper bounds and ^{3}J-coupling values with their counterparts calculated on the basis of the simulated ensembles. Moreover, we have critically compared the present results with the analogous results obtained with the GROMOS 45A3 (peptide 1) and 43A1 (peptide 2) force fields. We conclude that within the limits of conformational sampling employed here, the GROMOS 53A6 force field satisfactorily reproduces experimental findings regarding the behavior of short □-peptides, with accuracy that is comparable to but does not exceed that of the previous versions of the force field.

References: Phys. Chem. Chem. Phys. (2007) submitted

Title: On the calculation of atomic forces in classical simulation using the charge-on-spring method to explicitly treat electronic polarisation

Researchers: Daan P. Geerke
Wilfred F. van Gunsteren

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

Description:

An expression for the atomic forces in simulations using the charge-on-spring (COS) polarisable model is rederived. In previous implementations of COS-based models, contributions arising from the dependence of the induced dipoles (*i.e.* the positions of the charges-on-spring) on the coordinates of the other sites in the system were not taken into account. However, from calculations on gas-phase dimers we found a significant contribution of these terms. Errors in the forces when neglecting these contributions in condensed-phase calculations can be significantly reduced by choosing an appropriately large value for the size of the charge-on-spring.

References: J. Chem. Theory Comput. (2007) submitted

Title: Folding-unfolding equilibrium of methylene substituted beta-peptide

Researchers: Nathan Schmid
Bojan Zagrovic
Wilfred F. van Gunsteren

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

Description:

□-peptides possess the ability to fold into secondary structure elements and this property, together with resistance to biodegradation, makes these compounds interesting for pharmaceutical applications. Recently, a novel class of □-peptides containing a methylene moiety was described. The GROMOS 53A6 force field was used to simulate the folding equilibrium of a □^{3}-hexapeptide with methylene groups at all six CA carbons. Due to the rotational barriers induced by these methylene groups, the helical secondary structure elements, normally found in □^{3}-peptides, are disfavored in this molecule. Simulations, started from fully extended and 3_{14}-helical starting conformations, showed that the molecule adopts a complete 2_8-helix for about 5% of the time and partial 2_8-helical conformations for about 20% of the time. Yet, as suggested by experiment, the folding equilibrium is dominated by unfolded conformations.

References: Helv. Chem. Acta (2007) submitted

Title: A molecular dynamics study of the ASC and NALP1 Pyrin domains at low pH

Researchers: Zrinka Gattin
Wilfred F. van Gunsteren

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

Description:

The Pyrin domain is one out of four subfamilies of the death domain superfamily of proteins, of which all members share a similar three-dimensional fold, a six or five antiparallel □-helical structure. The Pyrin domain of the ASC (six-helical fold) and of the NALP1 (five-helical fold) proteins were simulated at two different pH-values, 3.7 and 6.5, with two different force-field parameter sets and the molecular dynamics simulation trajectories were compared to NMR experimental data. The two force fields used did not show very different results. The simulations of NALP1 at pH 6.5 did largely satisfy the experimental NOE atom-atom distance bounds measured at pH 6.5 and preserved its tertiary structure. The simulations at pH 3.7 showed a denaturation of the protein. The simulations of ASC at pH 3.7 only satisfied the experimental NOE atom-atom distance bounds measured at pH 3.7, if three acidic side chains, Asp48, Glu64 and Asp75, or only two, Glu64 and Asp75, were not protonated at pH 3.7. This indicates that at low pH the ASC tertiary structure is stabilized by salt bridges. A corresponding analysis for NALP1 at pH 3.7 only yielded one possible salt bridge, which, however, did not stabilize the tertiary structure at low pH. The results obtained show that the particular protonation states of acidic side chains in the protein interior may be crucial to a proper modelling of proteins at low pH.

References: ChemBioChem (2007) accepted

Title: On the conformational properties of □,□-dimethoxypolyethylene glycol

Researchers: Moritz Winger
Markus Christen
Wilfred F. van Gunsteren

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

Description:

A molecular dynamics (MD) study of □,□-dimethoxypolyethylene glycol has been carried out under various conditions with respect to solvent composition, ionic strength, chain length, force field and temperature. A previous MD study on a 15-mer of polyethyleneglycol (PEG) suggested a helical equilibrium structure that was stabilized by hydrogen bonding and bridging water molecules. Experiments show that PEG is highly soluble in water, and indicate that clustering is not favoured. In our simulations no helical structure was found, but formation of more or less compact random coils in aqueous solution due to hydrophobic interactions was observed. The two force fields used, GROMOS 45A3 and 53A6, perform similarly. Clusters of □,□-dimethoxypolyethylene glycol are stable for chain lengths between 6 and 23 ethylene glycol units. Molecules consisting of less than four PEG units do not form stable clusters. PEG shows no significant interaction with calcium or sulfate ions.

References: ChemPhysChem. (2007) submitted

Title: An Approach to Calculate the Free Energy of Dissolution of Salt Crystals from Molecular-Dynamics Simulations and its Application to Mixing of Lennard-Jones Liquids

Researchers: Daan P. Geerke
Fabienne Schwab
Wilfred F. van Gunsteren

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

Description:

For the purpose of optimizing force-field parameters for charged functional groups, a method is proposed to calculate the free-energy difference associated with the process of dissolving a salt crystal in water from molecular dynamics simulations using the thermodynamic-integration (TI) formalism. Even when applying a commonly used functional form to introduce softness into the nonbonded interactions at intermediate values for the TI coupling parameter λ in the employed Hamiltonian, a discontinuity in the obtained free-energy profile was observed which was associated with a phase transition. Also in simulations of the process of mixing two identical Lennard-Jones mixtures, the obtained free-energy curve was found to exhibit such a discontinuity, indicating that the strong electrostatic forces in the salt crystal can not be seen as the primary reason for the occurrence of the phase transition. Instead it was explained in terms of a two-state one-dimensional potential-energy surface for nonbonded interactions between a NaCl ion pair and a Lennard-Jones particle, occurring at intermediate values for λ. Suggestions are made to ensure a smooth transition between the two states, and their performance is tested via attempts to obtain a continuous free-energy profile for the mixing of two identical Lennard-Jones liquids.

References: ChemPhysChem. (2007) submitted

Title: QM-MM Interactions in Simulations of Liquid Water using Combined Semi-Empirical/Classical Hamiltonians

Researchers: Daan P. Geerke[1]
Stephan Thiel[2]
Walter Thiel[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim, Germany

Description:

Well-established semi-empirical quantum-mechanical methods such as AM1, PM3 and MNDO poorly describe hydrogen-bonding interactions. The recently developed OM1, OM2 and OM3 methods, which include explicit corrections in the one-electron terms of the Hamiltonian to counteract for the neglect of orthogonalization effects, show an improved description of hydrogen bonding. In the current work we compare the performance of the OMx models on the one hand and the AM1, PM3 and MNDO methods (as well as the SCC-DFTB method) on the other when used in combination with a classical force field in QM/MM calculations on a water dimer in the gas phase, and in QM/MM simulations of a QM water 'solute' in liquid MM water. It is found that when using the OMx methods to describe the QM water molecule, values for QM-MM interaction energies and the molecular dipole moment of the QM solute are significantly closer to experiment than when using the other semi-empirical methods. In addition, the compatibility of OM3 with the classical Hamiltonian improves upon explicitly including electronic polarization in the MM subsystem.

References: Phys. Chem. Chem. Phys. (2007) submitted

Title: Calculation of the Purcell Enhancement Factor using a vectorial, three-dimensional Finite-Element Method

Researchers: Bernd Witzigmann
Friedhard Römer
Dölf Aemmer

Institute/ Group: Integrated Systems Laboratory/
Computational Optoelectronics Group

Description:

Photonic crystal cavities facilitate novel applications demanding the efficient emission of incoherent light. This unique property arises when combining a relatively high quality factor of the cavity modes with a tight spatial constriction of the modes. A measure for the spontaneous emission enhancement is the local density of optical states (LDOS), which is a generalization of the classical Purcell enhancement factor. Due to the complicated three-dimensional geometry of photonic crystal cavities the LDOS quantity has to be computed numerically. In this project, we investigate the computation of the LDOS by means of a 3D Finite Element (FE) Maxwell Solver. The solver applies a sophisticated symmetry handling to reduce the problem size and provides perfectly matched layers to simulate open boundaries. Different photonic crystal cavity designs have been investigated for their spontaneous emission enhancement by means of this FE solver. The simulation results have been compared to photoluminescence characterizations of fabricated cavities. The excellent agreement of simulations and characterizations results confirms the performance and the accuracy of the 3D FE Maxwell Solver.

References:

F. Römer, Oscar Chinellato, P. Arbenz, and B. Witzigmann, 'Investigation of the Purcell Effect in Photonic Crystal Cavities with a 3D Finite Element Maxwell Solver', Journal of Optical and Quantum Electronics, published online June 2007 (0306-8919)

F. Intonti, S. Vignolini, F. Riboli, A. Vinattieri, D. S. Wiersma, M. Colocci, M. Guriolia, L. Balet, C. Monat, L. H. Li, N. Le Thomas, R. Houdre, A. Fiore, M. Francardi, A. Gerardino, F. Roemer, B. Witzigmann, 'Near-field mapping of quantum dot emission from single photonic crystal cavity modes', accepted for publication in Physica E.

Title: Automated data analysis for 3D protein NMR structure determination using the software MATCH, ASCAN and RADAR

Researchers: Torsten Herrmann
Jochen Volk
Francesco Fiorito
Pascal Bettendorff
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
This project is focused on automated NMR data analysis for three-dimensional structure determination of biological macromolecules in solution, with the prime objectives of increasing the efficiency and the reliability of protein structure determination by NMR. In this process, the presently used software for interactive analysis of multidimensional NMR spectra is being replaced by the fully automated routine RADAR. The software package RADAR will combine and tightly merge the functionalities of the two algorithms ATNOS for automated NOESY peak picking and CANDID for automated NOE assignment, and it should enable direct refinement of NMR structures of proteins against the raw NMR data.
Further developments include attempts to add automated sequence-specific assignment from minimal sets of NMR spectra using the software MATCH and ASCAN. MATCH is a new memetic algorithm for sequence-specific backbone resonance assignment applied to APSY input data. ASCAN introduces novel algorithms for automated sequence-specific side-chain resonance assignments extracted from NOESY data.

References:
Herrmann, T., Güntert, P. & Wüthrich, K
Protein NMR structure determination with automated NOE assignment using the new software CANDID and the torsion angle dynamics algorithm DYANA.
J. Mol. Biol. **319**(1) (2002) 209-227

Herrmann, T., Güntert, P. & Wüthrich, K.
Protein NMR structure determination with automated NOE-identification in the NOESY spectra using the new software ATNOS.
J. Biomol. NMR **24**(3) (2002) 171-189

Fiorito, F., Damberger, F. & Herrmann, T.
Novel algorithms for automated amino acid side-chain NMR assignment in proteins. (in preparation)

Volk, J., Herrmann, T. & Wüthrich, K
MATCH: A new memetic algorithm for sequence-specific protein NMR assignment: Application to APSY NMR data sets. (in preparation)

Title: Structural biology of mammalian and non-mammalian prion proteins

Researchers: Barbara Christen
Daniel Roberto Perez Lagos
Fred Damberger
Christine von Schroetter
Simone Hornemann
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
The prion protein (PrP) is a necessary factor in the development of transmissible spongiform encephalopathies (TSEs), such as Creutzfeldt-Jakob disease in humans, BSE ("mad cow disease") in cattle, and scrapie in sheep. PrP is a highly conserved glycoprotein in mammals, where it is predominantly expressed in neuronal tissue, and has also been found in birds and reptiles. We have solved three-dimensional structures of the recombinant “healthy” form of a selection of mammalian and non-mammalian prion proteins, and are analyzing similarities and differences that might bear on the function of the cellur form of PrP in healthy organisms and on the species barrier for infectious transmission of TSEs.
This line of work is continued with structure determinations of designed variants of murine PrP, of PrP from fish and other non-mammalian species, and of trans-membrane forms of PrP. Additional experiments bear on the mechanism of the conversion of the cellular prion protein into the disease-related scrapie form, which is still to be experimentally demonstrated and understood in detail. A special focus will lie on identifying potential interaction partners of the prion protein, and on induced up-regulation of cellular factors during onset of the disease.

References:
Lührs, T., Zhan, R. and Wüthrich, K.,
Amyloid formation by recombinant lull-length prion proteins in phospholipid bicelle solutions.
J. Mol Biol. **357** (2006), 833–841.

Lysek, D.A., Schorn, C., Nivon, L.G., Esteve-Moya, V., Christen, B., Calzolai, L., von Schroetter, C., Fiorito, F., Herrmann, T., Güntert, P. and Wüthrich, K.
Prion protein NMR structures of cats, dogs, pigs and sheep.
Proc. Natl. Acad. Sci. USA **102** (2005), 640–645

Gossert, A.D., Bonjour, S., Lysek, D.A., Fiorito, F. and Wüthrich, K.
Prion protein NMR structures of elk and mouse/elk hybrids.
Proc. Natl. Acad. Sci. USA **102** (2005), 646–650.

Calzolai, L., Lysek, D.A., Pérez, D.R., Güntert, P. and Wüthrich, K.
Prion protein NMR structures of chickens, turtles, and frogs.
Proc. Natl. Acad. Sci. USA **102** (2005), 651–655.

Title: NMR studies of insect pheromone-binding proteins

Researchers: Fred Damberger
Erich Michels
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
Odorant-binding proteins (OBPs) occur at high concentrations in the lymph of insect olfactory sensilla and transport the hydrophobic odorant molecules from the periphery of the sensillum to the olfactory receptors. The pheromone binding proteins (PBPs) are a subclass of the OBPs which bind pheromones used in insect communication. Our work so far shows that the pheromone binding protein from the silkmoth Bombyx mori (BmPBP) undergoes a pH-dependent conformational transition between two forms (BmPBPA observed at pH 4.5 and BmPBPB at pH 6.5), which is likely to relate to biological function. To obtain a more complete picture of the function of BmPBP, we have determined the solution structures at pH 4.5 and pH 6.5. Strikingly, the C-terminal dodecapeptide segment, which is disordered on the protein surface in BmPBPB and in the crystal structure of the BmPBP-bombykol complex, forms a regular alpha-helix in BmPBPA, which is inserted into the core of the protein and occupies the ligand binding site. This explains the absence of binding observed for BmPBP at pH 4.5. BmPBP represents a novel mechanism of intramolecular protein regulation involving regions distant in the sequence. We are following up on these initial results with further studies of BmPBP and designed variants of this protein under variable solution conditions, to provide further insight into structure-function correlations. It appears that the results thus obtained might bear on an entire class of proteins with pheromone-binding function.

References: Michel, E., Damberger, F.F., Chen, A.M., Ishida, Y., Leal, W.S. and Wüthrich, K. Assignments for the Bombyx mori pheromone-binding protein fragment BmPBP (1 – 128) at pH 6.5.
J. Biomol. NMR **31** (2005), 65.

Title: NMR studies of FimF

Researchers: Alvar Gossart
Francesco Fiorito
Torsten Herrmann
Rudi Glockshuber
Markus G. Grütter
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
Pilus assembly is a core project in the group of Prof. R. Glockshuber, and we try to support these studies with NMR structure determinations and investigations of protein-protein interactions. Type-1 pili ("Fimbrae") are large, heterooligomeric protein filaments of uropathogenic E. coli strains that are required for the attachment of the bacteria to host cell surfaces and that enable survival inside of macrophages. These pili are constituted by up to 2000 protein subunits, where FimA is the most abundant one (>98%), with FimF, FimI, FimG and the mannose-binding subunit FimH making up the rest. In a previous collaboration with the group of Prof. R. Glockshuber, we solved the solution structure of FimC, a periplasmic assembly factor which is not a structural component of the pili but is required for pilus assembly in vivo. The actual pilus assembly on the cell surface is performed by the membrane protein FimD. The application of new, TROSY-based NMR techniques provided insights into the structures of the different proteins involved in pilus assembly and their intermolecular interactions in solution, thus extending structural data obtained from X-ray crystallography. As a new target, the FimF subunit is currently being structurally characterized by NMR.

References:
Gossert, A.D., Hiller, S., Fiorito, F. and Wüthrich K.
NMR assignment of the E. coli type 1 pilus protein FimF.
J. Biolmol. NMR **38** (2007), 195.

Gossert, A.D., Bettendorff, P., Puorger, C., Vetsch, M., Herrmann, T., Glockshuber, R., and Wüthrich, K.
NMR structure of the E. coli type 1 pilus subunit FimF and its interactions with other pilus subunits.
J. Mol. Biol. (2007), (accepted).

Nishiyama, M., Horst, R., Eidam, O., Herrmann, T., Ignatov, O., Vetsch, M., Bettendorf, P., Jelesarov, I., Grütter, M.G., Wüthrich, K., Glockshuber, R. and Capitani, G.
Structural basis of chaperone–subunit complex recognition by the type 1 pilus assembly platform FimD.
EMBO J. **24** (2005), 2075–2086.

6

High-performance Hardware

6.1 C4: The Year in Review

The Competence Center for Computational Chemistry (C4) completed its second year with the new Steering Committee consisting of Profs. Wanda Andreoni (IBM Zürich Research), Jürg Hutter (University of Zürich), Wilfred F. van Gunsteren, and PD Dr. Hans P. Lüthi (both ETH Zürich).

The highlight of the past year was the 2006 C4 Workshop with the UC Berkeley Kenneth Pitzer Center for Theoretical Chemistry, represented by the entirety of its seven faculty members. During the three-day event, with lectures presented by the guest- and the host-team, there was an intense scientific exchange. This is reflected by the large attendance (close to one-hundred, even on a Saturday morning) and the fact that as many as 42 posters were presented by the C4 community. Honored by the presence of the ETH Vice Presidents for Research and for International Affairs, Profs. Dimos Poulikakos and Hans Thierstein, the event was an important step towards a formal exchange program between the two institutions.

As in the past year, C4 offered tutorials on advanced topics of molecular modeling and simulation. In October 2006, the second C4 Tutorial was on dynamical electron correlation, presented by Dr. David Tew and Prof Wim M. Klopper of the University of Karlsruhe. In August 2007, the topic of the third C4 Tutorial was the free energy calculation, presented by our colleagues J. Hutter, Philippe Hünenberger, and Wilfred van Gunsteren. Both tutorials, presented by leaders in the respective fields, gave the participants, close to 30 in number, insight into the state-of-the-art in these areas of method development. The course materials can be downloaded from www.c4.ethz.ch.

The actual “backbones” of C4, however, are the Seminar Program and the compute-resource. The C4 Seminar Program covered 13 lectures, some of them by leaders in their field. The seminar, that takes place every second Thursday during the semester, enjoys a remarkable popularity.

The new C4 compute-cluster Obélix, a 32 node IBM Opteron cluster with four CPUs each, was procured for method and code development, for the execution of resource-intense computations, and for computational campaigns. Operated by the ETH Informatikienste, Obélix delivered beyond ¾ million CPU hours worth of compute-cycles. Given the large demand, the number of “fat nodes” with sixteen GBytes of memory had to be expanded from four to eight. Also, the local disk storage was expanded. The science “produced” with Obélix will be the topic of the C4 2007 Workshop. The top-users will present their results with a focus on the computational science aspect (models, methods, algorithms),

The goals of C4, namely to seek new frontiers and opportunities in molecular modeling and simulation, to cater to the flow of know-how, and to serve as a platform for the interaction with external partners resulted in a “return on investment” of nearly 100 projects that are reported on in the 2005/06 C4 Annual Report. Some of these projects are expected to have considerable impact on modeling and simulation, or in the respective area of application.

We wish to thank the members and affiliates for their active participation, and we are looking forward to exciting trans-disciplinary collaboration between the C4 and CS&E community.

Hans P. Lüthi, Leiter C4
October 12, 2007

6.2 CSCS – Swiss National Supercomputing Centre

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Top class service for the national research community
As defined in it's mission statement and performance mandate, CSCS provides, develops and promotes technical and scientific services for the Swiss research community in the areas of high-performance computing and distributed high-throughput computing. It is a competence centre that pioneers and carries out it's own research in the area of computer science.

Serving Swiss research institutions of very high international standing it goes without saying, that CSCS' technical, HPC and computer science services must be of matching quality in order to be able to fulfill its users' needs.

Providing the national HPC facility and services
CSCS strives to offer a competitive edge to its customers by operating leading-edge supercomputing technology. As a small country Switzerland cannot afford to compete with the HPC facilities of larger countries based on the size of its installation. CSCS must therefore constantly strive to purchase the most innovative and advanced technology in order to give its customers a technical advantage. This strategy is further strengthened by constantly upgrading the purchased systems so they remain at the technical forefront over a number of years, thus maintaining the competitive edge until the next system is purchased. CSCS' technical infrastructure integrates a complex mixture of supercomputers, clusters, high-speed networks and data management resources as well as an extensive portfolio of application software.

CSCS' computing infrastructure
CSCS currently offers its customers supercomputing services on massively parallel processing and cluster environments.

The Cray XT3 massively parallel processing (MPP) computer system provides of 1664 2.6GHz AMD Opteron dual-core compute processors as well as a further 32 processors for service activities such as login access and parallel file system support. Following two upgrades, in July 2006 and April 2007, the system is now able to deliver a peak performance of 17 TFlop/s and a total of 3.3 Terabytes of memory. The processors are connected by the Cray SeaStar high-bandwidth, low-latency interconnect that uses a 3D torus typology. The parallel filesystem provides 23 Terabytes of temporary scratch storage with a peak data transfer rate of 4.5 Gigabytes per second.

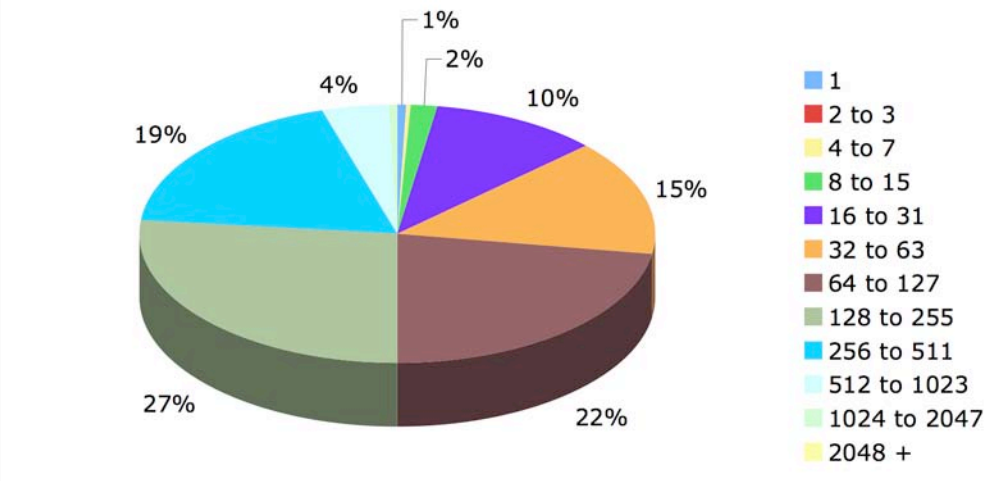
The IBM P5 that went into service production in January 2007, is a parallel constellation cluster consisting of 48 p5-575 SMP nodes with a total of 786 Power 5 CPUs and 1.5 Terabytes of main memory. This system offers a theoretical peak performance of 4.5 TFlop/s.

A dual-link 4X Infiniband interconnect links the nodes and provides a high-speed network for parallel computing. A peak data transfer rate of approximately 5 Gigabytes per second is available on the GPFS parallel file system where 17 Terabytes of storage are available.

Besides these two machines, CSCS also offers cluster computing capacity to the Swiss research community by means of the Tier-2 computing cluster it hosts for the Large Hadron Collider Computing Grid.

Since 2005 CSCS has made a strategic change towards massive parallel computing which is reflected in the distribution of job size on both of the current HPC servers.

Job size distribution on CSCS HPC servers (no. of CPU per job, aggregated by consumed CPU time)



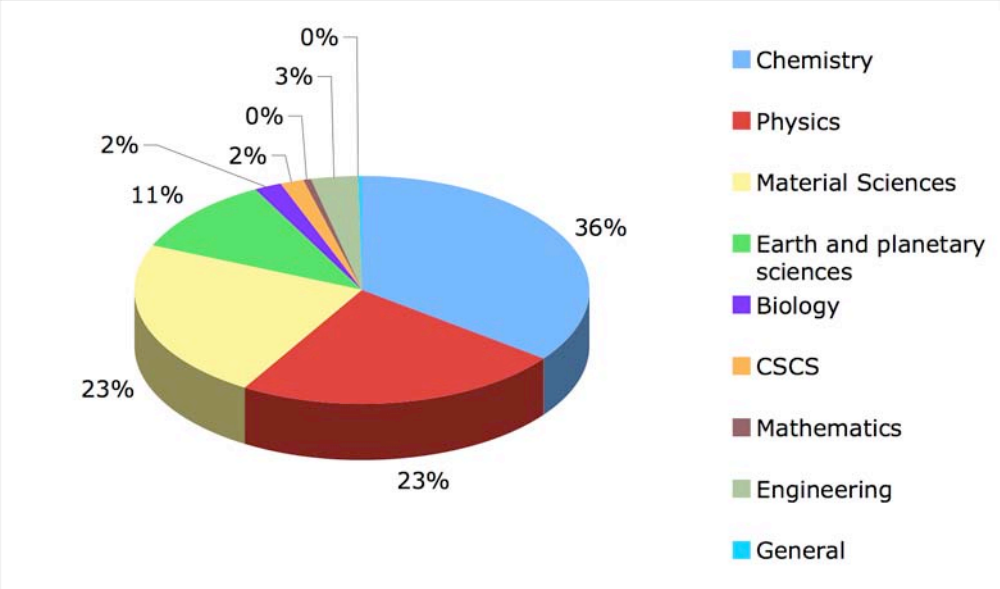
Data management facilities

CSCS recognizes the importance of the close integration of supercomputing with the data management services. 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 two high-capacity StorageTek "Powderhorn" tape silos with mixed SCSI/ FC tape drive technology; redundant Brocade switches ensure a fully-switched FiberChannel archive environment. A major upgrade of selected hardware and software components allowed users to benefit from the higher archive access performance and increased service availability, while still ensuring seamless growth of the archive capacity, currently exceeding 600TB.

Who uses CSCS' compute infrastructure?

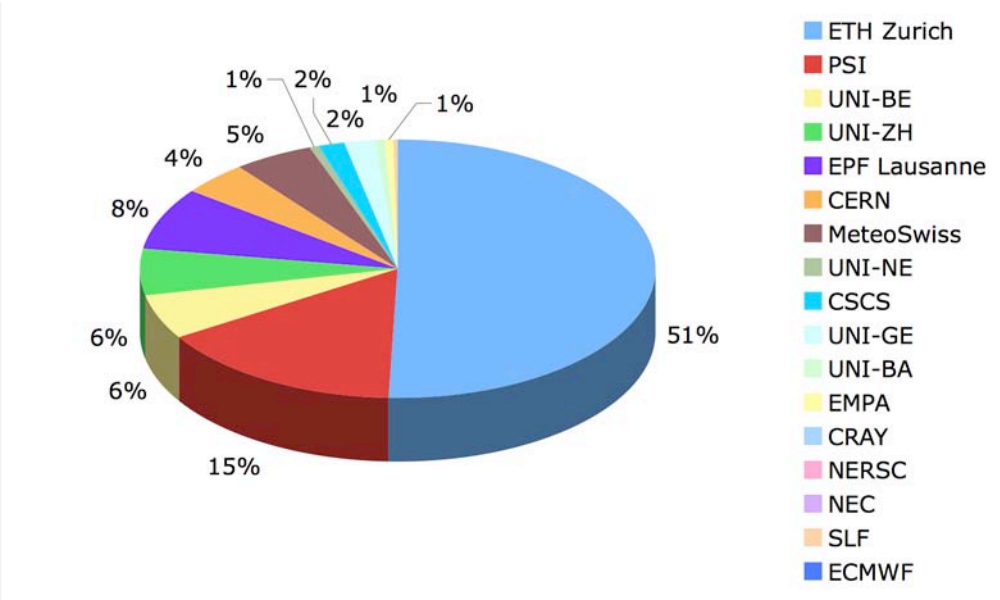
CSCS user base consists of researchers from the fields of chemistry, physics, material sciences, earth and planetary sciences and biosciences. Currently the vast majority of CSCS' resources are used by the fields of chemistry, physics and material sciences.

Usage of CSCS HPC resources by discipline



Of the produced CPU hours ETH Zurich consumes the largest part, followed by the Paul Scherrer Institute. The heavy ETH Zurich bias is due to the fact that all four ALPS grand challenge projects were awarded to scientist from this institution.

Usage of CSCS HPC resources by institution



High performance computing resources are allocated to research projects on a competitive basis. All applications undergo a technical and scientific review. Resources are distributed amongst projects based on their value to science, research, development and society. Projects are allocated time on a bi-annual basis. Below you may find the table of Large Projects and ALPS grand challenge projects that were granted during 2006.

ALPS Projects 2006

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 Altsheimer and HIV
Schär	Christoph	ETH Zurich	Investigate climate change on European and Alpine scales and possible future extreme weather events

Large Projects 2006

Aemmer	Doelf	ETH Zurich	Computational Science and Engineering in Nanoelectronics
Arbenz	Peter	ETH Zurich	Multi-level Micro-Finite Element Analysis for Human Bone Structures
Baiker	Alfons	ETH Zurich	Hydrogenation reactions in heterogeneous enantioselective catalysis and homgeneous catalysis in supercritical CO2
Bakowies	Dirk	ETH Zurich	Atomization energies from ab initio calculations without empirical corrections
Bey	Isabelle	EPF Lausanne	Coupling between tropospheric chemistry and aerosols in the general circulation model ECHAM5
Broennimann	Stefan	ETH Zurich	Climate and Stratospheric Ozone during the 20th century
Buergi	Thomas	UNI-NE	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper	W. Anthony	EPF Lausanne	Computation of Stellarator Coils, Equilibrium, Stability and Transport
De Forcrand	Philippe	ETH Zurich	Canonical approach to finite density QCD simulations
Deubel	Dirk V.	ETH Zurich	Quantum Chemical Studies of Transition Metal Anticancer Drugs
folini	doris	Empa	Inverse modeling to monitor source regions of air pollutants
Gervasio	Francesco	ETH Zurich	Charge transfer and oxidative damage to DNA
Goedecker	Stefan	UNI-BA	Atomistic simulations and atomic structure
Hasenfratz	Peter	UNI-BE	Full QCD with 2+ 1 Light Chiral Fermions
Hauser	Andreas	UNI-GE	Photophysics and photochemistry of transition metal compound
Helm	Lothar	EPF Lausanne	Magnetic interactions in extended systems
Hutter	Juerg	UNI-ZH	Development and Applications of ab initio Molecular Dynamics
Joos	Fortunat	UNI-BE	Modelling CARBOn Cycle CLIMate Feedbacks (CARBOCLIM)
Kleiser	Leonard	ETH Zurich	Numerical Simulation of Transitional, Turbulent and Multiphase Flow
Knechtli	Francesco	CERN	Simulations of gauge theories on an extra-dimension
Koumoutsakos	Petros	ETH Zurich	Multiphysics Simulations using Multiscale Particle Methods
Krajewski	Florian	ETH Zurich	Ab-initio simulation of the nucleation of silicon with novel linear scaling electronic structure method
Laeuchli	Andreas	EPF Lausanne	Computational Studies of Strongly Correlated Electron System
Leriche	Emmanuel	EPF Lausanne	Direct Numerical Simulation of the Buoyancy-Driven Turbulence in a Cavity: the DNSBDTC project
Luescher	Martin	CERN	Numerical lattice gauge theory
Maddocks	John	EPF Lausanne	Large-scale atomistic molecular dynamics simulations of DNA minicircles
Martonak	Roman	ETH Zurich	Crystal structure prediction from computer simulations
Meuwly	Markus	UNI-BA	Electronic Structur Calculations for Chemical Reactions involving Transition Metals

Oganov	Artem	ETH Zurich	Computational Mineral Physics and Crystallography
Parlange	Marc	EPF Lausanne	Large-eddy-simulation of flow and transport over complex terrain
Pasquarello	Alfredo	EPF Lausanne	Disordered Network-Forming Materials
Passerone	Daniele	UNI-ZH	Computational inverstigation of relevant photochemically active molecular switches
Poulikakos	Dimos	ETH Zurich	Biothermofluidics for Cerebrospinal Fluid Diagnostics and Control
Raible	Chistoph	UNI-BE	Modelling and Reconstruction of North Atlantic Climate System Variability (MONALISA)
Raiteri	paolo	ETH Zurich	Computational study of molecular nano-machines
Roethlisberger	Ursula	EPF Lausanne	Mixed Quantum Mechanical/Molecular mechanical (QM/MM) Studies of Systems of Biological Interest
Schaer	Christoph	ETH Zurich	Modeling Weather and Climate on European and Alpine scales
Schwierz	Cornelia	ETH Zurich	aLMo reanalysis and hindcast for the Alpine region
Sennhauser	Urs	EMPA	Reliability and degradation physics of ultrathin dielectrics (Nanoxide)
Sljivancanin	Zeljko	EPF Lausanne	Solid Surfaces and Interfaces
van Lenthe	Harry	UNI and ETH Zurich	What genetic loci are involved in the regulation of bone stregth?
Van Swygenhoven	Helena	PSI	The atomistic modeling of size effects in plasticity
Vogel	Viola	ETH Zurich	Developing High-resolution Models of How Mechanicanical Force changes Protein Function
Wild	Martin	ETH Zurich	Global Climate Change: Modelling Climate Dynamics on Decadal Time Scales

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, fluiddynamics, 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 Phoenics 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

- The Information Technology Services operate three Linux Clusters co-owned with the Departments Biology, Environmental Sciences, Physics, Mathematics, Material Sciences, Mechanical and Process Engineering and Computer Science:
    - “Hreidar” consists of 188 dual processor AMD Opteron 244 systems with 4 GB memory and Ethernet network

- "Brutus" consists of 192 dual processor dual core AMD Opteron 2220 systems with 16 GB memory and Ethernet network
- "Gonzales" consists of
  - 288 dual processor AMD Opteron 250 systems with 8 GB memory
  - 80 dual processor dual core AMD Opteron 2220 systems with 16 GB memory
  - Quadrics QsNet II High Bandwidth/Low Latency network

Parts of the clusters 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 Gonzales cluster is intended for parallel code (typically MPI based) needing high bandwidth and low latency communications, but not a globally shared memory. The Hreidar and Brutus clusters are intended for single node throughput computing and not communication intensive parallel jobs.

7

Outlook

This report documents the strength, scope and dynamics of CSE at the ETH.

Computational research is stimulated in two directions, by creating the organisation and means to foster interdisciplinary research on an ETH wide basis, and by strengthening in each field the research which uses computation as a major tool. In both directions we expect to see further development.
In the various departments of the ETH researchers in various fields of computation have been hired and we expect this trend to continue in the future.

This year the first ten students have obtained their Master Degree. Thus the full Bachelor and Master Program is in place and this was a moment to review the whole program and look to the future. The CSE Committee has decided to finally create a full three years **Bachelor curriculum** by adding the first year. Like this we hope that we can motivate high school students to start directly with studies in CSE rather than to choose one of the many curricula and then switch to CSE after the first year at ETH. Of course this possibility will stay open. It turned out that with a minor correction the first year of the Bachelor curriculum of the Department of Information Technology and Electrical Engineering is an excellent first year for CSE. In addition there will be no conflicts within the schedule. Further this change prepares the students much better and avoids certain repetitions, e.g. students from Mathematics and Physics had to do the *Introduction to Numerical Methods* in the 3rd semester, despite the fact they had already a similar, but much less computational course in their 2nd semester. For the **Master Program** we shall apply with the rector that all classes are held in **English** if there is one student who can not follow a course because it is taught in German. Currently the rector's office allows only students who have a C1 level in German. This requirement is forbidding for most students from non German speaking regions. As procedures for accepting students from outside ETH are now in place we shall start to advertise the Master program. We have set up a body to handle the admission of students from outside ETH. The tailoring of courses to the needs of students in CSE will continue.

Overall, we look optimistically into the future and are already looking forward to see the next annual report to find out about new exciting research happening at the ETH.

Zürich, November 28, 2007
Rolf Jeltsch

8

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